LIMITING DYNAMICS

IN

LARGE QUANTUM SYSTEMS

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Abstract

The aim of this thesis is a rigorous study of the dynamics of quantum systems in which some limiting parameter describing the size of the system (such as the number of particles or the mass of a single particle) is large. For a variety of systems and limiting regimes, we prove that the microscopic quantum time evolution is approximately described by a simpler, effective time evolution. Along the way, we also discuss some related mathematical problems.

In a first part, we study the dynamics of a finite number of quantum particles interacting with the quantized radiation field. Assuming that the particles are heavy and the number of photons is large, we prove that the quantum time evolution becomes classical in the sense that it is governed by the Newton-Maxwell equations. This provides an example of the emergence of classical behaviour in a quantum system. Our analysis of the limiting dynamics is based on a semiclassical argument due to Hepp.

In a second part, we study the limiting time evolution of various quantum lattice models. To begin with, we consider a general model of interacting quantum spins on a lattice, and study two limiting regimes: the large-spin limit and the continuum limit. In both cases, we identify the limiting dynamics as the Hamiltonian dynamics of a classical system of spins. This provides a rigorous derivation of Landau-Lifschitz-type equations from quantum dynamics. We extend these results to domains of infinite size and discuss as a special case the limiting dynamics of coherent spin states. Our proof is based on a perturbative expansion of the dynamics. In the large spin limit, we also prove the convergence of time-dependent correlation functions at some positive temperature. For high enough temperatures, we extend this result to an infinite lattice using a quantum cluster expansion. Finally, we study the related problem of the mean-field limit of time-dependent correlation functions of a lattice Bose gas.

In a third part, we consider the mean-field dynamics of quantum gases with a Coulomb interaction potential and a weak external potential. Our method is based on a perturbative graph expansion scheme for the dynamics of observables. We control the Coulomb singularity by counting graphs and by exploiting the dispersive nature of the free time evolution. First, we consider the mean-field limit of a Bose gas, and prove that the limiting time evolution is governed by the Hartree equation. Second, we consider the mean-field limit of a system of fermions describing for instance electrons in a large atom or molecule, and prove that their limiting time evolution is governed by the Hartree-Fock equation.

The last part of this thesis is devoted to the mean-field dynamics of coherent states in a Bose gas. Using a nonperturbative method based on a Grönwall-type argument, we strengthen and generalize many previously known results in two directions. First, we consider a large class of singular interaction potentials as well as strong, possibly time-dependent, external potentials. This allows us to deal for instance with the critical interaction potential $|x|^{-2}$ for nonrelativistic bosons, as well as strongly confining time-dependent traps. Second, we derive estimates on the rate of convergence to the mean-field limit. Thus we can for instance control the error in the mean-field approximation of a boson star. We also show that, if the mean-field dynamics satisfies a scattering condition, all error estimates are uniform in time. Moreover, we derive optimal bounds on the fraction of particles whose convergence to the mean-field limit can be controlled.

Résumé

Cette thèse se propose d'étudier de manière rigoureuse la dynamique de systèmes quantiques dans lesquels un paramètre décrivant la taille du système (tel que le nombre de particules ou la masse d'une particule) est grand. Pour un certain nombre de systèmes et régimes limite, nous démontrons que l'évolution temporelle quantique est approximativement décrite par une dynamique effective plus simple. En cours de route, nous étudions aussi certains problèmes mathématiques suggérés par cette analyse.

Dans un premier temps, nous étudions la dynamique d'un nombre fini de particules quantiques interagissant avec le champ quantique du rayonnement. Sous l'hypothèse que les particules sont lourdes et que le nombre de photons est grand, nous démontrons que l'évolution quantique devient classique, dans le sens où elle est régie par les équations de Newton-Maxwell. Ceci donne un exemple de l'émergence du comportement classique dans un système quantique. Notre analyse de la limite se base sur un argument semiclassique dû à Hepp.

Dans un deuxième temps, nous étudions la dynamique limite de divers modèles quantiques sur réseau. Pour commençer, nous considérons un modèle général de spins en interaction sur un réseau, et étudions deux cas limites: celui d'un grand spin et celui d'un réseau fin. Dans les deux cas, nous identifions la dynamique limite avec une dynamique Hamiltonienne d'un système de spins classiques. Ceci représente une dérivation rigoureuse d'équations du type Landau-Lifschitz à partir d'une dynamique quantique. Nous étendons ces résultats à des domaines de taille infinie et considérons comme cas particulier la dynamique d'états cohérents pour les spins. Notre démonstration se base sur un développement perturbatif de la dynamique. Dans la limite du grand spin, nous démontrons aussi la convergence des fonctions de corrélation dépendant du temps à température positive. Pour une température suffsamment élevée, nous étendons ce résultat à un réseau infini à l'aide d'un développement en amas quantique. Enfin, nous étudions le problème similaire de la limite du champ moyen de fonctions de corrélation dépendant du temps pour le baz de Bose sur réseau.

Dans un troisième temps, nous considérons la dynamique du champ moyen d'un gaz quantique interagissant par le biais d'un potentiel de Coulomb et soumis à un faible potentiel externe. Notre méthode se base sur un développement perturbatif de la dynamique des observables que nous exprimons à l'aide de graphes. Nous contrôlons la singularité du potentiel de Coulomb en estimant le nombre de graphes et en faisant appel au caractère dispersif de l'évolution temporelle libre. Tout d'abord, nous considérons la limite du champ moyen pour le gaz de Bose, et démontrons que l'évolution limite est régie par l'équation de Hartree. Nous considérons ensuite la limite du champ moyen pour un système de fermions décrivant par exemple des électrons dans un grand atome ou une grande molécule, et démontrons que l'évolution limite est régie par l'équation de Hartree-Fock.

La dernière partie de cette thèse est consacrée à la dynamique du champ moyen d'états cohérents du gaz de Bose. En utilisant une méthode non perturbative se basant sur un argument du type Grönwall, nous renforçons et généralisons plusieurs résultats existants dans deux directions. En premier lieu, nous admettons une grande classe de potentiels d'intéraction singuliers, ainsi que des potentiels externes forts qui peuvent être dépendant du temps. Ceci nous permet de traiter par exemple le potentiel d'interaction critique $|x|^{-2}$ dans le cas de bosons

non relativistes, ainsi que de puissants pièges à particules. En second lieu, nous dérivons des bornes sur la vitesse de convergence vers la limite du champ moyen. Ainsi nous pouvons par exemple contrôler l'erreur dans l'approximation du champ moyen pour une étoile à bosons. Nous montrons aussi que, si la dynamique du champ moyen satisfait une certaine condition de diffusion, toutes les estimations d'erreur sont uniformes dans le temps. De plus, nous dérivons des bornes optimales sur la fraction des particules pour laquelle la convergence vers la limite du champ moyen peut être contrôlée.

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Contents

Chapter 1

Introduction

Many physical systems consist of a large number of microscopic particles whose interactions are governed by the laws of quantum mechanics. Such systems often exhibit a comparatively simple, emergent macroscopic behaviour. Well-known examples are the semiclassical behaviour of heavy particles and the mean-field behaviour of systems such as Bose-Einstein condensates, plasmas, interstellar clouds of gas undergoing gravitational collapse, and globular star clusters. When trying to understand such systems it is of considerable interest to identify their macroscopic behaviour. Instead of a full microscopic description, one aims at a description that is not only simpler and therefore better suited for analytical and numerical analysis, but also less encumbered by tedious microscopic information. For instance, a typical sample of gas in a laboratory contains of the order 10^{23} particles. It is neither possible nor desirable to keep track of the position of each individual particle. Instead, one is interested in statistical quantities such as the density of particles and the two-particle correlation function. Using the effective macroscopic description one may obtain a clearer understanding of the collective behaviour of the system, and consequently address problems such as orbital stability and scattering behaviour of groups of particles, propagation of waves, and blow-up or collapse of clusters.

The aim of this thesis is a rigorous study of such limiting behaviour and some related mathematical problems. We focus mainly on the *dynamics* of large quantum systems, where one is interested in approximating the microscopic quantum-mechanical time evolution with some effective time evolution.

The general setup is as follows. The quantum (microscopic) dynamics is characterized by a limiting parameter that describes the "size" of the quantum system. Examples of such limiting parameters are the number of particles in a quantum gas, the total mass of a finite number of interacting quantum particles, and the magnitude of the spins in a quantum spin system. With each value of the limiting parameter is associated a quantum system, whose states are given by vectors in a Hilbert space and whose time evolution is given by a one-parameter group of unitary transformations. The limiting (macroscopic) dynamics is described by a classical Hamiltonian system. Classical states are points in phase space, and their time evolution is given by Hamilton's equation of motion. The goal is to show that, in some sense to be made precise, the quantum time evolution for a large limiting parameter is approximately described by the classical time evolution.

In order to make this asymptotic behaviour precise, one usually employs coherent states. A coherent state is a quantum state that is parametrized (in some suitable manner) by a classical state. For a classical state x, let $x(t)$ denote the classical time evolution of x up to time t. Then the above asymptotic behaviour may be formulated more precisely by saying that, in the limit of a large limiting parameter, the quantum time evolution of the coherent state around x is equal to the coherent state around $x(t)$. Thus, in the limit of a large limiting parameter, the quantum time evolution of a coherent state is again a coherent state, whose dynamics is governed by a classical Hamitonian system. In general, the family of coherent states is not invariant under quantum time evolution.

There are several cases of interest where the setup outlined above is too restrictive. One might for instance want to consider a larger class of states than coherent states, or even avoid the use of states altogether. Thus one is led to considering the quantum time evolution of *observables* instead of states. This may be interpreted as a passage from the Schrödinger picture of quantum mechanics to its Heisenberg picture. A further advantage of the observable picture is that it survives unscathed the process of taking the thermodynamic limit in various lattice models. In order to describe the limiting dynamics of observables, it is of great interest to interpret the macroscopic limit as the converse of a *quantization* of the classical Hamiltonian system. We outline the general procedure and refer to the examples in the following sections for more details.

The general framework is that of quantization of Poisson algebras. Let $\mathfrak{A}$ be a Poisson algebra, i.e. a commutative, associative algebra that is also a Lie algebra whose bracket $\{\cdot\,,\cdot\}$ satisfies $\{fg\,,h\} = f\{g\,,h\} + \{f\,,h\}g$. In most applications (and throughout this thesis) $\mathfrak{A}$ is a subalgebra of the algebra of smooth functions on a Poisson or even symplectic manifold. The elements of $\mathfrak{A}$ play the role of classical observables. As recognized already by Dirac, the process of quantization may be understood as a bijective linear mapping $\widehat{(\cdot)}_\varepsilon$ from $\mathfrak{A}$ into an algebra $\widehat{\mathfrak{A}}$ of operators on a Hilbert space, such that the commutator satisfies

$$[\widehat{f}_\varepsilon\,,\widehat{g}_\varepsilon] \;=\; \frac{\varepsilon}{\mathrm{i}}\widehat{\{f\,,g\}}_\varepsilon + O(\varepsilon^2) \tag{1.1}$$

for $\varepsilon \to 0$. Here ε plays the role of $\hbar$ in the usual quantization of a classical physical system. We call ε the *parameter* of the quantization $\widehat{(\cdot)}_\varepsilon$. As we shall soon see, ε^{-1} is the limiting parameter of the corresponding macroscopic limit.

It is sometimes useful to introduce a noncommutative *star product* $*_\varepsilon$ on $\mathfrak{A}$, defined as the "pull-back" of operator multiplication under the mapping $\widehat{(\cdot)}_\varepsilon$. Thus, we define

$$\widehat{(f *_\varepsilon g)}_\varepsilon \;:=\; \widehat{f}_\varepsilon\,\widehat{g}_\varepsilon\,. \tag{1.2}$$

Introducing the star product avoids the dramatic change in the nature of the objects after quantization[1].

Let us now return to the problem of understanding the limiting dynamics of observables. Take a Poisson algebra $\mathfrak{A}$ of classical observables. The dynamics is generated by a Hamilton function $H \in \mathfrak{A}$. Let $f \in \mathfrak{A}$ and denote by $f(t)$ its time evolution defined through its equation of motion

$$\partial_t f(t) \;=\; \{H\,, f(t)\}\,, \qquad f(0) \;=\; f\,. \tag{1.3}$$

Assume that we have a quantization $\widehat{(\cdot)}_\varepsilon$ of $\mathfrak{A}$, with associated star product $*_\varepsilon$. The quantized time evolution $f^\varepsilon(t)$ is defined through its equation of motion

$$\partial_t f^\varepsilon(t) \;=\; \frac{\mathrm{i}}{\varepsilon}[H\,, f^\varepsilon(t)]_\varepsilon\,, \qquad f^\varepsilon(0) \;=\; f\,, \tag{1.4}$$

where $[\cdot\,,\cdot]_\varepsilon$ is the commutator with respect to the star product $*_\varepsilon$. One would then like to show that $f(t) \approx f^\varepsilon(t)$ for small ε. Formally, (1.3) and (1.4) have the solutions

$$f(t) \;=\; \sum_{k\geqslant 0}\frac{t^k}{k!}\{H\,,f\}^{(k)}\,, \qquad f^\varepsilon(t) \;=\; \sum_{k\geqslant 0}\frac{t^k}{k!}\left(\frac{\mathrm{i}}{\varepsilon}\right)^k [H\,,f]_\varepsilon^{(k)}\,, \tag{1.5}$$

[1] This setup is the starting point of the theory of *deformation quantization*, where one is interested in the existence (in the weaker sense of formal power series in ε) of such star products on general Poisson algebras.

where $\{\cdot\,,\cdot\}^{(k)}$ is defined through $\{f\,,g\}^{(0)} = g$ and $\{f\,,g\}^{(k)} = \{f\,,\{f\,,g\}^{(k-1)}\}$; the multiple commutator $[\cdot\,,\cdot]_\varepsilon^{(k)}$ is defined similarly. Since the star product $*_\varepsilon$ satisfies $\mathrm{i}\varepsilon^{-1}\,[f\,,g]_\varepsilon \approx \{f\,,g\}$ for small ε, the representation (1.5) makes it plausible that $f^\varepsilon(t) \approx f(t)$ for small ε. This observation can in fact sometimes serve as the basis of a proof.

This limiting behaviour may be recast in terms of operators in $\widehat{\mathfrak{A}}$. Let us denote the map $f \mapsto f(t)$ defined in (1.3) by τ_t. Writing $F^\varepsilon(t) = \widehat{f^\varepsilon(t)}_\varepsilon$ and applying $\widehat{(\cdot)}_\varepsilon$ to (1.4) yields

$$\partial_t F^\varepsilon(t) \;=\; \frac{\mathrm{i}}{\varepsilon}[\widehat{H}_\varepsilon\,, F^\varepsilon(t)]\,, \qquad F^\varepsilon(0) \;=\; \widehat{(f)}_\varepsilon\,.$$

Denote the map $F \mapsto F(t)$ by $\widehat{\tau}_t^\varepsilon$. It follows that

$$\widehat{\tau}_t^\varepsilon F \;=\; \mathrm{e}^{\mathrm{i}\varepsilon^{-1}\widehat{H}_\varepsilon t}\, F\, \mathrm{e}^{-\mathrm{i}\varepsilon^{-1}\widehat{H}_\varepsilon t}\,.$$

The corresponding time evolution of a state $\Psi(t) = \mathrm{e}^{-\mathrm{i}\varepsilon^{-1}\widehat{H}_\varepsilon t}\Psi$ in the Schrödinger picture is therefore governed by the Schrödinger equation

$$\mathrm{i}\varepsilon\partial_t\Psi(t) \;=\; \widehat{H}_\varepsilon\Psi(t)\,.$$

That the classical and quantum dynamics approximately agree for small ε means that $f(t) \approx f^\varepsilon(t)$ for small ε. After applying $\widehat{(\cdot)}_\varepsilon$ this reads

$$\widehat{(\tau_t f)}_\varepsilon \;\approx\; \widehat{\tau}_t^\varepsilon\,\widehat{f}_\varepsilon \tag{1.6}$$

for small ε. Thus, the diagram

$$\begin{tikzcd}
\mathfrak{A} \arrow[r, "\tau_t"] \arrow[d, "\widehat{(\cdot)}_\varepsilon"'] & \mathfrak{A} \arrow[d, "\widehat{(\cdot)}_\varepsilon"] \\
\widehat{\mathfrak{A}} \arrow[r, "\widehat{\tau}_t^\varepsilon"'] & \widehat{\mathfrak{A}}
\end{tikzcd}$$

commutes for $\varepsilon \to 0$, i.e. quantization commutes with time evolution for $\varepsilon \to 0$. The first such result goes back to Egorov [Ego69], who gave a proof of the statement (1.6) in the context of canonical quantization of systems of a finite number of degrees of freedom. We call results of the form (1.6) Egorov-type theorems. Thus one may understand the semiclassical limit $\varepsilon \to 0$ as the converse of quantization. When studying the limiting dynamics of a quantum system with limiting parameter ε^{-1}, it is therefore of interest to identify the quantum system as a quantization with parameter ε of a classical Hamiltonian system. Here the classical system describes the limiting, macroscopic dynamics. As it turns out, this is a very general picture that describes a wide variety of limiting regimes. It is summarized in the following diagram.

$$\begin{tikzcd}
\boxed{\text{classical theory}} \arrow[r, shift left, "\text{quantization with parameter } \varepsilon"] & \boxed{\text{quantum theory}} \arrow[l, shift left, "\text{semiclassical limit } \varepsilon \to 0"]
\end{tikzcd}$$

Examples of physical systems whose limiting behaviours are well understood are listed in the following section.

1.1. Some examples

In this section we summarize three well-known limiting regimes: the semiclassical limit of a quantum system, the mean-field limit of a classical system, and the mean-field limit of a quantum system. We also outline how each limit may be understood as the converse of a quantization.

1.1.1. The semiclassical limit. We consider a classical system of a finite number, d, of degrees of freedom. The phase space is $\Gamma = \mathbb{R}^{2d}$. We write points in Γ as $x = (p, q) \in \Gamma$ with $p = (p_1, \dots, p_d)$ and $q = (q_1, \dots, q_d)$. The symplectic form of Γ is given by $\sum_{i=1}^d \mathrm{d}p_i \wedge \mathrm{d}q_i$, which gives rise to the Poisson bracket

$$\{p_i\,, q_j\} \;=\; \delta_{ij}\,, \qquad \{p_i\,, p_j\} \;=\; \{q_i\,, q_j\} \;=\; 0\,.$$

This may also be written as $\{x_i\,, x_j\} = J_{ij}$ with the $2d \times 2d$ matrix

$$J \;=\; \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix}.$$

Next, we introduce *Weyl quantization* with parameter ε. Consider the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^d, \mathrm{d}q_1 \cdots \mathrm{d}q_d)$ on which act the self-adjoint operators

$$P_i \;:=\; -\mathrm{i}\frac{\partial}{\partial q_i}\,, \qquad Q_i \;:=\; q_i\,.$$

The rescaled operators in the symmetric rescaling[2] are defined by $P_i^\varepsilon := \varepsilon^{1/2} P_i$ and $Q_i^\varepsilon := \varepsilon^{1/2} Q_i$. They satisfy the canonical commutation relations

$$[P_i^\varepsilon\,, Q_j^\varepsilon] \;=\; \frac{\varepsilon}{\mathrm{i}}\delta_{ij}\,, \qquad [P_i^\varepsilon\,, P_j^\varepsilon] \;=\; [Q_i^\varepsilon\,, Q_j^\varepsilon] \;=\; 0\,.$$

It is convenient to abbreviate $X = (P, Q)$ and $X^\varepsilon = (P^\varepsilon, Q^\varepsilon)$. Thus the canonical commutation relations become $[X_i^\varepsilon\,, X_j^\varepsilon] = -\mathrm{i}\varepsilon J_{ij}$. As our algebra of observables $\mathfrak{A}$ we take the space of smooth functions of at most polynomial growth. We define the Weyl quantization of $f \in \mathfrak{A}$ as

$$\widehat{f}_\varepsilon \;:=\; \int_{\mathbb{R}^{2d}} \mathrm{d}\xi\; \tilde{f}(\xi)\, \mathrm{e}^{\mathrm{i}\xi \cdot X^\varepsilon}\,, \tag{1.7}$$

where $\tilde{f}$ is the Fourier transform of f satisfying $f(x) = \int_{\mathbb{R}^{2d}} \mathrm{d}\xi\; \tilde{f}(\xi)\, \mathrm{e}^{\mathrm{i}\xi\cdot x}$. (The definition (1.7) makes sense as a quadratic form on $\mathcal{S}(\mathbb{R}^d) \subset \mathcal{H}$ because $f \in \mathfrak{A} \subset \mathcal{S}'(\mathbb{R}^{2d})$ is by assumption a tempered distribution and the mapping $\xi \mapsto \langle \Psi\,, \mathrm{e}^{\mathrm{i}\xi\cdot X^\varepsilon} \Psi\rangle$ is in $\mathcal{S}(\mathbb{R}^{2d})$ for $\Psi \in \mathcal{S}(\mathbb{R}^d)$.) From the definition (1.7) of Weyl quantization it is easy to infer the associated star product $*_\varepsilon$ on $\mathfrak{A}$. Indeed, we find

$$\widehat{f}_\varepsilon\, \widehat{g}_\varepsilon \;=\; \int \mathrm{d}\xi\, \mathrm{d}\zeta\; \tilde{f}(\xi)\tilde{g}(\zeta)\, \mathrm{e}^{\mathrm{i}\xi\cdot X^\varepsilon}\, \mathrm{e}^{\mathrm{i}\zeta\cdot X^\varepsilon} \;=\; \int \mathrm{d}\xi\, \mathrm{d}\zeta\; \tilde{f}(\xi)\tilde{g}(\zeta)\, \mathrm{e}^{\mathrm{i}(\xi+\zeta)\cdot X^\varepsilon}\, \mathrm{e}^{\mathrm{i}\varepsilon J_{ij}\xi_i\zeta_j/2}\,,$$

by the usual Weyl relations. Thus, $\widehat{f}_\varepsilon\, \widehat{g}_\varepsilon = \int \mathrm{d}\xi\; \tilde{h}(\xi)\, \mathrm{e}^{\mathrm{i}\xi\cdot X^\varepsilon}$ with

$$\tilde{h}(\xi) \;=\; \int \mathrm{d}\zeta\; \tilde{f}(\xi - \zeta)\tilde{g}(\zeta)\, \mathrm{e}^{\mathrm{i}\varepsilon J_{ij}(\xi_i - \zeta_i)\zeta_j/2}\,.$$

[2]For notational simplicity we adopt the somewhat unusual symmetric scaling. A simple unitary transformation of $\mathcal{H}$ maps P_i^ε to $\frac{\varepsilon}{\mathrm{i}}\frac{\partial}{\partial q_i}$ and Q_i^ε to q_i, thus recovering the usual scaling.

Taking the inverse Fourier transform yields the representation

$$(f *_\varepsilon g)(x) \;=\; h(x) \;=\; \exp\Big(\frac{\varepsilon}{2\mathrm{i}} J_{ij} \frac{\partial}{\partial y_i}\frac{\partial}{\partial z_j}\Big) f(y)g(z)\Big|_{y=z=x}\,,$$

the Moyal product of f and g.

Having dealt with the quantization of the classical system Γ, let us now turn to its time evolution. Consider a Hamilton function $H \in \mathfrak{A}$ of the form

$$H(p,q) \;=\; p \cdot Tp + V(q)\,,$$

where T is some positive matrix on $\mathbb{R}^d$ and V is a real function. Let $x \in \Gamma$ and consider the Hamiltonian equation of motion

$$\dot{x}(t) \;=\; -J\,\nabla H(x(t))\,, \qquad x(0) \;=\; x\,. \tag{1.8}$$

Under reasonable assumptions on V, the equation of motion (1.8) has a unique global solution $x(t)$.

The semiclassical regime of a quantum system is the regime where the typical action of the system (i.e. the integral $\int p_i \,\mathrm{d}q_i$ over a typical orbit) is large compared to Planck's constant $\hbar$ (1 in our units). In order to construct states with large action, it is convenient to use the Weyl operator

$$W(x) \;:=\; \mathrm{e}^{\mathrm{i}(p\cdot Q - q\cdot P)}\,,$$

for $x = (p,q) \in \Gamma$. The Weyl operator $W(x)$ implements a translation by x in classical phase space in the sense that

$$W(x)^*\,X\,W(x) \;=\; X + x\,.$$

To avoid unimportant technicalities, let us assume that $V \in C^3(\mathbb{R}^d)$ and ∇V is bounded. Then the equation of motion (1.8) has a unique global solution $x(t)$. Moreover, we have the following fundamental result due to Hepp [Hep74].

THEOREM 1.1. *For all $t \in \mathbb{R}$ and $\xi \in \Gamma$ we have*

$$\operatorname*{s-lim}_{\varepsilon\to 0} W(\varepsilon^{-1/2}x)^*\,\mathrm{e}^{\mathrm{i}\varepsilon^{-1}\widehat{H}_\varepsilon t}\,\mathrm{e}^{\mathrm{i}\xi\cdot X^\varepsilon}\,\mathrm{e}^{-\mathrm{i}\varepsilon^{-1}\widehat{H}_\varepsilon t}\,W(\varepsilon^{-1/2}x) \;=\; \mathrm{e}^{\mathrm{i}\xi\cdot x(t)}\,, \tag{1.9}$$

where $\widehat{H}_\varepsilon$ is the Weyl quantization (1.7) *of H.*

The meaning of theorem 1.1 becomes clear if we take the expectation of (1.9) in a state $\Psi \in \mathcal{H}$. In the state[3] $W(\varepsilon^{-1/2}x)\Psi$, the expectation of the operator X is asymptotically equal to $\varepsilon^{-1/2}x$, so that the typical action of the system is of order ε^{-1} and the semiclassical character of the limit is evident. The semiclassical limit is sometimes also referred to as the limit of heavy particles. The reason for this is best understood in the conventional rescaling of P and Q, where the Hamiltonian is obtained from $\widehat{H}_\varepsilon$ by conjugation with the ε-dependent unitary operator R_ε defined by $(R_\varepsilon\Psi)(q) := \varepsilon^{d/4}\Psi(\varepsilon^{1/2}q)$. Then the dynamics of the wave function $\Psi(t) \in \mathcal{H}$ is given by the Schrödinger equation

$$\mathrm{i}\partial_t\Psi(t) \;=\; \Big(\frac{1}{\varepsilon^{-1}}\,P\cdot TP + \varepsilon^{-1}V(Q)\Big)\Psi(t)\,.$$

[3] In fact, states of the form $W(x)\Omega$, where $\Omega(q) := \pi^{-d/4}\mathrm{e}^{|q|^2/2}$, constitute the traditional family of coherent states of a quantum system of a finite number of degrees of freedom. Thus, Theorem 1.1 describes as a special case the limiting dynamics of coherent states.

Thus we see that ε^{-1} plays the role of the mass of the particles. The potential V is also rescaled by ε^{-1}; this is clearly necessary to ensure that both sides of Newton's second law are of the same order.

Using Hepp's result we may easily derive a Egorov-type theorem for the semiclassical limit.

THEOREM 1.2. *Assume that V is smooth and ∇V is bounded. Let $f \in C_c^\infty(\mathbb{R}^{2d})$ and $t \in \mathbb{R}$. Then we have*

$$\operatorname*{s-lim}_{\varepsilon\to 0}\Big(\mathrm{e}^{\mathrm{i}\varepsilon^{-1}\widehat{H}_\varepsilon t}\,\widehat{f}_\varepsilon\,\mathrm{e}^{-\mathrm{i}\varepsilon^{-1}\widehat{H}_\varepsilon t} - (\widehat{f\circ\phi_t})_\varepsilon\Big) \;=\; 0\,,$$

where ϕ_t is the Hamiltonian flow on Γ.

PROOF. Setting $x = 0$, multiplying (1.9) by $\tilde{f}(\xi)$, and integrating over ξ yields

$$\operatorname*{s-lim}_{\varepsilon\to 0}\;\mathrm{e}^{\mathrm{i}\varepsilon^{-1}\widehat{H}_\varepsilon t}\,\widehat{f}_\varepsilon\,\mathrm{e}^{-\mathrm{i}\varepsilon^{-1}\widehat{H}_\varepsilon t} \;=\; (f\circ\phi_t)(0)\,,$$

by dominated convergence. Next, we note that by the theory of ordinary differential equations ϕ_t is smooth, so that $f\circ\phi_t \in C_c^\infty(\mathbb{R}^{2d})$. Setting $x = 0$, multiplying (1.9) at $t = 0$ by $(\widetilde{f\circ\phi_t})(\xi)$, and integrating over ξ yields

$$\operatorname*{s-lim}_{\varepsilon\to 0}\;(\widehat{f\circ\phi_t})_\varepsilon \;=\; (f\circ\phi_t)(0)\,,$$

by dominated convergence. The claim follows. $\square$

1.1.2. The mean-field limit in classical mechanics. In this section we review the mean-field limit in classical mechanics. Its physical heuristics may be understood as follows. Whenever many particles interact by means of weak two-body potentials, one expects that the potential felt by any one particle is given by an average potential generated by the mean particle density. This intuition turns out to be correct, and can be made precise by considering the *mean-field limit* of an N-body system.

We begin this section with a review of the traditional approach to the mean-field limit in classical mechanics. In a second part, we describe how the mean-field limit in classical mechanics may be interpreted as the semiclassical limit corresponding to a quantization of a classical Hamiltonian system, in line with the discussion at the beginning of this chapter.

The mean-field limit is a limit where the number of particles, N, tends to infinity. Consider a classical Hamiltonian system formulated on the phase space $\Gamma_N := \mathbb{R}^{2dN}$, where d is the number of spatial dimensions. We denote points in Γ_N by $X_N = (x_1, \dots, x_N)$, where $x_i = (p_i, q_i) \in \mathbb{R}^d \times \mathbb{R}^d$ for $i = 1, \dots, N$. The phase space carries the canonical symplectic form. The Hamilton function is given by

$$H_N(X_N) \;:=\; \sum_{i=1}^N \frac{p_i^2}{2m} + \frac{1}{N}\sum_{1\leqslant i<j\leqslant N} w(q_i - q_j)\,, \tag{1.10}$$

where $m > 0$ is the mass of each particle and w is an interaction potential that is assumed to be a real and even function. The scaling N^{-1} in front of the interaction potential characterizes the mean-field regime. This scaling is necessary for obtaining a well-defined limit when $N \to \infty$; it ensures that both the one-particle and the two-particle parts of H_N behave like $O(N)$ for $N \to \infty$. Thus we see that in the mean-field limit the interactions are weak and their range is of order 1.

The equation of motion for $X_N(t)$ is given by Hamilton's equation which we write in the form

$$\dot{p}_i(t) \;=\; -\frac{1}{N}\sum_j \nabla w\big(q_i(t) - q_j(t)\big)\,, \qquad \dot{q}_i(t) \;=\; \frac{p_i(t)}{m}\,. \tag{1.11}$$

We define the N-particle flow ϕ_t^N on Γ_N through $\phi_t^N(X_N) := X_N(t)$, where $X_N(t)$ is the solution of (1.11) with initial data X_N.

A simple rescaling of the equation of motion yields the rather appealing interpretation of the mean-field limit as the limit of a large number of light particles whose total mass is kept constant. Indeed, introducing the rescaled time variable $\tau = t/N$, we see that the equation of motion (1.11) is equivalent to

$$\partial_\tau p_i(\tau) \;=\; -\sum_j \nabla w\big(q_i(\tau) - q_j(\tau)\big)\,, \qquad \partial_\tau q_i(\tau) \;=\; \frac{p_i(\tau)}{mN^{-1}}\,.$$

It is convenient to replace the time evolution of points in phase space with the equivalent time evolution of N-particle densities on Γ_N. To that end, let ρ_N be a probability density on Γ_N. (In order to keep the notation simple through much of the following, we consider probability measures on Γ_N that have a density, but all of the following discussion is trivially valid for general probability measures on Γ_N.) We require that ρ_N be symmetric under permutation of its arguments $(x_1, \dots, x_N)$. This means that all particles are identically distributed. The time evolution of ρ_N is defined by $\rho_N(t, X_N) := \rho_N(\phi_{-t}^N(X_N))$. Then (1.11) implies that $\rho_N(t)$ satisfies the *Liouville equation*

$$\partial_t \rho_N(t, X_N) \;=\; -\sum_i \frac{p_i}{m} \cdot \frac{\partial \rho_N}{\partial q_i}(t, X_N) + \frac{1}{N}\sum_{i,j} \nabla w(q_i - q_j) \cdot \frac{\partial \rho_N}{\partial p_i}(t, X_N)\,. \tag{1.12}$$

Integrating out $N-k$ particles from ρ_N yields the k-particle marginal

$$\rho_N^{(k)}(x_1, \dots, x_k) \;:=\; \int \mathrm{d}x_{k+1} \cdots \mathrm{d}x_N \; \rho_N(x_1, \dots, x_N)\,,$$

a probability density on Γ_k. Thus we associate with each probability density ρ_N a sequence of marginals $(\rho_N^{(k)})_{k \in \mathbb{N}}$, whereby $\rho_N^{(k)}$ is by definition 0 if $k > N$. The marginals $\rho_N^{(k)}$ are useful objects when studying the mean-field limit because, unlike ρ_N, they act on a space that is independent of N so that questions related to their convergence make sense.

A simple calculation shows that the Liouville equation (1.12) is equivalent to the hierarchy of equations

$$\begin{aligned}
\partial_t \rho_N^{(k)}(t, x_1, \dots, x_k) \;=\; & -\sum_{i=1}^k \frac{p_i}{m} \cdot \frac{\partial \rho_N^{(k)}}{\partial q_i}(t, x_1, \dots, x_k) \\
& + \frac{1}{N} \sum_{1 \leqslant i,j \leqslant k} \nabla w(q_i - q_j) \cdot \frac{\partial \rho_N^{(k)}}{\partial p_i}(t, x_1, \dots, x_k) \\
& + \frac{N-k}{N} \sum_{i=1}^k \int \mathrm{d}x_{k+1} \nabla w(q_i - q_{k+1}) \cdot \frac{\partial \rho_N^{(k+1)}}{\partial p_i}(t, x_1, \dots, x_{k+1})\,,
\end{aligned} \tag{1.13}$$

the classical BBGKY hierarchy. Formally taking the limit $N \to \infty$ in (1.13) yields the *limiting hierarchy* for the sequence $\big(\rho_\infty^{(k)}(t)\big)_{k\in\mathbb{N}}$

$$\begin{aligned}\partial_t \rho_\infty^{(k)}(t,x_1,\dots,x_k) \;&=\; -\sum_{i=1}^k \frac{p_i}{m}\cdot\frac{\partial \rho_\infty^{(k)}}{\partial q_i}(t,x_1,\dots,x_k)\\ &\quad+\sum_{i=1}^k \int \mathrm{d}x_{k+1} \nabla w(q_i-q_{k+1})\cdot\frac{\partial \rho_\infty^{(k+1)}}{\partial p_i}(t,x_1,\dots,x_{k+1})\,. \end{aligned}\tag{1.14}$$

One therefore expects, for large N, that $\rho_N^{(k)}(t) \approx \rho_\infty^{(k)}(t)$ for all times t provided that $\rho_N^{(k)}(0) \approx \rho_\infty^{(k)}(0)$. As it turns out, this intuition is correct. However, as a tool for proving theorems, the BBGKY hierarchy is cumbersome, essentially because of the presence of derivatives which are hard to control. It is often more convenient to work on the one-particle phase space Γ_1.

To each probability density f on Γ_1 we may assign a sequence of marginals $(\rho_\infty^{(k)})_{k\in\mathbb{N}}$ with $\rho_\infty^{(k)} = f^{\otimes k}$. It is easy to see that the sequence $(\rho_\infty^{(k)}(t))_{k\in\mathbb{N}}$ satisfies the limiting hierarchy (1.14) if and only if $f(t)$ satisfies the *Vlasov equation*

$$\frac{\partial f}{\partial t}(t,x) \;=\; -\frac{p}{m}\cdot\frac{\partial f}{\partial q}(t,x) + \int \mathrm{d}x'\; f(t,x')\,\nabla w(q-q')\cdot\frac{\partial f}{\partial p}(t,x)\,. \tag{1.15}$$

It is of great interest to note that the Vlasov equation – when extended in the obvious way to measures on Γ_1 – describes as a special case the N-body classical dynamics governed by the Hamiltonian equation of motion (1.10). Indeed, a simple calculation shows that the probability measure $N^{-1}\sum_{i=1}^N \delta_{x_i(t)}$ is a solution of the Vlasov equation (1.15) if and only if $(x_1(t),\dots,x_N(t))$ is a solution of the Hamiltonian equation of motion (1.10). Under reasonable assumptions on the interaction potential w, (1.15) has a unique global solution for any initial data that is a finite measure (see Theorem 1.3 below). We conclude that solving the N-body problem (1.10) is equivalent to solving the Vlasov equation (1.15) with initial data of the form $N^{-1}\sum_i \delta_{x_i}$.

This picture of the mean-field limit of classical mechanics was first understood by Braun and Hepp [BH77] and, independently, by Neunzert [Neu75]. Let us outline their main results. As we work with probability measures on Γ_1, it is first necessary to introduce a notion of distance between probability measures. Particularly well suited for this task is the *BL-norm* (where "BL" stands for "bounded Lipschitz"). Denote by $\mathcal{M}$ the space of finite complex measures on Γ_1. The BL-norm is defined on $\mathcal{M}$ through

$$\|\mu\|_{\mathrm{BL}} \;:=\; \sup_{f\in\mathcal{D}}\left|\int \mathrm{d}\mu\; f\right|,$$

where

$$\mathcal{D} \;:=\; \Big\{f\in C(\Gamma_1)\;:\;|f(x)|\leqslant 1\,,\;|f(x)-f(y)|\leqslant|x-y|\Big\}\,.$$

Convergence in the BL-norm is equivalent to convergence in the weak topology of measures. In other words, $\|\mu_N-\mu\|_{\mathrm{BL}}\to 0$ if and only if $\int \mathrm{d}\mu_N\; f \to \int \mathrm{d}\mu\; f$ for all bounded and continuous functions f; see [Dud02].

The fundamental result about both the well-posedness of the Vlasov equation and the classical mean-field limit is the following theorem due to Neunzert [Neu75]; see also [Spo91].

THEOREM 1.3. *Let ∇w be bounded and Lipschitz continuous with a global Lipschitz constant. Then for each $\mu \in \mathcal{M}$ the Vlasov equation* (1.15) *has a unique solution $\mu(t) \in \mathcal{M}$ such that $\mu(0) = \mu$. Moreover, there is a constant K, depending only on w, such that*

$$\|\mu(t) - \nu(t)\|_{\mathrm{BL}} \;\leqslant\; \mathrm{e}^{K|t|}\|\mu(0) - \nu(0)\|_{\mathrm{BL}}\,.$$

Note that the assumptions of Theorem 1.3 are also sufficient for the Hamiltonian equation (1.10) to have unique global solutions. The proof of Theorem 1.3 is a more or less standard contraction mapping argument. The main idea is to rewrite the Vlasov equation using a self-consistent flow on Γ_1, to which standard methods for ordinary differential equations may be applied. See [Neu75] or [Spo91] for the full proof.

Theorem 1.3 makes it clear in what sense the mean-field limit in classical mechanics holds. Take a smooth probability density f on Γ_1 and a sequence of points $X = (x_i)_{i\in\mathbb{N}}$ that approximates f in the weak topology of measures, i.e. the measure

$$\mu_N^X \;:=\; \frac{1}{N}\sum_{i=1}^N \delta_{x_i} \tag{1.16}$$

satisfies $\text{w-lim}_N\, \mu_N^X = f$. Theorem 1.3 and the remark after (1.15) imply that $\text{w-lim}_N\, \mu_N^X(t) = f(t)$ for all t. Here $f(t)$ is the solution of the Vlasov equation (1.15) with initial data f, and

$$\mu_N^X(t) \;=\; \frac{1}{N}\sum_{i=1}^N \delta_{x_i(t)}\,,$$

where $(x_1(t), \dots, x_N(t)) = \phi_t^N(x_1, \dots, x_N)$.

The classical mean-field limit may also be interpreted as the "propagation of molecular chaos": In the mean-field limit factorized N-particle densities remain factorized under time evolution.

THEOREM 1.4. *Let μ be a probability measure on Γ_1. Then under the assumptions of Theorem 1.3 we have for all $t \in \mathbb{R}$ and $k \in \mathbb{N}$ that*

$$\operatorname*{w-lim}_{N\to\infty} \rho_N^{(k)}(t) \;=\; \mu(t)^{\otimes k}\,,$$

where $\rho_N(t)$ is solution of the Liouville equation (1.12) *with initial data $\rho_N(0) = \mu^{\otimes N}$, and $\mu(t)$ is the solution of the Vlasov equation* (1.15) *with initial data $\mu(0) = \mu$.*

PROOF. The proof relies on the strong law of large numbers. We work on the probability space $\Omega = \prod_{i\in\mathbb{N}} \Gamma_1$ with the product Borel algebra and probability measure $\bigotimes_{i\in\mathbb{N}} \mu$. We denote points in Ω by $X = (x_i)_{i\in\mathbb{N}}$. The measure (1.16) is now a random measure, and the strong law of large numbers implies that $\text{w-lim}_N\, \mu_N^X = \mu$ for almost all X. (One only needs to verify that proving weak convergence reduces to proving convergence of $\int \mathrm{d}\mu_N^X\, f$ for a countable family of bounded and continuous functions f.) Thus, Theorem 1.3 implies that

$$\operatorname*{w-lim}_N \mu_N^X(t) \;=\; \mu(t) \tag{1.17}$$

for almost all X and all t.

Next, by integrating with respect to a bounded and continuous test function, one finds

$$\mathbb{E}\Big[\mu_N^X(t, \mathrm{d}y_1) \cdots \mu_N^X(t, \mathrm{d}y_k)\Big] \;=\; \rho_N^{(k)}(t, \mathrm{d}y_1, \dots, \mathrm{d}y_k) + O(N^{-1})\,, \tag{1.18}$$

in the sense of weak convergence of measures. The claim now follows by taking the weak limit $N \to \infty$ in (1.18), using (1.17), and dominated convergence. $\square$

Using a De Finetti type representation theorem and the linearity of the limiting hierarchy (1.14), Theorem 1.4 may immediately be extended to general initial conditions that do not factorize; see [BH77]. Interestingly, we have proven that solutions of the classical BBGKY hierarchy (1.13) converge to solutions of the limiting hierarchy (1.14) without using the hierarchies themselves.

We conclude this section with a discussion on how the mean-field limit may be interpreted as the converse of a quantization, in line with the discussion at the beginning of this chapter. To this end, we show that the classical N-body dynamics is obtained by quantizing the Vlasov equation. We limit ourselves to solutions $\mu(t, \mathrm{d}x) = f(t,x)\,\mathrm{d}x$ that have a nonnegative density $f(t) \in L^1(\Gamma_1)$. The first step is to recognize the Vlasov dynamics generated by (1.15) as a Hamiltonian dynamics on an infinite-dimensional affine phase space Γ_{Vlasov}. To this end, we write $f(x) = \overline{\alpha}(x)\alpha(x)$, where $\overline{\alpha}(x)$ and $\alpha(x)$ are complex coordinates on Γ_{Vlasov}. For our purposes it is enough to say that Γ_{Vlasov} is a dense subspace of $L^2(\Gamma_1)$. The symplectic form of Γ_{Vlasov} is defined by

$$\omega \;=\; \mathrm{i}\int \mathrm{d}x\; \mathrm{d}\overline{\alpha}(x) \wedge \mathrm{d}\alpha(x)\,.$$

This yields the Poisson bracket

$$\{A, B\} \;=\; \mathrm{i}\int \mathrm{d}x\, \left(\frac{\delta A}{\delta\alpha(x)}\frac{\delta B}{\delta\overline{\alpha}(x)} - \frac{\delta B}{\delta\alpha(x)}\frac{\delta A}{\delta\overline{\alpha}(x)}\right),$$

which may be expressed in terms of operator kernels as

$$\{\alpha(x)\,,\overline{\alpha}(y)\} \;=\; \mathrm{i}\delta(x-y)\,, \qquad \{\alpha(x)\,,\alpha(y)\} \;=\; \{\overline{\alpha}(x)\,,\overline{\alpha}(y)\} \;=\; 0\,.$$

The Hamilton function on Γ_{Vlasov} is defined by

$$H(\alpha) \;:=\; -\mathrm{i}\int \mathrm{d}x\; \overline{\alpha}(x)\,\frac{p}{m}\cdot\frac{\partial}{\partial q}\,\alpha(x) + \mathrm{i}\int \mathrm{d}x\; \overline{\alpha}(x)\Big(\int \mathrm{d}x'\; |\alpha(x')|^2\, \nabla w(q-q')\Big)\cdot\frac{\partial}{\partial p}\,\alpha(x)\,.$$

Note that H is invariant under gauge transformations $\alpha(x) \mapsto \mathrm{e}^{-\mathrm{i}\theta}\alpha(x)$, $\overline{\alpha}(x) \mapsto \mathrm{e}^{\mathrm{i}\theta}\overline{\alpha}(x)$, which by Noether's theorem implies (at least formally) that $\int \mathrm{d}x\; |\alpha|^2$ is conserved. After a short calculation, we find that the Hamiltonian equation of motion, $\partial_t\alpha(t,x) = \{H\,, \alpha(t,x)\}$, is given by

$$\begin{aligned}\frac{\partial\alpha}{\partial t}(t,x) \;=\; -\frac{p}{m}\cdot\frac{\partial\alpha}{\partial q}(t,x) + \int \mathrm{d}x'\; |\alpha(t,x')|^2\, \nabla w(q-q')\cdot\frac{\partial\alpha}{\partial p}(t,x) \\ - \int \mathrm{d}x'\; \overline{\alpha}(t,x')\alpha(t,x)\, \nabla w(q-q')\cdot\frac{\partial\alpha}{\partial p'}(t,x')\,.\end{aligned} \tag{1.19}$$

Similarly, we find that $\overline{\alpha}(t,x)$ satisfies the complex conjugate equation. Therefore,

$$\begin{aligned}\frac{\partial}{\partial t}|\alpha(t,x)|^2 \;=\; -\frac{p}{m}\cdot\frac{\partial}{\partial q}|\alpha(t,x)|^2 + \int \mathrm{d}x'\; |\alpha(t,x')|^2\, \nabla w(q-q')\cdot\frac{\partial}{\partial p}|\alpha(t,x)|^2 \\ - |\alpha(t,x)|^2 \int \mathrm{d}x'\; \nabla w(q-q')\cdot\Big[\overline{\alpha}(t,x')\frac{\partial\alpha}{\partial p'}(t,x') + \alpha(t,x')\frac{\partial\overline{\alpha}}{\partial p'}(t,x')\Big]\,.\end{aligned} \tag{1.20}$$

We assume that

$$|\alpha(x)| \;=\; o(|x|^{-(d-1)/2})\,, \qquad |x| \to \infty\,. \tag{1.21}$$

We shall shortly see that this property is preserved under time evolution. By integration by parts we now find that the second line of (1.20) vanishes. Therefore $f(t,x) = |\alpha(t,x)|^2$ satisfies the Vlasov equation (1.15).

We comment briefly on the existence, uniqueness, and properties of solutions of the Hamiltonian equation of motion (1.19). We make the same assumptions on w as above, i.e. ∇w is bounded and Lipschitz continuous with a global Lipschitz constant. We use polar coordinates,

$$\alpha(t,x) \;=\; \beta(t,x)\,\mathrm{e}^{\mathrm{i}\varphi(t,x)}\,,$$

where $\beta(t,x) \geqslant 0$ and $\varphi(t,x) \in \mathbb{R}$. In the new coordinates β and φ the Hamiltonian equation of motion (1.19) reads

$$\frac{\partial \beta}{\partial t}(t,x) \;=\; -\frac{p}{m}\cdot\frac{\partial \beta}{\partial q}(t,x) + \int \mathrm{d}x'\;\beta(t,x')^2\,\nabla w(q-q')\cdot\frac{\partial \beta}{\partial p}(t,x)\,, \tag{1.22a}$$

$$\begin{aligned}\frac{\partial \varphi}{\partial t}(t,x) \;&=\; -\frac{p}{m}\cdot\frac{\partial \varphi}{\partial q}(t,x) + \int \mathrm{d}x'\;\beta(t,x')^2\,\nabla w(q-q')\cdot\frac{\partial \varphi}{\partial p}(t,x)\\ &\qquad - \int \mathrm{d}x'\;\beta(t,x')^2\,\nabla w(q-q')\cdot\frac{\partial \varphi}{\partial p'}(t,x')\,.\end{aligned} \tag{1.22b}$$

We consider two cases.

(i) $\varphi = 0$. In this case $\alpha = \beta$ and the equations of motion (1.22) are equivalent to the Vlasov equation (1.15) for $f = \beta^2$. The results of [Neu75] then yield a global well-posedness result.

(ii) $\varphi \neq 0$. The equation of motion (1.22a) is independent of φ. Case (i) implies that it has a unique global solution $\beta(t)$. In order to solve the linear equation (1.22b), we apply a contraction mapping argument. Consider the space $X := \{\varphi \in C(\mathbb{R}^6) \,:\, \nabla\varphi \in L^\infty(\mathbb{R}^6)\}$. Using Sobolev inequalities one finds that X, equipped with the norm $\|\varphi\|_X := |\varphi(0)| + \|\nabla\varphi\|_\infty$, is a Banach space. We rewrite (1.22b) as an integral equation using Duhamel's principle, and, using a standard contraction mapping argument on $C([0,T];X)$, show that it has a unique solution for small times T. Using conservation of $\int \mathrm{d}x\,\beta(t,x)^2$ we iterate this procedure to find a global solution. We omit the uninteresting details.

As noted in [BH77], the solution $\beta(t)$ can be written using a flow ϕ_t on the one-particle phase space: $\beta(t,x) = \beta(0,\phi_{-t}(x))$. The flow $\phi_t(x) = (p(t),q(t))$ satisfies

$$\begin{aligned}\dot p(t) \;&=\; -\int \mathrm{d}x'\;\beta(t,x')^2\,\nabla w(q(t)-q')\\ \dot q(t) \;&=\; \frac{p(t)}{m}\,.\end{aligned}$$

Using conservation of $\int \mathrm{d}x\,\beta(t,x)^2$ we find that there is a constant C such that $|\phi^{-t}(x)| \leqslant C(1+t)^2(1+|x|)$. In particular, the condition (1.21) holds for all times t provided that it holds at time $t=0$.

This completes our discussion on the Hamiltonian nature of the Vlasov equation. By a quantization, the Hamiltonian formulation of the Vlasov equation can serve as a starting point to recover the atomistic Hamiltonian mechanics of point particles. To this end, we canonically quantize the classical Hamiltonian system. The Hilbert space $\mathcal{H}$ is the bosonic Fock space over the one-particle Hilbert space $L^2(\Gamma_1)$. Denote by $a^*(x)$ and $a(x)$ the usual creation and annihilation operators on $\mathcal{H}$. It is convenient to introduce the rescaled creation and annihilation operators, $a_N(x) := N^{-1/2}\, a(x)$ and $a_N^*(x) := N^{-1/2}\, a^*(x)$, which satisfy the canonical commutation relations

$$\big[a_N(x), a_N^*(y)\big] \;=\; \frac{1}{N}\,\delta(x-y)\,, \qquad \big[a_N(x), a_N(y)\big] \;=\; \big[a_N^*(x), a_N^*(y)\big] \;=\; 0\,. \tag{1.23}$$

As our algebra $\mathfrak{A}$ of classical observables we take the polynomials[4] in α and $\overline{\alpha}$. Given $A \in \mathfrak{A}$, we define its quantization $\widehat{A}_N$ as the operator on $\mathcal{H}$ obtained from A by the replacement $\alpha \mapsto a_N$, $\overline{\alpha} \mapsto a_N^*$, followed by Wick ordering. It is easy to see that the map $A \mapsto \widehat{A}_N$ defines a quantization with parameter N^{-1}.

The Schrödinger dynamics of the quantized system is given by

$$\mathrm{i}N^{-1}\partial_t \Psi(t) \;=\; \widehat{H}_N \Psi(t)\,, \qquad \Psi(0) = \Psi\,, \tag{1.24}$$

where $\Psi(t) \in \mathcal{H}$. Let us consider initial data Ψ_N that lies in the N-particle subspace $\mathcal{H}^{(N)}$ of $\mathcal{H}$. Since $\widehat{H}_N$ is gauge invariant, the solution $\Psi(t)$ of (1.24) satisfies $\Psi_N(t) \in \mathcal{H}^{(N)}$. We now claim that $\rho_N(t) := |\Psi_N(t)|^2$ satisfies the Liouville equation (1.12). Let us outline the proof. Note first that $\Psi_N(t)$ may be written using creation operators as

$$\Psi_N(t) \;=\; \frac{N^{N/2}}{\sqrt{N!}} \int \mathrm{d}x_1 \cdots \mathrm{d}x_N\; \Psi_N(t, x_1, \dots, x_N)\, a_N^*(x_N) \cdots a_N^*(x_1)\, \Omega\,,$$

where Ω is the vacuum of $\mathcal{H}$. Then one finds after a simple calculation using the canonical commutation relations (1.23) that

$$\partial_t \Psi_N(t, x_1, \dots, x_N) \;=\; -\sum_{i=1}^N \frac{p_i}{m} \cdot \frac{\partial \Psi_N}{\partial q_i}(t, x_1, \dots, x_N) + \frac{1}{N} \sum_{i,j} \nabla w(q_i - q_j) \cdot \frac{\partial \Psi_N}{\partial p_i}(t, x_1, \dots, x_N)\,.$$

It now follows immediately that $\rho_N(t) = |\Psi_N(t)|^2$ satisfies the Liouville equation (1.12), as claimed. Thus we have shown that classical N-body dynamics can be interpreted as the quantization of the Vlasov dynamics: Atomism arises as the quantization with parameter N^{-1} of a continuum theory.

1.1.3. The mean-field limit in quantum mechanics. As our final example we give a short overview of the mean-field limit in quantum mechanics. This section differs slightly from the two previous ones in spirit. Since the quantum mean-field limit is a major topic in this thesis, we restrict the discussion in this introductory section to some background along with the traditional approach to the mean-field limit in quantum mechanics, the quantum BBGKY hierarchy. Other topics of interest (such as alternative methods, estimates on the rate of convergence, general potentials, and Egorov-type formulations) represent new results and are as such postponed to later chapters.

We consider a system of N identical quantum particles in d dimensions, whose state is given by a wave function $\Psi_N \in \mathcal{H}^{(N)} := L^2(\mathbb{R}^{dN}, \mathrm{d}x_1 \cdots \mathrm{d}x_N)$. The particles are indistinguishable, so that Ψ_N is either totally symmetric (in the case of bosons) or totally antisymmetric (in the case of fermions). That is,

$$\Psi_N(x_{\sigma(1)}, \dots, x_{\sigma(N)}) \;=\; (\pm 1)^\sigma\, \Psi_N(x_1, \dots, x_N)$$

[4]By a *polynomial* we mean a finite sum of mappings of the form $(\alpha, \overline{\alpha}) \mapsto \langle \alpha^{\otimes p}, a^{(p,q)} \alpha^{\otimes q} \rangle$, where $a^{(p,q)}$ is a closed operator from $L^2(\Gamma_q)$ to $L^2(\Gamma_p)$.

for all $\sigma \in S_N$, where $+$ stands for bosons and $-$ for fermions. In this section we assume that we are dealing with bosons, and denote by $\mathcal{H}_+^{(N)}$ the subspace of $\mathcal{H}^{(N)}$ consisting of symmetric wave functions (see Chapter 4 for more details on fermions). The Hamiltonian on $\mathcal{H}_+^{(N)}$ is given by

$$H_N \;=\; \sum_{i=1}^N h_i + \frac{1}{N} \sum_{1 \leqslant i<j \leqslant N} w(x_i - x_j)\,,$$

where h_i denotes a one-particle Hamiltonian h acting on the coordinate x_i, and w is an interaction potential, a real and even function. Typically, $h = -\frac{1}{2m}\Delta + v(x)$, where Δ is the Laplacian over $\mathbb{R}^d$ and v is a real function representing an external potential. Under reasonable assumptions on h and w, one shows that H_N gives rise to a self-adjoint operator on $\mathcal{H}_+^{(N)}$. The dynamics of the N-particle wave function $\Psi_N(t)$ is given by the Schrödinger equation

$$\mathrm{i}\partial_t \Psi_N(t) \;=\; H_N \Psi_N(t)\,, \qquad \Psi_N(0) \;=\; \Psi_N\,, \tag{1.25}$$

with solution

$$\Psi_N(t) \;=\; \mathrm{e}^{-\mathrm{i}tH_N}\Psi_N\,.$$

The interpretation of the factor $1/N$ in front of the interaction potential in H_N is exactly the same as in the previous section.

Next, let us consider factorized initial data $\Psi_N = \varphi^{\otimes N}$ for some $\varphi \in L^2(\mathbb{R}^d)$ satisfying the normalization condition $\|\varphi\|_{L^2(\mathbb{R}^d)} = 1$. Clearly, because of the interaction between the particles, the factorization of the wave function is not preserved by the time evolution. However, it turns out that for large N the interaction potential experienced by any single particle may be approximated by an effective mean-field potential, so that the wave function $\Psi_N(t)$ remains approximately factorized for all times. In other words we have that, in a sense to be made precise, $\Psi_N(t) \approx \varphi(t)^{\otimes N}$ for some appropriate $\varphi(t)$. This has the interpretation of "propagation of molecular chaos": For large N factorized states remain factorized under time evolution. A simple argument shows that in a product state $\varphi(t)^{\otimes N}$ the interaction potential experienced by a particle is approximately $w * |\varphi(t)|^2$, where $*$ denotes convolution. This implies that $\varphi(t)$ is a solution of the nonlinear *Hartree equation*

$$\mathrm{i}\partial_t \varphi(t) \;=\; h\varphi(t) + \big(w * |\varphi(t)|^2\big)\varphi(t)\,, \qquad \varphi(0) \;=\; \varphi\,. \tag{1.26}$$

Let us be a little more precise about what one means with $\Psi_N \approx \varphi^{\otimes N}$ (we omit the irrelevant time argument). One does not expect the L^2-distance $\big\|\Psi_N - \varphi^{\otimes N}\big\|_{L^2(\mathbb{R}^{Nd})}$ to become small as $N \to \infty$. A more useful, weaker, indicator of convergence should depend only on a finite, fixed number, k, of particles. This leads us to defining, in analogy to the reduced marginals $\rho_N^{(k)}$ of the previous section, the reduced k-particle density matrix

$$\gamma_N^{(k)} \;:=\; \mathrm{Tr}_{k+1,\dots,N}\, |\Psi_N\rangle\langle\Psi_N|\,,$$

where $\mathrm{Tr}_{k+1,\dots,N}$ denotes the partial trace over the coordinates $x_{k+1},\dots,x_N$, and $|\Psi_N\rangle\langle\Psi_N|$ denotes (in accordance with the usual Dirac notation) the orthogonal projector onto Ψ_N. In other words, $\gamma_N^{(k)}$ is the positive trace class operator on $L_+^2(\mathbb{R}^{kd}, \mathrm{d}x_1 \cdots \mathrm{d}x_k)$ with operator kernel

$$\gamma_N^{(k)}(x_1,\dots,x_k;y_1,\dots,y_k) \;=\; \int \mathrm{d}x_{k+1}\cdots \mathrm{d}x_N\; \Psi_N(x_1,\dots,x_N)\overline{\Psi_N(y_1,\dots,y_k,x_{k+1},\dots,x_N)}\,.$$

The reduced k-particle density matrix $\gamma_N^{(k)}$ embodies all the information contained in the full N-particle wave function that pertains to at most k particles. One expects that for each $k \in \mathbb{N}$ the reduced density matrix $\gamma_N^{(k)}(t)$ converges (in some appropriate topology) to the projector $(|\varphi(t)\rangle\langle\varphi(t)|)^{\otimes k}$ for all times t provided this holds at time 0.

As in the classical case, the time evolution of the reduced density matrices is given by a hierarchy of equations. Consider a solution $\Psi_N(t)$ of the Schrödinger equation (1.25). A straightforward computation shows that the associated sequence of density matrices $\big(\gamma_N^{(k)}(t)\big)_{k\in\mathbb{N}}$ satisfies the hierarchy

$$\begin{aligned} \mathrm{i}\partial_t \gamma_N^{(k)}(t) \;=\; & \sum_{i=1}^{k} \Big[h_i \,,\, \gamma_N^{(k)}(t)\Big] + \frac{1}{N} \sum_{1\leqslant i<j\leqslant k} \Big[w(x_i - x_j) \,,\, \gamma_N^{(k)}(t)\Big] \\ & + \frac{N-k}{N} \sum_{i=1}^{k} \mathrm{Tr}_{k+1} \Big[w(x_i - x_{k+1}) \,,\, \gamma_N^{(k+1)}(t)\Big] \,, \end{aligned} \tag{1.27}$$

the *quantum BBGKY hierarchy*. Formally taking the limit $N \to \infty$ in (1.27) yields the *limiting hierarchy* for the sequence $\big(\gamma_\infty^{(k)}(t)\big)_{k\in\mathbb{N}}$

$$\mathrm{i}\partial_t \gamma_\infty^{(k)}(t) \;=\; \sum_{i=1}^{k} \Big[h_i \,,\, \gamma_\infty^{(k)}(t)\Big] + \sum_{i=1}^{k} \mathrm{Tr}_{k+1} \Big[w(x_i - x_{k+1}) \,,\, \gamma_\infty^{(k+1)}(t)\Big] \,. \tag{1.28}$$

Thus one expects for large N that $\gamma_N^{(k)}(t) \approx \gamma_\infty^{(k)}(t)$ for all times t provided this holds at time 0. If we start in a product state $\gamma_N^{(k)}(0) = \gamma_\infty^{(k)}(0) \;=\; (|\varphi\rangle\langle\varphi|)^{\otimes k}$, this formulation of the mean-field limit is equivalent to the one in terms of the Hartree equation outlined above. Indeed, it is a simple computation to check that the sequence $\big((|\varphi(t)\rangle\langle\varphi(t)|)^{\otimes k}\big)_{k\in\mathbb{N}}$ solves the limiting hierarchy (1.28) if and only if $\varphi(t)$ solves the Hartree equation (1.26).

This general picture of the quantum mean-field limit was first understood by Hepp [Hep74] by using the semiclassical argument outlined in Section 1.1.1. Spohn [Spo80] realized the usefulness of the BBGKY hierarchy when dealing with the quantum mean-field limit, and strengthened the results of Hepp by proving the following theorem.

THEOREM 1.5. *Suppose that h is self-adjoint and w is bounded, i.e. $w \in L^\infty(\mathbb{R}^d)$. Take a one-particle wave function $\varphi \in L^2(\mathbb{R}^d)$ normalized as $\|\varphi\|_{L^2(\mathbb{R}^d)} = 1$. Then, for all $k \in \mathbb{N}$ and $t \in \mathbb{R}$, we have*

$$\lim_{N\to\infty} \mathrm{Tr}\Big|\gamma_N^{(k)}(t) - (|\varphi(t)\rangle\langle\varphi(t)|)^{\otimes k}\Big| \;=\; 0\,, \tag{1.29}$$

where $\varphi(t)$ is the solution of the Hartree equation (1.26) *and $\gamma_N^{(k)}(t)$ is the k-particle reduced density matrix of* $\mathrm{e}^{-\mathrm{i}tH_N}\varphi^{\otimes N}$.

Unlike the classical BBGKY hierarchy, its quantum counterpart is thus a powerful tool for proving theorems. The idea of Spohn's proof is to rewrite, using Duhamel's principle, the BBGKY hierarchy (1.27) as an integral equation, and iterate it to get a power series representation of $\gamma_N^{(k)}(t)$. Applying the same strategy to the limiting hierarchy (1.28) yields a power series expansion for $\gamma_\infty^{(k)}(t)$. Using standard trace inequalities, it is then easy to show that, for short times, $\mathrm{Tr}\big|\gamma_N^{(k)}(t) - \gamma_\infty^{(k)}(t)\big|$ vanishes as $N \to \infty$. The result is then extended to all times by iteration.

A different strategy for proving Theorem 1.5 was proposed in [BGM00, BEG$^+$00, EY01]. It turns out that, thanks to an abstract compactness argument, it is possible to entirely avoid the expansion of the BBGKY hierarchy, which is much more involved than the expansion of the limiting hierarchy. This strategy is especially useful in the case of singular interaction potentials (or singular scalings of the interaction potential for which the limiting dynamics is governed by the Gross-Pitaevskii equation), where controlling the expansion of the BBGKY hierarchy is an all but hopeless task. Let us denote by $\Gamma_N(t)$ the sequence $\big(\gamma_N^{(k)}(t)\big)_{k\in\mathbb{N}}$. The proof consists of three main steps.

(i) The sequence $\big(\Gamma_N(t)\big)_{N\in\mathbb{N}}$ is compact in an appropriate weak topology. This follows from an abstract argument using the Banach-Alaoglu theorem. Thus one infers that $\big(\Gamma_N(t)\big)_{N\in\mathbb{N}}$ has a weak limit point.

(ii) Any weak limit point of the sequence $\big(\Gamma_N(t)\big)_{N\in\mathbb{N}}$ satisfies the limiting hierarchy. To prove this one only needs to control the integral form of the BBGKY hierarchy (as opposed to its full expansion).

(iii) The limiting hierarchy has a unique solution. One shows this by expansion of the limiting hierarchy.

Putting the three steps together, one infers that $\Gamma_N(t)$ converges to $\Gamma_\infty(t) = \big(\gamma_\infty^{(k)}(t)\big)_{k\in\mathbb{N}}$ as $N \to \infty$ in the weak topology in which compactness was established. Using the fact that the limiting sequence $\big(\gamma_\infty^{(k)}(t)\big)_{k\in\mathbb{N}}$ consists of one-dimensional projections, one can then show (using Grümm's theorem; see [Sim05]) that the convergence holds in fact in the sense of (1.29).

We refer to Chapters 4 and 5 for more details about subsequent results on the quantum mean-field limit. A Egorov-type formulation of the quantum mean-field limit is given in Chapter 4.

1.2. Outline and summary of results

This thesis is organized as follows.

Chapter 2. In Chapter 2 we study the dynamics of a finite number of quantum particles coupled to the quantized radiation field. The time evolution is generated by the Pauli-Fierz Hamiltonian of nonrelativistic quantum electrodynamics. We consider the regime of heavy particles and strong radiation field, i.e. large photon number. We prove that the limiting dynamics is governed by the coupled Newton-Maxwell equations. We also establish global well-posedness of the Newton-Maxwell equations in appropriate spaces of solutions. Our analysis of the limiting dynamics is based on Hepp's semiclassical argument [Hep74].

Chapter 3. Chapter 3 is devoted to the study of limiting dynamics in various quantum lattice models. In a first part, we consider a general model of interacting quantum spins on a lattice, and study two limiting regimes: the large-spin limit and the continuum limit. In both cases, we identify the limiting dynamics as the Hamiltonian dynamics of a classical system of spins. This provides a rigorous derivation of the Landau-Lifschitz equation, in its various guises, from quantum dynamics. We extend our results to domains of infinite size and discuss as a special case the limiting dynamics of coherent spin states. Our proof is based on a perturbative expansion of the dynamics.

In a second part, we study time-dependent correlation functions of thermal states in the large-spin limit. We prove that a time-dependent correlation function at a fixed temperature converges to the corresponding time-dependent correlation function of a classical spin system. The main tool in our proof is an expansion in coherent spin states. For high enough temperatures, we extend this result to an infinite lattice using a quantum cluster expansion.

In a third part, we study the mean-field behaviour of time-dependent correlation functions of a Bose gas on a finite lattice. Compared to a quantum spin system, the lattice Bose gas presents additional difficulties arising from the fact that the density of particles is unbounded. In particular, more efforts are needed to control expansions.

Chapter 4. In Chapter 4 we study the mean-field dynamics of quantum gases with a Coulomb interaction potential and a weak external potential. Our method is based on a perturbative graph expansion scheme for the dynamics of observables. We control the Coulomb singularity by counting graphs and by exploiting the dispersive nature of the free time evolution. We first consider the mean-field limit of a Bose gas. We describe how the quantum N-body dynamics arises as the quantization of the Hartree equation, and prove a Egorov-type theorem. Next, we consider the mean-field limit of a system of fermions describing for instance electrons in a large atom or molecule. We prove that their limiting time evolution is governed by the Hartree-Fock equation. We also show how the N-body theory of the Fermi gas may be viewed as the quantization of a "superhamiltonian" system of anticommuting variables. This allows us to state and prove a Egorov-type theorem.

Chapter 5. Chapter 5 is devoted to the mean-field dynamics of coherent states in a Bose gas. Using a nonperturbative method that does not rely on the dispersive nature of the free time evolution, we strengthen and generalize many previously known results in two directions. First, we consider a large class of singular interaction potentials as well as strong, possibly time-dependent, external potentials. This allows us to deal for instance with the critical interaction potential $|x|^{-2}$ for nonrelativistic bosons, as well as strongly confining time-dependent traps. Second, we derive estimates on the rate of convergence to the mean-field limit. Thus we can for instance control the error in the mean-field approximation of a boson star. We also show that, if the mean-field dynamics satisfies a scattering condition, all error estimates are uniform in time. Moreover, we derive optimal bounds on the fraction of particles whose convergence to the mean-field limit can be controlled.

Appendices. For easy reference, we collect some standard results in the appendices. In Appendix A, we review cluster expansions and discuss their convergence using the Kotecký-Preiss criterion. Appendix B is devoted to integral inequalities, Lorentz spaces, and the real interpolation method. Finally, in Appendix C we list some Grönwall-type estimates useful for controlling time-dependent quantities.

1.3. Conventions and notations

Throughout this thesis we use "god-given" units in which the speed of light c and Planck's constant $\hbar$ are equal to 1. We use mostly standard mathematical notation. The following table lists mathematical symbols commonly used in this thesis.

List of symbols.

$\mathbb{N}_n$	$= \{1, \dots, n\}$
$\mathbb{1}_{\{\mathscr{A}\}}$	equal to 1 if $\mathscr{A}$ is true and 0 if $\mathscr{A}$ is false
C	a constant that can depend on fixed parameters
$a \lesssim b$	equivalent to $a \leqslant Cb$
$\mathcal{G}(A)$	the set of graphs with vertex set A
$\mathcal{G}_c(A)$	the set of connected graphs with vertex set A
$L^p(\Omega, \mathrm{d}\mu)$	the space of complex-valued functions f such that $\|f\|_{L^p(\Omega,\mathrm{d}\mu)} < \infty$, where $$\|f\|_{L^p(\Omega,\mathrm{d}\mu)} = \|f\|_{L^p} := \begin{cases} \left(\int \mathrm{d}\mu(x)\, \lvert f(x)\rvert^p\right)^{1/p} & \text{if } 0 < p < \infty \\ \operatorname{ess\,sup}_{x\in\Omega} \lvert f(x)\rvert & \text{if } p = \infty \end{cases}$$
$L^p(\Omega) = L^p$	$= L^p(\Omega, \mathrm{d}\mu)$
$L^p_w(\Omega) = L^p_w$	the weak L^p space; see Appendix B
$\hat{f}$	the Fourier transform of f, defined by $\hat{f}(k) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{d}x\, f(x)\, \mathrm{e}^{-\mathrm{i}k\cdot x}$
$H^s(\mathbb{R}^d) = H^s$	the Sobolev space of functions f on $\mathbb{R}^d$ such that $\|f\|_{H^s} < \infty$, where $$\|f\|_{H^s} := \left(\int \mathrm{d}x\, (1 + \lvert k\rvert^2)^{s/2} \lvert\hat{f}(k)\rvert^2\right)^{1/2}$$
$f * g$	the convolution $(f * g)(x) := \int \mathrm{d}y\, f(x-y)g(y)$
∇	the differential operator $\left(\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_d}\right)$
Δ	the Laplacian $\sum_{i=1}^d \frac{\partial^2}{\partial x_i^2}$
$\times$	the vector product on $\mathbb{R}^3$
$C^\infty(\mathbb{R}^d) = C^\infty$	the space of smooth functions on $\mathbb{R}^d$
$C^\infty_c(\mathbb{R}^d) = C^\infty_c$	the space of smooth functions with compact support on $\mathbb{R}^d$
$\mathcal{S}(\mathbb{R}^d) = \mathcal{S}$	the Schwartz space of smooth functions of rapid decrease on $\mathbb{R}^d$
$\mathcal{S}'(\mathbb{R}^d) = \mathcal{S}'$	the Schwartz space of tempered distributions on $\mathbb{R}^d$
$C(X;Y)$	the space of continuous functions from X to Y
$C^k(X;Y)$	the space of functions from X to Y that are k times continuously differentiable
$\mathcal{L}(X;Y)$	the space of linear, continuous mappings from X to Y
$\mathcal{L}(X) = \mathcal{L}$	$= \mathcal{L}(X;X)$
$\mathcal{H}$	a Hilbert space
$\langle\cdot,\cdot\rangle$	the scalar product of a Hilbert space, linear in the second argument
$[A, B]$	the commutator $AB - BA$
$\{\cdot,\cdot\}$	the Poisson bracket of a Poisson manifold
$\mathcal{L}^p(\mathcal{H}) = \mathcal{L}^p$	the space of operators $A \in \mathcal{L}(\mathcal{H})$ such that $\operatorname{Tr}\lvert A\rvert^p < \infty$
$\|\cdot\|_p$	the L^p-norm, $\|f\|_p = \|f\|_{L^p}$; the $\mathcal{L}^p$-norm, $\|A\|_p = \left(\operatorname{Tr}\lvert A\rvert^p\right)^{1/p}$

$\|\cdot\|$	the L^2-norm; the operator norm on $\mathcal{L}(X;Y)$
$\mathcal{D}(A)$	the operator domain of A
$\mathcal{Q}(A)$	the form domain of a semibounded operator A
$P_\pm$	the orthogonal projector onto the symmetric/antisymmetric subspace of $\mathcal{H}^{\otimes n}$, defined by linearity and $$P_\pm\,\psi_1\otimes\cdots\otimes\psi_n \;:=\; \frac{1}{n!}\sum_{\sigma\in S_n}(\pm 1)^\sigma\,\psi_{\sigma(1)}\otimes\cdots\otimes\psi_{\sigma(n)}$$
$\mathcal{H}_\pm^{(n)}$	$= P_\pm\mathcal{H}^{\otimes n}$
$\mathcal{F}_\pm(\mathcal{H})$	the symmetric/antisymmetric Fock space over $\mathcal{H}$, defined by $$\mathcal{F}_\pm(\mathcal{H}) \;:=\; \bigoplus_{n\in\mathbb{N}} P_\pm\mathcal{H}^{\otimes n}$$
$A_{i_1\cdots i_p}$	For an operator A on $\mathcal{H}^{\otimes p}$, $n\geqslant p$, and $1\leqslant i_1<\cdots<i_p\leqslant n$, the operator $A_{i_1\cdots i_p}$ on $\mathcal{H}^{\otimes n}$ is defined by letting A act on the factors $i_1,\dots,i_p$ of $\mathcal{H}^{\otimes n}$.
$\mathrm{Tr}_{p+1\cdots n}(\cdot)$	For $n>p$ the partial trace $$\mathrm{Tr}_{p+1\cdots n}\,:\,\mathcal{L}^1(\mathcal{H}^{\otimes n})\;\longrightarrow\;\mathcal{L}^1(\mathcal{H}^{\otimes p})\,,$$ is defined through $$\mathrm{Tr}\big((\mathrm{Tr}_{p+1\cdots n}\,A)B\big) \;:=\; \mathrm{Tr}\big(A(B\otimes\mathbb{1}^{(n-p)})\big)\,,$$ where $A\in\mathcal{L}^1(\mathcal{H}^{\otimes n})$, $B\in\mathcal{L}(\mathcal{H}^{\otimes p})$ and $\mathbb{1}^{(n-p)}\in\mathcal{L}(\mathcal{H}^{\otimes(n-p)})$ is the identity.
$X\cap Y$	For two Banach spaces X and Y contained in some topological vector space, $X\cap Y$ is the Banach space of vectors $u\in X\cap Y$ with norm $$\|u\|_{X\cap Y} \;:=\; \|u\|_X+\|u\|_Y\,.$$
$X+Y$	For two Banach spaces X and Y contained in some topological vector space, $X+Y$ is the Banach space of vectors u that can be written as $u=x+y$, where $x\in X$ and $y\in Y$; it carries the norm $$\|u\|_{X+Y} \;:=\; \inf_{u=x+y}\,(\|x\|_X+\|y\|_Y)\,.$$

Chapter 2

Heavy Particles Interacting with a Strong Quantized Radiation Field

In this chapter we consider the dynamics of a finite number of nonrelativistic quantum particles interacting with the quantized radiation field. We are interested in the limit of a strong field and heavy particles, where the number of photons and the mass of each particle are large. One expects that the quantum nature of the radiation field vanishes and the field becomes classical, and that the particles evolve according to the laws of classical mechanics. Indeed, our main result (Theorem 2.3) states that the limiting dynamics is given by the coupled (regularized) Newton-Maxwell equations.

2.1. The classical system

We start with a discussion of the classical dynamics of particles coupled to an electromagnetic field. It is well known that the coupled Newton-Maxwell equations make no sense. Indeed, the electromagnetic field generated by a point particle is singular at the particle's location, and hence leads to an ill-defined Lorentz force acting on the particle. This problem of self-interaction is traditionally removed by arguing that there is a physical cutoff in the smallness of a particle, which arises from a more refined theory. We therefore replace the point particles with particles whose charge density is smeared out over a small volume. To this end, let us choose a spherically symmetric function $\varphi \in C_c^\infty(\mathbb{R}^3)$ satisfying $\varphi(x) \geqslant 0$ and $\int \mathrm{d}x\, \varphi(x) = 1$. Let N denote the number of particles. Particle $i = 1, \dots, N$ is described by its position $q_i \in \mathbb{R}^3$, its momentum $p_i \in \mathbb{R}^3$, its mass $m_i > 0$, and its charge $e_i \in \mathbb{R}$. The electromagnetic field consists of the electric and magnetic fields $E, B : \mathbb{R}^3 \to \mathbb{R}^3$. Each particle i carries a smooth charge density $e_i \varphi(x - q_i)$. The dynamics of the particle-field system is then given by the regularized Newton-Maxwell equations, also called the *Abraham model*:

$$\begin{aligned}
\dot{B} &= -\nabla \times E\,, & \nabla \cdot B &= 0\,,\\
\dot{E} &= -j + \nabla \times B\,, & \nabla \cdot E &= \rho\,,\\
\dot{q}_i &= \frac{p_i}{m_i}\\
\dot{p}_i &= e_i\big((\varphi * E)(q_i) + \frac{p_i}{m_i} \times (\varphi * B)(q_i)\big)\,,
\end{aligned} \tag{2.1}$$

where

$$\rho(x) := \sum_{i=1}^N e_i\, \varphi(x - q_i)\,, \qquad j(x) := \sum_{i=1}^N e_i\, \frac{p_i}{m_i}\, \varphi(x - q_i) \tag{2.2}$$

are the charge and current densities, respectively. The two equations in the right-hand column of (2.1) are not equations of motion, but conditions on the fields E and B. If these conditions hold for some initial time, they hold for all times; this follows from the equations of motion (2.1) and the continuity equation $\dot\rho + \nabla \cdot j = 0$, an immediate consequence of (2.2).

For our purposes it convenient to replace the fields E and B by a single complex field α, representing the Fourier components of the electromagnetic vector potential in the Coulomb gauge. Let $\{\varepsilon_\lambda(k)\}_{k\in\mathbb{R}^3,\lambda\in\mathbb{N}_2}$ be a family of complex basis vectors such that $(k, \varepsilon_1(k), \varepsilon_2(k))$ is an orthonormal basis of $\mathbb{C}^3$ for each $k \in \mathbb{R}^3$. Define $\chi := \hat\varphi$. By assumption χ is smooth and decays faster than any power law. Let $\alpha : \mathbb{R}^3 \times \mathbb{N}_2 \to \mathbb{C}$ be a complex field and abbreviate $p = (p_1, \ldots, p_n) \in \mathbb{R}^{3N}$ as well as $q = (q_1, \ldots, q_N) \in \mathbb{R}^{3N}$. Consider the equation of motion for the triple (p, q, α) given by[1]

$$
\begin{aligned}
\partial_t p_i &= \frac{e_i}{m_i}\big(p_i - e_i A(q_i,\alpha)\big)_\mu \nabla_{q_i} A_\mu(q_i,\alpha) - \nabla_{q_i} V(q) \\
\partial_t q_i &= \frac{1}{m_i}\big(p_i - e_i A(q_i,\alpha)\big)\,, \\
\partial_t \alpha_\lambda(k) &= -\mathrm{i}|k|\alpha_\lambda(k) + \mathrm{i}\sum_{i=1}^N \frac{e_i}{m_i}\frac{\chi(k)}{(2\pi)^{3/2}\sqrt{2|k|}}\big(p_i - e_i A(q_i,\alpha)\big)\cdot\overline{\varepsilon}_\lambda(k)\mathrm{e}^{-\mathrm{i}k\cdot q_i}\,,
\end{aligned}
\tag{2.3}
$$

where

$$
A(x,\alpha) := \sum_\lambda \int \frac{\mathrm{d}k}{(2\pi)^{3/2}} \frac{\chi(k)}{\sqrt{2|k|}}\Big(\varepsilon_\lambda(k)\alpha_\lambda(k)\mathrm{e}^{\mathrm{i}k\cdot x} + \overline{\varepsilon}_\lambda(k)\overline{\alpha}_\lambda(k)\mathrm{e}^{-\mathrm{i}k\cdot x}\Big)
$$

and

$$
V(q) = \sum_{i<j} e_i e_j w(q_i - q_j)\,. \tag{2.4}
$$

Here $w = \varphi * \frac{1}{4\pi|\cdot|} * \varphi$ is the regularized Coulomb potential. It is a standard computation to show that (2.3) is equivalent to (2.1) with the identification

$$
\begin{aligned}
E(x) &= \mathrm{i}\sum_\lambda \int \frac{\mathrm{d}k}{(2\pi)^{3/2}}\frac{\sqrt{|k|}}{\sqrt{2}}\Big(\varepsilon_\lambda(k)\alpha_\lambda(k)\mathrm{e}^{\mathrm{i}k\cdot x} - \overline{\varepsilon}_\lambda(k)\overline{\alpha}_\lambda(k)\mathrm{e}^{-\mathrm{i}k\cdot x}\Big) - \sum_{i=1}^N \frac{e_i}{4\pi}\nabla\left[\frac{1}{|\cdot|} * \varphi\right](x - q_i)\,, \\
B(x) &= \nabla \times \sum_\lambda \int \frac{\mathrm{d}k}{(2\pi)^{3/2}}\frac{1}{\sqrt{2|k|}}\Big(\varepsilon_\lambda(k)\alpha_\lambda(k)\mathrm{e}^{\mathrm{i}k\cdot x} + \overline{\varepsilon}_\lambda(k)\overline{\alpha}_\lambda(k)\mathrm{e}^{-\mathrm{i}k\cdot x}\Big)\,.
\end{aligned}
$$

It is of considerable interest to note that the system (2.3) is Hamiltonian. The phase space is given (formally for now) by the space of points $u = (p, q, \alpha)$. We define the Poisson bracket $\{\cdot,\cdot\}$ through the relations

$$
\{p_{i\mu}, q_{j\nu}\} = \delta_{ij}\delta_{\mu\nu}\,, \qquad \{\alpha_\lambda(k), \overline{\alpha}_{\lambda'}(k')\} = \mathrm{i}\delta_{\lambda\lambda'}\delta(k - k')\,.
$$

By requiring that all other combinations vanish and that $\{\cdot,\cdot\}$ has the usual properties (bilinearity, derivation property in both arguments, and the Jacobi identity), $\{\cdot,\cdot\}$ is uniquely defined. The Hamilton function is given by

$$
H(p,q,\alpha) := \sum_{i=1}^N \frac{1}{2m_i}\big(p_i - e_i A(q_i,\alpha)\big)^2 + V(q) + \sum_\lambda \int \mathrm{d}k\,|k|\,\overline{\alpha}_\lambda(k)\alpha_\lambda(k)\,. \tag{2.5}
$$

[1] Here, and in the following, we use Einstein's summation convention where a summation over any index appearing twice is implied.

It is now a simple matter to check that (2.3) is indeed the Hamiltonian equation of motion of (2.5). Note that H has the physical interpretation of the energy of the system. Note also the ordering of the terms in the definition of H, which will play a role in the next section when the arguments of H do not commute.

Next, we note that at this stage it is possible to partially remove the regularization φ, namely in the Coulomb potential V. We make the following assumption on the electrostatic potential:

(H) Either

(Ha) $w = \varphi * \frac{1}{4\pi|\cdot|} * \varphi$,

or

(Hb) $w = \frac{1}{4\pi|\cdot|}$ and $e_i > 0$ for all i.

In order to solve the equation of motion (2.3), we introduce, for each $\sigma \in \mathbb{R}$, the norms

$$\|\alpha\|_{\dot{H}^\sigma} := \left(\sum_\lambda \int \mathrm{d}k\, |k|^{2\sigma} |\alpha_\lambda(k)|^2\right)^{1/2}, \qquad \|\alpha\|_{H^\sigma} := \left(\sum_\lambda \int \mathrm{d}k\, \left(1+|k|^2\right)^\sigma |\alpha_\lambda(k)|^2\right)^{1/2}.$$

We denote the corresponding Hilbert spaces by $\dot{H}^\sigma$ and H^σ, respectively. Abbreviate $u = (p, q, \alpha)$, and define the norms

$$\|u\|_{\dot{X}^\sigma} := \sum_{i=1}^N (|p_i| + |q_i|) + \|\alpha\|_{\dot{H}^\sigma}, \qquad \|u\|_{X^\sigma} := \sum_{i=1}^N (|p_i| + |q_i|) + \|\alpha\|_{H^\sigma},$$

which give rise to the spaces $\dot{X}^\sigma$ and X^σ, respectively. Note that if $u \in \dot{X}^{1/2}$ then the energy $H(u)$ is well-defined[2], and $\dot{X}^{1/2}$ is the largest space with this property. Thus, $\dot{X}^{1/2}$ is the *energy space* of (2.3).

LEMMA 2.1 (WELL-POSEDNESS IN ENERGY SPACE). *Let $u_0 \in \dot{X}^{1/2}$ and assume that* (H) *holds. Then* (2.3) *has a unique global solution*

$$u(\cdot) \in C(\mathbb{R}; \dot{X}^{1/2}) \cap C^1(\mathbb{R}; \dot{X}^{-1/2})$$

that satisfies $u(0) = u_0$. Moreover, the map $u_0 \mapsto u(t)$ is $\dot{X}^{1/2}$-continuous and the energy $H(u(t))$ is conserved.

LEMMA 2.2 (WELL-POSEDNESS IN X^σ). *Let $\sigma \geqslant 1/2$ and $u_0 \in X^\sigma$. Assume moreover that* (H) *holds. Then* (2.3) *has a unique global solution*

$$u(\cdot) \in C(\mathbb{R}; X^\sigma) \cap C^1(\mathbb{R}; X^{\sigma-1})$$

that satisfies $u(0) = u_0$. Moreover, the map $u_0 \mapsto u(t)$ is X^σ-continuous and the energy $H(u(t))$ is conserved.

[2] In the case (Hb), we of course exclude initial data satisfying $q_i = q_j$ for some $i \neq j$. It is easy to see that the energy conservation shown in Lemma 2.1 implies that such configurations never appear as a result of time evolution.

Proof of Lemmas 2.1 and 2.2. We first outline the method of proof. Local existence follows in both cases from a standard contraction mapping argument. In a second step, we show that the energy $H(u(t))$ is conserved for $\dot{X}^{1/2}$-solutions, from which we infer global existence of $\dot{X}^{1/2}$-solutions using Assumption (H). Finally, we show global existence of X^σ-solutions by deriving an a-priori estimate on $\|u(t)\|_{X^\sigma}$ from energy conservation.

Using Duhamel's principle, we write (2.3) abstractly as

$$u(t) \;=\; \mathrm{e}^{Dt}u_0 + \int_0^t \mathrm{d}s\, \mathrm{e}^{D(t-s)} F(u(s))\,. \tag{2.6}$$

Here $F = (F_p, F_q, F_\alpha)$, with

$$\begin{aligned}
(F_p)_i(u) \;&=\; \frac{e_i}{m_i}\big(p_i - e_i A(q_i,\alpha)\big)_\mu \nabla_{q_i} A_\mu(q_i,\alpha) - \nabla_{q_i} V(q)\,,\\
(F_q)_i(u) \;&=\; \frac{1}{m_i}\big(p_i - e_i A(q_i,\alpha)\big)\,,\\
(F_\alpha(u))_\lambda(k) \;&=\; \sum_{i=1}^N \frac{e_i}{m_i}\frac{\chi(k)}{(2\pi)^{3/2}\sqrt{2|k|}}\big(p_i - e_i A(q_i,\alpha)\big)\cdot \bar{\varepsilon}_\lambda(k)\mathrm{e}^{-\mathrm{i}k\cdot q_i}\,.
\end{aligned}$$

Also, D is the multiplication operator $D \;=\; (0,0,-\mathrm{i}|k|)$. Clearly, e^{Dt} is an isometry on $\dot{H}^\rho$ and H^ρ for all $\rho \in \mathbb{R}$. By the standard theory of semilinear evolution equations (see e.g. [CH98]), it suffices to prove the existence of a unique solution $u(\cdot)$ of (2.6) in the space $C(\mathbb{R};\dot{X}^{1/2})$ (in the case of Lemma 2.1) or $C(\mathbb{R};X^\sigma)$ (in the case of Lemma 2.2).

Next, note that

$$|A(q,\alpha)| \;\leqslant\; \sqrt{2}\sum_\lambda \int \frac{\mathrm{d}k}{(2\pi)^{3/2}}\frac{\chi(k)}{|k|^{1/2+\rho}}\,|k|^\rho |a_\lambda(k)| \;\leqslant\; 2\bigg(\int \mathrm{d}k\, \frac{\chi^2(k)}{(2\pi)^3|k|^{1+2\rho}}\bigg)^{1/2} \|\alpha\|_{\dot{H}^\rho}\,.$$

Thus

$$|A(q,\alpha)| \;\lesssim\; \|\alpha\|_{\dot{H}^\rho}\,, \qquad \rho < 1\,. \tag{2.7}$$

Similarly, one finds

$$|\nabla_q^s A(q,\alpha)| \;\lesssim\; \|\alpha\|_{\dot{H}^\rho}\,, \qquad \rho < 1+s\,. \tag{2.8}$$

Let us now assume that $0 \leqslant \rho < 1$ and $\sigma \geqslant 0$. Using (2.7) and (2.8) it is easy to see that

$$|F_p(u)| \;\lesssim\; \sum_i \big(|p_i| + \|\alpha\|_{\dot{H}^\rho}\big)\|\alpha\|_{\dot{H}^\rho} + \sum_i \big|\nabla_{q_i} V(q)\big|\,, \tag{2.9a}$$

$$|F_q(u)| \;\lesssim\; \sum_i \big(|p_i| + \|\alpha\|_{\dot{H}^\rho}\big)\,, \tag{2.9b}$$

$$\|F_\alpha(u)\|_{\dot{H}^\sigma} \;\lesssim\; \sum_i \big(|p_i| + \|\alpha\|_{\dot{H}^\rho}\big)\,, \tag{2.9c}$$

A similar, slightly lengthier, calculation yields

$$|F_p(u) - F_p(\tilde{u})| \;\lesssim\; \|u-\tilde{u}\|_{\dot{X}^\rho}\big(1 + |p| + |\tilde{p}| + \|\alpha\|_{\dot{H}^\rho} + \|\tilde{\alpha}\|_{\dot{H}^\rho}\big)^2 + \sum_i \big|\nabla_{q_i} V(q) - \nabla_{\tilde{q}_i} V(\tilde{q})\big| \tag{2.10a}$$

$$|F_q(u) - F_q(\tilde{u})| \;\lesssim\; \|u-\tilde{u}\|_{\dot{X}^\rho}\big(1 + \|\alpha\|_{\dot{H}^\rho} + \|\tilde{\alpha}\|_{\dot{H}^\rho}\big)\,, \tag{2.10b}$$

$$\|F_\alpha(u) - F_\alpha(\tilde{u})\|_{\dot{H}^\sigma} \;\lesssim\; \|u-\tilde{u}\|_{\dot{X}^\rho}\big(1 + |p| + |\tilde{p}| + \|\alpha\|_{\dot{H}^\rho} + \|\tilde{\alpha}\|_{\dot{H}^\rho}\big)\,. \tag{2.10c}$$

The potential V is locally Lipschitz. Therefore a standard contraction mapping argument, using the estimates (2.9) and (2.10) with $0 \leqslant \sigma = \rho < 1$, implies that (2.6) is locally well-posed in the space $\dot{X}^\rho$. In other words, there is a unique solution $u(\cdot) \in C([0,T); \dot{X}^\rho)$ up to some finite time $T > 0$, and the solution map $u_0 \mapsto u(t)$ is continuous. Moreover, it is easy to see directly from (2.6) that $u(\cdot) \in C^1([0,T); \dot{X}^{\rho-1})$.

More generally, we infer from (2.9) and (2.10) local well-posedness in the space $\dot{X}^\rho \cap \dot{X}^\sigma$, where $0 \leqslant \rho < 1$ and $\sigma \geqslant 0$. The solution $u(\cdot)$ also satisfies $u(\cdot) \in C^1([0,T); \dot{X}^{\rho-1} \cap \dot{X}^{\sigma-1})$.

Next, we show conservation of energy. Unfortunately $t \mapsto H(u(t))$ is not differentiable for $u(t) \in \dot{X}^{1/2}$. To overcome this problem we consider solutions of higher regularity. Let $u_0 \in \dot{X}^{1/2} \cap \dot{X}^{3/2}$. We have shown that $u(\cdot)$ exists and satisfies

$$u(\cdot) \;\in\; C([0,T); \dot{X}^{1/2} \cap \dot{X}^{3/2}) \cap C^1([0,T); \dot{X}^{-1/2} \cap \dot{X}^{1/2})\,.$$

It is then easy to see that $t \mapsto H(u(t))$ is differentiable and a short calculation shows that $\frac{\mathrm{d}}{\mathrm{d}t} H(u(t)) = 0$, i.e. $H(u(t)) = H(u_0)$. In the case $u_0 \in \dot{X}^{1/2}$ we use an approximating sequence $(u_0^n)_{n \in \mathbb{N}}$ in $\dot{X}^{1/2} \cap \dot{X}^{3/2}$ converging in $\dot{X}^{1/2}$ to u_0 (Such a sequence exists because $\dot{X}^{1/2} \cap \dot{X}^{3/2}$ is dense in $\dot{X}^{1/2}$). It is easy to see that $u \mapsto H(u)$ is $\dot{X}^{1/2}$-continuous. Therefore taking the limit $n \to \infty$ in $H(u^n(t)) = H(u_0^n)$ yields $H(u(t)) = H(u_0)$.

We now exploit the energy conservation to prove global existence in energy space. By Assumption (H), $V(q)$ is bounded from below. Thus, by conservation of energy, the quantity

$$\sum_{i=1}^N \frac{1}{2m_i} \big(p_i - e_i A(q_i, \alpha)\big)^2 + \sum_\lambda \int \mathrm{d}k\, |k|\, |\alpha_\lambda(k)|^2$$

is bounded by some constant K depending only on the energy $H(u_0)$. We conclude that $\|\alpha\|_{\dot{H}^{1/2}}^2 \leqslant K$. Moreover, recalling (2.7), we see that $|p| \lesssim K$.

Next, we remark that we may assume that the potential $V(q)$ has bounded second derivatives. Indeed, if (Ha) holds this is already true, and if (Hb) holds we use energy conservation $0 \leqslant V(q) \leqslant H(u_0)$ to ensure that we may smooth out the Coulomb singularity at a small distance δ that depends only on the energy $H(u_0)$. In particular ∇V has a global Lipschitz constant.

Next, we note that by standard arguments (see e.g. the presentation of [CH98]) we have the blow-up alternative: either $T = \infty$ or $\lim_{t \uparrow T} \|u(t)\|_{\dot{X}^{1/2}} = \infty$. But it was shown above that the latter is impossible. Hence the solution exists for all times. This concludes the proof of Lemma 2.1.

In order to complete the proof of Lemma 2.2 we need to show that the solution in X^σ is global in time. Note that $H^\sigma \cong \dot{H}^0 \cap \dot{H}^\sigma$, so that we have local well-posedness and the blow-up alternative: either $T = \infty$ or $\lim_{t \uparrow T} \|u(t)\|_{X^\sigma} = \infty$. To show that the latter is impossible we again use energy conservation. As shown above, as a $\dot{X}^{1/2}$-solution, $u(t)$ exists for all times, and $|p|$ and $\|\alpha\|_{\dot{H}^{1/2}}$ are bounded in time. Thus using the estimate (2.9) with $\rho = 1/2$ in (2.6) yields the a-priori estimate

$$\|u(t)\|_{X^\sigma} \;\leqslant\; \|u_0\|_{X^\sigma} + Ct\,,$$

for some constant C. Here we also used that, as shown above, $|\nabla_{q_i} V(q)|$ is bounded in time. This concludes the proof of Lemma 2.2. $\square$

2.2. The quantum system

The quantum system is described by the Pauli-Fierz model of nonrelativistic quantum electrodynamics. It is obtained by canonical quantization of the Abraham model.

The Hilbert space is given by

$$\mathcal{H} := \mathcal{H}_{\text{particles}} \otimes \mathcal{H}_{\text{field}} \tag{2.11}$$

with

$$\mathcal{H}_{\text{particles}} := L^2(\mathbb{R}^{3N}), \qquad \mathcal{H}_{\text{field}} := \mathcal{F}_+\big(L^2(\mathbb{R}^3 \times \mathbb{N}_2)\big).$$

Here $\mathbb{R}^3 \times \mathbb{N}_2$, indexing the momentum $k \in \mathbb{R}^3$ and polarization $\lambda \in \mathbb{N}_2$ of a photon, is equipped with the natural product measure.

Vectors in $\mathcal{H}_{\text{particles}}$ are wave functions in the variable $X = (X_1, \dots, X_N) \in \mathbb{R}^{3N}$. Define the self-adjoint operators $P = (P_1, \dots, P_N)$ and $Q = (Q_1, \dots, Q_N)$ through

$$P_i := -\mathrm{i}\frac{\partial}{\partial X_i}\,\cdot \qquad Q_i := X_i\,\cdot\,.$$

Next, on $\mathcal{H}_{\text{field}}$ we have the usual creation and annihilation operators, $a^*_\lambda(k)$ and $a_\lambda(k)$, which satisfy the canonical commutation relations

$$[a_\lambda(k), a_{\lambda'}(k')] = [a^*_\lambda(k), a^*_{\lambda'}(k')] = 0, \qquad [a_\lambda(k), a^*_{\lambda'}(k')] = \delta_{\lambda\lambda'}\,\delta(k-k').$$

Let us abbreviate $U := (P, Q, a)$. The Hamiltonian is given by

$$H(U) = \sum_{i=1}^N \frac{1}{2m_i}\big(P_i - e_i A(Q_i, a)\big)^2 + V(Q) + \sum_\lambda \int \mathrm{d}k\, |k|\, a^*_\lambda(k) a_\lambda(k), \tag{2.12}$$

where, we recall,

$$A(Q_i, a) = \sum_\lambda \int \frac{\mathrm{d}k}{(2\pi)^{3/2}} \frac{\chi(k)}{\sqrt{2|k|}} \Big(\varepsilon_\lambda(k) a_\lambda(k) \mathrm{e}^{\mathrm{i}k\cdot Q_i} + \overline{\varepsilon}_\lambda(k) a^*_\lambda(k) \mathrm{e}^{-\mathrm{i}k\cdot Q_i}\Big).$$

Note the importance of the ordering of the terms in the definition (2.5) of H.

The self-adjointness of $H(U)$ is a well-known result, first derived by Nelson [Nel]; see also [Hir02].

2.3. The limit

We now move on to the main subject of this chapter, the limiting dynamics of the Pauli-Fierz model.

2.3.1. The scaling. We start with a heuristic discussion and physical motivation of our choice of scaling. We are interested in the limit of heavy particles and many photons. We choose a scaling parameter $\varepsilon > 0$, and require that the mass of each particle and the number of photons be of order ε^{-1} for $\varepsilon \to 0$. Denote by m_i^ε the physical mass of particle i, and by $\Psi_0^\varepsilon \in \mathcal{H}$ the initial state of the coupled matter-radiation system. We therefore require that

$$m_i^\varepsilon \;=\; O(\varepsilon^{-1})\,, \qquad \left\langle \Psi_0^\varepsilon\,,\, \sum_\lambda \int \mathrm{d}k\, a_\lambda^*(k) a_\lambda(k)\, \Psi_0^\varepsilon \right\rangle \;=\; O(\varepsilon^{-1})\,. \tag{2.13}$$

Position and time are unrescaled.

The scaling behaviour of all other physical quantities is now uniquely determined. Note first that (2.13) implies that the electromagnetic field satisfies

$$\big\langle \Psi_0^\varepsilon, A(Q_i,a)\, \Psi_0^\varepsilon \big\rangle \;=\; O(\varepsilon^{-1/2})\,. \tag{2.14}$$

Let V^ε denote the physical interaction potential, and e_i^ε the physical charge of particle i. Since position and time are unrescaled, the velocity of particle i,

$$v_i \;=\; \left\langle \Psi_0^\varepsilon\,,\, \frac{1}{2m_i^\varepsilon}\big(P_i - e_i^\varepsilon A(Q_i,a)\big)\Psi_0^\varepsilon \right\rangle,$$

is of order one. This means that $\langle \Psi_0^\varepsilon, P_i \Psi_0^\varepsilon\rangle = O(\varepsilon^{-1})$ and, recalling (2.14), that $e_i^\varepsilon = O(\varepsilon^{-1/2})$. Next, recalling the definition (2.4), we see that $V^\varepsilon = O(\varepsilon^{-1})$.

Let us summarize. The Hamiltonian with the physical (rescaled) quantities reads

$$\begin{aligned}
\widehat{H}^\varepsilon \;&:=\; \sum_{i=1}^N \frac{1}{2m_i^\varepsilon}\big(P_i - e_i^\varepsilon A(Q_i,a)\big)^2 + V^\varepsilon(Q) + \sum_\lambda \int \mathrm{d}k\, |k|\, a_\lambda^*(k) a_\lambda(k)\\
&=\; \sum_{i=1}^N \frac{\varepsilon}{2m_i}\big(P_i - \varepsilon^{-1/2} e_i A(Q_i,a)\big)^2 + \varepsilon^{-1} V(Q) + \sum_\lambda \int \mathrm{d}k\, |k|\, a_\lambda^*(k) a_\lambda(k)\,.
\end{aligned}$$

It acts on initial states $\Psi_0^\varepsilon \in \mathcal{H}$ satisfying

$$\langle \Psi_0^\varepsilon, P\Psi_0^\varepsilon\rangle \;=\; O(\varepsilon^{-1})\,, \qquad \langle \Psi_0^\varepsilon, Q\Psi_0^\varepsilon\rangle \;=\; O(1)\,, \qquad \langle \Psi_0^\varepsilon, a\Psi_0^\varepsilon\rangle \;=\; O(\varepsilon^{-1/2})\,. \tag{2.15}$$

It is useful to rewrite the condition (2.15) as

$$\langle \Psi_0^\varepsilon, P\Psi_0^\varepsilon\rangle \;\sim\; \varepsilon^{-1} p\,, \qquad \langle \Psi_0^\varepsilon, Q\Psi_0^\varepsilon\rangle \;\sim\; q\,, \qquad \langle \Psi_0^\varepsilon, a\Psi_0^\varepsilon\rangle \;\sim\; \varepsilon^{-1/2}\alpha\,, \tag{2.16}$$

for some triple (p,q,α).

For computations it is convenient to introduce the rescaled operators

$$P^\varepsilon \;:=\; \varepsilon^{1/2} P\,, \qquad Q^\varepsilon \;:=\; \varepsilon^{1/2} Q\,, \qquad a^\varepsilon \;:=\; \varepsilon^{1/2} a$$

and to set

$$H^\varepsilon \;:=\; \varepsilon^{-1} H(U^\varepsilon)\,.$$

Then we have

$$\widehat{H}^\varepsilon \;=\; R_\varepsilon\, H^\varepsilon R_\varepsilon^*\,,$$

where $R_\varepsilon \in \mathcal{L}(\mathcal{H})$ is defined as the unitary map that rescales the argument X of the particle wave function with $\varepsilon^{1/2}$. It satisfies

$$R_\varepsilon^* P R_\varepsilon \;=\; \varepsilon^{1/2} P\,, \qquad R_\varepsilon^* Q R_\varepsilon \;=\; \varepsilon^{-1/2} Q\,, \qquad R_\varepsilon^* a R_\varepsilon \;=\; a\,,$$

2.3.2. Weyl operators. A convenient way to construct states Ψ_0^ε satisfying the condition (2.16) is by using Weyl operators. Introduce the shorthands

$$\begin{aligned} \langle Q\,, p\rangle \;&=\; \sum_{i=1}^N Q_i \cdot p_i\,, &\qquad \langle P\,, q\rangle \;&=\; \sum_{i=1}^N P_i \cdot q_i\,, \\ \langle a\,, \alpha\rangle \;&=\; \sum_\lambda \int \mathrm{d}k\; \alpha_\lambda(k) a_\lambda^*(k)\,, &\qquad \langle \alpha\,, a\rangle \;&=\; \sum_\lambda \int \mathrm{d}k\; \overline{\alpha}_\lambda(k) a_\lambda(k)\,. \end{aligned}$$

For $U = (P, Q, a)$ and $u = (p, q, \alpha)$ we abbreviate

$$\langle U\,, u\rangle \;:=\; \mathrm{i}\langle Q\,, p\rangle - \mathrm{i}\langle P\,, q\rangle + \langle a\,, \alpha\rangle - \langle \alpha\,, a\rangle\,. \tag{2.17}$$

For each $u \in X^0$ we define the *Weyl operator*

$$W(u) \;:=\; \mathrm{e}^{\langle U\,, u\rangle}\,.$$

It is easy to show that $W(u)$ is unitary and satisfies

$$W(u)^*\, U\, W(u) \;=\; U + u\,. \tag{2.18}$$

Next, let Ψ_0 be an arbitrary state and define

$$\Psi_0^{\varepsilon, u} \;:=\; R_\varepsilon^*\, W(\varepsilon^{-1/2} u)\Psi_0\,. \tag{2.19}$$

It follows that $\Psi_0^{\varepsilon,u}$ satisfies (2.16).

2.3.3. Main result. Denote the quantum mechanical propagator by

$$U^\varepsilon(t) \;:=\; \mathrm{e}^{-\mathrm{i}H^\varepsilon t}\,.$$

We may now state our main result.

THEOREM 2.3. *Let $v \in X^0$ and $u_0 \in X^1$. Let $u(\cdot)$ be the solution of (2.3) with initial data u_0. Then for all $t \in \mathbb{R}$ we have*

$$\operatorname*{s-lim}_{\varepsilon \to 0} W(\varepsilon^{-1/2} u_0)^*\, U^\varepsilon(t)^*\, \mathrm{e}^{\langle U^\varepsilon\,, v\rangle}\, U^\varepsilon(t)\, W(\varepsilon^{-1/2} u_0) \;=\; \mathrm{e}^{\langle u(t)\,, v\rangle}\,.$$

REMARK 2.4. *Theorem 2.3 may be rewritten in the original scaling of Section 2.3.1:*

$$\operatorname*{s-lim}_{\varepsilon \to 0} W(\varepsilon^{-1/2} u_0)^*\, R_\varepsilon\, \mathrm{e}^{\mathrm{i}\varepsilon^{-1} H(\widehat{U}^\varepsilon)}\, \mathrm{e}^{\langle \widehat{U}^\varepsilon\,, v\rangle}\, \mathrm{e}^{-\mathrm{i}\varepsilon^{-1} H(\widehat{U}^\varepsilon)}\, R_\varepsilon^*\, W(\varepsilon^{-1/2} u_0) \;=\; \mathrm{e}^{\langle u(t)\,, v\rangle}\,,$$

where the variables $\widehat{U}^\varepsilon = (\widehat{P}^\varepsilon, \widehat{Q}^\varepsilon, \widehat{a}^\varepsilon) := (\varepsilon P, Q, \varepsilon^{1/2} a)$ are rescaled so that $\langle \Psi_0^{\varepsilon,u}\,, \widehat{U}^\varepsilon \Psi_0^{\varepsilon,u}\rangle = O(1)$, where $\Psi_0^{\varepsilon,u}$ is defined in (2.19) In a state of the form (2.19) we have therefore

$$\lim_{\varepsilon \to 0} \Big\langle \mathrm{e}^{-\mathrm{i}t\widehat{H}^\varepsilon}\, \Psi_0^{\varepsilon,u}\,,\, \mathrm{e}^{\langle \widehat{U}^\varepsilon\,, v\rangle}\, \mathrm{e}^{-\mathrm{i}t\widehat{H}^\varepsilon}\, \Psi_0^{\varepsilon,u} \Big\rangle \;=\; \mathrm{e}^{\langle u(t)\,, v\rangle}\,,$$

REMARK 2.5. *Theorem 2.3 is stated in terms of Weyl operators, but by superposition it may be applied for instance to generic classical observables $f(p, q)$ depending on the position and momentum of the particles. Assume that the Fourier transform $\tilde{f} \in L^1(\mathbb{R}^{6N})$ so that we may write*

$$f(p, q) \;=\; \int \mathrm{d}\xi\, \mathrm{d}\pi\; \tilde{f}(\xi, \pi)\, \mathrm{e}^{\mathrm{i}\langle q\,, \pi\rangle - \mathrm{i}\langle p\,, \xi\rangle}\,.$$

The Weyl quantization of f is by definition

$$\widehat{f}_\varepsilon \;:=\; \int \mathrm{d}\xi\,\mathrm{d}\pi\;\tilde{f}(\xi,\pi)\,\mathrm{e}^{\mathrm{i}\langle Q^\varepsilon,\pi\rangle - \mathrm{i}\langle P^\varepsilon,\xi\rangle}\,.$$

Setting $v = (\pi, \xi, 0)$ in Theorem 2.3, multiplying both sides by $\tilde{f}(\xi,\pi)$, and integrating over ξ and π yields (by dominated convergence)

$$\operatorname*{s-lim}_{\varepsilon\to 0} W(\varepsilon^{-1/2}u_0)^*\,U^\varepsilon(t)^*\,\widehat{f}_\varepsilon\,U^\varepsilon(t)\,W(\varepsilon^{-1/2}u_0) \;=\; f(p(t),q(t))\,. \tag{2.20}$$

REMARK 2.6. *The previous remark may serve as a starting point for a Egorov-type formulation of Theorem 2.3. This formulation is not entirely satisfying in that the electromagnetic field is treated as an external parameter which must vanish at time $t = 0$.*

On the classical phase space of the particles, $\mathbb{R}^{6N}$, we introduce the flow ϕ_t, defined through $\phi_t(p,q) = (p(t),q(t))$ where $(p(t),q(t),\alpha(t))$ is the solution of (2.3) with initial data $u_0 = (p,q,0)$. Next, we need some smoothness of the map ϕ_t. To this end, we prove that $\nabla^k\phi_t$ exists for all t and $k \in \mathbb{N}$ by differentiating the equation of motion (2.3) in the initial data, and by applying a contraction mapping argument in the style of Lemma 2.2 to the resulting equation of motion for $\nabla^k\phi_t(p,q)$; we omit the details.

Thus we find that ϕ_t is smooth. In particular, $f\circ\phi_t \in C_c^\infty(\mathbb{R}^{6N})$ if $f \in C_c^\infty(\mathbb{R}^{6N})$ and Theorem 2.3 yields, as in Remark 2.5,

$$\operatorname*{s-lim}_{\varepsilon\to 0} W(\varepsilon^{-1/2}u_0)^*\,\big(\widehat{f\circ\phi_t}\big)_\varepsilon\,W(\varepsilon^{-1/2}u_0) \;=\; f(p(t),q(t))\,.$$

Subtracting this from (2.20) and setting $u_0 = 0$ yields

$$\operatorname*{s-lim}_{\varepsilon\to 0}\Big(U^\varepsilon(t)^*\,\widehat{f}_\varepsilon\,U^\varepsilon(t) - \big(\widehat{f\circ\phi_t}\big)_\varepsilon\Big) \;=\; 0\,.$$

2.3.4. Outline of the proof of Theorem 2.3. The proof of Theorem 2.3 is based on a semiclassical argument due to Hepp [Hep74]. The main technical difficulties arise from unbounded operators acting on vectors of the form $V(t,s)\Psi$ (see below for the definition of $V(t,s)$). The key tool for dealing with these difficulties a Dyson expansion for $V(t,s)$. This approach is better suited for infinite-dimensional phase spaces, such as X^1, than the approach of [Hep74] using symplectic transformations. The drawback is that controlling decay and regularity of the wave function of the particles requires more effort.

We start with a state of the form $\Phi_0^{\varepsilon,u_0} := W(\varepsilon^{-1/2}u_0)\Psi$ for some $\Psi \in \mathcal{H}$. Its time evolution is given by $\Phi^{\varepsilon,u_0}(t) := U^\varepsilon(t)\Phi_0^{\varepsilon,u_0}$. The idea of Hepp is to consider the quantum fluctuations around the classical orbit $u(\cdot)$. It is motivated by the following heuristics. We expect that

$$\big\langle \Phi^{\varepsilon,u_0}(t)\,,U\,\Phi^{\varepsilon,u_0}(t)\big\rangle \;=\; O(\varepsilon^{-1/2})\,,$$

while the quantum fluctuations, described by $U - \varepsilon^{-1/2}u(t)$, satisfy

$$\big\langle \Phi^{\varepsilon,u_0}(t)\,,\big(U - \varepsilon^{-1/2}u(t)\big)\,\Phi^{\varepsilon,u_0}(t)\big\rangle \;=\; O(1)\,.$$

For technical reasons, it is convenient to study the fluctuations using the bounded Weyl operator

$$\mathrm{e}^{\langle U - \varepsilon^{-1/2}u(t)\,,v\rangle}\,,$$

where $v \in X^0$. Its expectation in the state $\Phi^{\varepsilon,u_0}(t)$ is equal to

$$\big\langle \Psi \,, W(\varepsilon^{-1/2}u_0)^* \, U^\varepsilon(t)^* \, \mathrm{e}^{\langle U - \varepsilon^{-1/2}u(t) \,, v\rangle} \, U^\varepsilon(t) \, W(\varepsilon^{-1/2}u_0)\Psi \big\rangle \,.$$

Next, we note that

$$W(\varepsilon^{-1/2}u_0)^* \, U^\varepsilon(t)^* \, \mathrm{e}^{\langle U - \varepsilon^{-1/2}u(t) \,, v\rangle} \, U^\varepsilon(t) \, W(\varepsilon^{-1/2}u_0) \;=\; V^\varepsilon(t,0)^* \, \mathrm{e}^{\langle U \,, v\rangle} \, V^\varepsilon(t,0) \,,$$

where

$$V^\varepsilon(t,s) \;:=\; W(\varepsilon^{-1/2}u(t))^* \, U^\varepsilon(t-s) \, W(\varepsilon^{-1/2}u(s)) \, \mathrm{e}^{\mathrm{i}\varepsilon^{-1}\int_s^t \beta}$$

and β is any phase. The unitary family $V^\varepsilon(t,s)$ satisfies $V^\varepsilon(t,s)V^\varepsilon(s,r) = V^\varepsilon(t,r)$ and $V^\varepsilon(t,t) = \mathbb{1}$. In order to understand its limiting behaviour for $\varepsilon \to 0$, we compute its generator (see Lemma 2.10 below):

$$\frac{\mathrm{d}}{\mathrm{d}s} V^\varepsilon(t,s) \;=\; V^\varepsilon(t,s) D^\varepsilon(s) \,,$$

where, provided the phase β is chosen appropriately, we have

$$D^\varepsilon(t) \;:=\; \mathrm{i}\varepsilon^{-1} H(u(t) + U^\varepsilon) - \mathrm{i}\varepsilon^{-1} H(u(t)) - \mathrm{i}\varepsilon^{-1} \frac{\mathrm{d}}{\mathrm{d}\xi} H(u(t) + \xi U^\varepsilon)\Big|_{\xi=0} \,.$$

Using Taylor's formula we therefore find

$$D^\varepsilon(t) \;=\; \mathrm{i}\varepsilon^{-1} \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} H\big(u(t) + \xi U^\varepsilon\big)\Big|_{\xi=0} + \mathrm{i}\varepsilon^{-1} O(\varepsilon^{3/2}) \;=\; \mathrm{i}H(t) + O(\varepsilon^{1/2}) \,,$$

where

$$H(t) \;:=\; \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} H\big(u(t) + \xi U\big)\Big|_{\xi=0}$$

is a quadratic Hamiltonian independent of ε. (Recall that $U^\varepsilon = \varepsilon^{1/2} U$.) Thus we have that $D^\varepsilon(t) \to \mathrm{i}H(t)$ as $\varepsilon \to 0$. We therefore expect that $V^\varepsilon(t,s) \to V(t,s)$ as $\varepsilon \to 0$, where $V(t,s)$ is the propagator generated by $H(t)$, i.e.

$$\mathrm{i}\partial_t V(t,s) \;=\; H(t) V(t,s) \,, \qquad V(s,s) \;=\; \mathbb{1} \,.$$

In order to show this we estimate, using the fundamental theorem of calculus,

$$\big\| V(t,0)\Psi - V^\varepsilon(t,0)\Psi \big\| \;\leqslant\; \int_0^t \mathrm{d}s \, \big\| V^\varepsilon(t,s)\big(D^\varepsilon(s) - \mathrm{i}H(s)\big)V(s,0)\Psi \big\| \,.$$

The main work (Lemma 2.11 below) is to show that $\big\| \big(D^\varepsilon(s) - \mathrm{i}H(s)\big)V(s,0)\Psi \big\| \to 0$ as $\varepsilon \to 0$. This shows that the quantum fluctuations around the classical orbit, measured by the expectation of $U - \varepsilon^{-1/2}u(t)$, are of order one. Hence the expectation of $U^\varepsilon - u(t)$ is of order $\varepsilon^{1/2}$, from which the claim may be easily derived.

2.3.5. Proof of Theorem 2.3. We start by recalling the natural isomorphism

$$\mathcal{F}_+(\mathbb{C}^{3N}) \;\cong\; L^2(\mathbb{R}^{3N})\,,$$

given by identifying the vacuum of $\mathcal{F}_+(\mathbb{C}^{3N})$ with the Gaussian $f(X) = \pi^{-3N/4}\mathrm{e}^{-|X|^2/2}$ in $L^2(\mathbb{R}^{3N})$, as well as the identification

$$P_{i\mu} \;=\; -\mathrm{i}\frac{\partial}{\partial X_{i\mu}}\,\cdot \;=\; \frac{1}{\sqrt{2}\mathrm{i}}(a_{i\mu} - a^*_{i\mu})\,, \qquad Q_{i\mu} \;=\; X_{i\mu}\,\cdot \;=\; \frac{1}{\sqrt{2}}(a_{i\mu} + a^*_{i\mu})\,;$$

see e.g. [RS75]. Together with the identity $\mathcal{F}_+(\mathfrak{h}_1 \oplus \mathfrak{h}_2) \cong \mathcal{F}_+(\mathfrak{h}_1) \otimes \mathcal{F}_+(\mathfrak{h}_2)$ this implies

$$\mathcal{H} \;\cong\; \mathcal{F}_+(\mathfrak{h})\,, \qquad \mathfrak{h} \;:=\; \mathbb{C}^{3N} \oplus L^2(\mathbb{R}^3 \times \mathbb{N}_2)\,.$$

In the following we tacitly identify $\mathcal{H}$ with $\mathcal{F}_+(\mathfrak{h})$. We denote by Ω the vacuum of $\mathcal{H}$.

Much of the following is simplified by writing $\mathfrak{h}$ as an L^2-space and adopting a unified notation for $a_{i\mu}$ and $a_\lambda(k)$. To this end, we note that

$$\mathfrak{h} \;=\; L^2\big(M, \mathrm{d}z\big)\,, \qquad M \;:=\; \mathbb{N}_N \times \mathbb{N}_3 \;\cup\; \mathbb{R}^3 \times \mathbb{N}_2\,,$$

where the measure $\mathrm{d}z$ on M is defined in the natural way: $\mathbb{R}^3$ carries the Lebesgue measure and $\mathbb{N}_j$ the counting measure. We adopt the unified notation $a^*(z)$ and $a(z)$ for the creation and annihilation operators on $\mathcal{H}$:

$$a(z) \;=\; \begin{cases} a_{i\mu} & \text{if } z = (i,\mu) \in \mathbb{N}_N \times \mathbb{N}_3 \\ a_\lambda(k) & \text{if } z = (k,\lambda) \in \mathbb{R}^3 \times \mathbb{N}_2\,. \end{cases}$$

We have the canonical commutation relations

$$[a(z), a(z')] \;=\; [a^*(z), a^*(z')] \;=\; 0\,, \qquad [a(z), a^*(z')] \;=\; \delta(z - z')\,, \tag{2.21}$$

where δ is the delta function on M with respect to the measure $\mathrm{d}z$.

Let $n \in \mathbb{N}$ and define the subspace $\mathcal{H}^{\leqslant n} \subset \mathcal{H}$ through $\mathcal{H}^{\leqslant n} \;:=\; \bigoplus_{m=0}^n P_+ \mathfrak{h}^{\otimes m}$. Clearly, the union

$$\mathcal{H}^0 \;:=\; \bigcup_{n \geqslant 0} \mathcal{H}^{\leqslant n}$$

is dense in $\mathcal{H}$. The following lemma gives a bound (with the sharp constant) on the norm of a "second quantized" operator.

LEMMA 2.7. *Let $p, q \in \mathbb{N}$ and $B \in \mathcal{L}(P_+\mathfrak{h}^{\otimes q}; P_+\mathfrak{h}^{\otimes p})$. Then for any $n \in \mathbb{N}$ and $\Psi \in \mathcal{H}^{\leqslant n}$ we have*

$$\bigg\| \int \mathrm{d}z_1 \cdots \mathrm{d}z_p\, \mathrm{d}z'_1 \cdots \mathrm{d}z'_q\, B(z_1, \dots, z_p; z'_1, \dots, z'_q)\, a^*(z_1) \cdots a^*(z_p)\, a(z'_1) \cdots a(z'_q)\, \Psi \bigg\| \leqslant \frac{\sqrt{n!(n+p-q)!}}{(n-q)!}\, \|B\|\, \|\Psi\|\,, \tag{2.22}$$

where $B(z_1, \dots, z_p; z'_1, \dots, z'_q)$ is the operator kernel of B.

PROOF. Denote by $\mathrm{d}\Gamma(B)\Psi$ the expression inside the norm on the left-hand side of (2.22). It is enough to show the claim for $\Psi = (0, \dots, 0, \Psi^{(n)}, 0, \dots)$ where $\Psi^{(n)} \in P_+\mathfrak{h}^{\otimes n}$. Note first that $\langle \Phi, \mathrm{d}\Gamma(B)\Psi\rangle$ only depends on $\Phi^{(n+p-q)} \in P_+\mathfrak{h}^{\oplus(n+p-q)}$; without loss of generality we assume that other components of Φ vanish. Let us write

$$\Psi = \frac{1}{\sqrt{n!}} \int \mathrm{d}z_1 \cdots \mathrm{d}z_n \, \Psi^{(n)}(z_1, \dots, z_n)\, a^*(z_1) \cdots a^*(z_n)\, \Omega\,,$$
$$\Phi = \frac{1}{\sqrt{(n+p-q)!}} \int \mathrm{d}z_1 \cdots \mathrm{d}z_{n+p-q} \, \Phi^{(n+p-q)}(z_1, \dots, z_{n+q-q})\, a^*(z_1) \cdots a^*(z_{n+p-q})\, \Omega\,.$$

Then a simple combinatorial argument using the canonical commutation relations (2.21) yields

$$\langle \Phi, \mathrm{d}\Gamma(B)\Psi\rangle = \binom{n}{q}\binom{n+p-q}{p} p!q! \frac{(n-q)!}{\sqrt{n!(n+p-q)!}} \big\langle \Phi^{(n+p-q)}, \big(B \otimes \mathbb{1}^{\otimes(n-q)}\big)\Psi^{(n)}\big\rangle\,.$$

Taking the absolute value followed by the supremum over Φ yields the claim. $\square$

Quadratic fluctuations around the classical orbit are described by the Hamiltonian

$$H(t) := \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} H\big(u(t) + \xi U\big)\Big|_{\xi=0}\,.$$

Let us abbreviate

$$\nabla^k V(q) \cdot Q^k := \frac{\partial^k}{\partial q_{i_1\mu_1} \cdots \partial q_{i_k\mu_k}} V(q)\, Q_{i_1\mu_1} \cdots Q_{i_k\mu_k}\,, \tag{2.23}$$

where a summation over all indices is implied. We get the explicit expression

$$H(t) = T + \widetilde{H}(t)$$

where

$$T := \sum_\lambda \int \mathrm{d}k\, |k|\, a^*_\lambda(k) a_\lambda(k) \tag{2.24}$$

and

$$\widetilde{H}(t) := \nabla^2 V(q(t)) \cdot Q^2 + \sum_{i=1}^N \frac{1}{m_i}\Big(Y_i(t) \cdot Y_i''(t) + Y_i'(t) \cdot Y_i'(t)\Big)\,.$$

Here the vectors $Y_i(t)$, $Y_i'(t)$ and $Y_i''(t)$ are defined by

$$Y_i(t) := p_i(t) - e_i \sum_\lambda \int \frac{\mathrm{d}k}{(2\pi)^{3/2}} \frac{\chi(k)}{\sqrt{2|k|}} \Big[\varepsilon_\lambda(k)\alpha_\lambda(t,k)\mathrm{e}^{\mathrm{i}k\cdot q_i(t)} + \mathrm{H.c.}\Big]$$
$$Y_i'(t) := P_i - e_i \sum_\lambda \int \frac{\mathrm{d}k}{(2\pi)^{3/2}} \frac{\chi(k)}{\sqrt{2|k|}} \Big[\varepsilon_\lambda(k)\mathrm{e}^{\mathrm{i}k\cdot q_i(t)}\big(a_\lambda(k) + \mathrm{i}\alpha_\lambda(t,k) k \cdot Q_i\big) + \mathrm{H.c.}\Big]$$
$$Y_i''(t) := -e_i \sum_\lambda \int \frac{\mathrm{d}k}{(2\pi)^{3/2}} \frac{\chi(k)}{\sqrt{2|k|}} \Big[\varepsilon_\lambda(k)\mathrm{e}^{\mathrm{i}k\cdot q_i(t)}\big(2\mathrm{i}a_\lambda(k)\, k \cdot Q_i - \alpha_\lambda(t,k)(k \cdot Q_i)^2\big) + \mathrm{H.c.}\Big]\,,$$

where “H.c.” denotes Hermitian conjugate. The propagator $V(t,s)$ satisfies

$$\mathrm{i}\partial_t V(t,s) = H(t)V(t,s)\,, \qquad V(s,s) = \mathbb{1}\,. \tag{2.25}$$

We show its existence using its strongly convergent Dyson series. To this end, we record the following estimate.

LEMMA 2.8. *Let $u_0 \in \dot{X}^{1/2}$. Then for $n \in \mathbb{N}$ we have*

$$\widetilde{H}(t) \,:\, \mathcal{H}^{\leqslant n} \longrightarrow \mathcal{H}^{\leqslant (n+2)}$$

and

$$\Big\| \widetilde{H}(t)\big|_{\mathcal{H}^{\leqslant n}} \Big\| \leqslant M(n+2)$$

for some constant M depending only on u_0.

PROOF. Since $H(t)$ is quadratic in $a(z), a^*(z)$, the first statement follows immediately. In order to show the second, let $\Psi \in \mathcal{H}^{\leqslant n}$. From now on, we tacitly apply Lemma 2.7. The first term of $\widetilde{H}(t)$ is easily estimated:

$$\big\| \nabla^2 V(q(t)) \cdot Q^2 \, \Psi \big\| \lesssim \big| \nabla^2 V(q(t)) \big| \, (n+2) \|\Psi\| \,.$$

In order to bound the second, we note that

$$|Y_i(t)| \lesssim |p_i(t)| + \|\alpha(t)\|_{\dot{H}^{1/2}}$$

as well as

$$\|Y_i''(t)\Psi\| \lesssim \big(1 + \|\alpha(t)\|_{\dot{H}^{1/2}}\big)(n+2)\|\Psi\| \,.$$

Finally, we find

$$\|Y_i'(t)\Psi\| \lesssim \sqrt{n+1}\big(1 + \|\alpha(t)\|_{\dot{H}^{1/2}}\big) \,.$$

Thus,

$$\|Y_i'(t) \cdot Y_i'(t)\Psi\| \lesssim \sqrt{n+2}\sqrt{n+1}\big(1 + \|\alpha(t)\|_{\dot{H}^{1/2}}\big)^2 \,.$$

By Lemma 2.1, $\sup_{t \in \mathbb{R}} \|\alpha(t)\|_{\dot{H}^{1/2}} < \infty$ and the proof is complete. □

The Dyson series for $V(t,s)\Psi$, where $\Psi \in \mathcal{H}^{\leqslant n}$, reads

$$\sum_{k \geqslant 0} \int_0^\infty \mathrm{d}r_0 \cdots \int_0^\infty \mathrm{d}r_k \; \delta(t - s - r_0 - \cdots - r_k)$$
$$\times \mathrm{e}^{\mathrm{i}Tr_k} \widetilde{H}(s + r_0 + \cdots + r_{k-1}) \mathrm{e}^{-\mathrm{i}Tr_{k-1}} \cdots \widetilde{H}(s + r_0 + r_1) \mathrm{e}^{-\mathrm{i}Tr_1} \widetilde{H}(s + r_0) \mathrm{e}^{-\mathrm{i}Tr_0} \Psi \,. \tag{2.26}$$

Since $\mathrm{e}^{-\mathrm{i}Tr}$ is an isometry that preserves the particle number, Lemma 2.8 implies that (2.26) is bounded by

$$\sum_{k \geqslant 0} \frac{1}{k!} |t-s|^k \, M^k (n+2)(n+4) \cdots (n+2k) \, \|\Psi\| \leqslant 2^n \sum_{k \geqslant 0} \big(4|t-s|M\big)^k \,.$$

Thus (2.26) converges in norm for $|t-s| < (4M)^{-1}$. By unitarity of $V(t,s)$ and density of $\mathcal{H}^0$ in $\mathcal{H}$, it follows that $V(t,s)$ exists for all times t, s.

Next, we compute the time derivative of $W(u(t))$.

LEMMA 2.9. *Let $u_0 \in X^1$ and $\Psi \in \mathcal{H}^0$. Then $W(u(t))\Psi$ is differentiable in t and*

$$\frac{\mathrm{d}}{\mathrm{d}t} W(u(t))\Psi = \Big\langle U - \frac{u(t)}{2} \,,\, \dot{u}(t) \Big\rangle W(u(t))\Psi \,.$$

Proof. Abbreviate

$$A_\delta \ := \ \langle U\,, u(t+\delta)\rangle$$

and write $W(u(t+\delta)) = \mathrm{e}^{A_0 + (A_\delta - A_0)}$. This yields, for each $K \in \mathbb{N}$, the Dyson series

$$\begin{aligned}
&W(u(t+\delta))\Psi \\
&\quad = \sum_{k=0}^{K-1} \int_0^1 \mathrm{d}x_0 \cdots \mathrm{d}x_k \; \delta\Bigl(1 - \sum_{i=0}^{k} x_i\Bigr)\; \mathrm{e}^{A_0 x_k}(A_\delta - A_0)\mathrm{e}^{A_0 x_{k-1}} \cdots \mathrm{e}^{A_0 x_1}(A_\delta - A_0)\mathrm{e}^{A_0 x_0}\Psi \\
&\qquad + \int_0^1 \mathrm{d}x_0 \cdots \mathrm{d}x_K \; \delta\Bigl(1 - \sum_{i=0}^{K} x_i\Bigr)\; \mathrm{e}^{A_\delta x_K}(A_\delta - A_0)\mathrm{e}^{A_0 x_{K-1}} \cdots \mathrm{e}^{A_0 x_1}(A_\delta - A_0)\mathrm{e}^{A_0 x_0}\Psi\,. \qquad (2.27)
\end{aligned}$$

By (2.18), the k'th term is equal to

$$\int_0^1 \mathrm{d}x_0 \cdots \mathrm{d}x_k \; \delta\Bigl(1 - \sum_{i=0}^{k} x_i\Bigr)\mathrm{e}^{A_0} B_\delta(x_0 + \cdots + x_{k-1}) \cdots B_\delta(x_0 + x_1) B_\delta(x_0)\Psi\,, \qquad (2.28)$$

where

$$B_\delta(x) \ := \ \bigl\langle U + x u(t)\,, u(t+\delta) - u(t)\bigr\rangle\,.$$

Let us assume that $\Psi \in \mathcal{H}^{\leqslant n}$. Then Lemma 2.7 yields

$$\|B_\delta(x)\Psi\| \ \leqslant \ 2\bigl(\sqrt{n+1} + \|u(t)\|_{X^0}\bigr)\bigl\|u(t+\delta) - u(t)\bigr\|_{X^0}\|\Psi\|\,.$$

Since $B_\delta : \mathcal{H}^{\leqslant n} \to \mathcal{H}^{\leqslant (n+1)}$ and e^{A_0} is unitary, we therefore find that (2.28) is bounded in norm by

$$\frac{1}{k!} 2^k \bigl(\sqrt{n+k+1} + \|u(t)\|_{X^0}\bigr)^k \bigl\|u(t+\delta) - u(t)\bigr\|_{X^0}^k \|\Psi\| \ \leqslant \ \frac{C^k}{\sqrt{k!}}\|\Psi\|\,.$$

The same estimate applies for the rest term in (2.27). Therefore the Dyson series (2.27) with $K = \infty$ converges in norm.

Next, we observe that by Lemma 2.7 the map

$$X^0 \to \mathcal{H}^0 \qquad u \mapsto \langle U\,, u\rangle\Psi\,,$$

where $\Psi \in \mathcal{H}^0$, is continuous for all $\Psi \in \mathcal{H}^0$. Therefore, by assumption and Lemma 2.2, $B_\delta(x)\Psi$ is strongly differentiable in ε. A straightforward modification of the above estimate of the Dyson series shows that, when computing $\frac{\mathrm{d}}{\mathrm{d}\delta}W(u(t+\delta))\Psi$, one may exchange the order of the differentiation and the summation/integration. Thus, $W(u(t+\delta))\Psi$ is strongly differentiable with respect to δ at 0, and only the term $k = 1$ survives in its derivative at $\delta = 0$. We thus find

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\delta} W(u(t+\delta))\Psi\Big|_{\delta=0} \ &= \ \int_0^1 \mathrm{d}x \; \mathrm{e}^{A_0} \frac{\mathrm{d}}{\mathrm{d}\delta} B_\delta(x)\Psi\Big|_{\delta=0} \\
&= \ \int_0^1 \mathrm{d}x \; \mathrm{e}^{A_0} \langle U + x u(t)\,, \dot{u}(t)\rangle\Psi \\
&= \ \Bigl\langle U - \frac{u(t)}{2}\,,\, \dot{u}(t)\Bigr\rangle\Psi\,,
\end{aligned}$$

where in the last step we used (2.18). ☐

We now move on to discussing the quantum fluctuations around the classical orbit. Let $v \in X^0$ and $u_0 \in X^1$, and consider the solution $u(t)$ of (2.3). Note first that we may write

$$W(\varepsilon^{-1/2}u_0)^* \, U^\varepsilon(t)^* \, \mathrm{e}^{\langle U - \varepsilon^{-1/2}u(t)\,, v\rangle} \, U^\varepsilon(t) \, W(\varepsilon^{-1/2}u_0) \;=\; V^\varepsilon(t,0)^* \, \mathrm{e}^{\langle U\,, v\rangle} \, V^\varepsilon(t,0) \,. \tag{2.29}$$

Here

$$V^\varepsilon(t,s) \;:=\; W(\varepsilon^{-1/2}u(t))^* \, U^\varepsilon(t-s) \, W(\varepsilon^{-1/2}u(s)) \, \mathrm{e}^{\mathrm{i}\varepsilon^{-1}\int_s^t \beta} \,,$$

where

$$\beta(t) \;:=\; H(u(t)) - \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\xi} H(u(t) + \xi u(t))\Big|_{\xi=0}$$

is a phase. It is easy to see that $V^\varepsilon(t,s)$ is unitary and satisfies

$$V^\varepsilon(t,s)V^\varepsilon(s,r) \;=\; V^\varepsilon(t,r)\,, \qquad V^\varepsilon(t,t) \;=\; \mathbb{1}\,.$$

Next, we compute the generator of $V^\varepsilon(t,s)$.

LEMMA 2.10. *Let $u_0 \in X^1$ and $\Psi \in \mathcal{H}^0 \cap \mathcal{D}(T)$. Then $V^\varepsilon(t,s)\Psi$ is strongly differentiable with respect to s and we have*

$$\frac{\mathrm{d}}{\mathrm{d}s} V^\varepsilon(t,s)\Psi \;=\; V^\varepsilon(t,s) D^\varepsilon(s)\Psi \,,$$

where

$$D^\varepsilon(s) \;:=\; \mathrm{i}\varepsilon^{-1} H(u(s) + U^\varepsilon) - \mathrm{i}\varepsilon^{-1} H(u(s)) - \mathrm{i}\varepsilon^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi} H(u(s) + \xi U^\varepsilon)\Big|_{\xi=0} \,. \tag{2.30}$$

PROOF. Note first that (2.18) implies that $W(\varepsilon^{-1/2}u(s))\Psi$ is in the domain of $H(U^\varepsilon)$. Therefore Lemma 2.9 implies that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}s} V^\varepsilon(t,s)\Psi \;&=\; W(\varepsilon^{-1/2}u(t))^* \, U^\varepsilon(t-s) \\ &\times \left(\mathrm{i}\varepsilon^{-1} H(U^\varepsilon) + \varepsilon^{-1}\left\langle U^\varepsilon - \frac{u(s)}{2}\,,\, \dot u(s)\right\rangle - \mathrm{i}\varepsilon^{-1}\beta(s)\right) W(\varepsilon^{-1/2}u(s)) \, \mathrm{e}^{\mathrm{i}\varepsilon^{-1}\int_s^t \beta} \, \Psi \,.\end{aligned}$$

Using (2.18) we get therefore

$$\frac{\mathrm{d}}{\mathrm{d}s} V^\varepsilon(t,s)\Psi \;=\; V^\varepsilon(t,s)\left(\mathrm{i}\varepsilon^{-1} H(U^\varepsilon + u(s)) + \varepsilon^{-1}\left\langle U^\varepsilon + \frac{u(s)}{2}\,,\, \dot u(s)\right\rangle - \mathrm{i}\varepsilon^{-1}\beta(s)\right)\Psi \,. \tag{2.31}$$

Next, note that $u(t)$ satisfies the Hamiltonian equations of motion

$$\begin{aligned}\dot p(s) \;&=\; -\frac{\partial H}{\partial q}(u(s))\,, & \dot q(s) \;&=\; \frac{\partial H}{\partial p}(u(s))\,, \\ \dot\alpha(s) \;&=\; -\mathrm{i}\frac{\partial H}{\partial \overline{\alpha}}(u(s))\,, & \dot{\overline{\alpha}}(s) \;&=\; -\mathrm{i}\frac{\partial H}{\partial \alpha}(u(s))\,.\end{aligned}$$

Recalling the definition (2.17), we therefore get

$$\langle U\,, \dot u(s)\rangle \;=\; -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\xi} H(u(s) + \xi U)\Big|_{\xi=0} \,.$$

Inserting this into (2.31) yields

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}s}V^\varepsilon(t,s)\Psi &= V^\varepsilon(t,s)\bigg(\mathrm{i}\varepsilon^{-1}H(U^\varepsilon+u(s)) - \mathrm{i}\varepsilon^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}H(u(s)+\xi U^\varepsilon)\Big|_{\xi=0} \\ &\qquad - \frac{\mathrm{i}\varepsilon^{-1}}{2}\frac{\mathrm{d}}{\mathrm{d}\xi}H(u(s)+\xi u(s))\Big|_{\xi=0} - \mathrm{i}\varepsilon^{-1}\beta(s)\bigg)\Psi \\ &= V^\varepsilon(t,s)\bigg(\mathrm{i}\varepsilon^{-1}H(U^\varepsilon+u(s)) - \mathrm{i}\varepsilon^{-1}H(u(s)) - \mathrm{i}\varepsilon^{-1}\frac{\mathrm{d}}{\mathrm{d}\xi}H(u(s)+\xi U^\varepsilon)\Big|_{\xi=0}\bigg)\Psi\,,\end{aligned}$$

which is the claim. □

After these preparations we may prove our main lemma.

LEMMA 2.11. *Let $u_0 \in X^1$, $\Psi \in \mathcal{H}$ and $t, s \in \mathbb{R}$. Then*

$$\lim_{\varepsilon\to 0}\big\|V^\varepsilon(t,s)\Psi - V(t,s)\Psi\big\| \;=\; 0\,.$$

PROOF. By density, is suffices to prove the claim for $\Psi \in \mathcal{H}^{\leqslant n} \cap \mathcal{D}(T)$, which we assume from now on. Also, since both $V(t,s)$ and $V^\varepsilon(t,s)$ are unitary, it suffices to prove the claim for $|t-s| < (4M)^{-1}$, where M is the constant from Lemma 2.8. To simplify notation, let us assume that $s = 0$ and $0 \leqslant t < (4M)^{-1}$.

The idea of the proof is to write, at least formally,

$$V(t,0)\Psi - V^\varepsilon(t,0)\Psi \;=\; \int_0^t \mathrm{d}s\,\frac{\mathrm{d}}{\mathrm{d}s}V^\varepsilon(t,s)V(s,0)\Psi\,, \tag{2.32}$$

and use Lemma 2.10 to get

$$V(t,0)\Psi - V^\varepsilon(t,0)\Psi \;=\; \int_0^t V^\varepsilon(t,s)\big(D^\varepsilon(s) - \mathrm{i}H(s)\big)V(s,0)\Psi\,. \tag{2.33}$$

Let us now justify the formal identity (2.32). In order to show that $V^\varepsilon(t,s)V(s,0)\Psi$ is strongly differentiable in s, it suffices to show that $V(s,0)\Psi$ is in the domains of $H(s)$ and $D^\varepsilon(s)$. (That Lemma 2.10 is applicable follows from a simple argument using the strongly convergent Dyson series (2.26)).

We start by showing $V(s,0)\Psi \in \mathcal{D}(H(s))$. The Dyson series (2.26), combined with Lemma 2.8, immediately shows that $V(s,0)\Psi \in \mathcal{D}(\widetilde{H}(s))$. It remains to ensure that $V(s,0)\Psi \in \mathcal{D}(T)$. To this end we define the sequence of vectors

$$\Psi^{(0)} \;:=\; \mathrm{e}^{-\mathrm{i}Tr_0}\Psi\,, \qquad \Psi^{(k)} \;=\; \mathrm{e}^{-\mathrm{i}Tr_k}\widetilde{H}(r_0+\cdots+r_{k-1})\Psi^{(k-1)}\,,$$

which depend on a sequence of real numbers $r_0, r_1, \ldots$. Lemma 2.8 implies that

$$\Psi^{(k)} \in \mathcal{H}^{\leqslant(n+2k)}\,, \qquad \|\Psi^{(k)}\| \;\leqslant\; M^k(n+2)(n+4)\cdots(n+2k)\|\Psi\|\,. \tag{2.34}$$

We may now rewrite the Dyson series (2.26) as

$$V(s,0)\Psi \;=\; \sum_{k\geqslant 0}\int_0^\infty \mathrm{d}r_0\cdots\int_0^\infty \mathrm{d}r_k\;\delta(s-r_0-\cdots r_k)\Psi^{(k)}\,. \tag{2.35}$$

Next, write

$$T\Psi^{(k)} \;=\; \mathrm{e}^{-\mathrm{i}Tr_k}\big[T, \widetilde{H}(r_0+\cdots+r_{k-1})\big]\Psi^{(k-1)} + \mathrm{e}^{-\mathrm{i}Tr_k}\widetilde{H}(r_0+\cdots+r_{k-1})T\Psi^{(k-1)}\,.$$

A straightforward calculation using the canonical commutation relations (2.21) and Lemma 2.7 yields the bound

$$\big\|[T\,,\widetilde{H}(t)]\big|_{\mathcal{H}^{\leqslant m}}\big\| \;\leqslant\; C(m+2)\,,$$

where the constant C depends only on $H(u_0)$. This yields

$$\begin{aligned}\big\|T\Psi^{(k)}\big\| \;&\leqslant\; C(n+2k)\big\|\Psi^{(k-1)}\big\| + \big\|\widetilde{H}(r_0+\cdots+r_{k-1})T\Psi^{(k-1)}\big\|\\ &\leqslant\; CM^{k-1}(n+2)(n+4)\cdots(n+2k)\big\|\Psi\big\| + M(n+2k)\big\|T\Psi^{(k-1)}\big\|\,,\end{aligned}$$

where in the last step we used Lemma 2.8. Iterating this estimate yields

$$\begin{aligned}\big\|T\Psi^{(k)}\big\| \;&\leqslant\; kCM^{k-1}(n+2)(n+4)\cdots(n+2k)\|\Psi\| + M^k(n+2)(n+4)\cdots(n+2k)\|T\Psi\|\\ &\leqslant\; 2^n\bigg(\frac{kC}{M}\|\Psi\|+\|T\Psi\|\bigg)(4M)^k k!\,.\end{aligned}$$

Inserting this into (2.35) yields

$$\|T\,V(s,0)\Psi\| \;\leqslant\; \sum_{k\geqslant 0} 2^n\bigg(\frac{kC}{M}\|\Psi\|+\|T\Psi\|\bigg)(4Ms)^k \;<\; \infty\,,$$

by assumption. This concludes the proof of $V(s,0)\Psi\in\mathcal{D}(T)$.

We now move on to showing that $V(s,0)\Psi\in\mathcal{D}(D^\varepsilon(s))$, where $D^\varepsilon(s)$ is given by (2.30). The second term of $D^\varepsilon(s)$ is bounded uniformly in time. Its third term is easily seen to be finite when applied to the Dyson series (2.35), as it is linear in $a(z), a^*(z)$. Let us therefore concentrate on the term $\mathrm{i}\varepsilon^{-1}H(u(s)+U^\varepsilon)$. It is easy to see, using the Dyson series (2.35), that $V(s,0)\Psi$ lies in the domain of

$$\sum_{i=1}^N \frac{1}{2m_i}\big(p_i(s)+P^\varepsilon - e_iA(q_i(s)+Q^\varepsilon,\alpha(s)+a^\varepsilon)\big)^2\,.$$

Similarly, since $\alpha(s)\in X^1$ and $V(s,0)\Psi\in\mathcal{D}(T)$ as shown above, it follows that $V(s,0)\Psi$ is in the domain of

$$\sum_\lambda\int \mathrm{d}k\,|k|\,\big(\overline{\alpha_\lambda}(s,k)+a_\lambda^{\varepsilon *}(k)\big)\big(\alpha_\lambda(s,k)+a_\lambda^\varepsilon(k)\big)\,.$$

It therefore remains to show that $V(s,0)\Psi$ is in the domain of

$$V(q(s)+Q^\varepsilon) \;=\; \sum_{i<j} e_ie_j w(q_i(s)-q_j(s)+Q_i^\varepsilon-Q_j^\varepsilon)\,.$$

If (Ha) holds then w is bounded and the claim follows immediately. If (Hb) holds, we use Hardy's inequality

$$\langle\psi\,,|x|^{-2}\psi\rangle \;\lesssim\; -\langle\psi\,,\Delta\psi\rangle\,,$$

valid in $L^2(\mathbb{R}^3)$, to get

$$\bigg\|\frac{1}{\big|q_i(s)-q_j(s)+Q_i^\varepsilon-Q_j^\varepsilon\big|}\Phi\bigg\| \;\lesssim\; \varepsilon^{-1/2}\,\|P_i\Phi\|. \tag{2.36}$$

Hence,

$$\big\|V(q(s)+Q^\varepsilon)V(s,0)\Psi\big\| \;\lesssim\; \varepsilon^{-1/2}\sum_{i=1}^N\|P_iV(s,0)\Psi\|\,. \tag{2.37}$$

It is now easy to conclude from the Dyson series (2.35) that the right-hand side of (2.37) is finite. This concludes the proof of $V(s,0)\Psi \in \mathcal{D}(D^\varepsilon(s))$, and hence of (2.33).

Let us summarize. We have shown that

$$V(t,0)\Psi - V^\varepsilon(t,0)\Psi \;=\; \int_0^t V^\varepsilon(t,s)L^\varepsilon(s)V(s,0)\Psi\,, \tag{2.38}$$

where

$$L^\varepsilon(s) \;:=\; \mathrm{i}\varepsilon^{-1}\left[H_w(u(s)+U^\varepsilon) - H_w(u(s)) - \frac{\mathrm{d}}{\mathrm{d}\xi}H_w(u(s)+\xi U^\varepsilon)\Big|_{\xi=0} - \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}H_w\big(u(s)+\xi U^\varepsilon\big)\Big|_{\xi=0}\right]$$

and

$$H_w(p,q,\alpha) \;:=\; \sum_{i=1}^N \frac{1}{2m_i}\big(p_i - e_i A(q_i,\alpha)\big)^2 + V(q)\,. \tag{2.39}$$

Here we used that all terms that are quadratic in U^ε vanish in $D^\varepsilon(s) - \mathrm{i}H(s)$, so that they may be omitted from H. It is sometimes convenient to rewrite this as

$$L^\varepsilon(s) \;=\; F(1) - F(0) - F'(0) - \frac{1}{2}F''(0) \;=\; \frac{1}{2}\int_0^1 \mathrm{d}\xi\; F'''(\xi)(1-\xi)^2\,, \tag{2.40}$$

where

$$F(\xi) \;:=\; \mathrm{i}\varepsilon^{-1}H_w(u(s)+\xi U^\varepsilon)\,.$$

Next, we decompose $L^\varepsilon(s) = L_1^\varepsilon(s) + L_2^\varepsilon(s)$ into two terms corresponding to the two terms of (2.39). Let us start by estimating $\big\|L_2^\varepsilon V(s,0)\Psi\big\|$. Explicitly,

$$\begin{aligned} L_2^\varepsilon(s) \;&=\; \mathrm{i}\varepsilon^{-1}\Big(V\big(q(s)+Q^\varepsilon\big) - V(q(s)) - \nabla V(q(s))\cdot Q^\varepsilon - \frac{1}{2}\nabla^2 V(q(s))\cdot (Q^\varepsilon)^2\Big) &(2.41)\\ &=\; \frac{\mathrm{i}\varepsilon^{-1}}{2}\int_0^1 \mathrm{d}\xi\;(1-\xi)^2\,\nabla^3 V\big(q(s)+\xi Q^\varepsilon\big)\cdot (Q^\varepsilon)^3 &(2.42)\end{aligned}$$

in the notation of (2.23). Let us assume fist that (Ha) holds. Then $\|\nabla^3 V\|_\infty < \infty$ and (2.42) yields

$$\big\|L_2^\varepsilon(s)V(s,0)\Psi\big\| \;\leqslant\; \varepsilon^{1/2}\|\nabla^3 V\|_\infty \||Q|^3 V(s,0)\Psi\|\,.$$

Using the Dyson series (2.35), we therefore get

$$\lim_{\varepsilon\to 0}\big\|L_2^\varepsilon(s)V(s,0)\Psi\big\| \;=\; 0\,.$$

The case (Hb) requires a little more work. Note first that there is a $\sigma > 0$ such that, in the σ-neighbourhood of the trajectory $\{q(s)\}_{s\in\mathbb{R}}$, $V(q)$ has bounded derivatives of any order. Choose a smooth cutoff function $\zeta : \mathbb{R} \to [0,1]$ such that $\zeta(x) = 0$ for $x \leqslant 1/2$ and $\zeta(x) = 1$ for $x \geqslant 1$. Abbreviate $\overline{\zeta} := 1 - \zeta$ and partition

$$\mathbb{1} \;=\; \zeta(|Q^\varepsilon|/\sigma) + \overline{\zeta}(|Q^\varepsilon|/\sigma)\,.$$

The first resulting term, $\big\|\zeta(|Q^\varepsilon|/\sigma)L_2^\varepsilon V(s,0)\Psi\big\|$, vanishes faster than any power of ε. To show this, consider for instance the second term of (2.41). We have for any M

$$\begin{aligned} &\varepsilon^{-1}\big\|\zeta(|Q^\varepsilon|/\sigma)\,V(q(s))\,V(s,0)\Psi\big\|\\ \leqslant\;& \varepsilon^{-1}\sup_r|V(q(r))|\,\big\|\zeta(|Q^\varepsilon|/\sigma)\,V(s,0)\Psi\big\|\\ \lesssim\;& \varepsilon^{M-1}\big\|\zeta(|Q^\varepsilon|/\sigma)\,\varepsilon^{-M}\,V(s,0)\Psi\big\|\\ \leqslant\;& \varepsilon^{M-1}\Big(\frac{2}{\sigma}\Big)^{2M}\big\||Q|^{2M}\,V(s,0)\Psi\big\|\,, \end{aligned} \tag{2.43}$$

where in the last step we used that $\varepsilon^{-1/2} \leqslant 2\sigma^{-1}|Q|$ on the support of $\zeta(|Q^\varepsilon|/\sigma)$. By the Dyson series (2.35), the right-hand side of (2.43) is finite. The second and third terms of (2.41) are handled in the same way. In order to estimate the first term of (2.41) we start as in (2.43):

$$\varepsilon^{-1}\big\|\zeta(|Q^\varepsilon|/\sigma)\, V(q(s)+Q^\varepsilon)\, V(s,0)\Psi\big\| \;\lesssim\; \varepsilon^{M-1}\big\|V(q(s)+Q^\varepsilon)\,\zeta(|Q^\varepsilon|/\sigma)\,|Q|^{2M}\, V(s,0)\Psi\big\|\,.$$

In a second step, we apply Hardy's inequality (2.36) to get

$$\begin{aligned}
&\varepsilon^{-1}\big\|\zeta(|Q^\varepsilon|/\sigma)\, V(q(s)+Q^\varepsilon)\, V(s,0)\Psi\big\| \\
\lesssim\;& \varepsilon^{M-3/2}\sum_{i=1}^{N}\big\|P_i\,\zeta(|Q^\varepsilon|/\sigma)\,|Q|^{2M}\, V(s,0)\Psi\big\| \\
\leqslant\;& \varepsilon^{M-3/2}\sum_{i=1}^{N}\Big(\frac{\varepsilon^{1/2}}{\sigma}\sup_x|\zeta'(x)|\big\||Q|^{2M}\, V(s,0)\Psi\big\| + \big\|P_i\,|Q|^{2M}\, V(s,0)\Psi\big\|\Big)\,,
\end{aligned}$$

where the right-hand side is finite by the Dyson series (2.35). This concludes the proof of

$$\lim_{\varepsilon\to 0}\big\|\zeta(|Q^\varepsilon|/\sigma)L_2^\varepsilon V(s,0)\Psi\big\| \;=\; 0$$

in the case (Hb). Let us now consider

$$\big\|\overline{\zeta}(|Q^\varepsilon|/\sigma)L_2^\varepsilon V(s,0)\Psi\big\| \;\leqslant\; \big\|\mathbb{1}_{\{|Q^\varepsilon|\leqslant\sigma\}}L_2^\varepsilon V(s,0)\Psi\big\|\,.$$

From (2.42) and by assumption on σ, we get

$$\big\|\mathbb{1}_{\{|Q^\varepsilon|\leqslant\sigma\}}L_2^\varepsilon V(s,0)\Psi\big\| \;\leqslant\; \frac{\varepsilon^{1/2}}{2}\int_0^1 \mathrm{d}\xi\; C(1-\xi)^2\big\||Q|^3 V(s,0)\Psi\big\|\,.$$

This concludes the proof of

$$\lim_{\varepsilon\to 0}\big\|L_2^\varepsilon V(s,0)\Psi\big\| \;=\; 0$$

in the case (Hb).

Consider now

$$\begin{aligned}
L_1^\varepsilon(s) \;&=\; \frac{\mathrm{i}\varepsilon^{-1}}{2}\int_0^1 \mathrm{d}\xi\;(1-\xi)^2\frac{\mathrm{d}^3}{\mathrm{d}\xi^3}H_w(u(s)+\xi U^\varepsilon) \\
&=\; \frac{\mathrm{i}\varepsilon^{-1}}{2}\int_0^1 \mathrm{d}\xi\;(1-\xi)^2\sum_{i=1}^{N}\frac{1}{2m_i} \\
&\qquad\times\big(Y_i'''(\xi)\cdot Y_i(\xi) + 3Y_i''(\xi)\cdot Y_i'(\xi) + 3Y_i'(\xi)\cdot Y_i''(\xi) + Y_i(\xi)\cdot Y_i'''(\xi)\big)\,;
\end{aligned} \tag{2.44}$$

here

$$Y_i(\xi) \;:=\; P_i(\xi) - e_i\sum_\lambda\int\frac{\mathrm{d}k}{(2\pi)^{3/2}}\frac{\chi(k)}{\sqrt{2|k|}}\Big[\varepsilon_\lambda(k)a_\lambda(\xi,k)\mathrm{e}^{\mathrm{i}k\cdot Q_i(\xi)} + \mathrm{H.c.}\Big]\,,$$

with the shorthands

$$P(\xi) \;:=\; p(s)+\xi P^\varepsilon\,,\qquad Q(\xi) \;:=\; q(s)+\xi Q^\varepsilon\,,\qquad a(\xi) \;:=\; \alpha(s)+\xi a^\varepsilon\,.$$

We get the somewhat unwieldy explicit expressions

$$
\begin{aligned}
Y_i'(\xi) &= P_i^\varepsilon(\xi) - e_i \sum_\lambda \int \frac{\mathrm{d}k}{(2\pi)^{3/2}} \frac{\chi(k)}{\sqrt{2|k|}} \Big[\varepsilon_\lambda(k) \mathrm{e}^{\mathrm{i}k\cdot Q_i(\xi)} \Big(a_\lambda^\varepsilon(k) + \mathrm{i}k \cdot Q_i^\varepsilon \, a_\lambda(\xi,k)\Big) + \text{H.c.}\Big] \,, \\
Y_i''(\xi) &= -e_i \sum_\lambda \int \frac{\mathrm{d}k}{(2\pi)^{3/2}} \frac{\chi(k)}{\sqrt{2|k|}} \\
&\qquad \times \Big[\varepsilon_\lambda(k) \mathrm{e}^{\mathrm{i}k\cdot Q_i(\xi)} \Big(2\mathrm{i}k \cdot Q_i^\varepsilon \, a_\lambda^\varepsilon(k) + a_\lambda(\xi,k) \big(\mathrm{i}k \cdot Q_i^\varepsilon\big)^2\Big) + \text{H.c.}\Big] \,, \\
Y_i'''(\xi) &= -e_i \sum_\lambda \int \frac{\mathrm{d}k}{(2\pi)^{3/2}} \frac{\chi(k)}{\sqrt{2|k|}} \\
&\qquad \times \Big[\varepsilon_\lambda(k) \mathrm{e}^{\mathrm{i}k\cdot Q_i(\xi)} \Big(3a_\lambda^\varepsilon(k) \big(\mathrm{i}k \cdot Q_i^\varepsilon\big)^2 + a_\lambda(\xi,k) \big(\mathrm{i}k \cdot Q_i^\varepsilon\big)^3\Big) + \text{H.c.}\Big] \,.
\end{aligned}
$$

Next, let $\Phi \in \mathcal{H}^{\leqslant m}$. Let us estimate for example $\|Y_i(\xi) \cdot Y_i'''(\xi)\Phi\|$ (the other terms in (2.44) are dealt with in the same way). Write

$$
\begin{aligned}
Y_i(\xi) \cdot Y_i'''(\xi)\Phi &= \big(Y_i(\xi) - P_i(\xi)\big) \cdot Y_i'''(\xi)\Phi + P_i(\xi) \cdot Y_i'''(\xi)\Phi \\
&= \big(Y_i(\xi) - P_i(\xi)\big) \cdot Y_i'''(\xi)\Phi + Y_i'''(\xi) \cdot P_i(\xi)\Phi \,,
\end{aligned} \tag{2.45}
$$

where the second step follows from a simple calculation using $k \cdot \varepsilon_\lambda(k) = 0$. Let us assume without loss of generality that $\varepsilon \leqslant 1$. Then, using Lemma 2.7, we may bound the second term of (2.45) by

$$
C\varepsilon^{3/2}(m+5)^{5/2}\|\Phi\| \,, \tag{2.46}
$$

where C depends only on $H(u_0)$. Writing all factors of the form $\mathrm{e}^{\mathrm{i}k\cdot Q_i(\xi)}$ on the left and applying Lemma 2.7 implies similarly that the first term of (2.45) is bounded by (2.46). Thus we have shown that

$$
\big\|L_1^\varepsilon(s)\Phi\big\| \;\leqslant\; C\varepsilon^{1/2}(m+5)^{5/2}\|\Phi\| \,.
$$

Hence the Dyson series (2.35) implies

$$
\big\|L_1^\varepsilon(s)V(s,0)\Psi\big\| \;\leqslant\; C\varepsilon^{1/2} \,.
$$

Let us summarize: We have shown that

$$
\lim_{\varepsilon\to 0}\big\|L^\varepsilon(s)V(s,0)\Psi\big\| \;=\; 0 \,.
$$

Also, note that $V^\varepsilon(t,s)$ is unitary and, as shown above, we have the bound

$$
\big\|L^\varepsilon(s)V(s,0)\Psi\big\| \;\leqslant\; C
$$

for all $\varepsilon \leqslant 1$. Thus, the claim follows by applying dominated convergence (for strong vector-valued integrals) in (2.38). $\square$

We may now complete the proof of Theorem 2.3. Let $\Psi \in \mathcal{H}$. We find

$$
\begin{aligned}
&\big\|W(\varepsilon^{-1/2}u_0)^* \, U^\varepsilon(t)^* \, \mathrm{e}^{\langle U^\varepsilon, v\rangle} \, U^\varepsilon(t) \, W(\varepsilon^{-1/2}u_0)\Psi - \mathrm{e}^{\langle u(t), v\rangle}\Psi\big\| \\
&= \big\|W(\varepsilon^{-1/2}u_0)^* \, U^\varepsilon(t)^* \, \mathrm{e}^{\langle U^\varepsilon - u(t), v\rangle} \, U^\varepsilon(t) \, W(\varepsilon^{-1/2}u_0)\Psi - \Psi\big\| \\
&= \big\|V^\varepsilon(t,0)^* \, \mathrm{e}^{\varepsilon^{1/2}\langle U, v\rangle} \, V^\varepsilon(t,0)\Psi - \Psi\big\| \,,
\end{aligned}
$$

by (2.29). Since $\text{s-lim}_\varepsilon V^\varepsilon(t,0) = V(t,0)$ by Lemma 2.11, and $\text{s-lim}_\varepsilon \mathrm{e}^{\varepsilon^{1/2}\langle U, v\rangle} = \mathbb{1}$, the claim follows.

Chapter 3

Limiting Dynamics in Quantum Lattice Models

In this chapter we study the limiting dynamics of various quantum lattice models.

Sections 3.1 and 3.2 are similar in spirit. In Section 3.1 we consider the large-spin limit of a quantum spin system on a lattice; the limiting/quantization parameter is the inverse magnitude of the spins. In Section 3.2 we consider the continuum limit of a quantum spin system, where the magnitude of the spins remains fixed but the lattice spacing converges to zero; the limiting/quantization parameter is a power of the lattice spacing. The strategy is similar for both sections. We start by introducing a large class of quantum spin systems, as well as the corresponding class of classical spin systems. We prove a Egorov-type theorem, which we also extend to domains of infinite size. Our proof relies on a perturbative expansion of the dynamics. As an application, we discuss the limiting dynamics of coherent spin states. The physical interpretation in both cases is similar: In a macroscopic regime where quantum spins form large clusters whose constituents cannot be observed individually, the spins behave classically.

In Section 3.3 we extend the results of Section 3.1 to cover the limiting behaviour of time-dependent correlation functions at a positive temperature. We prove that, in the large-spin limit, correlation functions of the quantum spin system converge to correlation functions of the corresponding classical spin system. The main ingredient of our proof is an expansion in coherent spin states. Assuming the temperature is high enough (thus in particular ruling out phase transitions), we extend this result to domains of infinite size using a quantum cluster expansion.

Finally, in Section 3.4 we consider a Bose gas on a finite lattice, and prove results analogous to those of Section 3.3. The limiting parameter is the inverse of the mean density of the Bose gas; this corresponds to a mean-field limit. Although our strategy is similar to that of Section 3.3, we have to deal with additional technical difficulties arising from the unboundedness of the particle density.

3.1. Spins on a lattice: the large-spin limit

In this section we consider spins on an arbitrary, fixed lattice. We study their dynamics in the limit where their magnitude tends to infinity. In this limit the behaviour of a quantum spin becomes classical in the sense that its Cartesian components commute and take on continuous values on the unit sphere. Thus one expects that the dynamics of the quantum spin system should be governed by an equation of motion of a classical spin system. A typical example of such an equation is the *Landau-Lifschitz equation*

$$\partial_t M(t,x) \;=\; M(t,x) \times H_M(t,x)\,, \tag{3.1}$$

where M denotes a classical spin field with values on the unit 2-sphere, x a point in the lattice, and $\times$ the vector product on $\mathbb{R}^3$. The "exchange field" H is some (nonlocal) function of the spin field M. It is responsible for the interactions between different spins. Equations of the type (3.1) are widely used in the study of ferromagnetism and describe for instance the propagation of spins waves in a ferromagnet. A standard choice for the exchange field is $H_M = J\Delta M$, where $J \in \mathbb{R}$ is a coupling constant and Δ is the Laplacian. In this case (and its continuum analogue, see Section 3.2), the evolution equation (3.1) has been studied in the mathematical literature; see for instance [GKT07, KP06] and references given there.

Historically, the first mathematical results on the large-spin limit concerned aspects independent of time, such as the classical limit of quantum partition functions for spin systems [Lie73, Sim80]. Here we consider the dynamical evolution of quantum spin systems in limiting regimes; see [MPS99, Vui80] for earlier results in this direction.

3.1.1. A system of classical spins. We start by introducing a system of classical spins. Consider the infinite lattice[1] $\mathbb{Z}^d$, where $d \geqslant 1$. Let $\Lambda \subset \mathbb{Z}^d$ be a finite subset. A *classical spin system* on Λ is formulated on the phase space

$$\Gamma_\Lambda \;:=\; \prod_{x\in\Lambda} \mathbb{S}^2\,,$$

where $\mathbb{S}^2 \subset \mathbb{R}^3$ is the unit two-sphere. It is well known that Γ_Λ is a symplectic manifold with symplectic 2-form

$$\omega \;=\; -\sum_{x\in\Lambda}\sum_{i,j,k=1}^{3} \varepsilon_{ijk}\, M_i(x)\, \mathrm{d}M_j(x) \otimes \mathrm{d}M_k(x)\,, \tag{3.2}$$

where $\{M_i(x)\}_{x\in\Lambda, i=1,2,3}$ are the Cartesian coordinate functions on Γ_Λ. Here ε_{ijk} is the totally antisymmetric symbol.

For our purposes it is convenient to work on the larger space

$$\Xi_\Lambda \;:=\; \prod_{x\in\Lambda} \overline{B_1(0)}\,,$$

where $\overline{B_1(0)} \subset \mathbb{R}^3$ is the closed unit ball. We also replace the coordinates $\{M_i(x)\}_{x\in\Lambda,i=1,2,3}$ with

$$M_\pm(x) \;:=\; \frac{1}{\sqrt{2}}\big(M_1(x) \pm \mathrm{i} M_2(x)\big)\,, \qquad M_z(x) \;:=\; M_3(x)\,. \tag{3.3}$$

Thus, Ξ_Λ is a Poisson manifold with Poisson bracket given by

$$\big\{M_i(x)\,, M_j(y)\big\} \;=\; \mathrm{i}\sum_{k\in I} \tilde{\varepsilon}_{ijk}\, \delta(x,y)\, M_k(x)\,, \tag{3.4}$$

where $i,j \in I$ with $I := \{+, z, -\}$. Here $\tilde{\varepsilon}_{ijk}$ is defined by $\tilde{\varepsilon}_{\pm\mp z} = \pm 1$, $\tilde{\varepsilon}_{\pm z \pm} = \mp 1$, $\tilde{\varepsilon}_{z\pm\pm} = \pm 1$, and $\tilde{\varepsilon}_{ijk} = 0$ otherwise. It is a simple matter to check that (3.4), when restricted to Γ_Λ, agrees with the Poisson bracket of (3.2). One finds immediately that

$$|M_i(x)| \;\leqslant\; 1\,, \qquad x \in \Lambda\,,\; i \in I\,. \tag{3.5}$$

[1] We choose $\mathbb{Z}^d$ for simplicity of presentation, but our results hold for any lattice.

Here $|\cdot|$ denotes the Euclidean norm on $\mathbb{R}^3$.

Let us denote by $\mathfrak{A}_\Lambda$ the space of polynomials in the variables $\{M_i(x)\}_{x\in\Lambda, i\in I}$. Thus, $\mathfrak{A}_\Lambda$ is Poisson algebra with Poisson bracket given by (3.4). We equip $\mathfrak{A}_\Lambda$ with the norm

$$\|A\|_\infty \;:=\; \sup_{M\in\Xi_\Lambda} |A(M)|\,.$$

By the Stone-Weierstrass theorem, $\mathfrak{A}_\Lambda$ is dense in the set $\overline{\mathfrak{A}}_\Lambda$ of continuous functions on Ξ_Λ.

If $\Lambda_1 \subset \Lambda_2$, a function $A_1 \in \mathfrak{A}_{\Lambda_1}$ may be identified in the usual fashion with a function $A_2 \in \mathfrak{A}_{\Lambda_2}$ by setting $A_2 = A_1 \otimes 1_{\Lambda_2\setminus\Lambda_1}$, where $1_{\Lambda_2\setminus\Lambda_1}$ is the unit function. In the following we tacitly make use of this identification.

3.1.2. A system of quantum spins. The quantum analogue of the classical spin system described above is formulated on the finite-dimensional Hilbert space

$$\mathcal{H}^s_\Lambda \;:=\; \bigotimes_{x\in\Lambda} \mathcal{H}^s_x\,,$$

where $s = \frac{1}{2}, 1, \frac{3}{2}, \dots$ denotes the magnitude of the spins. Here $\mathcal{H}^s_x := \mathbb{C}^{2s+1}$ carries the irreducible s-representation of su(2), with generators $S^s_1(x), S^s_2(x), S^s_3(x)$. In the following we drop the superscript s when it is not needed. The basis transformation defined by (3.3), when applied to $S_1(x), S_2(x), S_3(x)$, yields the generators $S_+(x), S_z(x), S_-(x)$. Define the rescaled generators

$$\widehat{S}_i(x) \;:=\; \frac{1}{s} S_i(x)\,, \qquad i\in I\,,\, x\in\Lambda\,.$$

The rescaling by s^{-1} may be interpreted as semiclassical. Indeed, $\widehat{S}$ has the physical meaning of an angular momentum that possesses a well-defined limit as $s\to\infty$, and s^{-1} plays the role of $\hbar$.

It follows $\{\widehat{S}_i(x)\}$ satisfy the commutation relations

$$\big[\widehat{S}_i(x)\,, \widehat{S}_j(y)\big] \;=\; \frac{1}{s}\sum_{k\in I} \tilde{\varepsilon}_{ijk}\, \delta(x,y)\, \widehat{S}_k(x)\,, \tag{3.6}$$

where $i,j\in I$. A simple computation shows that

$$\big\|\widehat{S}_i(x)\big\| \;\leqslant\; \begin{cases} 1 & \text{if } s\geqslant 1 \\ \sqrt{2} & \text{if } s=\frac{1}{2}\,. \end{cases} \tag{3.7}$$

Here $\|\cdot\|$ denotes operator norm. As we are interested in the limit $s\to\infty$, we assume from now on that $s\geqslant 1$. This avoids having to treat the case $s=1/2$ separately when applying (3.7).

In analogy to $\mathfrak{A}_\Lambda$, we denote by $\widehat{\mathfrak{A}}_\Lambda$ the set of polynomials in the variables $\{\widehat{S}_i(x)\}_{x\in\Lambda,i\in I}$. Using Schur's lemma and von Neumann's bicommutant theorem we see that $\widehat{\mathfrak{A}}_\Lambda$ is in fact equal to $\mathcal{L}(\mathcal{H}_\Lambda)$, the space of operators on $\mathcal{H}_\Lambda$.

If $\Lambda_1\subset\Lambda_2$, an operator $\mathbf{A}_1 \in \widehat{\mathfrak{A}}_{\Lambda_1}$ may be identified with an operator $\mathbf{A}_2 \in \widehat{\mathfrak{A}}_{\Lambda_2}$ by setting $\mathbf{A}_2 = \mathbf{A}_1 \otimes \mathbb{1}_{\Lambda_2\setminus\Lambda_1}$. In the following we tacitly make use of this identification.

3.1.3. Quantization. We now introduce a quantization mapping from $\mathfrak{A}_\Lambda$ to $\widehat{\mathfrak{A}}_\Lambda$. Since the generators $\{\widehat{S}_i(x)\}$ of $\widehat{\mathfrak{A}}_\Lambda$ do not commute, we introduce an ordering prescription for products of generators. We say that a monomial $\widehat{S}_{i_1}(x_1)\cdots\widehat{S}_{i_p}(x_p)$ is *normal-ordered* if $i_k < i_l \Rightarrow k < l$, where $<$ is defined on I through $+ < z < -$. We then define *normal ordering* $:\cdot:$ by

$$:\widehat{S}_{i_1}(x_1)\cdots\widehat{S}_{i_p}(x_p): \;=\; \widehat{S}_{i_{\sigma(1)}}(x_{\sigma(1)})\cdots\widehat{S}_{i_{\sigma(p)}}(x_{\sigma(p)})\,,$$

where $\sigma \in S_p$ is a permutation such that the monomial on the right-hand side is normal-ordered. We extend $:\cdot:$ to polynomials by linearity.

Next, we define *quantization* $\widehat{(\cdot)} : \mathfrak{A}_\Lambda \to \widehat{\mathfrak{A}}_\Lambda$ as the formal replacement $M_i(x) \mapsto \widehat{S}_i(x)$ followed by normal ordering. We also set $\widehat{1} = \mathbb{1}$. Note that, by definition, $\widehat{(\cdot)}$ is a linear map (but, of course, not an algebra homomorphism) and satisfies $(\widehat{A})^* = \widehat{\overline{A}}$. It is also easy to see that, for $A, B \in \mathfrak{A}_\Lambda$, we have

$$[\widehat{A}, \widehat{B}] \;=\; -\frac{\mathrm{i}}{s}\widehat{\{A, B\}} + O(s^{-2})\,,$$

so that s^{-1} is the parameter of $\widehat{(\cdot)}$.

We also remark that, while natural, the above choice of normal ordering is by no means unique. Our results remain valid for any choice of normal ordering. It is sometimes useful to also consider other orderings; we use the notation $Q(\widehat{S}^\alpha)$ to denote an ordering of a monomial $\widehat{S}^\alpha$ defined by Q.

3.1.4. Hamilton function and dynamics. A fairly general class of Hamilton functions H_Λ on Ξ_Λ may be conveniently written using multi-indices $\alpha \in \mathbb{N}^{I\times\mathbb{Z}^d}$, which we write as $\alpha = (\alpha_i(x))_{x\in\mathbb{Z}^d, i\in I}$. We only consider multi-indices α satisfying $|\alpha| < \infty$, where

$$|\alpha| \;:=\; \sum_{x\in\mathbb{Z}^d}\sum_{i\in I}\alpha_i(x)\,.$$

The concept of the *support* of α,

$$[\alpha] \;:=\; \big\{x \in \mathbb{Z}^d \,:\, \exists i \in I \;\alpha_i(x) \neq 0\big\}\,,$$

is sometimes useful.

Next, we associate with each multi-index α the monomial

$$M^\alpha \;:=\; \prod_{x\in\Lambda}\prod_{i\in I} M_i(x)^{\alpha_i(x)}\,. \tag{3.8}$$

Consider a family $(V(\alpha))_{\alpha\in\mathbb{N}^{I\times\mathbb{Z}^d}}$ of complex numbers. The associated Hamilton function H_Λ on Ξ_Λ is defined through

$$H_\Lambda \;:=\; \sum_{\alpha\,:\,[\alpha]\subset\Lambda} V(\alpha)\, M^\alpha\,. \tag{3.9}$$

We impose the following conditions on the family $(V(\alpha))$. First, we require that $\overline{V(\alpha)} = V(\overline{\alpha})$. Here the "conjugate" $\overline{\alpha}$ of a multi-index α is defined as $\overline{\alpha}_i(x) := \alpha_{\overline{i}}(x)$, where the action of $\overline{\cdot}$ on I is defined by $(+, z, -) \mapsto (-, z, +)$. This condition ensures that H_Λ is a real function. Second, we assume that there is an $r > 0$ such that

$$\|V\|_r \;:=\; \sum_{n\in\mathbb{N}}\sup_{x\in\mathbb{Z}^d}\sum_{\substack{\alpha\,:\,|\alpha|=n\,,\\ [\alpha]\ni x}} |V(\alpha)|\,\mathrm{e}^{rn} \;<\; \infty\,. \tag{3.10}$$

If the condition (3.10) holds, it is easy to see that (3.9) converges in $\|\cdot\|_\infty$ for any finite Λ. After a short calculation, we find that the Hamiltonian equation of motion reads

$$\frac{\mathrm{d}}{\mathrm{d}t} M_i(x) \;=\; \sum_{\alpha\,:\,[\alpha]\subset\Lambda} V(\alpha) \sum_{j,k} \mathrm{i}\tilde{\varepsilon}_{jik}\, \alpha_j(x)\, M^{\alpha-\delta_j(x)+\delta_k(x)}\,, \tag{3.11}$$

where the multi-index $\delta_i(x)$ is defined by $[\delta_i(x)]_j(y) := \delta_{ij}\delta(x,y)$. We record the following well-posedness result for the dynamics generated by the class of Hamiltonians introduced above.

LEMMA 3.1. *Let Λ be a (possibly infinite) subset of $\mathbb{Z}^d$. Let $M_0 \in \Xi_\Lambda$. Then* (3.11) *has a unique global-in-time solution $M \in C^1(\mathbb{R};\Xi_\Lambda)$ that satisfies $M(0) = M_0$. Here Ξ_Λ carries the l^∞-norm. Moreover, we have the pointwise conservation law $|M(t,x)| = |M(0,x)|$ for all t.*

PROOF. Local-in-time existence and uniqueness follows from a simple contraction mapping argument for the integral equation associated with (3.11). We omit the details. Also, continuous dependence on M_0 is a direct consequence of the contraction mapping argument. Finally, the claim that $|M(0,x)| = |M(t,x)|$ for all t can be easily verified by using (3.11), which implies that $\frac{\mathrm{d}}{\mathrm{d}t}M(t,x)$ is perpendicular to $M(t,x)$. $\square$

REMARK 3.2. *Under our assumptions,* (3.11) *also makes sense for infinite $\Lambda \subset \mathbb{Z}^d$, whereas the Hamiltonian H_Λ does not have a limit when $|\Lambda| \to \infty$.*

REMARK 3.3. *The last statement of Lemma 3.1 implies that the magnitude of each spin remains constant in time, i.e. the spins precess. In particular, if $M_0 \in \Gamma_\Lambda$, it follows that $M(t) \in \Gamma_\Lambda$ for all t. Mathematically, this is simply the statement that the symplectic leaves of the Poisson manifold Ξ_Λ remain invariant under the Hamiltonian flow.*

REMARK 3.4. *Time-dependent potentials $V(t,\alpha)$ may be treated without complications, provided that the map $t \mapsto V(t)$ is $\|\cdot\|_r$-continuous and $\sup_x$ in* (3.10) *is replaced by $\sup_{x,t}$. The weaker assumption that $t \mapsto V(t,\alpha)$ is continuous for all α implies Lemma 3.1 with the slightly weaker statement that $M \in C(\mathbb{R},\Xi_\Lambda)$ is a classical solution of* (3.11).

EXAMPLE 3.5. *Consider the Hamiltonian*

$$H_\Lambda(t) \;=\; -\sum_{x\in\Lambda} h(t,x)\cdot M(x) - \frac{1}{2}\sum_{x,y\in\Lambda} J(x,y)\, M(x)\cdot M(y)\,, \tag{3.12}$$

where $M(x) = (M_1(x), M_2(x), M_3(x))$. Here $h(t,x) \in \mathbb{R}^3$ is an "external magnetic field" satisfying $\sup_{t\in\mathbb{R},x\in\mathbb{Z}^d}|h(t,x)| < \infty$. We also require the map $t \mapsto h(t,x)$ to be continuous for all $x \in \mathbb{Z}^d$. The exchange coupling $J : \mathbb{Z}^d \times \mathbb{Z}^d \to \mathbb{R}$ is assumed to be symmetric and to satisfy $J(x,x) = 0$ for all x. Finally we assume, in accordance with condition (3.10), *that $\sup_{x\in\mathbb{Z}^d}\sum_{y\in\mathbb{Z}^d}|J(x,y)| < \infty$. The corresponding equation of motion for $M(t,x)$ is given by*

$$\frac{\mathrm{d}}{\mathrm{d}t} M(t,x) \;=\; M(t,x) \times \Big[h(t,x) + \sum_{y\in\Lambda} J(x,y) M(t,y)\Big]\,, \tag{3.13}$$

the Landau-Lifschitz equation *for a classical lattice spin system.*

Next, we move on to discussing the dynamics of the quantum spin system. Its dynamics is generated by the Hamiltonian $\widehat{H}_\Lambda$ defined as the quantization of H_Λ. More precisely, we set

$$\widehat{H}_\Lambda \;:=\; \sum_{\alpha\,:\,[\alpha]\subset\Lambda} V(\alpha) : \widehat{S}^{\,\alpha} : \;, \tag{3.14}$$

and note that the sum converges in operator norm. One easily checks that H_Λ is a (bounded) self-adjoint operator on $\mathcal{H}_\Lambda$. Denote by $U_\Lambda(t)$ the unitary propagator satisfying

$$\mathrm{i}s^{-1}\partial_t U_\Lambda(t) \;=\; \widehat{H}_\Lambda(t)U_\Lambda(t)\,, \qquad U_\Lambda(0) \;=\; \mathbb{1}\,.$$

If H_Λ is time-independent then $U_\Lambda(t) = \mathrm{e}^{-\mathrm{i}s\widehat{H}_\Lambda t}$.

Finally, we introduce a convenient shorthand for the time evolution of observables. For $A \in \mathfrak{A}_\Lambda$ and $\mathbf{A} \in \widehat{\mathfrak{A}}_\Lambda$ define

$$\begin{aligned}(\tau_\Lambda^t A)(M_0) \;&:=\; A(M(t))\,,\\ \widehat{\tau}_\Lambda^t \mathbf{A} \;&:=\; U_\Lambda(t)^*\,\mathbf{A}\,U_\Lambda(t)\,,\end{aligned}$$

where $M(t)$ is the solution of (3.11) with initial data M_0. Note that both τ_Λ^t and $\widehat{\tau}_\Lambda^t$ are norm-preserving.

3.1.5. Dynamics in the large-spin limit. We are now ready to tackle the main subject of this section: the convergence of the quantum dynamics. The following lemma is the main technical result from which everything else follows easily.

LEMMA 3.6. *Let $\varepsilon > 0$, $t \in \mathbb{R}$ and $A \in \mathfrak{A}_{\mathbb{Z}^d}$. Then there exists a finite set B of multi-indices and a family $(v_\alpha)_{\alpha \in B}$ of complex numbers with the following properties:*

$$\Bigg\|\tau_\Lambda^t A - \sum_{\alpha \in B} \mathbb{1}_{\{[\alpha] \subset \Lambda\}}\, v_\alpha\, M^\alpha\Bigg\|_\infty \;\leqslant\; \varepsilon\,, \tag{3.15a}$$

$$\Bigg\|\widehat{\tau}_\Lambda^t \widehat{A} - \sum_{\alpha \in B} \mathbb{1}_{\{[\alpha] \subset \Lambda\}}\, v_\alpha\, Q_\alpha\big(\widehat{S}^\alpha\big)\Bigg\| \;\leqslant\; \varepsilon\,, \tag{3.15b}$$

for all $s = 1, \frac{3}{2}, \dots$ and all finite Λ satisfying $A \in \mathfrak{A}_\Lambda$. Here $Q_\alpha\big(\widehat{S}^\alpha\big)$ is some ordering of the monomial $\widehat{S}^\alpha$.

PROOF. Let Λ be finite and satisfy $A \in \mathfrak{A}_\Lambda$. For simplicity of notation we also assume, here and in the following proofs, that H_Λ is time-independent. The main tool in the proof is the (formal) Schwinger-Dyson expansion

$$\tau_\Lambda^t A \;=\; \sum_{l \geqslant 0} \frac{t^l}{l!}\,\{H_\Lambda\,, A\}^{(l)}\,, \tag{3.16}$$

where $\{A, B\}^{(0)} := B$ and $\{A, B\}^{(l)} := \big\{A, \{A, B\}^{(l-1)}\big\}$. Without loss of generality we assume that $A = M^\beta$ for some multi-index $\beta \in \mathbb{N}^{I \times \Lambda}$. In order to compute the nested Poisson brackets we observe that

$$\{M^\alpha, M^\beta\} \;=\; \sum_{x \in \Lambda} \sum_{i,j,k \in I} \mathrm{i}\tilde{\varepsilon}_{ijk}\, \alpha_i(x)\, \beta_j(x)\, M^{\alpha+\beta-\delta_i(x)-\delta_j(x)+\delta_k(x)}\,, \tag{3.17}$$

as can be seen after a short calculation. (We recall that the multi-index $\delta_i(x)$ is defined by $[\delta_i(x)]_j(y) = \delta_{ij}\delta(x,y)$.) Iterating this identity yields

$$\begin{aligned}\big\{H_\Lambda, A\big\}^{(l)} \;=\; \mathrm{i}^l &\sum_{\alpha^1,\dots,\alpha^l} \sum_{x_1,\dots,x_l} \sum_{i_1,\dots,i_l} \sum_{j_1,\dots,j_l} \sum_{k_1,\dots,k_l} \mathbb{1}_{\{[\alpha^1] \subset \Lambda\}} \cdots \mathbb{1}_{\{[\alpha^l] \subset \Lambda\}}\\ &\left[\prod_{q=1}^{l} \tilde{\varepsilon}_{i_q j_q k_q}\, V(\alpha^q)\, \alpha^q_{i_q}(x_q) \left[\beta + \sum_{r=1}^{q-1} \big(\alpha^r - \delta_{i_r}(x_r) - \delta_{j_r}(x_r) + \delta_{k_r}(x_r)\big)\right]_{j_q}(x_q)\right]\\ &M^{\beta + \sum_{r=1}^{l} \left(\alpha^r - \delta_{i_r}(x_r) - \delta_{j_r}(x_r) + \delta_{k_r}(x_r)\right)}\,.\end{aligned} \tag{3.18}$$

This is manifestly of the form $\sum_{\alpha\in D} \mathbb{1}_{\{[\alpha]\subset\Lambda\}}\, c_\alpha\, M^\alpha$ for a countable set D.

In order to estimate $\sum_{\alpha\in D}|c_\alpha|$, we rewrite (3.18) using that

$$\sum_{\alpha^1,\dots,\alpha^l} = \sum_{n_1,\dots n_l=1}^{\infty} \sum_{|\alpha^1|=n_1} \cdots \sum_{|\alpha^l|=n_l} .$$

We then proceed recursively, starting with the sum over $\alpha^l, x_l, i_l, j_l, k_l$ and, at each step, using that

$$\sum_{|\alpha|=n} \sum_x \sum_{i,j,k} |\tilde{\varepsilon}_{ijk}|\, \alpha_i(x)\, \gamma_j(x)\, |V(\alpha)| \;\leqslant\; |\gamma|\, \|V\|^{(n)} ,$$

where

$$\|V\|^{(n)} \;:=\; n \sup_{x\in\mathbb{Z}^d} \sum_{\substack{\alpha\,:\,|\alpha|=n\\ [\alpha]\ni x}} |V(\alpha)| .$$

In this manner we find that

$$\begin{aligned}
\sum_{\alpha\in D}|c_\alpha| \;&\leqslant\; \sum_{n_1,\dots,n_l=1}^{\infty} |\beta|(|\beta|+n_1)\cdots(|\beta|+n_1+\cdots+n_{l-1})\, \|V\|^{(n_1)}\cdots\|V\|^{(n_l)} \\
&\leqslant\; \frac{1}{\rho^l} \sum_{n_1,\dots,n_l=1}^{\infty} \rho^l\, (|\beta|+n_1+\cdots+n_l)^l\, \|V\|^{(n_1)}\cdots\|V\|^{(n_l)} \\
&\leqslant\; \frac{l!}{\rho^l} \sum_{n_1,\dots,n_l=1}^{\infty} \mathrm{e}^{\rho(|\beta|+n_1+\cdots+n_l)}\, \|V\|^{(n_1)}\cdots\|V\|^{(n_l)} \\
&\leqslant\; C\frac{l!}{\rho^l}\, \mathrm{e}^{\rho|\beta|}\, \|V\|_r^l ,
\end{aligned}$$

for any $\rho < r$. Therefore we find that the series on the right-hand side of (3.16) is equal to

$$\sum_{\alpha\in\widetilde{D}} v_\alpha(t) \mathbb{1}_{\{[\alpha]\subset\Lambda\}} M^\alpha$$

for some countable set $\widetilde{D}$, where the coefficients $v_\alpha(t)$ satisfy

$$\sum_{\alpha\in\widetilde{D}} |v_\alpha(t)| \;<\; \infty$$

provided that $|t| < C(\|V\|_r)$. Thus the estimate (3.5) implies that the right-hand side of (3.16) converges in $\|\cdot\|_\infty$ provided that $|t| < C(\|V\|_r)$. An analogous estimate for the remainder of the Lie-Schwinger expansion of $\tau_\Lambda^t A$ shows that equality holds in (3.16) provided that $|t| < C(\|V\|_r)$. This proves (3.15a) for small times.

The quantum-mechanical case is similar. Consider the (formal) Schwinger-Dyson series for the time evolution of the quantum spin system:

$$\widehat{\tau}_\Lambda^t \widehat{A} \;=\; \sum_{l=0}^{\infty} \frac{t^l}{l!}\, (\mathrm{i}s)^l\, \big[\widehat{H}_\Lambda, \widehat{A}\big]^{(l)} , \tag{3.19}$$

where $[\mathbf{A}, \mathbf{B}]^{(0)} := \mathbf{B}$ and $[\mathbf{A}, \mathbf{B}]^{(l)} := \big[\mathbf{A}, [\mathbf{A}, \mathbf{B}]^{(l-1)}\big]$. In order to estimate the multiple commutators, we note, from (3.4) and (3.6) and the fact that both $\{\cdot\,,\cdot\}$ and $\mathrm{i}s[\cdot\,,\cdot]$ are derivations in both arguments, that $(\mathrm{i}s)^l\big[\widehat{H}_\Lambda, \widehat{A}\big]^{(l)}$ is equal to the expression obtained from $\big\{H_\Lambda, A\big\}^{(l)}$ by reordering the factors of each monomial appropriately and by replacing $M_i(x)$ with $\widehat{S}_i(x)$. Therefore, repeating the above analysis almost to the letter, we see that the series on the right-hand side of (3.19) is equal to

$$\sum_{\alpha\in\widetilde{D}} v_\alpha(t)\mathbb{1}_{\{[\alpha]\subset\Lambda\}} Q_\alpha\big(\widehat{S}^\alpha\big)\,, \tag{3.20}$$

for some family of orderings $(Q_\alpha)_\alpha$. Recalling the estimate (3.7), we see that if $|t| < C(\|V\|_r)$ then the right-hand side of (3.19) converges in norm and equality holds in (3.19). This proves (3.15b) for small times.

In order to extend the result to arbitrary times we proceed by iteration. The crucial observations that enable this process are that the convergence radius of the Schwinger-Dyson series is independent of β, and that τ_Λ^t and $\widehat{\tau}_\Lambda^t$ are norm-preserving. Let us assume that $t < C(\|V\|_r)$, so that both Schwinger-Dyson series converge. Choose $\varepsilon > 0$ and write

$$\tau_\Lambda^{2t} A \;=\; \tau_\Lambda^t \sum_{\alpha\in B} \mathbb{1}_{\{[\alpha]\in\Lambda\}} v_\alpha M^\alpha + \tau_\Lambda^t R_1\,, \tag{3.21}$$

where we used (3.15a) for small times. Here $\|R_1\|_\infty \leqslant \varepsilon$ and hence $\|\tau_\Lambda^t R\|_\infty \leqslant \varepsilon$. The first term of (3.21) may now be expanded using the Schwinger-Dyson series, so that we get

$$\tau_\Lambda^{2t} \;=\; \sum_{\alpha\in B'} \mathbb{1}_{\{[\alpha]\in\Lambda\}} v'_\alpha M^\alpha + \tau_\Lambda^t R_1 + R_2\,,$$

where $\|R_2\|_\infty \leqslant \varepsilon$. A similar iteration of the quantum Schwinger-Dyson expansion yields

$$\widehat{\tau}_\Lambda^{2t} \;=\; \sum_{\alpha\in B'} \mathbb{1}_{\{[\alpha]\in\Lambda\}} v'_\alpha Q'_\alpha\big(\widehat{S}^\alpha\big) + \widehat{\tau}_\Lambda^t \mathbf{R}_1 + \mathbf{R}_2\,,$$

where $\|\mathbf{R}_2\|, \|\widehat{\tau}_\Lambda^t \mathbf{R}_1\| \leqslant \varepsilon$. This proves the claim for the time $2t$. A straightforward extension of this procedure yields the claim for arbitrary times. ☐

We may now state and prove our main result for the case of a finite lattice Λ. Roughly it states that time evolution and quantization commute in the limit $s \to \infty$.

THEOREM 3.7. *Let $A \in \mathfrak{A}_\Lambda$. Then for any $\varepsilon > 0$ there exists a function $A_\varepsilon(t) \in \mathfrak{A}_\Lambda$ such that*

$$\sup_{t\in\mathbb{R}} \|\tau_\Lambda^t A - A_\varepsilon(t)\|_\infty \;\leqslant\; \varepsilon\,, \tag{3.22}$$

and, for any $t \in \mathbb{R}$,

$$\big\|\widehat{\tau}_\Lambda^t \widehat{A} - \widehat{A_\varepsilon(t)}\big\| \;\leqslant\; \varepsilon + \frac{C(t,\varepsilon)}{s}\,. \tag{3.23}$$

REMARK 3.8. *The "intermediate function" $A_\varepsilon(t)$ is necessary, as τ_Λ^t does not leave $\mathfrak{A}_\Lambda$ invariant.*

PROOF. The proof of Theorem 3.7 is an easy consequence of Lemma 3.6. For each $t \in \mathbb{R}$ set

$$A_\varepsilon(t) \;:=\; \sum_{\alpha\in B} \mathbb{1}_{\{[\alpha]\subset\Lambda\}}\, v_\alpha\, M^\alpha$$

(in the notation of Lemma 3.6). Thus (3.22) holds trivially, and (3.23) follows from

$$\left\|\sum_{\alpha\in B} \mathbb{1}_{\{[\alpha]\subset\Lambda\}}\, v_\alpha\, Q_\alpha\big(\widehat{S}^\alpha\big) - \sum_{\alpha\in B} \mathbb{1}_{\{[\alpha]\subset\Lambda\}}\, v_\alpha \;:\widehat{S}^\alpha:\right\| \;\leqslant\; \frac{C(t,\varepsilon)}{s}\,,$$

which itself follows readily from the commutation relations (3.6). ☐

3.1.6. The thermodynamic limit. The above analysis was done for a finite subset Λ, but the obtained uniformity in Λ allows for a statement of the result directly in the limit $\Lambda \to \mathbb{Z}^d$. Here $\Lambda \to \mathbb{Z}^d$ means convergence in the sense of nets, where finite subsets $\Lambda \subset \mathbb{Z}^d$ are ordered by inclusion. We pause to describe how this works.

Concentrate first on the quantum case. Recall that, for $\Lambda_1 \subset \Lambda_2$, we have the norm-preserving mapping $\widehat{\mathfrak{A}}_{\Lambda_1} \to \widehat{\mathfrak{A}}_{\Lambda_2}$ of the abstract C^*-algebras and the isotony relation $\widehat{\mathfrak{A}}_{\Lambda_1} \subset \widehat{\mathfrak{A}}_{\Lambda_2}$. Observables of the quantum spin system in the thermodynamic limit are elements of the *quasi-local algebra*

$$\widehat{\mathfrak{A}} := \overline{\bigvee_{\Lambda \subset \mathbb{Z}^d \text{ finite}} \widehat{\mathfrak{A}}_\Lambda}\,,$$

which is the C^*-algebra defined as the closure of the normed algebra generated by the union of all $\widehat{\mathfrak{A}}_\Lambda$'s, where Λ is finite. The spins are represented on $\widehat{\mathfrak{A}}$ by a family $\{\widehat{S}_i(x) : i \in I, x \in \mathbb{Z}^\nu\}$ of operators.

The dynamics of the system is determined by a one-parameter group $(\widehat{\tau}^t)_{t\in\mathbb{R}}$ of automorphisms of $\widehat{\mathfrak{A}}$. Its existence is an easy consequence of the proof of Lemma 3.6.

LEMMA 3.9. *Let $\mathbf{A} \in \widehat{\mathfrak{A}}_{\Lambda_0}$ for some finite $\Lambda_0 \subset \mathbb{Z}^d$ and $t \in \mathbb{R}$. Then the following limit exists in the norm sense:*

$$\lim_{\Lambda \to \mathbb{Z}^d} \widehat{\tau}^t_\Lambda \mathbf{A} =: \widehat{\tau}^t \mathbf{A}\,.$$

By continuity, $\widehat{\tau}^t$ extends to a strongly continuous one-parameter group $(\widehat{\tau}^t)_{t\in\mathbb{R}}$ of automorphisms of $\widehat{\mathfrak{A}}$.

PROOF. For small t, the Schwinger-Dyson series (3.19) is bounded in norm, uniformly in Λ, and the representation (3.20) immediately implies that $\widehat{\tau}^t_\Lambda \mathbf{A}$ converges as $\Lambda \to \mathbb{Z}^d$. Thus $\widehat{\tau}^t \mathbf{A}$ is well-defined for any polynomial $\mathbf{A}$. By continuity, $\widehat{\tau}^t$ extends to an automorphism of $\widehat{\mathfrak{A}}$. Since $\widehat{\tau}^t \mathbf{A} \in \widehat{\mathfrak{A}}$ and $\widehat{\tau}^t$ is a one-parameter group, we may extend it to all times by iteration. Strong continuity follows since $\widehat{\tau}^t \mathbf{A}$, for small t and polynomial $\mathbf{A}$, is defined through a convergent power series:

$$\lim_{t \to 0} \|\widehat{\tau}^t \mathbf{A} - \mathbf{A}\| = 0\,.$$

By continuity, this remains true for all $\mathbf{A} \in \widehat{\mathfrak{A}}$. ☐

For classical spin systems and finite Λ we recall that $\overline{\mathfrak{A}}_\Lambda = C\big(\prod_{x\in\Lambda} \overline{B_1(0)}; \mathbb{C}\big)$, a commutative C^*-algebra with norm $\|\cdot\|_\infty$. As above, for $\Lambda_1 \subset \Lambda_2$ we have a norm-preserving mapping $\mathfrak{A}_{\Lambda_1} \to \mathfrak{A}_{\Lambda_2}$ of the abstract C^*-algebras and the relation $\mathfrak{A}_{\Lambda_1} \subset \mathfrak{A}_{\Lambda_2}$. Define the algebra of polynomials in the thermodynamic limit as

$$\mathfrak{A} := \bigvee_{\Lambda \subset \mathbb{Z}^d \text{ finite}} \mathfrak{A}_\Lambda\,,$$

and denote by $\overline{\mathfrak{A}}$ its closure in $\|\cdot\|_\infty$. The classical quasi-local algebra $\overline{\mathfrak{A}}$ is equal to the space of complex functions on $\prod_{x\in\mathbb{Z}^d} \overline{B_1(0)}$ that are continuous in the product topology (this is an immediate consequence of the Tychonoff and Stone-Weierstrass theorems).

The spins are represented on $\overline{\mathfrak{A}}$ by a family $\{M_i(x) : i \in I, x \in \mathbb{Z}^\nu\}$ of functions. Existence of the dynamics follows exactly as above.

LEMMA 3.10. *Let $A \in \mathfrak{A}_{\Lambda_0}$ for some finite $\Lambda_0 \subset \mathbb{Z}^d$ and $t \in \mathbb{R}$. Then the following limit exists in $\|\cdot\|_\infty$:*

$$\lim_{\Lambda \to \mathbb{Z}^d} \tau^t_\Lambda A =: \tau^t A\,.$$

By continuity this extends to a strongly continuous one-parameter group $(\tau^t)_{t\in\mathbb{R}}$ *of automorphisms of* $\overline{\mathfrak{A}}$. *Furthermore,* $\tau^t A = A\circ\phi^t$, *where* ϕ^t *is the classical flow on* $\Xi_{\mathbb{Z}^d}$ *generated by the equation of motion* (3.11).

Then the proof of Theorem 3.7 may be easily extended to the thermodynamics limit.

THEOREM 3.11. *Let* $A\in\mathfrak{A}$. *Then for any* $\varepsilon>0$ *there exists a function* $A_\varepsilon(t)\in\mathfrak{A}$ *such that*

$$\sup_{t\in\mathbb{R}} \|\tau^t A - A_\varepsilon(t)\|_\infty \;\leqslant\; \varepsilon\,, \tag{3.24}$$

and, for any $t\in\mathbb{R}$,

$$\big\|\widehat{\tau}^t\widehat{A} - \widehat{A_\varepsilon(t)}\big\| \;\leqslant\; \varepsilon + \frac{C(\varepsilon,t)}{s}\,. \tag{3.25}$$

REMARK. *In particular, the result applies to classical equations of motion of the form* (3.13) *where the sum over* y *ranges over* $\mathbb{Z}^d$.

3.1.7. Coherent spin states. We now move on to discussing coherent spins states. Aside from providing a "down to earth" interpretation of Theorem 3.11, they are a powerful tool for proving theorems.

Recall that $S_i = s\widehat{S}_i$ is the unscaled spin operator in the spin-s-representation of su(2). A coherent state is generated by the skew-adjoint operator $A(\theta,\varphi)$ on $\mathbb{C}^{2s+1}$, defined through

$$A(\theta,\varphi) \;:=\; \frac{\theta}{\sqrt{2}}\Big(\mathrm{e}^{\mathrm{i}\varphi}\,S_- - \mathrm{e}^{-\mathrm{i}\varphi}\,S_+\Big)\,.$$

For the polar angles[2] $(\theta,\varphi)\in[0,\pi]\times[0,2\pi)$ corresponding to the unit vector $M\in\mathbb{S}^2$ we define the *coherent state*

$$W_M \;:=\; U(\theta,\varphi)|s\rangle\,, \qquad U(\theta,\varphi) \;:=\; \mathrm{e}^{A(\theta,\varphi)}\,. \tag{3.26}$$

Here $|s\rangle$ is the normalized highest weight state in $\mathbb{C}^{2s+1}$, characterized (uniquely up to a phase) by $S_z|s\rangle = s\,|s\rangle$. The properties of coherent spin states that are of interest to us are summarized in the following Lemma.

LEMMA 3.12. *(i) The coherent spin states form a complete set in* $\mathbb{C}^{2s+1}$, *in the sense that*

$$\frac{2s+1}{4\pi}\int \mathrm{d}M\;|W_M\rangle\langle W_M| \;=\; \mathbb{1}\,. \tag{3.27}$$

In particular,

$$\operatorname{Tr}\mathbf{A} \;=\; \frac{2s+1}{4\pi}\int \mathrm{d}M\;\langle W_M\,,\mathbf{A}\,W_M\rangle\,. \tag{3.28}$$

(ii) For any unit vector $M\in\mathbb{S}^2$, *we have*

$$\Big|\langle W_M\,,\widehat{S}_{i_1}\cdots\widehat{S}_{i_p}\,W_M\rangle - M_{i_1}\cdots M_{i_p}\Big| \;\leqslant\; \frac{p}{\sqrt{s}}\,. \tag{3.29}$$

[2] We use the convention where the "latitude" θ is measured down from the north pole; see (3.32).

PROOF. For (i), see [ACGT72]. In order to show (ii), we note that

$$U^* S_i U = \sum_{k\geqslant 0} \frac{1}{k!} [\dots[S_i, A], \dots, A]$$

yields the expressions

$$\begin{aligned} U^* S_1 U &= \sin\theta\cos\varphi\, S_z + \frac{1}{\sqrt{2}}\cos^2\frac{\theta}{2}\,(S_+ + S_-) - \frac{1}{\sqrt{2}}\sin^2\frac{\theta}{2}\left(\mathrm{e}^{-2\mathrm{i}\varphi}S_+ + \mathrm{e}^{2\mathrm{i}\varphi}S_-\right), \\ U^* S_2 U &= \sin\theta\sin\varphi\, S_z + \frac{1}{\sqrt{2}\mathrm{i}}\cos^2\frac{\theta}{2}\,(S_+ - S_-) - \frac{1}{\sqrt{2}\mathrm{i}}\sin^2\frac{\theta}{2}\left(\mathrm{e}^{2\mathrm{i}\varphi}S_+ - \mathrm{e}^{-2\mathrm{i}\varphi}S_-\right), \\ U^* S_3 U &= \cos\theta\, S_z - \frac{1}{\sqrt{2}}\sin\theta\left(\mathrm{e}^{-\mathrm{i}\varphi}S_+ + \mathrm{e}^{\mathrm{i}\varphi}S_-\right). \end{aligned} \tag{3.30}$$

We start by showing

$$\widehat{S}_i W_M = M_i W_M + R_i , \tag{3.31}$$

where $\|R_i\| \leqslant 1/\sqrt{s}$. Note first that $S_- |s\rangle = \sqrt{s}\,|s-1\rangle$, where $|s-1\rangle$ is a unit vector satisfying $S_z|s-1\rangle = (s-1)|s-1\rangle$; see e.g. [Mes00]. Thus, for any unit vector $v \in \mathbb{R}^3$, (3.30) implies

$$R_i = \frac{\sqrt{s}}{s}\, a_i\, U|s-1\rangle ,$$

where

$$a = \frac{1}{\sqrt{2}}\left(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}\, e^{2\mathrm{i}\varphi}\,,\, \mathrm{i}\cos^2\frac{\theta}{2} - \mathrm{i}\sin^2\frac{\theta}{2}\, e^{-2\mathrm{i}\varphi}\,,\, -\sin\varphi\, e^{-\mathrm{i}\varphi}\right).$$

Therefore $|a_i| \leqslant 1$, and (3.31) follows. To conclude the proof, we note that (3.29) follows immediately from (3.31). □

Another noteworthy consequence of (3.30) is

$$\langle W_M\,, \widehat{S}\, W_M\rangle = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix} = M\,. \tag{3.32}$$

3.1.8. Time evolution of coherent spin states. Let $M : \mathbb{Z}^d \to \mathbb{S}^2$ be a configuration of classical spins on the infinite lattice. Then M defines a state ρ_M on $\widehat{\mathfrak{A}}$ as follows. For finite Λ, consider the product state

$$W_{M,\Lambda} := \bigotimes_{x\in\Lambda} W_{M(x)} \in \mathcal{H}_\Lambda\,.$$

Then, for $\mathbf{A} \in \widehat{\mathfrak{A}}_\Lambda$, we set

$$\rho_M(\mathbf{A}) := \langle W_{M,\Lambda}\,, \mathbf{A}\, W_{M,\Lambda}\rangle\,,$$

and extend the definition of ρ_M to arbitrary $\mathbf{A} \in \widehat{\mathfrak{A}}$ by continuity.

Let $M : \mathbb{R}\times\mathbb{Z}^d \to \mathbb{S}^2$ be the solution of the Hamiltonian equation of motion (3.11) with initial conditions $M(0,x) = M(x)$. The following result links the quantum time evolution for coherent spin states with the corresponding classical configuration in the large-spin limit.

THEOREM 3.13. *Let $t \in \mathbb{R}$, $A \in \mathfrak{A}$ and $M : \mathbb{Z}^d \to \mathbb{S}^2$. Then*

$$\lim_{s\to\infty} \rho_M(\widehat{\tau}^t \widehat{A}) = A(M(t))\,,$$

uniformly in t on compact time intervals.

PROOF. By Lemma 3.6, it is enough to show that

$$\lim_{s\to\infty}\left|\sum_{\alpha\in B} v_\alpha M^\alpha - \rho_M\left(\sum_{\alpha\in B} v_\alpha Q_\alpha\big(\widehat{S}^\alpha\big)\right)\right| \;=\; 0\,.$$

But this follows immediately from Lemma 3.12 (ii). The uniformity in t on compacts is a simple consequence of the form of time-dependence of the coefficients v_α. □

3.2. Spins on a lattice: the continuum limit

This section is devoted to the dynamics of a quantum spin system in the continuum (or mean-field) limit. More precisely, we consider a system of quantum spins on a cubic lattice with spacing $h > 0$. The magnitude s of the spins is fixed and we take the limit $h \to 0$. In order to obtain quantities that are well-defined in the limit $h \to 0$, we smear out the spin operators with continuous test functions on $\mathbb{R}^d$. One expects the smeared-out spin observables to behave classically in the limit $h \to 0$, in the sense that their Cartesian components commute. Indeed, the contribution of products of spins on the same lattice site is subleading. Thus one expects that the dynamics of the quantum spin system should be governed by a classical equation of motion for continuous spin fields. A typical example is the continuum Landau-Lifschitz equation

$$\partial_t M(t,x) \;=\; M(t,x)\times H_M(t,x)\,, \tag{3.33}$$

where M denotes a classical continuous spin field and $x \in \mathbb{R}^d$. An example of exchange interaction H_M is $H_M = J\Delta M$, where Δ is the Laplacian. In this thesis we consider the Landau-Lifschitz equation with an exchange field H_M given by an integral operator applied to M, along with nonlinear generalizations thereof. Equation (3.33) then takes the form

$$\partial_t M(t,x) = M(t,x)\times\int J(x,y)\,M(t,y)\,\mathrm{d}y\,. \tag{3.34}$$

The integral kernel $J(x,y)$ describes the exchange interactions between classical spins beyond the nearest-neighbour approximation in the continuum limit. In a formal way, the Landau-Lifschitz equation $\partial_t M = JM\times\Delta M$ can be obtained from (3.34) with $J = J(|x-y|)$ by Taylor expanding $M(t,y)$ up to second order in $y-x$. This leads to $\partial_t M = JM\times\Delta M$ after rescaling time according to $t\mapsto\lambda t$, where $\lambda = \frac{1}{2d}\int J(|x|)|x|^2\,\mathrm{d}x$.

Our main result is again a Egorov-type theorem: The quantum dynamics approaches the dynamics of a classical spin system defined on a continuum. This provides a rigorous justification of the observation that, at scales large compared to the lattice size, spin systems such as ferromagnets behave classically. The limiting/quantization parameter is h^d/s, where d is the number of spatial dimensions. As in the previous section, we also discuss the thermodynamic limit and the time evolution of coherent states.

3.2.1. A system of quantum spins on a lattice. We start by describing the quantum spin system, which is very similar to the system of Section 3.1.2. Let $\Lambda\subset\mathbb{R}^d$ be bounded and open. We assign to each spacing $h > 0$ the finite lattice

$$\Lambda^{(h)} := h\mathbb{Z}^d\cap\Lambda.$$

At each lattice site $x \in \Lambda^{(h)}$ there is a spin of (fixed) magnitude $s = \frac{1}{2}, 1, \frac{3}{2}, \dots$. The Hilbert space of this quantum system is

$$\mathcal{H}_\Lambda^{(h)} := \bigotimes_{x \in \Lambda^{(h)}} \mathbb{C}^{2s+1} .$$

The algebra of bounded operators on $\mathcal{H}_\Lambda^{(h)}$ is denoted by $\widehat{\mathfrak{A}}_\Lambda^{(h)}$.

The spins are represented on $\mathcal{H}_\Lambda^{(h)}$ by a family $\{\widehat{S}_i(x) : i = 1,2,3,\ x \in \Lambda^{(h)}\}$ of operators, where $\widehat{S}_i(x)$ is the i'th generator of the spin-s-representation of su(2), rescaled by h^d/s. As in Section 3.1.4, we replace the coordinates $(\widehat{S}_1, \widehat{S}_2, \widehat{S}_3)$ with $(\widehat{S}_+, \widehat{S}_z, \widehat{S}_-)$ defined through the basis transformation (3.3). The new coordinates satisfy the bounds

$$\|\widehat{S}_i\| \leqslant \begin{cases} h^d & \text{if } s \geqslant 1 \\ \sqrt{2} h^d & \text{if } s = \frac{1}{2} . \end{cases}$$

for $i \in I$, where, we recall, $I = \{+, z, -\}$. The canonical commutation relations read

$$\big[\widehat{S}_i(x), \widehat{S}_j(y)\big] = \frac{h^d}{s} \tilde{\varepsilon}_{ijk}\, \delta(x,y)\, \widehat{S}_k(x) , \tag{3.35}$$

for $i, j, k \in I$.

3.2.2. A continuum theory of spins. We now move on to discussing the continuum theory of classical spin fields. Let $\Lambda \subset \mathbb{R}^d$ be a bounded and open. A system of classical spins on Λ is represented in terms of the Poisson "phase space"[3]

$$\Xi_\Lambda := \big\{ M \in L^\infty(\Lambda; \mathbb{R}^3) : \|M\|_\infty \leqslant 1 \big\} ,$$

where $\mathbb{R}^3$ carries the Euclidean norm. As in Section 3.1.1, we replace the Cartesian coordinates (M_1, M_2, M_3) with the complex coordinates (M_+, M_z, M_-), defined through the basis transformation (3.3). The Poisson bracket on Ξ_Λ is defined by

$$\big\{ M_i(x), M_j(y) \big\} = \mathrm{i}\, \tilde{\varepsilon}_{ijk}\, \delta(x-y)\, M_k(x) , \tag{3.36}$$

for $i, j, k \in I$.

3.2.3. Classical observables. In order to describe a useful class of observables on Ξ_Λ, we introduce the space $\mathscr{B}^{(p)}$, $p \in \mathbb{N}$, which consists of all functions f in $C(\mathbb{R}^{pd}; \mathbb{C}^{3^p})$ that are symmetric in their arguments, in the sense that $Pf = f$, where

$$(Pf)_{i_1 \dots i_p}(x_1, \dots, x_p) := \frac{1}{p!} \sum_{\sigma \in S_p} f_{i_{\sigma(1)} \dots i_{\sigma(p)}}(x_{\sigma(1)}, \dots, x_{\sigma(p)}) .$$

On the space $\mathscr{B}^{(p)}$ we introduce the norms

$$\|f\|_1^{(h)} := h^{pd} \sum_{i_1, \dots, i_p \in I} \sum_{x_1, \dots, x_p \in h\mathbb{Z}^d} |f_{i_1 \dots i_p}(x_1, \dots, x_p)| ,$$

$$\|f\|_{\infty,1}^{(h)} := \sup_x \sum_{i_1, \dots, i_p \in I} h^{(p-1)d} \sum_{x_2, \dots, x_p \in h\mathbb{Z}^d} |f_{i_1 \dots i_p}(x, x_2, \dots, x_p)| .$$

[3] As in the previous section, one may introduce a symplectic phase space Γ_Λ consisting of all $M \in \Xi_\Lambda$ such that $|M(x)| = 1$ a.e.

We are interested in observables associated with functions $f \in \mathscr{B}^{(p)}$ satisfying

$$\limsup_{h \to 0} \|f\|_1^{(h)} \;<\; \infty\,. \tag{3.37}$$

Note that Fatou's lemma implies that $\|f\|_1 \leqslant \limsup_{h\to 0} \|f\|_1^{(h)}$.

We define $\mathfrak{A}_\Lambda$ as the "polynomial" algebra of functions on Ξ_Λ generated by functions of the form

$$M_\Lambda(f) \;:=\; \sum_{i_1,\dots,i_p} \int_{\Lambda^p} \mathrm{d}x_1 \cdots \mathrm{d}x_p\; f_{i_1\dots i_p}(x_1,\dots,x_p)\, M_{i_1}(x_1)\cdots M_{i_p}(x_p)\,,$$

where $f \in \mathscr{B}^{(p)}$ satisfies (3.37). $\mathfrak{A}_\Lambda$ is clearly a Poisson algebra. We equip it with the norm $\|A\|_\infty \;:=\; \sup_{M\in\Xi_\Lambda}|A(M)|$ so that

$$\|M_\Lambda(f)\|_\infty \;\leqslant\; \|f\|_1\,. \tag{3.38}$$

3.2.4. Quantization and quantum observables. For $f \in \mathscr{B}^{(p)}$ let us define

$$\widehat{S}_\Lambda(f) \;:=\; \sum_{i_1,\dots,i_p} \sum_{x_1,\dots,x_p\in\Lambda^{(h)}} f_{i_1\dots i_p}(x_1,\dots,x_p)\, \widehat{S}_{i_1}(x_1)\cdots \widehat{S}_{i_p}(x_p)\,. \tag{3.39}$$

If f satisfies (3.37), we find that

$$\|\widehat{S}_\Lambda(f)\| \;\leqslant\; \|f\|_1^{(h)}\,. \tag{3.40}$$

As above, quantization $\widehat{(\cdot)} : \mathfrak{A}_\Lambda \to \widehat{\mathfrak{A}}_\Lambda^{(h)}$ is defined by $\widehat{M_\Lambda(f)} = \;:\widehat{S}_\Lambda(f):\;$ and linearity. Here $:\cdot:$ denotes the normal-ordering of the spin operators introduced in Section 3.1.3. Also, we set $\widehat{1} = \mathbb{1}$. Again, $(\widehat{A})^* = \widehat{\overline{A}}$. Furthermore one sees readily that h^d/s is the parameter of $\widehat{(\cdot)}$.

3.2.5. Hamilton function and dynamics. Let us now introduce a Hamiltonian for the classical spin system. Consider a family $V = \big(V^{(n)}\big)_{n=1}^\infty$ of functions, where $V^{(n)} \in \mathscr{B}^{(p)}$ satisfies

$$\overline{V^{(n)}_{i_1\dots i_n}(x_1,\dots,x_n)} \;=\; V^{(n)}_{\bar{i}_1\dots\bar{i}_n}(x_1,\dots,x_n)\,,$$

where, we recall, $\bar{\cdot}$ on I maps $(+,z,-)$ to $(-,z,+)$. We define the Hamilton function on Ξ_Λ through

$$H_\Lambda \;:=\; \sum_{n=1}^\infty M_\Lambda(V^{(n)})\,. \tag{3.41}$$

Set

$$\|V\|^{(h)} \;:=\; \sum_{n=1}^\infty n\mathrm{e}^n\, \|V^{(n)}\|_{\infty,1}^{(h)}\,. \tag{3.42}$$

We impose the condition $\|V\| := \limsup_{h\to 0}\|V\|^{(h)} \;<\; \infty$. (Note that, as in Section 3.1.4, one may generalize the class of allowed potentials by replacing $n\mathrm{e}^n$ in (3.42) with e^{rn} for some $r > 0$.)

In the continuum limit, we observe that

$$\sum_{n=1}^\infty n\mathrm{e}^n \sup_x \sum_{i_1,\dots,i_n} \int \mathrm{d}x_2\cdots\mathrm{d}x_n \big|V^{(n)}_{i_1\dots i_n}(x,x_2,\dots,x_n)\big| \;\leqslant\; \|V\|\,, \tag{3.43}$$

as can be seen using Fatou's lemma. It now follows easily that, for each bounded set Λ, the sum (3.41) converges in $\|\cdot\|_\infty$ on Ξ_Λ and yields a well-defined real Hamilton function H_Λ.

The Hamiltonian equation of motion reads

$$\frac{\mathrm{d}}{\mathrm{d}t} M_i(t,x) \;=\; \mathrm{i} \sum_{n=1}^{\infty} n \sum_{i_1,\dots,i_n,j} \int \mathrm{d}x_2 \cdots \mathrm{d}x_n \, V^{(n)}_{i_1\dots i_n}(x,x_2,\dots,x_n)$$
$$\tilde{\varepsilon}_{i_1 i j}\, M_j(t,x)\, M_{i_2}(t,x_2) \cdots M_{i_n}(t,x_n)\,. \qquad (3.44)$$

By a standard contraction mapping argument, we find the following global well-posedness result for the equation of motion (3.44).

LEMMA 3.14. *Let $\Lambda \subset \mathbb{R}^d$ by an open (not necessarily bounded) subset of $\mathbb{R}^d$ and $M_0 \in \Xi_\Lambda$. Then (3.44) has a unique solution $M \in C^1(\mathbb{R}, \Xi_\Lambda)$ that satisfies $M(0) = M_0$. Here Ξ_Λ is equipped with the L^∞-norm. Moreover, we have the pointwise conservation law $|M(t,x)| = |M(0,x)|$ for all t.*

REMARK 3.15. *Time-dependent potentials $V(t)$ may be treated exactly as in Remark 3.4.*

EXAMPLE 3.16. *Consider*

$$H_\Lambda \;=\; -\int_\Lambda \mathrm{d}x\, h(t,x) \cdot M(x) - \frac{1}{2} \int_{\Lambda\times\Lambda} \mathrm{d}x\, \mathrm{d}y\, J(x,y)\, M(x) \cdot M(y)\,,$$

which yields the Landau-Lifschitz equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t} M(t,x) \;=\; M(t,x) \times \left[h(t,x) + \int_\Lambda \mathrm{d}y\; J(x,y) M(t,y) \right]$$

with continuous integral kernel.

The quantum dynamics is generated by the Hamiltonian $\widehat{H}_\Lambda \in \widehat{\mathfrak{A}}^{(h)}_\Lambda$ defined as the quantization of H_Λ. More precisely, each term of H_Λ is quantized and it may be easily verified that the resulting series converges in operator norm. The fact that H_Λ is real immediately implies that $\widehat{H}_\Lambda$ is self-adjoint. As above we introduce the short-hand notation

$$\begin{aligned} \tau^t_\Lambda A \;&:=\; A \circ \phi^t_\Lambda\,, \qquad A \in \mathfrak{A}_\Lambda, \\ \widehat{\tau}^t_\Lambda \mathbf{A} \;&:=\; U_\Lambda(t)^* \,\mathbf{A}\, U_\Lambda(t)\,, \qquad \mathbf{A} \in \widehat{\mathfrak{A}}^{(h)}_\Lambda. \end{aligned}$$

Here, ϕ^t_Λ is the flow on Ξ_Λ generated by (3.44), and $U_\Lambda(t)$ is the quantum mechanical propagator, equal to $\mathrm{e}^{\mathrm{i}sh^{-d}\widehat{H}_\Lambda t}$ if $\widehat{H}_\Lambda$ is time-independent.

3.2.6. The continuum limit. We are now in a position to state our main result on the mean-field dynamics of the quantum system on the finite lattice $\Lambda^{(h)}$ in the continuum limit, as $h \to 0$.

THEOREM 3.17. *Let $\Lambda \subset \mathbb{R}^d$ be open and bounded, $s = \frac{1}{2}, 1, \frac{3}{2}, \dots$ fixed, and $A \in \mathfrak{A}_\Lambda$. Then for any $\varepsilon > 0$ there exists a function $A_\varepsilon(t) \in \mathfrak{A}_\Lambda$ such that*

$$\sup_{t\in\mathbb{R}} \|\tau^t_\Lambda A - A_\varepsilon(t)\|_\infty \;\leqslant\; \varepsilon\,, \qquad (3.45)$$

and, for any $t \in \mathbb{R}$,

$$\left\|\widehat{\tau}^t_\Lambda \widehat{A} - \widehat{A_\varepsilon(t)}\right\| \;\leqslant\; \varepsilon + C(\varepsilon,t)\, h^d\,. \qquad (3.46)$$

PROOF. One finds, for $f \in \mathscr{B}^{(p)}$ and $g \in \mathscr{B}^{(q)}$,

$$\big\{M_\Lambda(f), M_\Lambda(g)\big\} = pq\, M_\Lambda(f \rightharpoonup g) \tag{3.47}$$

where $f \rightharpoonup g \in \mathscr{B}^{(p+q-1)}$ is defined by

$$\begin{aligned}(f \rightharpoonup g)_{i_1 \dots i_{p+q-1}}&(x_1, \dots, x_{p+q-1}) \\ &:= \mathrm{i}P \sum_{i,j} \tilde{\varepsilon}_{iji_1} f_{ii_2 \dots i_p}(x_1, \dots x_p)\, g_{ji_{p+1} \dots i_{p+q-1}}(x_1, x_{p+1}, \dots, x_{p+q-1})\,. \end{aligned} \tag{3.48}$$

We have the estimate

$$\|f \rightharpoonup g\|_1 \;\leqslant\; \|f\|_{\infty,1}\, \|g\|_1\,, \tag{3.49}$$

where

$$\|f\|_{\infty,1} \;:=\; \sup_x \sum_{i_1, \dots, i_p} \int \mathrm{d}x_2 \dots \mathrm{d}x_p\, |f_{i_1 \dots i_p}(x, x_2, \dots x_p)|\,.$$

Without loss of generality, we assume that $A = M_\Lambda(f)$ for some $f \in \mathscr{B}^{(p)}$ satisfying the bound (3.37). Iterating

$$\big\{H_\Lambda, M_\Lambda(f)\big\} \;=\; \sum_{n=1}^\infty np\, M_\Lambda(V^{(n)} \rightharpoonup f)$$

we obtain that

$$\begin{aligned}\big\{H_\Lambda, M_\Lambda(f)\big\}^{(l)} \;=\; \sum_{n_1, \dots, n_l = 1}^\infty &\big[pn_1\big]\, \big[(p + n_1 - 1)n_2\big] \cdots \big[(p + n_1 + \dots + n_{l-1} - l + 1)n_l\big] \\ &M_\Lambda\Big(V^{(n_l)} \rightharpoonup \big(V^{(n_{l-1})} \rightharpoonup \dots (V^{(n_1)} \rightharpoonup f)\big)\Big)\,,\end{aligned}$$

with norm

$$\begin{aligned}\big\|\big\{H_\Lambda, M_\Lambda(f)\big\}^{(l)}\big\|_\infty \;&\leqslant\; \sum_{n_1, \dots, n_l} \big[pn_1\big]\, \big[(p + n_1 - 1)n_2\big] \cdots \big[(p + n_1 + \dots + n_{l-1} - l + 1)n_l\big] \\ &\qquad \|V^{(n_l)}\|_{\infty,1} \cdots \|V^{(n_1)}\|_{\infty,1}\, \|f\|_1 \\ &\leqslant\; l! \sum_{n_1, \dots, n_l} \frac{(p + n_1 + \dots + n_l)^l}{l!}\, n_1 \cdots n_l\, \|V^{(n_l)}\|_{\infty,1} \cdots \|V^{(n_1)}\|_{\infty,1}\, \|f\|_1 \\ &\leqslant\; \mathrm{e}^p\, \|f\|_1\, l! \left[\sum_n n\mathrm{e}^n\, \|V^{(n)}\|_{\infty,1}\right]^l \\ &\leqslant\; \mathrm{e}^p\, \|f\|_1\, l!\, \|V\|^l\,,\end{aligned} \tag{3.50}$$

by (3.43). Therefore, for $|t| < \|V\|^{-1}$, the series

$$\sum_{l=0}^\infty \frac{t^l}{l!} \big\{H_\Lambda, A\big\}^{(l)} \tag{3.51}$$

converges in $\|\cdot\|_\infty$ to $\tau_\Lambda^t A$.

The quantum case is dealt with in a similar fashion, with the additional complication caused by the ordering of the generators $\{\widehat{S}_i(x)\}$. This does not trouble us, however, as an exact knowledge of the ordering is not required. It is easy to see that, for f and g as above,

$$\mathrm{i}sh^{-d}\Big[\widehat{S}_\Lambda(f), \widehat{S}_\Lambda(g)\Big]$$

is equal, up to a reordering of the spin operators, to $pq\widehat{S}_\Lambda(f \rightharpoonup g)$. Iterating this shows that

$$(\mathrm{i}sh^{-d})^l \left[\widehat{H}_\Lambda, \widehat{A}\right]^{(l)}$$

is equal, up to a reordering of the spin operators, to

$$\sum_{n_1,\dots,n_l=1}^{\infty} \big[pn_1\big]\,\big[(p+n_1-1)n_2\big]\cdots\big[(p+n_1+\cdots+n_{l-1}-l+1)n_l\big]$$
$$\widehat{S}_\Lambda\Big(V^{(n_l)} \rightharpoonup \big(V^{(n_{l-1})} \rightharpoonup \dots (V^{(n_1)} \rightharpoonup f)\big)\Big)\,,$$

Consequently an estimate analogous to (3.50) yields, for $s \geqslant 1$,

$$\big\|(\mathrm{i}sh^{-d})^l \left[\widehat{H}_\Lambda, \widehat{A}\right]^{(l)}\big\| \;\leqslant\; \mathrm{e}^p\, \|f\|_1^{(h)}\, l!\, (\|V\|^{(h)})^l\,,$$

which readily implies the bound

$$\Big\|\sum_{l=0}^{\infty}\frac{t^l}{l!}(\mathrm{i}sh^{-d})^l \left[\widehat{H}_\Lambda, \widehat{A}\right]^{(l)}\Big\| \leqslant \mathrm{e}^p\, \|f\|_1^{(h)} \sum_{l=0}^{\infty}(|t|\, \|V\|^{(h)})^l\,. \tag{3.52}$$

If $s = 1/2$, the first line of (3.50) gets the additional factor $\sqrt{2}^{n_1+\cdots+n_l+p}$. This may be dealt with by replacing the factor $(p+n_1+\cdots+n_l)^l$ in the second line of (3.50) with $(rp+rn_1+\cdots+rn_l)^l/r^l$. The desired bound then follows for $0 < r \leqslant 1-\frac{1}{2}\log 2$. Note that in this case the convergence radius for t is reduced to $r\|V\|^{-1}$. For ease of notation, we restrict the following analysis to the case $s \geqslant 1$, while bearing in mind that the extension to $s = 1/2$ follows by using the above rescaling trick.

Now, by definition of $\|V\|$, for any $|t| < \|V\|^{-1}$ there is an h_0 such that (3.52) converges in norm to $\widehat{\tau}_\Lambda^t\widehat{A}$ for all $h \leqslant h_0$, uniformly in h and Λ.

In order to establish the statement of the theorem for short times $|t| < \|V\|^{-1}$, we remark that the commutation relations (3.35) imply the bound

$$\big\|\mathbf{A}-\mathbf{B}\big\| \;\leqslant\; \frac{h^d}{s}\,p^2\, \|f\|_1^{(h)}\,,$$

for arbitrary reorderings, $\mathbf{A}$ and $\mathbf{B}$, of the same operator $\widehat{S}_\Lambda(f)$, with $f \in \mathscr{B}^{(p)}$ for some $p < \infty$.

If we define $\widehat{\tau_\Lambda^t A}$ through its norm-convergent power series, we therefore get

$$
\begin{aligned}
&\|\widehat{\tau}_\Lambda^t \widehat{A} - \widehat{\tau_\Lambda^t A}\| \\
&\leqslant \frac{h^d}{s} \sum_{l=0}^{\infty} \frac{|t|^l}{l!} \sum_{n_1,\dots,n_l} \big[pn_1\big] \big[(p+n_1-1)n_2\big] \cdots \big[(p+n_1+\cdots+n_{l-1}-l+1)n_l\big] \\
&\qquad (n_1+\cdots+n_l-l+1)^2 \, \|V^{(n_l)}\|_{\infty,1}^{(h)} \cdots \|V^{(n_1)}\|_{\infty,1}^{(h)} \, \|f\|_1^{(h)} \\
&\leqslant \frac{h^d}{s} \sum_{l=0}^{\infty} |t|^l \sum_{n_1,\dots,n_l} \frac{(p+n_1+\cdots+n_l)^{l+2}}{l!} n_1 \cdots n_l \, \|V^{(n_l)}\|_{\infty,1}^{(h)} \cdots \|V^{(n_1)}\|_{\infty,1}^{(h)} \, \|f\|_1^{(h)} \\
&\leqslant \frac{h^d}{s} \sum_{l=0}^{\infty} |t|^l \mathrm{e}^p \, \|f\|_1^{(h)} \, (l+2)(l+1) \left[\sum_n n\mathrm{e}^n \, \|V^{(n_1)}\|_{\infty,1}^{(h)}\right]^l \\
&\leqslant \frac{h^d}{s} \, \mathrm{e}^p \, \|f\|_1^{(h)} \sum_{l=0}^{\infty} (l+2)(l+1) \, (|t| \, \|V\|^{(h)})^l \\
&= O(h^d) \,,
\end{aligned}
$$

where in the last step we have used the fact that the sum convergences uniformly in h, for h small enough, as seen above.

Arbitrary times are reached by iteration of the above result, exactly as in the proof of Lemma 3.6. □

3.2.7. The thermodynamic limit. The above result may again be formulated in the thermodynamic limit as $\Lambda \to \mathbb{R}^d$. Here the convergence $\Lambda \to \mathbb{R}^d$ is understood in the sense of nets, where subsets $\Lambda \subset \mathbb{R}^d$ are ordered by inclusion. We only sketch the arguments, which are almost identical to those of Section 3.1.6.

The quantum quasi-local algebra is

$$
\widehat{\mathfrak{A}}^{(h)} := \overline{\bigvee_{\Lambda \subset \mathbb{R}^d \text{ bounded}} \widehat{\mathfrak{A}}_\Lambda^{(h)}} \,,
$$

The existence of dynamics is guaranteed by the following lemma.

Lemma 3.18. *Let $h > 0$ and suppose $\mathbf{A} \in \widehat{\mathfrak{A}}_{\Lambda_0}^{(h)}$ for some open and bounded $\Lambda_0 \subset \mathbb{R}^d$. Then, for any $t \in \mathbb{R}$, the following limit exists in the norm sense:*

$$
\lim_{\Lambda \to \mathbb{R}^d} \widehat{\tau}_\Lambda^t \mathbf{A} =: \widehat{\tau}^t \mathbf{A} \,,
$$

By continuity this extends to a strongly continuous one-parameter group $(\widehat{\tau}^t)_{t \in \mathbb{R}}$ of automorphisms of $\widehat{\mathfrak{A}}^{(h)}$.

The classical quasi-local algebra is

$$
\overline{\mathfrak{A}} := \overline{\bigvee_{\Lambda \subset \mathbb{R}^d \text{ bounded}} \mathfrak{A}_\Lambda} \,.
$$

Lemma 3.19. *Let $A \in \mathfrak{A}_{\Lambda_0}$ for some open and bounded $\Lambda_0 \subset \mathbb{R}^d$. Then, for any $t \in \mathbb{R}$, the following limit exists in $\|\cdot\|_\infty$:*

$$
\lim_{\Lambda \to \mathbb{R}^d} \tau_\Lambda^t A =: \tau^t A \,,
$$

By continuity this extends to a strongly continuous one-parameter group $(\tau^t)_{t\in\mathbb{R}}$ of automorphisms of $\mathfrak{A}$. Furthermore, $\tau^t A = A\circ\phi^t$, where ϕ^t is the flow on $\Xi_{\mathbb{R}^d}$ defined by the Hamiltonian equation of motion (3.44)*.*

Now, for $f \in \mathscr{B}^{(p)}$, $M(f)$ and $\widehat{S}(f)$ are well-defined in the obvious way. Define $\mathfrak{A}$ as the algebra generated by functions of the form $M(f)$, where f satisfies (3.37).

THEOREM 3.20. *Let $A \in \mathfrak{A}$. Then for any $\varepsilon > 0$ there exists a function $A_\varepsilon(t) \in \mathfrak{A}$ such that*

$$\sup_{t\in\mathbb{R}} \|\tau^t A - A_\varepsilon(t)\|_\infty \;\leqslant\; \varepsilon\,, \tag{3.53}$$

and, for any $t \in \mathbb{R}$,

$$\big\|\widehat{\tau}^t \widehat{A} - \widehat{A_\varepsilon(t)}\big\| \;\leqslant\; \varepsilon + C(\varepsilon, t)\, h^d\,. \tag{3.54}$$

3.2.8. Evolution of coherent states. As an application of Theorem 3.20, we consider the time evolution of coherent states. From now on we assume that test functions f have compact support, i.e. belong to the space

$$\mathscr{B}_c^{(p)} \;:=\; \mathscr{B}^{(p)} \cap C_c(\mathbb{R}^{pd}; \mathbb{C}^{3^p})\,.$$

In addition, we require the interaction potential V to be of finite range in the sense that there exists a sequence $R_n > 0$ such that if $|x_i - x_j| > R_n$ for some pair (i,j) then $V^{(n)}_{i_1\dots i_n}(x_1,\dots,x_n) = 0$.

Next, we take some initial classical spin configuration $M \in C(\mathbb{R}^d; \mathbb{S}^2)$, or, more generally, a function $M : \mathbb{R}^d \to \mathbb{S}^2$ whose points of discontinuity form a null set. We shall study the time evolution of product states ρ_M on $\widehat{\mathfrak{A}}^{(h)}$ that reproduce the given classical state M. For open and bounded $\Lambda \subset \mathbb{R}^d$, we define the product state

$$W_{M,\Lambda} \;:=\; \bigotimes_{x\in\Lambda^{(h)}} W_{M(x)}\,,$$

where $W_{M(x)}$ is the coherent spin state corresponding to the unit vector $M(x)$. For $\mathbf{A} \in \widehat{\mathfrak{A}}_\Lambda^{(h)}$, define

$$\rho_M\big(\mathbf{A}\big) \;:=\; \langle W_{M,\Lambda}\,, \mathbf{A}\, W_{M,\Lambda}\rangle\,,$$

which we extend to arbitrary $\mathbf{A} \in \widehat{\mathfrak{A}}^{(h)}$ by continuity.

For our main result on the time evolution of coherent states, we first record the following auxiliary result.

LEMMA 3.21. *Let $f \in \mathscr{B}_c^{(p)}$ satisfy* (3.37)*. Then*

$$\lim_{h\to 0} \rho_M\big(\widehat{S}(f)\big) \;=\; M(f)\,. \tag{3.55}$$

PROOF. We first show the claim for $f = f_1 \otimes \cdots \otimes f_p$. Thus $\widehat{S}(f) = \widehat{S}(f_1)\dots\widehat{S}(f_p)$. We proceed by induction on p. The assertion for $p = 1$ follows easily from (3.32) and the fact that f has compact support. Consider now

$$\begin{aligned}
&\rho_M\big(\widehat{S}(f_1)\cdots\widehat{S}(f_{p+1})\big)\\
&\quad= \sum_{x_1,\dots x_{p+1}} \rho_M\big(f_1(x_1)\cdot\widehat{S}(x_1)\cdots f_{p+1}(x_{p+1})\cdot\widehat{S}(x_{p+1})\big)\\
&\quad= \sum_{x_1,\dots x_p}\ \sum_{x_{p+1}\notin\{x_1,\dots,x_p\}} \rho_M\big(f_1(x_1)\cdot\widehat{S}(x_1)\cdots f_{p+1}(x_{p+1})\cdot\widehat{S}(x_{p+1})\big)\\
&\qquad+ \sum_{x_1,\dots x_p}\ \sum_{x_{p+1}\in\{x_1,\dots,x_p\}} \rho_M\big(f_1(x_1)\cdot\widehat{S}(x_1)\cdots f_{p+1}(x_{p+1})\cdot\widehat{S}(x_{p+1})\big)\,.
\end{aligned}$$

The second term is bounded by

$$h^d\,p\,\|f_{p+1}\|_\infty \prod_{q=1}^p\bigg(h^d\sum_{x\in h\mathbb{Z}^d}|f_q(x)|_1\bigg)\,.$$

Using the fact that f has compact support we see that the product converges to $\prod_q\|f_q\|_1$, so that the whole expression is of order $O(h^d)$. Since ρ_M is a product state, we thus get

$$\begin{aligned}
&\rho_M\big(\widehat{S}(f_1)\cdots\widehat{S}(f_{p+1})\big)\\
&\quad= \sum_{x_1,\dots x_p}\ \sum_{x_{p+1}\notin\{x_1,\dots,x_p\}} \rho_M\big(f_1(x_1)\cdot\widehat{S}(x_1)\cdots f_p(x_p)\cdot\widehat{S}(x_p)\big)\\
&\qquad\qquad \rho_M\big(f_{p+1}(x_{p+1})\cdot\widehat{S}(x_{p+1})\big)+O(h^d)\\
&\quad= \sum_{x_1,\dots x_p}\ \sum_{x_{p+1}} \rho_M\big(f_1(x_1)\cdot\widehat{S}(x_1)\cdots f_p(x_p)\cdot\widehat{S}(x_p)\big)\\
&\qquad\qquad \rho_M\big(f_{p+1}(x_{p+1})\cdot\widehat{S}(x_{p+1})\big)+O(h^d)\\
&\quad= \rho_M\big(\widehat{S}(f_1)\cdots\widehat{S}(f_p)\big)\,\rho_M\big(\widehat{S}(f_{p+1})\big)+O(h^d)\,,
\end{aligned}$$

where the second equality follows along the same lines as the previous estimate. From the case $p=1$ we get therefore

$$\rho_M\big(\widehat{S}(f_1)\cdots\widehat{S}(f_{p+1})\big) \;=\; \rho_M\big(\widehat{S}(f_1)\cdots\widehat{S}(f_p)\big)\,M_\Lambda(f_{p+1})+o(1)\,.$$

In a second step, we approximate a general $f\in\mathscr{B}_c^{(p)}$ by product functions. Let $\varepsilon>0$. There is a function

$$\tilde{f} \;=\; \sum_\alpha f_1^\alpha\otimes\cdots\otimes f_p^\alpha,$$

where α ranges over a finite set and $f_q^\alpha\in\mathscr{B}_c^{(1)}$, such that $\|f-\tilde{f}\|_1\leqslant\varepsilon$. Furthermore, from (3.40) we get

$$\big|\rho_M\big(\widehat{S}(f)\big)-\rho_M\big(\widehat{S}(\tilde{f})\big)\big| \;\leqslant\; \|f-\tilde{f}\|_1\,.$$

Since both f and $\tilde{f}$ have compact support, is is easy to see that there is an $h_1>0$ such that

$$h\leqslant h_1 \quad\Longrightarrow\quad \|f-\tilde{f}\|_1 \;\leqslant\; \|f-\tilde{f}\|_1+\varepsilon\leqslant 2\varepsilon\,.$$

From (3.38) we also get

$$|M_\Lambda(f)-M_\Lambda(\tilde{f})| \;\leqslant\; \varepsilon\,.$$

Finally, the previous step implies that there is an $h_2 > 0$, independent of Λ, such that

$$h \leqslant h_2 \quad \Longrightarrow \quad |\rho_M\big(\widehat{S}(\tilde{f})\big) - M_\Lambda(\tilde{f})| \;\leqslant\; \varepsilon\,.$$

Therefore for $h \leqslant \min(h_1, h_2)$ we have

$$|\rho_M\big(\widehat{S}(f)\big) - M_\Lambda(f)| \;\leqslant\; 4\varepsilon\,. \qquad \square$$

We may now state our main result for coherent spin states.

THEOREM 3.22. *Let $t \in \mathbb{R}$, $A \in \mathfrak{A}$, and M as above. Let $M(t)$ be the solution of* (3.44) *on $\mathbb{R}^d$ with initial configuration M. Then*

$$\lim_{h \to 0} \rho_M\big(\widehat{\tau}^t \widehat{A}\big) \;=\; A(M(t))\,,$$

uniformly in t on compact time intervals.

PROOF. The proof is a corollary of the proof of Theorem 3.17. First, let $|t| < \|V\|^{-1}$ and pick an $\varepsilon > 0$. Choose a cutoff such that the tails of the thermodynamic limits of the series (3.51) and (3.52) are bounded by ε. We therefore have to estimate a finite sum of terms of the form

$$\big|\rho_M\big(\widehat{S}(g)\big) - M(g)\big|\,,$$

where $g \in \mathscr{B}_c^{(p(g))}$ because of our assumptions on V. By Lemma 3.21, for h small enough, these are all bounded by ε, and the claim for small times follows. Finally, by iteration, we extend the result to arbitrary times. $\square$

3.3. Time-dependent correlation functions in the large-spin limit

In this section we consider the quantum spin system introduced in Section 3.1. We consider time-dependent correlation functions of the quantum spin system at some finite temperature, and prove that they converge to time-dependent correlation functions of the corresponding classical spin system. Our method relies on the Schwinger-Dyson expansion for the time evolution of observables (Lemma 3.6) and an expansion in coherent spin states. Using a quantum cluster expansion, we extend this result to an infinite lattice provided the temperature is high enough.

3.3.1. Time-dependent correlation functions and main result. From now on we use the notations and definitions of Section 3.1 without further comment. Let $\Lambda \subset \mathbb{Z}^d$ be finite. For a function A on Γ_Λ we set

$$\langle A \rangle_\Lambda \;:=\; \frac{1}{(4\pi)^{|\Lambda|}} \int_{\Gamma_\Lambda} \mathrm{d}M \; A(M)\,.$$

Here $\mathrm{d}M = \prod_{x \in \Lambda} \mathrm{d}M(x)$, where $\mathrm{d}M(x)$ is the uniform measure on $\mathbb{S}^2$. Similarly, for an operator $\mathbf{A}$ on $\mathcal{H}_\Lambda$ we set

$$\langle \mathbf{A} \rangle_\Lambda \;:=\; \frac{1}{(2s+1)^{|\Lambda|}} \, \mathrm{Tr}_{\mathcal{H}_\Lambda} \mathbf{A}\,.$$

Then $\langle\cdot\rangle_\Lambda$ in both cases is a state, i.e. a positive linear functional satisfying $\langle\mathbb{1}\rangle_\Lambda = 1$ (here $\mathbb{1}$ denotes the function $\mathbb{1}(M) = 1$ or the unit operator respectively). Moreover, we have the estimates

$$|\langle A\rangle_\Lambda| \leqslant \|A\|_\infty\,, \qquad |\langle \mathbf{A}\rangle_\Lambda| \leqslant \|\mathbf{A}\|\,. \tag{3.56}$$

Next, let $\beta > 0$, $\Lambda \subset \mathbb{Z}^d$ be finite, $A_1, \dots, A_n \in \mathfrak{A}_\Lambda$, and $t_1, \dots, t_n \in \mathbb{R}$. Then we define the time-dependent correlation function of the classical spin system

$$\rho_{\beta,\Lambda}\big((A_i, t_i)_{i=1}^n\big) \;:=\; \frac{1}{Z_{\beta,\Lambda}}\Big\langle(\tau_\Lambda^{t_1} A_1)\cdots(\tau_\Lambda^{t_n} A_n)\,\mathrm{e}^{-\beta H_\Lambda}\Big\rangle_\Lambda\,, \tag{3.57}$$

where

$$Z_{\beta,\Lambda} \;:=\; \big\langle \mathrm{e}^{-\beta H_\Lambda}\big\rangle_\Lambda$$

is the classical partition function.

The time-dependent correlation function of the quantum system is defined similarly. Let $s = \frac{1}{2}, 1, \frac{3}{2}, \dots$ be given, and define the time-dependent correlation function of the quantum spin system

$$\widehat{\rho}^{\,s}_{\beta,\Lambda}\big((A_i, t_i)_{i=1}^n\big) \;:=\; \frac{1}{\widehat{Z}^s_{\beta,\Lambda}}\Big\langle\big(\widehat{\tau}_\Lambda^{t_1} \widehat{A}_1\big)\cdots\big(\widehat{\tau}_\Lambda^{t_n} \widehat{A}_n\big)\,\mathrm{e}^{-\beta \widehat{H}_\Lambda}\Big\rangle_\Lambda\,,$$

where

$$\widehat{Z}^s_{\beta,\Lambda} \;:=\; \big\langle \mathrm{e}^{-\beta \widehat{H}_\Lambda}\big\rangle_\Lambda$$

is the quantum partition function. As before, we usually refrain from indicating the explicit s-dependence when it is not needed.

We may now formulate our main result. Set $\|\alpha\| := |[\alpha]|$, where $|\cdot|$ denotes cardinality.

Theorem 3.23. *Assume that* (3.10) *holds,* $\beta > 0$*,* $\Lambda \subset \mathbb{Z}^d$ *is finite,* $A_1, \dots, A_n \in \mathfrak{A}_\Lambda$*, and* $t_1, \dots, t_n \in \mathbb{R}$*. Then we have*

$$\lim_{s\to\infty} \widehat{\rho}^{\,s}_{\beta,\Lambda}\big((A_i, t_i)_{i=1}^n\big) \;=\; \rho_{\beta,\Lambda}\big((A_i, t_i)_{i=1}^n\big)\,. \tag{3.58}$$

Moreover, if β *satisfies*

$$\beta \sup_{x\in\mathbb{Z}^d} \sum_{\alpha\,:\,[\alpha]\ni x} |V(\alpha)|\,\mathrm{e}^{2a\|\alpha\|} \;\leqslant\; a \tag{3.59}$$

for some $a > 0$ *then the limits*

$$\lim_{\Lambda\to\mathbb{Z}^d} \widehat{\rho}^{\,s}_{\beta,\Lambda}\big((A_i, t_i)_{i=1}^n\big)\,, \qquad \lim_{\Lambda\to\mathbb{Z}^d} \rho_{\beta,\Lambda}\big((A_i, t_i)_{i=1}^n\big) \tag{3.60}$$

exist and satisfy

$$\lim_{s\to\infty}\lim_{\Lambda\to\mathbb{Z}^d} \widehat{\rho}^{\,s}_{\beta,\Lambda}\big((A_i, t_i)_{i=1}^n\big) \;=\; \lim_{\Lambda\to\mathbb{Z}^d} \rho_{\beta,\Lambda}\big((A_i, t_i)_{i=1}^n\big)\,. \tag{3.61}$$

Here $\Lambda \to \mathbb{Z}^d$ *means convergence in the sense of nets, where the finite subsets* $\Lambda \subset \mathbb{Z}^d$ *are ordered by inclusion.*

Remark 3.24. *One readily sees that, assuming* (3.10)*, the left-hand side of* (3.59) *is finite for* $a = r/2$*. Hence, it is always possible to find* β *and* a *such that* (3.59) *holds.*

Remark 3.25. *In the definition of* $A \mapsto \widehat{A}$ *we impose normal ordering of the spin variables. However,* (3.6) *immediately implies that Theorem 3.23 holds if normal ordering in the definition of* $\widehat{A}$ *is replaced by any other ordering.*

REMARK 3.26. *To keep the presentation of the cluster expansion in the proof of Theorem 3.23 simple, we require the unnecessarily strong convergence condition* (3.59)*. It may in fact be replaced with the weaker condition*

$$\beta \sup_{x\in\mathbb{Z}^d} \sum_{\alpha\,:\,[\alpha]\ni x\,,\,\|\alpha\|\geqslant 2} |V(\alpha)|\, \mathrm{e}^{2a\|\alpha\|} \;\leqslant\; a \tag{3.62}$$

for some $a > 0$*.*

We sketch the (minor) modifications needed in the cluster expansion of Section 3.3.2 below. Split

$$H_\Lambda \;=\; H_\Lambda^0 + V_\Lambda\,,$$

where H_Λ^0 *contains all one-site interactions, i.e. contains the terms of the form* $V(\alpha)M^\alpha$ *where* $[\alpha]$ *consists of a single lattice point. Without loss of generality, we assume that* H_Λ^0 *and* $\widehat{H}_\Lambda^0$ *are nonnegative. We then proceed as in Section 3.3.2, but instead of the full expansion* (3.69) *we use the Dyson series*

$$\widehat{Z}_{\beta,\Lambda} \;=\; 1+\sum_{n\geqslant 1}(-1)^n\int_0^\infty \mathrm{d}t_0\cdots\int_0^\infty \mathrm{d}t_n\,\delta(\beta-t_0-\cdots-t_n)$$
$$\times\left\langle \mathrm{e}^{-t_0\widehat{H}_\Lambda^0}\widehat{V}_\Lambda \mathrm{e}^{-t_1\widehat{H}_\Lambda^0}\widehat{V}_\Lambda\cdots \mathrm{e}^{-t_{n-1}\widehat{H}_\Lambda^0}\widehat{V}_\Lambda \mathrm{e}^{-t_n\widehat{H}_\Lambda^0}\right\rangle_\Lambda .$$

Using the fact that $\widehat{H}_\Lambda^0$ *leaves* $\mathcal{L}(\mathcal{H}_X)$ *invariant for all* $X\subset\Lambda$*, we may follow the derivation of Section 3.3.2 to get the cluster expansion* (3.73) *with "interaction picture" polymer weights*

$$\widehat{w}(X) \;=\; \sum_{m\geqslant 1}(-1)^m \sum_{\substack{\alpha_1,\dots,\alpha_m\\ X\text{-connected}\\ \|\alpha_i\|\geqslant 2\,\forall i}} \int_0^\infty \mathrm{d}t_0\cdots\int_0^\infty \mathrm{d}t_m\,\delta(\beta-t_0-\cdots-t_m)$$
$$\times\left\langle \mathrm{e}^{-t_0\widehat{H}_\Lambda^0}\,\Phi(\alpha_1)\,\mathrm{e}^{-t_1\widehat{H}_\Lambda^0}\Phi(\alpha_2)\cdots \mathrm{e}^{-t_{n-1}\widehat{H}_\Lambda^0}\,\Phi(\alpha_m)\,\mathrm{e}^{-t_m\widehat{H}_\Lambda^0}\right\rangle_X ;$$

see Section 3.3.2 for an explanation of notations.

The rest of the proof follows as in Section 3.3.2.

EXAMPLE 3.27. *Consider Example 3.5, i.e.*

$$H_\Lambda \;:=\; -\sum_{x\in\Lambda} h(x)\cdot M(x) - \frac{1}{2}\sum_{x,y\in\Lambda} J(x,y)\,M(x)\cdot M(y)$$

where we use the notation $M(x) = (M_1(x), M_2(x), M_3(x))$*. We assume that* $h(x)$ *and* $J(x,y)$ *are real functions satisfying*

$$\sup_{x\in\mathbb{Z}^d} h(x) \;<\; \infty\,, \qquad J(x,y) \;=\; J(y,x)\,, \qquad \|J\|_{\infty,1} \;:=\; \sup_{x\in\mathbb{Z}^d}\sum_{y\in\mathbb{Z}^d}|J(x,y)| \;<\; \infty\,.$$

This corresponds to the Heisenberg model*. Condition* (3.10) *is satisfied for all* $r > 0$*. Condition* (3.62) *reads in this case*

$$\beta\, 3\mathrm{e}^{4a}\|J\|_{\infty,1} \;\leqslant\; a\,.$$

Optimizing in a*, we find that* (3.62)*, and hence* (3.61)*, holds provided that*

$$\beta \;\leqslant\; \frac{1}{12\mathrm{e}\,\|J\|_{\infty,1}}\,.$$

3.3.2. Proof of Theorem 3.23. We start by proving the statement on a finite lattice, i.e. (3.58).

Convergence for finite Λ. The main idea is to approximate, uniformly in s, functions in ρ and $\widehat{\rho}$ with polynomials, whose limit may be handled with Lemma 3.12. After eventually adding a constant to H_Λ and $\widehat{H}_\Lambda$, we may assume that both are nonnegative. Moreover, without loss of generality we assume that $A_j = M^{\alpha_j}$ for $j = 1, \dots, n$. Clearly, it suffices to show

$$\lim_{s\to\infty} \Big\langle \big(\widehat{\tau}_\Lambda^{t_1} \widehat{A}_1\big) \cdots \big(\widehat{\tau}_\Lambda^{t_n} \widehat{A}_n\big) \, \mathrm{e}^{-\beta \widehat{H}_\Lambda} \Big\rangle_\Lambda \;=\; \Big\langle (\tau_\Lambda^{t_1} A_1) \cdots (\tau_\Lambda^{t_n} A_n) \, \mathrm{e}^{-\beta H_\Lambda(M)} \Big\rangle_\Lambda . \tag{3.63}$$

Let $\varepsilon > 0$. Lemma 3.6 implies, for each $j = 1, \dots, n$,

$$\widehat{\tau}_\Lambda^{t_j} \widehat{A}_j \;=\; \mathbf{P}_j + \mathbf{R}_j \,,$$

where

$$\mathbf{P}_j \;=\; \sum_{\alpha \in B_j} \mathbb{1}_{\{[\alpha] \subset \Lambda\}} \, v_\alpha^j \, Q_\alpha^j\big(\widehat{S}^\alpha\big) \,, \qquad \|\mathbf{R}_j\| \;\leqslant\; \varepsilon \,.$$

Thus,

$$\big\| \big(\widehat{\tau}_\Lambda^{t_1} \widehat{A}_1\big) \cdots \big(\widehat{\tau}_\Lambda^{t_n} \widehat{A}_n\big) - \mathbf{P}_1 \cdots \mathbf{P}_n \big\| \;\leqslant\; 2^n (1+\varepsilon)^{n-1} \varepsilon \,, \tag{3.64}$$

so that

$$\Big| \Big\langle \big(\widehat{\tau}_\Lambda^{t_1} \widehat{A}_1\big) \cdots \big(\widehat{\tau}_\Lambda^{t_n} \widehat{A}_n\big) \, \mathrm{e}^{-\beta \widehat{H}_\Lambda} \Big\rangle_\Lambda - \Big\langle \mathbf{P}_1 \cdots \mathbf{P}_n \, \mathrm{e}^{-\beta \widehat{H}_\Lambda} \Big\rangle_\Lambda \Big| \;\leqslant\; 2^n (1+\varepsilon)^{n-1} \varepsilon \,.$$

Similarly, we find

$$\tau_\Lambda^{t_j} A_j \;=\; P_j + R_j \,,$$

where

$$P_j \;=\; \sum_{\alpha \in B_j} \mathbb{1}_{\{[\alpha] \subset \Lambda\}} \, v_\alpha^j \, M^\alpha \,, \qquad \|R_j\|_\infty \;\leqslant\; \varepsilon \,.$$

Therefore, in order to show (3.63), it suffices to show

$$\lim_{s\to\infty} \big\langle \mathbf{P}_1 \cdots \mathbf{P}_n \, \mathrm{e}^{-\beta \widehat{H}_\Lambda} \big\rangle_\Lambda \;=\; \big\langle P_1 \cdots P_n \, \mathrm{e}^{-\beta H_\Lambda} \big\rangle_\Lambda \,.$$

Since H_Λ and $\widehat{H}_\Lambda$ are both bounded, we may expand the exponential on both sides. By dominated convergence, it suffices to show

$$\lim_{s\to\infty} \big\langle \mathbf{P}_1 \cdots \mathbf{P}_n \, \widehat{H}_\Lambda^k \big\rangle_\Lambda \;=\; \big\langle P_1 \cdots P_n \, H_\Lambda^k \big\rangle_\Lambda \,.$$

Next, let us write

$$H_\Lambda \;=\; \sum_{\alpha \in C} V(\alpha) M^\alpha + E \,, \qquad \widehat{H}_\Lambda \;=\; \sum_{\alpha \in C} V(\alpha) :\widehat{S}^\alpha: + \widehat{E}$$

where C is finite, $\|E\|_\infty \leqslant \varepsilon$ and $\|\widehat{E}\| \leqslant \varepsilon$ for all s. Thus,

$$\Bigg| \big\langle \mathbf{P}_1 \cdots \mathbf{P}_n \, \widehat{H}_\Lambda^k \big\rangle_\Lambda - \Bigg\langle \mathbf{P}_1 \cdots \mathbf{P}_n \Bigg(\sum_{\alpha \in C} V(\alpha) :\widehat{S}^\alpha: \Bigg)^k \Bigg\rangle_\Lambda \Bigg| \;\leqslant\; (1+\varepsilon)^n \, 2^k \, (\|\widehat{H}_\Lambda\| + \varepsilon)^{k-1} \, \varepsilon \,,$$

for all s. A similar estimate holds for the corresponding classical expression. We conclude that it suffices to show

$$\lim_{s\to\infty} \big\langle Q(\widehat{S}^\alpha) \big\rangle_\Lambda \;=\; \big\langle M^\alpha \big\rangle_\Lambda \,, \tag{3.65}$$

for an arbitrary multi-index α and ordering Q.

We show (3.65) using coherent spin states. For $M \in \Gamma_\Lambda$ define the coherent product state

$$W_M \;:=\; \bigotimes_{x\in\Lambda} W_{M(x)} \in \mathcal{H}_\Lambda\,,$$

where $W_{M(x)}$ is the coherent state (3.26). From (3.28) we get

$$\frac{1}{(2s+1)^{|\Lambda|}}\operatorname{Tr}_{\mathcal{H}^s_\Lambda}\big(Q(\widehat{S}^\alpha)\big) \;=\; \frac{1}{(4\pi)^{|\Lambda|}}\int_{\Gamma_\Lambda} \mathrm{d}M\,\big\langle W_M\,, \big(Q(\widehat{S}^\alpha)\big)\,W_M\big\rangle\,.$$

Now (3.29) implies

$$\lim_{s\to\infty}\big\langle W_M\,, Q(\widehat{S}^\alpha)\,W_M\big\rangle \;=\; M^\alpha\,.$$

Therefore (3.65) follows by dominated convergence, and the proof of (3.58) is complete.

The thermodynamic limit. We now move on to showing the existence of the limits (3.60) as well as the convergence (3.61). Let $\varepsilon > 0$. Arguing as in the proof of Lemma 3.6 (see (3.64)), we find that there is a finite set B such that

$$\bigg\|(\tau^{t_1}_\Lambda A_1)\cdots(\tau^{t_n}_\Lambda A_n) - \sum_{\alpha\in B}\mathbb{1}_{\{[\alpha]\subset\Lambda\}}\,v_\alpha\,M^\alpha\bigg\|_\infty \;\leqslant\; \varepsilon\,,$$

$$\bigg\|(\widehat{\tau}^{t_1}_\Lambda \widehat{A}_1)\cdots(\widehat{\tau}^{t_n}_\Lambda \widehat{A}_n) - \sum_{\alpha\in B}\mathbb{1}_{\{[\alpha]\subset\Lambda\}}\,v_\alpha\,Q_\alpha\big(\widehat{S}^\alpha\big)\bigg\| \;\leqslant\; \varepsilon\,,$$

for all s and Λ large enough. Let us choose Λ_0 so that $[\alpha]\subset\Lambda_0$ for all $\alpha\in B$. Then we have

$$\bigg|\rho_{\beta,\Lambda}\big((A_i,t_i)_{i=1}^n\big) - \sum_{\alpha\in B} v_\alpha\,\frac{1}{Z_{\beta,\Lambda}}\big\langle M^\alpha \mathrm{e}^{-\beta H_\Lambda}\big\rangle_\Lambda\bigg| \;\leqslant\; \varepsilon\,,$$

$$\bigg|\widehat{\rho}_{\beta,\Lambda}\big((A_i,t_i)_{i=1}^n\big) - \sum_{\alpha\in B} v_\alpha\,\frac{1}{\widehat{Z}_{\beta,\Lambda}}\big\langle Q_\alpha\big(\widehat{S}^\alpha\big) \mathrm{e}^{-\beta \widehat{H}_\Lambda}\big\rangle_\Lambda\bigg| \;\leqslant\; \varepsilon\,,$$

for all s and $\Lambda\supset\Lambda_0$. We conclude that it suffices to show that, for any multi-index α, the limits

$$\lim_{\Lambda\to\mathbb{Z}^d}\frac{1}{Z_{\beta,\Lambda}}\big\langle M^\alpha\,\mathrm{e}^{-\beta H_\Lambda}\big\rangle_\Lambda\,,\qquad \lim_{\Lambda\to\mathbb{Z}^d}\frac{1}{\widehat{Z}_{\beta,\Lambda}}\big\langle\, :\widehat{S}^\alpha:\,\mathrm{e}^{-\beta \widehat{H}_\Lambda}\big\rangle_\Lambda \tag{3.66}$$

exist and satisfy

$$\lim_{s\to\infty}\lim_{\Lambda\to\mathbb{Z}^d}\frac{1}{\widehat{Z}_{\beta,\Lambda}}\big\langle\, :\widehat{S}^\alpha:\,\mathrm{e}^{-\beta \widehat{H}_\Lambda}\big\rangle_\Lambda \;=\; \lim_{\Lambda\to\mathbb{Z}^d}\frac{1}{Z_{\beta,\Lambda}}\big\langle M^\alpha\,\mathrm{e}^{-\beta H_\Lambda}\big\rangle_\Lambda\,. \tag{3.67}$$

We do this with a quantum cluster expansion.

Setting up the cluster expansion. Let us concentrate on the quantum spin system; the classical spin system is handled in the same way. Let $\Lambda\subset\mathbb{Z}^d$ be finite. Note that $\langle\cdot\rangle_\Lambda$ satisfies the factorization property

$$\langle AB\rangle_\Lambda \;=\; \langle A\rangle_\Lambda\langle B\rangle_\Lambda\,, \tag{3.68}$$

whenever the supports of A and B are disjoint in Λ, i.e. whenever there exist disjoint sets $X,Y\subset\Lambda$ such that $A\in\mathcal{L}(\mathcal{H}_X)$ and $B\in\mathcal{L}(\mathcal{H}_Y)$.

Abbreviate

$$\Phi(\alpha) \;:=\; V(\alpha) : \widehat{S}^\alpha :$$

and consider the partition function

$$\widehat{Z}_{\beta,\Lambda} \;=\; \big\langle \mathrm{e}^{-\beta \widehat{H}_\Lambda} \big\rangle_\Lambda \;=\; 1 + \sum_{n \geqslant 1} \frac{(-\beta)^n}{n!} \sum_{\alpha_1, \dots, \alpha_n} \big\langle \Phi(\alpha_1) \cdots \Phi(\alpha_n) \big\rangle_\Lambda \,, \tag{3.69}$$

where the sum ranges over α_i satisfying $[\alpha_i] \subset \Lambda$. In order to get a cluster expansion with polymers given by the subsets $X \subset \Lambda$, we decompose $\bigcup_{i=1}^n [\alpha_i]$ in view of using the factorization property (3.68).

We start with some notation. Define $\mathbb{N}_n := \{1, \dots, n\}$. We use the symbol $\uplus$ to denote disjoint union of sets. We use $\mathcal{G}(A)$ to denote the set of graphs on the vertex set A and $\mathcal{G}_c(A) \subset \mathcal{G}(A)$ to denote the subset of connected graphs. The set of edges of a graph G, i.e. a set of unordered pairs of vertices, is denoted by $E(G)$. When writing $A = I_1 \uplus \cdots \uplus I_k$ for a partition of the set A into k subsets, we always mean that $I_l \neq \emptyset$ for $l = 1, \dots, k$.

Next, define

$$\xi(X, Y) \;:=\; \begin{cases} 1 & \text{if } X \cap Y \neq \emptyset \\ 0 & \text{otherwise}\,. \end{cases}$$

We also use the abbreviation $X \nsim Y$ to mean $X \cap Y \neq \emptyset$. To avoid cluttering the notation, we omit the brackets $[\cdot]$ around multi-indices in expressions like $\xi(\alpha, X)$ and $\alpha \nsim X$. Now, for any sequence $\alpha_1, \dots, \alpha_n$, we have

$$1 \;=\; \sum_{G \in \mathcal{G}(\mathbb{N}_n)} \prod_{\{i,j\} \in E(G)} \xi(\alpha_i, \alpha_j) \prod_{\{i,j\} \notin E(G)} \big(1 - \xi(\alpha_i, \alpha_j)\big) \,, \tag{3.70}$$

since the summand is equal to 1 for exactly one G and 0 otherwise. Let us decompose the sum over G into a sum over partitions of the vertex set $\mathbb{N}_n = I_1 \uplus \cdots \uplus I_k$, followed by a sum over connected subgraphs within each partition. This yields

$$\begin{aligned} 1 \;=\; \sum_{k \geqslant 1} \frac{1}{k!} \sum_{I_1 \uplus \cdots \uplus I_k = \mathbb{N}_n} & D_{I_1, \dots, I_k}(\alpha_1, \dots, \alpha_n) \\ & \times \prod_{l=1}^k \left[\sum_{G \in \mathcal{G}_c(I_l)} \prod_{\{i,j\} \in E(G)} \xi(\alpha_i, \alpha_j) \prod_{\{i,j\} \notin E(G)} \big(1 - \xi(\alpha_i, \alpha_j)\big) \right] \,, \end{aligned} \tag{3.71}$$

where

$$D_{I_1, \dots, I_k}(\alpha_1, \dots, \alpha_n) \;:=\; \prod_{1 \leqslant l < l' \leqslant k} \prod_{i \in I_l} \prod_{j \in I_{l'}} \big(1 - \xi(\alpha_i, \alpha_j)\big) \,. \tag{3.72}$$

The following definitions will prove useful. We say that $\alpha_1, \dots, \alpha_n$ are *connected* if

$$\sum_{G \in \mathcal{G}_c(\mathbb{N}_n)} \prod_{\{i,j\} \in E(G)} \xi(\alpha_i, \alpha_j) \prod_{\{i,j\} \notin E(G)} \big(1 - \xi(\alpha_i, \alpha_j)\big) \;=\; 1 \,;$$

compare this with (3.70). If $\alpha_1, \dots, \alpha_n$ are connected and $X = [\alpha_1] \cup \cdots \cup [\alpha_n]$ we say that $\alpha_1, \dots, \alpha_n$ are *X-connected*. Thus,

$$\begin{aligned} \widehat{Z}_{\beta,\Lambda} \;=\; 1 + \sum_{n \geqslant 1} \frac{(-\beta)^n}{n!} \sum_{k \geqslant 1} \frac{1}{k!} & \sum_{I_1 \uplus \cdots \uplus I_k = \mathbb{N}_n} \\ & \times \sum_{\alpha_1, \dots, \alpha_n} D_{I_1, \dots, I_k}(\alpha_1, \dots, \alpha_n) \big\langle \Phi(\alpha_1) \cdots \Phi(\alpha_n) \big\rangle_\Lambda \prod_{l=1}^k \mathbb{1}_{\{(\alpha_i)_{i \in I_l} \text{ connected}\}} \,. \end{aligned}$$

By definition of $D_{I_1,\dots,I_k}(\alpha_1,\dots,\alpha_n)$ and the factorization property (3.68) we have

$$D_{I_1,\dots,I_k}(\alpha_1,\dots,\alpha_n)\,\big\langle\Phi(\alpha_1)\cdots\Phi(\alpha_n)\big\rangle_\Lambda \;=\; D_{I_1,\dots,I_k}(\alpha_1,\dots,\alpha_n)\prod_{l=1}^k\Bigg\langle\prod_{i\in I_l}\Phi(\alpha_i)\Bigg\rangle_\Lambda\,,$$

where the product inside $\langle\cdot\rangle_\Lambda$ is in the same order as on the left-hand side. This yields

$$\begin{aligned}\widehat{Z}_{\beta,\Lambda} \;&=\; 1+\sum_{n\geqslant 1}\frac{(-\beta)^n}{n!}\sum_{k\geqslant 1}\frac{1}{k!}\sum_{I_1\uplus\cdots\uplus I_k=\mathbb{N}_n}\;\sum_{X_1,\dots,X_k}\\ &\qquad\times\sum_{\alpha_1,\dots,\alpha_n}D_{I_1,\dots,I_k}(\alpha_1,\dots,\alpha_n)\prod_{l=1}^k\Bigg(\mathbb{1}_{\{(\alpha_i)_{i\in I_l}\ X_l\text{-connected}\}}\Bigg\langle\prod_{i\in I_l}\Phi(\alpha_i)\Bigg\rangle_\Lambda\Bigg)\\ &=\; 1+\sum_{n\geqslant 1}\frac{(-\beta)^n}{n!}\sum_{k\geqslant 1}\frac{1}{k!}\sum_{I_1\uplus\cdots\uplus I_k=\mathbb{N}_n}\;\sum_{\substack{X_1,\dots,X_k\\ \text{disjoint}}}\\ &\qquad\times\sum_{\alpha_1,\dots,\alpha_n}\prod_{l=1}^k\Bigg(\mathbb{1}_{\{(\alpha_i)_{i\in I_l}\ X_l\text{-connected}\}}\Bigg\langle\prod_{i\in I_l}\Phi(\alpha_i)\Bigg\rangle_\Lambda\Bigg)\,,\end{aligned}$$

by definition of $D_{I_1,\dots,I_k}(\alpha_1,\dots,\alpha_n)$. Using the renaming $(\alpha_i)_{i\in I_l}\mapsto(\alpha_i)_{i=1}^{|I_l|}$ we get

$$\begin{aligned}\widehat{Z}_{\beta,\Lambda} \;&=\; 1+\sum_{n\geqslant 1}\frac{(-\beta)^n}{n!}\sum_{k\geqslant 1}\frac{1}{k!}\sum_{I_1\uplus\cdots\uplus I_k=\mathbb{N}_n}\;\sum_{\substack{X_1,\dots,X_k\\ \text{disjoint}}}\prod_{l=1}^k\Bigg(\sum_{\substack{\alpha_1,\dots,\alpha_{|I_l|}\\ X_l\text{-connected}}}\big\langle\Phi(\alpha_1)\cdots\Phi(\alpha_{|I_l|})\big\rangle_\Lambda\Bigg)\\ &=\; 1+\sum_{n\geqslant 1}\frac{(-\beta)^n}{n!}\sum_{k\geqslant 1}\frac{1}{k!}\sum_{m_1+\cdots+m_k=n}\;\sum_{\substack{I_1\uplus\cdots\uplus I_k=\mathbb{N}_n:\\ |I_l|=m_l\ \forall l}}\;\sum_{\substack{X_1,\dots,X_k\\ \text{disjoint}}}\prod_{l=1}^k\Bigg(\sum_{\substack{\alpha_1,\dots,\alpha_{m_l}\\ X_l\text{-connected}}}\big\langle\Phi(\alpha_1)\cdots\Phi(\alpha_{m_l})\big\rangle_\Lambda\Bigg)\\ &=\; 1+\sum_{n\geqslant 1}\frac{(-\beta)^n}{n!}\sum_{k\geqslant 1}\frac{1}{k!}\sum_{m_1+\cdots+m_k=n}\frac{n!}{m_1!\cdots m_k!}\sum_{\substack{X_1,\dots,X_k\\ \text{disjoint}}}\prod_{l=1}^k\Bigg(\sum_{\substack{\alpha_1,\dots,\alpha_{m_l}\\ X_l\text{-connected}}}\big\langle\Phi(\alpha_1)\cdots\Phi(\alpha_{m_l})\big\rangle_\Lambda\Bigg)\,.\end{aligned}$$

This yields the cluster expansion

$$\widehat{Z}_{\beta,\Lambda} \;=\; 1+\sum_{k\geqslant 1}\frac{1}{k!}\sum_{\substack{X_1,\dots,X_k\\ \text{disjoint}}}\prod_{l=1}^k\widehat{w}(X_l)\,, \tag{3.73}$$

where the summation is restricted to $X_l\subset\Lambda$. The polymer weights are given by

$$\widehat{w}(X) \;:=\; \sum_{m\geqslant 1}\frac{(-\beta)^m}{m!}\sum_{\substack{\alpha_1,\dots,\alpha_m\\ X\text{-connected}}}\big\langle\Phi(\alpha_1)\cdots\Phi(\alpha_m)\big\rangle_X\,. \tag{3.74}$$

Using the definition

$$\zeta(X,Y) \;:=\; -\xi(X,Y)\,.$$

and renaming indices we may write (3.73) as

$$\widehat{Z}_{\beta,\Lambda} \;=\; 1+\sum_{n\geqslant 1}\frac{1}{n!}\sum_{X_1,\dots,X_n\subset\Lambda}\prod_{i=1}^n\widehat{w}(X_i)\prod_{1\leqslant i<j\leqslant n}(1+\zeta(X_i,X_j))\,. \tag{3.75}$$

It is then well known (see Appendix A) that, at least as a formal power series,

$$\log \widehat{Z}_{\beta,\Lambda} \;=\; \sum_{n\geqslant 1} \frac{1}{n!} \sum_{X_1,\dots,X_n \subset \Lambda} \varphi(X_1,\dots,X_n) \prod_{i=1}^{n} \widehat{w}(X_i)\,, \tag{3.76}$$

where

$$\varphi(X_1,\dots,X_n) \;:=\; \begin{cases} 1 & \text{if } n=1 \\ \sum_{G\in\mathcal{G}_c(\mathbb{N}_n)} \prod_{\{i,j\}\in E(G)} \zeta(X_i,X_j) & \text{if } n \geqslant 2\,. \end{cases}$$

Convergence of the cluster expansion. A convenient way to address the convergence of (3.76) is the *Kotecký-Preiss* criterion [KP86, Uel04]

$$\sum_{Y \nsim X} |\widehat{w}(Y)|\, \mathrm{e}^{a|Y|} \;\leqslant\; a|X| \qquad \forall X\,, \tag{3.77}$$

for some $a > 0$. The following Lemma is the main tool for controlling cluster expansions.

LEMMA 3.28. *Let $\widehat{w}$ satisfy* (3.77)*. Then for all X_1 we have*

$$1 + \sum_{n\geqslant 2} \frac{1}{(n-1)!} \sum_{X_2,\dots,X_n} |\varphi(X_1,\dots,X_2)||\widehat{w}(X_2)|\cdots|\widehat{w}(X_n)| \;\leqslant\; \mathrm{e}^{a|X_1|}\,.$$

PROOF. See Theorem A.1 in Appendix A. ◻

In order to show (3.77), we note that the expression (3.74) for $\widehat{w}(X)$ has the approximate structure of a cluster expansion. It is therefore natural to estimate it using methods similar to those employed to prove the convergence of cluster expansions. Let us abbreviate

$$V_a(\alpha) \;:=\; |V(\alpha)|\, \mathrm{e}^{a\|\alpha\|}\,.$$

The criterion (3.59) is equivalent to

$$\beta \sum_{\alpha \nsim X} V_a(\alpha)\, \mathrm{e}^{a\|\alpha\|} \;\leqslant\; a|X| \qquad \forall X\,. \tag{3.78}$$

LEMMA 3.29. *Let V satisfy* (3.59)*. Then for all α_1 we have*

$$1 + \sum_{n\geqslant 2} \frac{\beta^{n-1}}{(n-1)!} \sum_{\substack{\alpha_2,\dots,\alpha_n :\\ \alpha_1,\dots,\alpha_n \text{ connected}}} V_a(\alpha_2)\cdots V_a(\alpha_n) \;\leqslant\; \mathrm{e}^{a\|\alpha_1\|}\,.$$

PROOF. Define

$$K_N(\alpha_1) \;:=\; 1 + \sum_{n=2}^{N+1} \frac{\beta^{n-1}}{(n-1)!} \sum_{\substack{\alpha_2,\dots,\alpha_n :\\ \alpha_1,\dots,\alpha_n \text{ connected}}} V_a(\alpha_2)\cdots V_a(\alpha_n)\,.$$

We need to show that $K_N(\alpha_1) \leqslant \mathrm{e}^{a\|\alpha_1\|}$ for all α_1 and N. We do this by induction on N.

Note first that if $K_N(\alpha_1) \leqslant \mathrm{e}^{a\|\alpha_1\|}$ then we have for all X

$$\begin{aligned}
&\sum_{n=1}^{N+1} \frac{\beta^n}{n!} \sum_{\substack{\alpha_1,\dots,\alpha_n \\ \text{connected}}} \sum_{i=1}^{n} \xi(X,\alpha_i) V_a(\alpha_1)\cdots V_a(\alpha_n) \\
&\quad = \sum_{n=1}^{N+1} \frac{\beta^n}{(n-1)!} \sum_{\substack{\alpha_1,\dots,\alpha_n \\ \text{connected}}} \xi(X,\alpha_1) V_a(\alpha_1)\cdots V_a(\alpha_n) \\
&\quad = \sum_{\alpha_1} \xi(X,\alpha_1)\beta V_a(\alpha_1) K_N(\alpha_1) \\
&\quad \leqslant \sum_{\alpha_1} \xi(X,\alpha_1)\beta V_a(\alpha_1) \mathrm{e}^{a\|\alpha_1\|} \\
&\quad \leqslant a|X|,
\end{aligned} \tag{3.79}$$

where the last step follows from (3.78).

Clearly, the claim $K_N(\alpha_1) \leqslant \mathrm{e}^{a\|\alpha_1\|}$ is true for $N = 0$. For the induction step it is convenient to rename the variables,

$$K_N(\alpha_0) \;=\; 1 + \sum_{n=1}^{N} \frac{\beta^n}{n!} \sum_{\substack{\alpha_1,\dots,\alpha_n : \\ \alpha_0,\dots,\alpha_n \text{ connected}}} V_a(\alpha_1)\cdots V_a(\alpha_n)\,.$$

The idea of the induction step is as follows (see also [Uel04]). One considers the connectivity graph of $\alpha_0, \dots, \alpha_n$, i.e. the graph on $\{0, \dots, n\}$ that contains the edge $\{i, j\}$ if and only if $\alpha_i \nsim \alpha_j$. Removing the vertex 0 yields a graph that is in general no longer connected. One then decomposes this graph into its connected components and applies the induction hypothesis on each connected subgraph.

Using (3.71), we find for all α_0

$$\begin{aligned}
K_N(\alpha_0) \;&=\; 1 + \sum_{n=1}^{N} \frac{\beta^n}{n!} \sum_{\substack{\alpha_1,\dots,\alpha_n : \\ \alpha_0,\dots,\alpha_n \text{ connected}}} V_a(\alpha_1)\cdots V_a(\alpha_n) \\
&\qquad \times \sum_{k \geqslant 1} \frac{1}{k!} \sum_{I_1 \uplus \cdots \uplus I_k = \mathbb{N}_n} D_{I_1,\dots,I_k}(\alpha_1,\dots,\alpha_n) \prod_{l=1}^{k} \mathbb{1}_{\{(\alpha_i)_{i\in I_l} \text{ connected}\}} \\
&\leqslant\; 1 + \sum_{n=1}^{N} \frac{\beta^n}{n!} \sum_{\substack{\alpha_1,\dots,\alpha_n : \\ \alpha_0,\dots,\alpha_n \text{ connected}}} V_a(\alpha_1)\cdots V_a(\alpha_n) \\
&\qquad \times \sum_{k \geqslant 1} \frac{1}{k!} \sum_{I_1 \uplus \cdots \uplus I_k = \mathbb{N}_n} \prod_{l=1}^{k} \big[\mathbb{1}_{\{\exists i \in I_l \,:\, \alpha_i \nsim \alpha_0\}} \mathbb{1}_{\{(\alpha_i)_{i\in I_l} \text{ connected}\}}\big] \\
&\leqslant\; 1 + \sum_{n=1}^{N} \frac{\beta^n}{n!} \sum_{k \geqslant 1} \frac{1}{k!} \sum_{m_1 + \cdots + m_k = n} \sum_{\substack{I_1 \uplus \cdots \uplus I_k = \mathbb{N}_n : \\ |I_l| = m_l \ \forall l}} \\
&\qquad \times \prod_{l=1}^{k} \Bigg[\sum_{\alpha_1,\dots,\alpha_{m_l}} \mathbb{1}_{\{\exists i \in \mathbb{N}_{m_l} \,:\, \alpha_i \nsim \alpha_0\}} \mathbb{1}_{\{(\alpha_1,\dots,\alpha_{m_l}) \text{ connected}\}} V_a(\alpha_1)\cdots V_a(\alpha_{m_l}) \Bigg],
\end{aligned}$$

by relaxing the connectedness condition on $\alpha_0, \dots, \alpha_n$. Thus,

$$
\begin{aligned}
K_N(\alpha_0) \;&\leqslant\; 1 + \sum_{n=1}^{N} \frac{\beta^n}{n!} \sum_{k\geqslant 1} \frac{1}{k!} \sum_{m_1+\dots+m_k=n} \frac{n!}{m_1! \cdots m_k!} \\
&\qquad \times \prod_{l=1}^{k} \Bigg[\sum_{\substack{\alpha_1,\dots,\alpha_{m_l} \\ \text{connected}}} \mathbb{1}_{\{\exists i\in\mathbb{N}_{m_l} \,:\, \alpha_i \nsim \alpha_0\}} V_a(\alpha_1)\cdots V_a(\alpha_{m_l}) \Bigg] \\
&\leqslant\; 1 + \sum_{k\geqslant 1} \frac{1}{k!} \Bigg[\sum_{m=1}^{N} \frac{\beta^m}{m!} \sum_{\substack{\alpha_1,\dots,\alpha_m \\ \text{connected}}} \mathbb{1}_{\{\exists i\in\mathbb{N}_m \,:\, \alpha_i \nsim \alpha_0\}} V_a(\alpha_1)\cdots V_a(\alpha_m) \Bigg]^k .
\end{aligned}
$$

By the induction hypothesis, $K_{N-1}(\alpha_0) \leqslant \mathrm{e}^{a\|\alpha_0\|}$ for all α_0. Thus, (3.79) yields

$$
\begin{aligned}
K_N(\alpha_0) \;&\leqslant\; \exp\Bigg[\sum_{m=1}^{N} \frac{\beta^m}{m!} \sum_{\substack{\alpha_1,\dots,\alpha_m \\ \text{connected}}} \mathbb{1}_{\{\exists i\in\mathbb{N}_m \,:\, \alpha_i \nsim \alpha_0\}} V_a(\alpha_1)\cdots V_a(\alpha_m) \Bigg] \\
&\leqslant\; \exp\Bigg[\sum_{m=1}^{N} \frac{\beta^m}{m!} \sum_{\substack{\alpha_1,\dots,\alpha_m \\ \text{connected}}} \sum_{i=1}^{m} \xi(\alpha_0,\alpha_i) V_a(\alpha_1)\cdots V_a(\alpha_m) \Bigg] \\
&\leqslant\; \mathrm{e}^{a\|\alpha_0\|} .
\end{aligned}
$$

□

LEMMA 3.30. *Assume* (3.59). *Then the Kotecký-Preiss criterion* (3.77) *holds.*

PROOF. This is a simple consequence of Lemma 3.29. Note first that (3.79) implies

$$
\sum_{n\geqslant 1} \frac{\beta^n}{n!} \sum_{\substack{\alpha_1,\dots,\alpha_n \\ \text{connected}}} \sum_{i=1}^{n} \xi(X,\alpha_i) V_a(\alpha_1)\cdots V_a(\alpha_n) \;\leqslant\; a|X| .
$$

Thus,

$$
\begin{aligned}
\sum_{Y \nsim X} |\widehat{w}(Y)|\, \mathrm{e}^{a|Y|} \;&\leqslant\; \sum_{Y\nsim X} \sum_{n\geqslant 1} \frac{\beta^n}{n!} \sum_{\substack{\alpha_1,\dots,\alpha_n \\ Y\text{-connected}}} |V(\alpha_1)| \cdots |V(\alpha_n)|\, \mathrm{e}^{a|Y|} \\
&\leqslant\; \sum_{Y\nsim X} \sum_{n\geqslant 1} \frac{\beta^n}{n!} \sum_{\substack{\alpha_1,\dots,\alpha_n \\ Y\text{-connected}}} V_a(\alpha_1)\cdots V_a(\alpha_n) \\
&=\; \sum_{n\geqslant 1} \frac{\beta^n}{n!} \sum_{\substack{\alpha_1,\dots,\alpha_n \\ \text{connected}}} \mathbb{1}_{\{\exists i\in\mathbb{N}_n \,:\, \alpha_i \nsim X\}} V_a(\alpha_1)\cdots V_a(\alpha_n) \\
&\leqslant\; \sum_{n\geqslant 1} \frac{\beta^n}{n!} \sum_{\substack{\alpha_1,\dots,\alpha_n \\ \text{connected}}} \sum_{i=1}^{n} \xi(X,\alpha_i) V_a(\alpha_1)\cdots V_a(\alpha_n) \\
&\leqslant\; a|X| .
\end{aligned}
$$

□

Expectation values in the thermodynamic limit. The quantum cluster expansion (3.76) with polymer weights

$$
\widehat{w}(X) \;=\; \sum_{m\geqslant 1} \frac{(-\beta)^m}{m!} \sum_{\substack{\alpha_1,\dots,\alpha_m \\ X\text{-connected}}} V(\alpha_1)\cdots V(\alpha_m) \big\langle :\widehat{S}^{\alpha_1}: \,\cdots\, :\widehat{S}^{\alpha_m}: \big\rangle_X \tag{3.80}
$$

has the classical analogue

$$\log Z_{\beta,\Lambda} \;=\; 1 + \sum_{n\geqslant 1} \frac{1}{n!} \sum_{X_1,\dots,X_n \subset \Lambda} \varphi(X_1,\dots,X_n) \prod_{i=1}^{n} w(X_i)\,, \tag{3.81}$$

with classical polymer weights

$$w(X) \;:=\; \sum_{m\geqslant 1} \frac{(-\beta)^m}{m!} \sum_{\substack{\alpha_1,\dots,\alpha_m \\ X\text{-connected}}} V(\alpha_1)\cdots V(\alpha_m) \big\langle M^{\alpha_1}\cdots M^{\alpha_m}\big\rangle_X\,. \tag{3.82}$$

The derivation is identical to the above derivation of the quantum cluster expansion. Moreover, the bound (3.77) and Lemma 3.28 hold with $\widehat{w}$ replaced by w.

Expectations of observables are conveniently computed by defining the perturbed Hamiltonian $\widehat{H}_\Lambda(\lambda) := \widehat{H}_\Lambda + \lambda : \widehat{S}^\alpha :$. Recall the identity

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\bigg|_{\lambda=0} \mathrm{e}^{A(\lambda)} \;=\; \int_0^1 \mathrm{d}x\; \mathrm{e}^{xA}\, A'\, \mathrm{e}^{(1-x)A}\,,$$

where $A = A(0)$ and $A' = \mathrm{d}A(0)/\mathrm{d}\lambda$. Thus, by cyclicity of the trace, we find

$$-\frac{1}{\beta}\frac{\mathrm{d}}{\mathrm{d}\lambda}\bigg|_{\lambda=0} \log\big\langle \mathrm{e}^{-\beta \widehat{H}_\Lambda(\lambda)}\big\rangle_\Lambda \;=\; \frac{1}{\widehat{Z}_{\beta,\Lambda}} \big\langle : \widehat{S}^\alpha : \,\mathrm{e}^{-\beta\widehat{H}_\Lambda}\big\rangle_\Lambda\,.$$

Also, from (3.76) we get

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\lambda}\bigg|_{\lambda=0} \log\big\langle \mathrm{e}^{-\beta \widehat{H}_\Lambda(\lambda)}\big\rangle_\Lambda \;&=\; \sum_{n\geqslant 1} \frac{1}{n!} \sum_{X_1,\dots,X_n \subset \Lambda} \varphi(X_1,\dots,X_n) \frac{\mathrm{d}}{\mathrm{d}\lambda}\bigg|_{\lambda=0} \prod_{i=1}^{n} \widehat{w}(X_i) \\
&=\; \sum_{n\geqslant 1} \frac{1}{(n-1)!} \sum_{X_1,\dots,X_n \subset \Lambda} \varphi(X_1,\dots,X_n)\, \widehat{w}'(X_1) \prod_{i=2}^{n} \widehat{w}(X_i)\,,
\end{aligned} \tag{3.83}$$

by symmetry of φ. Let us therefore define

$$\widehat{F}\big(: \widehat{S}^\alpha : \big) \;:=\; \sum_{n\geqslant 1} \frac{1}{(n-1)!} \sum_{X_1,\dots,X_n \subset \mathbb{Z}^d} \varphi(X_1,\dots,X_n)\, \widehat{w}'(X_1) \prod_{i=2}^{n} \widehat{w}(X_i)\,. \tag{3.84}$$

Similarly, using the perturbed classical Hamilton function $H_\Lambda(\lambda) := H_\Lambda + \lambda M^\alpha$, we define

$$F(M^\alpha) \;:=\; \sum_{n\geqslant 1} \frac{1}{(n-1)!} \sum_{X_1,\dots,X_n \subset \mathbb{Z}^d} \varphi(X_1,\dots,X_n)\, w'(X_1) \prod_{i=2}^{n} w(X_i)\,. \tag{3.85}$$

LEMMA 3.31. *If* (3.59) *holds, then the right-hand side of* (3.84) *converges absolutely and uniformly in s, and the right-hand side of* (3.85) *converges absolutely. Moreover,*

$$\lim_{\Lambda\to\mathbb{Z}^d} \frac{1}{\widehat{Z}_{\beta,\Lambda}} \big\langle : \widehat{S}^\alpha : \,\mathrm{e}^{-\beta\widehat{H}_\Lambda}\big\rangle_\Lambda \;=\; -\frac{1}{\beta}\widehat{F}\big(: \widehat{S}^\alpha : \big)\,, \tag{3.86a}$$

$$\lim_{\Lambda\to\mathbb{Z}^d} \frac{1}{Z_{\beta,\Lambda}} \big\langle M^\alpha\, \mathrm{e}^{-\beta H_\Lambda}\big\rangle_\Lambda \;=\; -\frac{1}{\beta}F\big(M^\alpha\big)\,. \tag{3.86b}$$

PROOF. We only show the claims concerning $\widehat{F}$. We show that the right-hand side of (3.84) converges absolutely and uniformly in s. Then (3.86a) follows immediately from the representation (3.83) and (3.84).

The right-hand side of (3.84) is bounded in absolute value by

$$\begin{aligned}
&\sum_{n\geqslant 1}\frac{1}{(n-1)!}\sum_{X_1,\dots,X_n}|\varphi(X_1,\dots,X_n)|\,|\widehat{w}'(X_1)|\prod_{i=2}^{n}|\widehat{w}(X_i)|\\
&=\ \sum_{X_1}|\widehat{w}'(X_1)|\left(1+\sum_{n\geqslant 2}\frac{1}{(n-1)!}\sum_{X_2,\dots,X_n}|\varphi(X_1,\dots,X_n)|\prod_{i=2}^{n}|\widehat{w}(X_i)|\right)\\
&\leqslant\ \sum_{X_1}|\widehat{w}'(X_1)|\,\mathrm{e}^{a|X_1|}\,,
\end{aligned}$$

where in the last step we used Lemma 3.28. Let us therefore estimate

$$\sum_{X}|\widehat{w}'(X)|\,\mathrm{e}^{a|X|}\ \leqslant\ \sum_{X}\mathrm{e}^{a|X|}\sum_{m\geqslant 1}\frac{\beta^m}{(m-1)!}\sum_{\substack{\alpha_1,\dots,\alpha_m\\ X\text{-connected}}}|V'(\alpha_1)|\prod_{i=2}^{m}|V(\alpha_i)|\,.$$

Using $V'(\alpha_1)=\mathbb{1}_{\{\alpha_1=\alpha\}}$ and $|X|\leqslant\|\alpha_1\|+\cdots+\|\alpha_m\|$ we get the bound

$$\begin{aligned}
&\sum_{X}\beta\mathrm{e}^{a\|\alpha\|}\sum_{m\geqslant 1}\frac{\beta^{m-1}}{(m-1)!}\sum_{\substack{\alpha_1,\dots,\alpha_m\\ X\text{-connected}}}\mathbb{1}_{\{\alpha_1=\alpha\}}\prod_{i=2}^{m}V_a(\alpha_i)\\
&\leqslant\ \beta\,\mathrm{e}^{a\|\alpha\|}\sum_{m\geqslant 1}\frac{\beta^{m-1}}{(m-1)!}\sum_{\substack{\alpha_1,\dots,\alpha_m\\ \text{connected}}}\mathbb{1}_{\{\alpha_1=\alpha\}}\prod_{i=2}^{m}V_a(\alpha_i)\\
&=\ \beta\,\mathrm{e}^{a\|\alpha\|}\left(1+\sum_{m\geqslant 2}\frac{\beta^{m-1}}{(m-1)!}\sum_{\substack{\alpha_2,\dots,\alpha_m:\\ \alpha,\alpha_2,\dots,\alpha_n\ \text{connected}}}\prod_{i=2}^{m}V_a(\alpha_i)\right)\\
&\leqslant\ \beta\,\mathrm{e}^{2a\|\alpha\|}\,,
\end{aligned}$$

where in the last step we used Lemma 3.29. □

We may now complete the proof of Theorem 3.23. What remains is to show that

$$\lim_{s\to\infty}\widehat{F}(\,:\widehat{S}^{\alpha}:\,)\ =\ F(M^{\alpha})\,.$$

By Lemma 3.31 and dominated convergence, it suffices to prove that

$$\lim_{s\to\infty}\widehat{w}(X)\ =\ w(X)\,,\qquad \lim_{s\to\infty}\widehat{w}'(X)\ =\ w'(X)\,,$$

for all finite X. We only show the first equality; the proof of the second follows along the same lines. Using (3.10), one readily sees that the sum (3.80) is absolutely convergent, uniformly in s; similarly the sum (3.82) is absolutely convergent. By dominated convergence, it is therefore enough to show that

$$\lim_{s\to\infty}\big\langle\,:\widehat{S}^{\alpha_1}:\,\cdots\,:\widehat{S}^{\alpha_m}:\big\rangle_X\ =\ \big\langle M^{\alpha_1}\cdots M^{\alpha_m}\big\rangle_X\,.$$

But this is (3.65), which we have already proven. Thus the proof of Theorem 3.23 is complete.

3.4. Time-dependent correlation functions of a lattice Bose gas

In this section we consider an interacting Bose gas on a finite lattice Λ, and prove a result analogous to Theorem 3.23. We consider a regime where the density tends to infinity, which corresponds to a mean-field regime.

Throughout this section we work on a fixed, finite subset $\Lambda \subset \mathbb{Z}^d$. As Λ is fixed throughout the following, we systematically omit the subscript Λ.

3.4.1. The lattice Bose gas. The one-particle Hilbert space is

$$\mathcal{H} \; := \; l^2(\Lambda)\,.$$

The n-particle space is the symmetric tensor product

$$\mathcal{H}^{(n)} \; := \; P_+ \mathcal{H}^{\otimes n}\,,$$

where P_+ is the orthogonal projection onto the subspace of symmetric tensors. Vectors in $\mathcal{H}^{(n)}$ are wave functions $\Psi^{(n)}(x_1, \dots, x_n)$ that are symmetric in their arguments $x_1, \dots, x_n \in \Lambda$.

The many-body problem is formulated on the bosonic Fock space $\mathcal{F} \; := \; \bigoplus_{n \geqslant 0} \mathcal{H}^{(n)}$. A vector $\Psi \in \mathcal{F}$ is a sequence $(\Psi^{(n)})_{n \geqslant 0}$, where $\Psi^{(n)} \in \mathcal{H}^{(n)}$. The space $\mathcal{H}^{(0)} \cong \mathbb{C}$ is spanned by a single unit vector, Ω, the vacuum. The Fock space $\mathcal{F}$ is a Hilbert space with scalar product

$$\langle \Psi_1 \,, \Psi_2 \rangle \; = \; \sum_{n \geqslant 0} \sum_{x_1, \dots, x_n \in \Lambda} \overline{\Psi_1^{(n)}(x_1, \dots, x_n)}\, \Psi_2^{(n)}(x_1, \dots, x_n)\,.$$

On $\mathcal{F}$ we have the creation and annihilation operators, $a^*(x)$ and $a(x)$. They are defined by

$$(a^*(x)\Psi)^{(n)}(x_1, \dots, x_n) \; := \; \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \delta(x - x_1) \Psi^{(n-1)}(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)\,,$$

where $\delta(x) := \mathbb{1}_{\{x=0\}}$ is the discrete delta function; also,

$$(a(x)\Psi)^{(n)}(x_1, \dots, x_n) \; := \; \sqrt{n+1}\, \Psi^{(n+1)}(x, x_1, \dots, x_n)\,.$$

It is not hard to check that $a^*(x)$ and $a(x)$ are both closable and each other's adjoints (see e.g. [BR02]). Moreover, they satisfy the canonical commutation relations

$$[a(x) \,, a^*(y)] \; = \; \delta(x - y)\,, \qquad [a(x) \,, a(y)] \; = \; [a^*(x) \,, a^*(y)] \; = \; 0\,.$$

In the following the notation is somewhat streamlined by introducing the rescaled creation and annihilation operators

$$a_N^*(x) \; := \; \frac{1}{\sqrt{N}}\, a^*(x)\,, \qquad a_N(x) \; := \; \frac{1}{\sqrt{N}}\, a(x)\,,$$

where $N > 0$. They satisfy the commutation relations

$$[a_N(x) \,, a_N^*(y)] \; = \; \frac{1}{N}\, \delta(x - y)\,, \qquad [a_N(x) \,, a_N(y)] \; = \; [a_N^*(x) \,, a_N^*(y)] \; = \; 0\,. \tag{3.87}$$

Let $p \in \mathbb{N}$ and $b^{(p)} \in \mathcal{L}(\mathcal{H}^{(p)})$ be a p-particle operator, with kernel $b^{(p)}(x_1, \dots, x_p; y_1, \dots, y_p)$. Define its second quantization

$$\widehat{\mathrm{A}}_N(b^{(p)}) \;:=\; \sum_{x_1,\dots,x_p} \sum_{y_1,\dots,y_p} b^{(p)}(x_1, \dots, x_p; y_1, \dots, y_p)\, a_N^*(x_1) \cdots a_N^*(x_p) a_N(y_1) \cdots a_N(y_p)\,.$$

It is easy to check that $\widehat{\mathrm{A}}_N(b^{(p)})$ is a closable operator on $\mathcal{F}$, whose action on the n-particle sector is given by

$$\widehat{\mathrm{A}}_N(b^{(p)})\big|_{\mathcal{H}^{(n)}} \;=\; \begin{cases} \frac{p!}{N^p}\binom{n}{p} P_+\big(b^{(p)} \otimes \mathbb{1}^{(n-p)}\big) P_+ & \text{if } n \geqslant p \\ 0 & \text{otherwise}\,. \end{cases} \tag{3.88}$$

The operation $\widehat{\mathrm{A}}_N(\cdot)$ has the following important properties whose simple proofs we omit.

(i) If $b^{(p)} \in \mathcal{L}(\mathcal{H}^{(p)})$ and $c^{(q)} \in \mathcal{L}(\mathcal{H}^{(q)})$, then

$$\widehat{\mathrm{A}}_N(b^{(p)})\, \widehat{\mathrm{A}}_N(c^{(q)}) \;=\; \sum_r \binom{p}{r}\binom{q}{r} \frac{r!}{N^r}\, \widehat{\mathrm{A}}_N\big(b^{(p)} \bullet_r c^{(q)}\big)\,, \tag{3.89}$$

where

$$b^{(p)} \bullet_r c^{(q)} \;:=\; P_+\,(b^{(p)} \otimes \mathbb{1}^{(q-r)})\,(\mathbb{1}^{(p-r)} \otimes c^{(q)})\,P_+ \;\in\; \mathcal{L}(\mathcal{H}^{(p+q-r)})\,. \tag{3.90}$$

Here we adopt the convention that $\binom{n}{k} = 0$ for $k \notin \{0, \dots, n\}$.

(ii) The operator $\widehat{\mathrm{A}}_N(b^{(p)})$ leaves the n-particle subspaces $\mathcal{H}_\pm^{(n)}$ invariant.

(ii) If $b^{(p)} \in \mathcal{L}(\mathcal{H}^{(p)})$ then

$$\Big\|\widehat{\mathrm{A}}_N(b^{(p)})\big|_{\mathcal{H}^{(n)}}\Big\| \;\leqslant\; \left(\frac{n}{N}\right)^p \|b^{(p)}\|\,. \tag{3.91}$$

We introduce the notation

$$\big[b^{(p)}, c^{(q)}\big]_r \;:=\; b^{(p)} \bullet_r c^{(q)} - c^{(q)} \bullet_r b^{(p)}\,. \tag{3.92}$$

Note that $\big[b^{(p)}, c^{(q)}\big]_0 = 0$. Thus,

$$\big[\widehat{\mathrm{A}}_N(b^{(p)}), \widehat{\mathrm{A}}_N(c^{(q)})\big] \;=\; \sum_{r \geqslant 1} \binom{p}{r}\binom{q}{r} \frac{r!}{N^r}\, \widehat{\mathrm{A}}_N\big(\big[b^{(p)}, c^{(q)}\big]_r\big)\,. \tag{3.93}$$

Next, we discuss the dynamics. As we are interested in the large-density limit of the Bose gas, it is of some interest to consider a Hamiltonian with many-body interactions. Consider a family $V = \big(V^{(k)}\big)_{k \geqslant 1}$ of self-adjoint operators with $V^{(k)} \in \mathcal{L}(\mathcal{H}^{(k)})$. Define a Hamiltonian through

$$\widehat{H}_N \;:=\; \sum_{k \geqslant 1} \frac{1}{k!}\, \widehat{\mathrm{A}}_N\big(V^{(k)}\big)\,. \tag{3.94}$$

We impose the condition

$$\|V\|_r \;:=\; \sum_{k \geqslant 1} \mathrm{e}^{rk}\, \big\|V^{(k)}\big\| \;<\; \infty\,, \tag{3.95}$$

for all $r > 0$.

Using Nelson's analytic vector theorem (see e.g. [RS75]) on the set of vectors of finite particle number, it is not hard to see that $\widehat{H}_N$ is self-adjoint on $\mathcal{F}$. The quantum time evolution of observables is defined by

$$\widehat{\tau}^t \mathbf{A} \;:=\; \mathrm{e}^{\mathrm{i}N\widehat{H}_N t}\, \mathbf{A}\, \mathrm{e}^{-\mathrm{i}N\widehat{H}_N t}\,.$$

3.4.2. The classical lattice gas. The theory of a classical gas on the finite lattice Λ is formulated on the phase space

$$\Gamma \;:=\; l^2(\Lambda)\,,$$

whose points we denote by α. We denote by $\|\alpha\|$ the l^2-norm of α. The symplectic form on Γ is given by

$$w \;=\; \mathrm{i}\sum_{x\in\Lambda} \mathrm{d}\overline{\alpha}(x)\wedge \mathrm{d}\alpha(x)\,,$$

which yields the Poisson bracket

$$\{\alpha(x)\,,\overline{\alpha}(y)\} \;=\; \mathrm{i}\delta(x-y)\,,\qquad \{\alpha(x)\,,\alpha(y)\} \;=\; \{\overline{\alpha}(x)\,,\overline{\alpha}(y)\} \;=\; 0\,.$$

In analogy to the second quantization $\widehat{\mathrm{A}}_N$, we define the function $\mathrm{A}(b^{(p)}) \,:\, \Gamma\to\mathbb{C}$ through

$$\mathrm{A}(b^{(p)})(\alpha) \;:=\; \sum_{x_1,\dots,x_p}\sum_{y_1,\dots,y_p} b^{(p)}(x_1,\dots,x_p;y_1,\dots,y_p)\overline{\alpha}(x_1)\cdots\overline{\alpha}(x_p)\alpha(y_1)\cdots\alpha(y_p)\,.$$

We record the following properties of A.

(i) If $b^{(p)}\in\mathcal{L}(\mathcal{H}^{(p)})$ and $c^{(q)}\in\mathcal{L}(\mathcal{H}^{(q)})$ then

$$\big\{\mathrm{A}(b^{(p)})\,,\mathrm{A}(c^{(q)})\big\} \;=\; \mathrm{i}pq\mathrm{A}\big(\big[b^{(p)}\,,c^{(q)}\big]_1\big)\,. \tag{3.96}$$

(ii) If $b^{(p)}\in\mathcal{L}(\mathcal{H}^{(p)})$ then

$$\big|\mathrm{A}(b^{(p)})(\alpha)\big| \;\leqslant\; \|b^{(p)}\|\|\alpha\|^{2p}\,. \tag{3.97}$$

The dynamics is generated by the Hamilton function

$$H \;:=\; \sum_{k\geqslant 1}\frac{1}{k!}\mathrm{A}(V^{(k)})\,.$$

The Hamiltonian equation of motion,

$$\mathrm{i}\partial_t\alpha \;=\; \partial_{\overline{\alpha}}H(\alpha)\,, \tag{3.98}$$

has a globally well-defined solution for all initial data, as one easily sees using a standard contraction mapping argument. (We omit further details; see also Lemma 3.36, whose proof by expansion also yields a proof of the well-posedness of (3.98).) Moreover, it is easy to see that $\|\alpha\|$ is conserved under time evolution.

For a function $A(\alpha)$ on Γ we abbreviate

$$(\tau^t A)(\alpha) \;:=\; A(\alpha(t))\,,$$

where $\alpha(t)$ is the solution of (3.98) with initial data α.

3.4.3. Main result. We start with some notation. For a function A on Γ we set

$$\langle A \rangle \; := \; \frac{1}{\pi^{|\Lambda|}} \int_\Gamma \mathrm{d}\alpha \; A(\alpha) \,,$$

where $\mathrm{d}\alpha := \prod_{x \in \Lambda} \mathrm{d}(\operatorname{Re} \alpha(x)) \, \mathrm{d}(\operatorname{Im} \alpha(x))$. Similarly, for an operator $\mathbf{A} \in \mathcal{L}^1(\mathcal{F})$ we set

$$\langle \mathbf{A} \rangle \; := \; \frac{1}{N^{|\Lambda|}} \operatorname{Tr} \mathbf{A} \,.$$

Assume that H and $\widehat{H}_N$ are nonnegative, for all $N > 0$. Denote by $\mathcal{N}$ the function $\mathcal{N}(\alpha) \; := \; \sum_{x \in \Lambda} |\alpha(x)|^2$. Similarly, define the rescaled particle number operator $\widehat{\mathcal{N}}_N \; := \; \sum_{x \in \Lambda} a_N^*(x) a_N(x)$.

Let $\beta > 0$, $0 < z < 1$ and $t_1, \dots, t_n \in \mathbb{R}$. Moreover, let $p_1, \dots, p_n \in \mathbb{N}$ and $b_i \in \mathcal{H}^{(p_i)}$ for $i = 1, \dots, n$. Then we define the time-dependent correlation function of the classical lattice gas, at inverse temperature β and fugacity z, through

$$\rho_{\beta,z}\big((b_i, t_i)_{i=1}^n\big) \; := \; \frac{1}{Z_{\beta,z}} \Big\langle \big(\tau^{t_1} \mathrm{A}(b_1)\big) \cdots \big(\tau^{t_n} \mathrm{A}(b_n)\big) \, \mathrm{e}^{-\beta H} z^{\mathcal{N}} \Big\rangle \,, \tag{3.99}$$

where

$$Z_{\beta,z} \; := \; \big\langle \mathrm{e}^{-\beta H} z^{\mathcal{N}} \big\rangle$$

is the classical partition function. Similarly, we define the time-dependent correlation function of the quantum Bose gas, at inverse temperature β and fugacity z, through

$$\widehat{\rho}^{N}_{\beta,z}\big((b_i, t_i)_{i=1}^n\big) \; := \; \frac{1}{\widehat{Z}^N_{\beta,z}} \Big\langle \big(\widehat{\tau}^{t_1} \widehat{\mathrm{A}}_N(b_1)\big) \cdots \big(\widehat{\tau}^{t_n} \widehat{\mathrm{A}}_N(b_n)\big) \, \mathrm{e}^{-\beta \widehat{H}_N} z^{\widehat{\mathcal{N}}_N} \Big\rangle \,, \tag{3.100}$$

where

$$\widehat{Z}^N_{\beta,z} \; := \; \big\langle \mathrm{e}^{-\beta \widehat{H}_N} z^{\widehat{\mathcal{N}}_N} \big\rangle$$

is the quantum partition function.

We may now state our main result.

THEOREM 3.32. *Let $\Lambda \subset \mathbb{Z}^d$ be finite. Let $\beta > 0$, $0 < z < 1$ and $t_1, \dots, t_n \in \mathbb{R}$. Moreover, let $p_1, \dots, p_n \in \mathbb{N}$ and $b_i \in \mathcal{H}^{(p_i)}$ for $i = 1, \dots, n$. Then we have*

$$\lim_{N \to \infty} \widehat{\rho}^N_{\beta,z}\big((b_i, t_i)_{i=1}^n\big) \; = \; \rho_{\beta,z}\big((b_i, t_i)_{i=1}^n\big) \,.$$

REMARK 3.33. *This is a result on the mean-field limit of the quantum Bose gas, in a regime where the density of particles grows like N. Indeed, for large N the state*

$$\mathbf{A} \; \longmapsto \; \frac{1}{\widehat{Z}^N_{\beta,z}} \big\langle \mathbf{A} \, \mathrm{e}^{-\beta \widehat{H}_N} z^{\widehat{\mathcal{N}}_N} \big\rangle$$

has an expected number of particles proportional to N. This is an immediate corollary of Theorem 3.32: The rescaled particle number operator $\widehat{\mathcal{N}}_N = N^{-1} \sum_{x \in \Lambda} a^*(x) a(x)$ has expectation of order one. Heuristically, this behaviour is already apparent in the case $\widehat{H}_N = 0$ and $|\Lambda| = 1$, where the expected number of particles is given by

$$\frac{\sum_{n \geqslant 0} n z^{n/N}}{\sum_{n \geqslant 0} z^{n/N}} \; = \; \frac{1}{z^{-1/N} - 1} \; = \; \frac{1}{-\log z} N + O(1) \,.$$

REMARK 3.34. *By the previous remark, the typical configuration in the above state has $n \sim N$ particles. Thus,* (3.88) *implies that the expectation of $\widehat{A}_N(b^{(p)})$ is of order one for all $b^{(p)} \in \mathcal{H}^{(p)}$. In particular, all terms of the Hamiltonian $\widehat{H}_N$ have expectation of order one.*

EXAMPLE 3.35. *Consider $V^{(1)} = -\Delta + v(x)$, where Δ is the discrete Laplacian (with arbitrary boundary conditions) and v is some external potential. Set furthermore $V^{(2)} = w(x_1 - x_2)$, where the interaction potential w is an even function. Set $V^{(k)} = 0$ for $k \geqslant 3$. This describes a lattice Bose gas with two-body interactions. The classical equation of motion is*

$$\mathrm{i}\partial_t \alpha(x) = (-\Delta + v(x))\alpha(x) + \sum_{y \in \Lambda} w(x-y)|\alpha(y)|^2 \alpha(x)\,,$$

the discrete Hartree equation.

3.4.4. Proof of Theorem 3.32.

Preliminaries. We start with some notation. For $n \in \mathbb{N}$ write

$$\mathcal{H}^{(\leqslant n)} \;:=\; \bigoplus_{i=0}^{n} \mathcal{H}^{(i)}\,.$$

Also, for $\zeta > 0$ define the ball

$$B_\zeta \;:=\; \big\{\alpha \in \Gamma \,:\, \|\alpha\|^2 \leqslant \zeta\big\}\,.$$

We control the time evolution with a Schwinger-Dyson-type expansion.

LEMMA 3.36. *Let $\varepsilon > 0$, $t \in \mathbb{R}$, $\zeta > 0$ and $b^{(p)} \in \mathcal{H}^{(p)}$ for some $p \in \mathbb{N}$. Then there exists an $L \in \mathbb{N}$ and a finite sequence $(e^{(l)})_{l=0}^{L}$, where $e^{(l)} \in \mathcal{H}^{(l)}$, such that*

$$\bigg\|\tau^t \mathrm{A}(b^{(p)}) - \sum_{l=0}^{L} \mathrm{A}(e^{(l)})\bigg\|_{L^\infty(B_\zeta)} \;\leqslant\; \varepsilon\,, \tag{3.101a}$$

$$\bigg\|\bigg(\widehat{\tau}^t \widehat{\mathrm{A}}_N(b^{(p)}) - \sum_{l=0}^{L} \widehat{\mathrm{A}}_N(e^{(l)})\bigg)\bigg|_{\mathcal{H}^{(\leqslant \zeta N)}}\bigg\| \;\leqslant\; \varepsilon\,, \tag{3.101b}$$

for all N large enough.

PROOF. We use a "one-loop" expansion for the quantum evolution. The fundamental theorem of calculus yields

$$\begin{aligned}
\widehat{\tau}^t \widehat{\mathrm{A}}_N(b^{(p)}) \;&=\; \widehat{\mathrm{A}}_N(b^{(p)}) + \int_0^t \mathrm{d}s\; \mathrm{e}^{\mathrm{i}sN\widehat{H}_N}\, \mathrm{i}N\big[\widehat{H}_N\,, \widehat{\mathrm{A}}_N(b^{(p)})\big]\, \mathrm{e}^{-\mathrm{i}sN\widehat{H}_N} \\
&=\; \widehat{\mathrm{A}}_N(b^{(p)}) + \sum_{k \geqslant 1} \frac{1}{k!} \int_0^t \mathrm{d}s\; \mathrm{e}^{\mathrm{i}sN\widehat{H}_N}\, \mathrm{i}N\big[\widehat{\mathrm{A}}_N(V^{(k)}), \widehat{\mathrm{A}}_N(b^{(p)})\big]\, \mathrm{e}^{-\mathrm{i}sN\widehat{H}_N} \\
&=\; \widehat{\mathrm{A}}_N(b^{(p)}) + \sum_{k \geqslant 1} \frac{1}{k!} \int_0^t \mathrm{d}s\; \mathrm{i}kp\, \widehat{\tau}^s \widehat{A}_N\big(\big[V^{(k)}, b^{(p)}\big]_1\big) \\
&\qquad + \sum_{k \geqslant 1} \frac{1}{k!} \sum_{r \geqslant 2} \int_0^t \mathrm{d}s\; \frac{\mathrm{i}}{N^{r-1}} \binom{k}{r} \binom{p}{r} r!\, \widehat{\tau}^s \widehat{A}_N\big(\big[V^{(k)}, b^{(p)}\big]_r\big)\,,
\end{aligned} \tag{3.102}$$

where the last step follows from (3.93). We now iterate this identity by applying it to the second term on the right-hand side. This gives the series expansion

$$\widehat{\tau}^t \widehat{\mathrm{A}}_N(b^{(p)}) \;=\; \widehat{T}^t_N(b^{(p)}) + \widehat{L}^t_N(b^{(p)}) \,,$$

where

$$\begin{aligned}\widehat{T}^t_N(b^{(p)}) \;:=\; &\sum_{l\geqslant 0} \frac{t^l}{l!} \sum_{k_1\geqslant 1} \frac{1}{k_1!} \cdots \sum_{k_l\geqslant 1} \frac{1}{k_l!} k_1 \cdots k_l \\ &\times \mathrm{i}^l p(p+k_1-1)\cdots\big(p+(k_1-1)+\cdots+(k_{l-1}-1)\big)\, \widehat{A}_N\big(\big[V^{(k_l)},\dots \big[V^{(k_1)},b^{(p)}\big]_1\cdots\big]_1\big)\,,\end{aligned} \tag{3.103}$$

and

$$\begin{aligned}\widehat{L}^t_N(b^{(p)}) \;:=\; &\sum_{l\geqslant 1}\sum_{k_1\geqslant 1} \frac{1}{k_1!} \cdots \sum_{k_l\geqslant 1} \frac{1}{k_l!} \sum_{r\geqslant 2} \int_0^t \mathrm{d}s_1 \cdots \int_0^{s_{l-1}} \mathrm{d}s_l \; k_1\cdots k_{l-1} \frac{1}{N^{r-1}} \\ \times \mathrm{i}^l p(p+k_1-1)\cdots\big(p+(k_1-1)&+\cdots+(k_{l-2}-1)\big) \binom{k_l}{r}\binom{p+(k_1-1)+\cdots+(k_{l-1}-1)}{r} r! \\ &\times \widehat{\tau}^{s_l}\widehat{A}_N\big(\big[V^{(k_l)},\big[V^{(k_{l-1})},\dots\big[V^{(k_1)},b^{(p)}\big]_1\cdots\big]_1\big]_r\big)\,,\end{aligned} \tag{3.104}$$

where the term $l=1$ is understood to be the last line of (3.102). To simplify presentation, we do not consider the rest term arising from a finite number of iterations; the following estimates showing the convergence of (3.103) and (3.104), together with the fact that the time evolutions are norm-preserving, also imply that the rest terms vanish.

In order to estimate the sums in (3.103) and (3.104) on the space $\mathcal{H}^{(\leqslant \zeta N)}$, assume without loss of generality that $\zeta \geqslant 1$. Then, using (3.91), we find that the right-hand side of (3.103) is bounded by

$$\begin{aligned}&\sum_{l\geqslant 0}|t|^l \sum_{k_1\geqslant 1}\frac{1}{(k_1-1)!}\cdots\sum_{k_l\geqslant 1}\frac{1}{(k_l-1)!}\frac{(p+k_1+\cdots+k_l)^l}{l!}\, 2^l\, \zeta^{p+k_1+\cdots+k_l}\, \|V^{(k_1)}\|\cdots\|V^{(k_l)}\|\|b^{(p)}\| \\ &\qquad\leqslant\; \mathrm{e}^p\zeta^p\|b^{(p)}\|\sum_{l\geqslant 0}|t|^l 2^l\Bigg(\sum_{k\geqslant 1}\frac{1}{(k-1)!}\mathrm{e}^k\zeta^k\|V^{(k)}\|\Bigg)^l\,.\end{aligned} \tag{3.105}$$

By assumption, the quantity in parentheses is finite, so that the sum converges for $|t|$ small enough. Similarly, we estimate the right-hand side of (3.104), restricted to the space $\mathcal{H}^{(\leqslant \zeta N)}$. Since $\widehat{\tau}^t$ preserves the operator norm, we get the bound

$$\begin{aligned}&\frac{1}{N}\sum_{l\geqslant 1}\frac{|t|^l}{l!}\sum_{k_1\geqslant 1}\frac{1}{(k_1-1)!}\cdots\sum_{k_{l-1}\geqslant 1}\frac{1}{(k_{l-1}-1)!}\sum_{k_l\geqslant 1}\frac{1}{k_l!}\,(p+k_1+\cdots+k_l)^l \\ &\times\sum_{r\geqslant 2}\binom{k_l}{r}\binom{p+k_1+\cdots+k_l}{r} r!\, 2^l\, \|V^{(k_1)}\|\cdots\|V^{(k_l)}\|\|b^{(p)}\|\,\zeta^{p+k_1+\cdots+k_l} \\ \leqslant\; &\frac{1}{N}\sum_{l\geqslant 1}|t|^l\sum_{k_1\geqslant 1}\frac{1}{(k_1-1)!}\cdots\sum_{k_{l-1}\geqslant 1}\frac{1}{(k_{l-1}-1)!}\sum_{k_l\geqslant 1}\mathrm{e}^{p+k_1+\cdots+k_l} \\ &\times 2^{k_l}2^{p+k_1+\cdots+k_l}\,2^l\,\|V^{(k_1)}\|\cdots\|V^{(k_l)}\|\|b^{(p)}\|\,\zeta^{p+k_1+\cdots+k_l}\,,\end{aligned}$$

where we used $r \leqslant k_l$ and $\sum_r \binom{n}{r} = 2^n$. Thus we get the bound

$$\frac{1}{N} \mathrm{e}^p 2^p \zeta^p \|b^{(p)}\| \sum_{l \geqslant 1} |t|^l \left(\sum_{k \geqslant 1} \frac{1}{(k-1)!} \mathrm{e}^k 2^k \zeta^k \|V^{(k)}\| \right)^{l-1} \left(\sum_{k \geqslant 1} \mathrm{e}^k 4^k \zeta^k \|V\|^{(k)} \right). \tag{3.106}$$

By assumption, both terms in parentheses are finite, and the series converges for small t. Thus all series converge if $|t| < \rho(\zeta)$, for some positive convergence radius $\rho(\zeta)$. Let us assume that $|t| < \rho(\zeta)$ and introduce a cutoff $l \leqslant L$ in the series (3.103) such that the corresponding tail in (3.105) is bounded by $\varepsilon/2$. Choosing N large enough that (3.106) is bounded by $\varepsilon/2$ yields the claim (3.101b)

For $|t| < \rho(\zeta)$, the classical Schwinger-Dyson expansion (3.101a) is shown similarly. Iterating

$$\tau^t \mathrm{A}(b^{(p)}) \;=\; \mathrm{A}(b^{(p)}) + \int_0^t \mathrm{d}s \, \tau^s \{H, \mathrm{A}(b^{(p)})\}$$

and recalling (3.96), we find

$$\begin{aligned} \tau^t \mathrm{A}(b^{(p)}) \;=\; & \sum_{l \geqslant 0} \frac{t^l}{l!} \sum_{k_1 \geqslant 1} \frac{1}{k_1!} \cdots \sum_{k_l \geqslant 1} \frac{1}{k_l!} k_1 \cdots k_l \\ & \times \mathrm{i}^l p(p + k_1 - 1) \cdots \big(p + (k_1 - 1) + \cdots + (k_{l-1} - 1)\big) \, A\big(\big[V^{(k_l)}, \ldots \big[V^{(k_1)}, b^{(p)}\big]_1 \cdots\big]_1\big). \end{aligned}$$

Using (3.97) and the estimate (3.105), we see that this series converges in $L^\infty(B_\zeta)$ provided that $|t| < \rho(\zeta)$. Therefore (3.101a) is proven for small times.

The extension to arbitrary times is done by iteration, as in the proof of Lemma 3.6. One uses norm conservation, $\|\widehat{\tau}^t \mathbf{A}|_{\mathcal{H}(\leqslant \zeta N)}\| = \|\mathbf{A}|_{\mathcal{H}(\leqslant \zeta N)}\|$ and $\|\tau^t A\|_{L^\infty(B_\zeta)} = \|A\|_{L^\infty(B_\zeta)}$, as well as the fact that the convergence radius $\rho(\zeta)$ is independent of p. We omit the uninteresting details. $\square$

Next, we introduce and recall the key properties of two convenient families of basis vectors. Let $n = (n(x))_{x \in \Lambda}$ be a family of nonnegative integers. Define the occupation number state

$$B_n \;:=\; \prod_{x \in \Lambda} \frac{1}{\sqrt{n(x)!}} \big(a^*(x)\big)^{n(x)} \, \Omega\,. \tag{3.107}$$

It is not hard to see that $\{B_n\}_{n \in \mathbb{N}^\Lambda}$ is an orthonormal basis of $\mathcal{F}$. It satisfies

$$\widehat{\mathcal{N}}_N B_n \;=\; \frac{\|n\|_1}{N} B_n\,, \tag{3.108}$$

where

$$\|n\|_1 \;:=\; \sum_{x \in \Lambda} n(x)\,.$$

Coherent states are another useful family of vectors; we refer to [Gla63] for proofs and details. For $\alpha \in \Gamma$ define $a(\alpha) := \sum_{x \in \Lambda} \overline{\alpha}(x) a(x)$; $a^*(\alpha)$ is the adjoint of $a(\alpha)$. Define the coherent state

$$W_\alpha \;:=\; \mathrm{e}^{a^*(\alpha) - a(\alpha)} \, \Omega \;=\; \mathrm{e}^{-\|\alpha\|^2/2} \mathrm{e}^{a^*(\alpha)} \, \Omega\,.$$

Coherent states form a complete set in $\mathcal{F}$ in the sense that

$$\frac{1}{\pi^{|\Lambda|}} \int_\Gamma \mathrm{d}\alpha \, |W_\alpha\rangle\langle W_\alpha| \;=\; \mathbb{1}\,,$$

where, we recall, $\mathrm{d}\alpha := \prod_{x\in\Lambda} \mathrm{d}(\operatorname{Re}\alpha(x))\,\mathrm{d}(\operatorname{Im}\alpha(x))$. In particular,

$$\operatorname{Tr}\mathbf{A} \;=\; \frac{1}{\pi^{|\Lambda|}}\int_\Gamma \mathrm{d}\alpha\;\langle W_\alpha\,,\mathbf{A}W_\alpha\rangle\,. \tag{3.109}$$

Coherent states also have the property

$$a(x)W_\alpha \;=\; \alpha(x)W_\alpha\,. \tag{3.110}$$

Finally, we have

$$\langle B_n\,,W_\alpha\rangle \;=\; \mathrm{e}^{-\|\alpha\|^2/2}\prod_{x\in\Lambda}\frac{\alpha(x)^{n(x)}}{\sqrt{n(x)!}}\,. \tag{3.111}$$

Proof of convergence. We now have all the necessary tools to prove Theorem 3.32. Clearly, it suffices to show

$$\lim_{N\to\infty}\Big\langle\big(\widehat{\tau}^{t_1}\widehat{\mathrm{A}}_N(b_1)\big)\cdots\big(\widehat{\tau}^{t_n}\widehat{\mathrm{A}}_N(b_n)\big)\,\mathrm{e}^{-\beta\widehat{H}_N}z^{\widehat{\mathcal{N}}_N}\Big\rangle \;=\; \Big\langle\big(\tau^{t_1}\mathrm{A}(b_1)\big)\cdots\big(\tau^{t_n}\mathrm{A}(b_n)\big)\,\mathrm{e}^{-\beta H}z^{\mathcal{N}}\Big\rangle\,. \tag{3.112}$$

Let $\varepsilon>0$. We begin by introducing a cutoff of order ζ in the rescaled number of particles. To this end, let χ be a continuous function on $\mathbb{R}$ satisfying $\chi(x)\in[0,1]$, $\chi(x)=1$ for $x\leqslant 1/2$ and $\chi(x)=0$ for $x\geqslant 1$. Set $\overline{\chi}:=1-\chi$.

LEMMA 3.37. *There is a $\zeta>0$ such that*

$$\Big|\Big\langle\big(\tau^{t_1}\mathrm{A}(b_1)\big)\cdots\big(\tau^{t_n}\mathrm{A}(b_n)\big)\,\mathrm{e}^{-\beta H}z^{\mathcal{N}}\overline{\chi}(\mathcal{N}/\zeta)\Big\rangle\Big| \;\leqslant\; \varepsilon\,, \tag{3.113a}$$

$$\Big|\Big\langle\big(\widehat{\tau}^{t_1}\widehat{\mathrm{A}}_N(b_1)\big)\cdots\big(\widehat{\tau}^{t_n}\widehat{\mathrm{A}}_N(b_n)\big)\,\mathrm{e}^{-\beta\widehat{H}_N}z^{\widehat{\mathcal{N}}_N}\overline{\chi}(\widehat{\mathcal{N}}_N/\zeta)\Big\rangle\Big| \;\leqslant\; \varepsilon\,, \tag{3.113b}$$

for all N.

PROOF. Let us start with (3.113b). Since $\widehat{H}_N$ and b_i are gauge invariant (i.e. they commute with $\widehat{\mathcal{N}}_N$), we find that the left-hand side of (3.113b) is equal to

$$\Big|\Big\langle\widehat{\tau}^{t_1}\big((\mathbb{1}+\widehat{\mathcal{N}}_N)^{-p_1}\widehat{\mathrm{A}}_N(b_1)\big)\cdots\widehat{\tau}^{t_n}\big((\mathbb{1}+\widehat{\mathcal{N}}_N)^{-p_n}\widehat{\mathrm{A}}_N(b_n)\big) \\ \times\,\mathrm{e}_N^{-\beta\widehat{H}}\big(\mathbb{1}+\widehat{\mathcal{N}}_N\big)^{p_1+\cdots+p_n}z^{\widehat{\mathcal{N}}_N}\overline{\chi}(\widehat{\mathcal{N}}_N/\zeta)\Big\rangle\Big|\,.$$

Note that (3.88) implies

$$\big\|(\mathbb{1}+\widehat{\mathcal{N}}_N)^{-p_i}\widehat{\mathrm{A}}_N(b_i)\big\| \;\leqslant\; \|b_i\|$$

for $i=1,\dots,n$. Recall also the inequality $\operatorname{Tr}(\mathbf{AB})\leqslant\|\mathbf{A}\|\|\mathbf{B}\|_1$. Since $\widehat{\tau}^t$ preserves the operator norm we therefore get the bound

$$\|b_1\|\cdots\|b_n\|\frac{1}{N^{|\Lambda|}}\operatorname{Tr}\Big|\big(\mathbb{1}+\widehat{\mathcal{N}}_N\big)^{p_1+\cdots+p_n}z^{\widehat{\mathcal{N}}_N}\overline{\chi}(\widehat{\mathcal{N}}_N/\zeta)\Big| \\ =\; \|b_1\|\cdots\|b_n\|\frac{1}{N^{|\Lambda|}}\operatorname{Tr}\Big(\big(\mathbb{1}+\widehat{\mathcal{N}}_N\big)^{p_1+\cdots+p_n}z^{\widehat{\mathcal{N}}_N}\overline{\chi}(\widehat{\mathcal{N}}_N/\zeta)\Big)\,.$$

Let us abbreviate

$$f_\zeta(\lambda) \;:=\; (1+\lambda)^{p_1+\cdots+p_n}\,z^\lambda\,\overline{\chi}(\lambda/\zeta)\,.$$

Thus we need a bound on

$$S_N(\zeta) \;:=\; \frac{1}{N^{|\Lambda|}}\operatorname{Tr}f_\zeta(\widehat{\mathcal{N}}_N) \;=\; \sum_{n\in\mathbb{N}^\Lambda}\frac{1}{N^{|\Lambda|}}f_\zeta(\|n\|_1/N)\,,$$

where we used the basis (3.107) for computing the trace. Then (3.113b) follows if we can show that $\lim_{\zeta\to\infty} S_N(\zeta) = 0$ uniformly in N. We do this by showing that, for all $\zeta > 0$, we have

$$\lim_{N\to\infty} S_N(\zeta) \;=\; S_\infty(\zeta) \;:=\; \int_0^\infty \cdots \int_0^\infty \prod_{x\in\Lambda} \mathrm{d}u(x)\; f_\zeta(\|u\|_1)\,, \tag{3.114}$$

where $u = (u(x))_{x\in\Lambda}$ and $\|u\|_1 = \sum_{x\in\Lambda}|u(x)|$. Thus, since clearly $\lim_{\zeta\to\infty} S_\infty(\zeta) = 0$, we find that (3.114) implies (3.113b).

In order to show (3.114) we note that $S_N(\zeta)$ is a Riemann sum with mesh size N^{-1}. The somewhat delicate convergence of a Riemann sum on an infinite domain may in our case be easily dealt with by using the fact that f_ζ is monotone nonincreasing for large enough arguments. For $u = (u(x))_{x\in\Lambda}$ define $[u]_N = ([u]_N(x))_{x\in\Lambda}$ by setting $[u]_N(x)$ equal to the integer multiple of N^{-1} nearest to $u(x)$. Thus,

$$S_N(\zeta) \;=\; \int_0^\infty \cdots \int_0^\infty \prod_{x\in\Lambda} \mathrm{d}u(x)\; f_\zeta(\|[u]_N\|_1)\,.$$

Since clearly $f_\zeta(\|[u]_N\|_1) \to f_\zeta(\|u\|_1)$ pointwise, (3.114) follows by dominated convergence if we can find a function g such that $f_\zeta(\|[u]_N\|_1) \leqslant g(\|u\|_1)$ for large enough N, and $u \mapsto g(\|u\|_1)$ is integrable. Choose $\kappa > 0$ large enough that $f_\zeta(\lambda)$ is nonincreasing on $[\kappa-1,\infty)$ and set

$$g(\lambda) \;:=\; \begin{cases} \sup_{[0,\kappa]} f_\zeta & \text{if } \lambda \leqslant \kappa \\ f_\zeta(\lambda-1) & \text{if } \lambda > \kappa\,. \end{cases}$$

It is easy to see that g has the desired properties. Hence the proof of (3.113b) is complete.

The proof of (3.113a) is similar to (in fact easier than) the proof of (3.113b). The claim follows from $\lim_{\zeta\to\infty} S_\infty(\zeta) = 0$. ☐

By Lemma 3.37, Theorem 3.32 follows if we can prove

$$\begin{aligned}\lim_{N\to\infty} \Big\langle \big(\widehat{\tau}^{t_1}\widehat{\mathrm{A}}_N(b_1)\big)\cdots\big(\widehat{\tau}^{t_n}\widehat{\mathrm{A}}_N(b_n)\big)\,\mathrm{e}^{-\beta\widehat{H}_N}\, z^{\widehat{\mathcal{N}}_N}\chi(\widehat{\mathcal{N}}_N/\zeta)\Big\rangle \\ = \Big\langle \big(\tau^{t_1}\mathrm{A}(b_1)\big)\cdots\big(\tau^{t_n}\mathrm{A}(b_n)\big)\,\mathrm{e}^{-\beta H}\, z^{\mathcal{N}}\chi(\mathcal{N}/\zeta)\Big\rangle \end{aligned} \tag{3.115}$$

for arbitrary $\zeta > 0$. Let us consider the left-hand side of (3.115). Since $\chi(\widehat{\mathcal{N}}_N/\zeta)$ commutes with all other factors, we may use Lemma 3.36 to expand the factors $\widehat{\tau}^{t_i}\widehat{\mathrm{A}}_N(b_i)$ to get, just like in Section 3.3.2,

$$\begin{aligned}&\Big\langle \big(\widehat{\tau}^{t_1}\widehat{\mathrm{A}}_N(b_1)\big)\cdots\big(\widehat{\tau}^{t_n}\widehat{\mathrm{A}}_N(b_n)\big)\,\mathrm{e}^{-\beta\widehat{H}_N}\, z^{\widehat{\mathcal{N}}_N}\chi(\widehat{\mathcal{N}}_N/\zeta)\Big\rangle \\ &\qquad = \sum_{l_1=0}^{L_1}\cdots\sum_{l_n=0}^{L_n} \Big\langle \widehat{\mathrm{A}}_N(e_1^{(l_1)})\cdots\widehat{\mathrm{A}}_N(e_n^{(l_n)})\,\mathrm{e}^{-\beta\widehat{H}_N}\, z^{\widehat{\mathcal{N}}_N}\,\chi(\widehat{\mathcal{N}}_N/\zeta)\Big\rangle + R_N\,, \end{aligned} \tag{3.116}$$

with $|R_N| \leqslant \varepsilon$ for N large enough. Next, (3.91) implies that, on the range of $\chi(\widehat{\mathcal{N}}_N/\zeta)$, the Hamiltonian $\widehat{H}_N$ is bounded uniformly in N. Thus we may expand $\mathrm{e}^{-\beta\widehat{H}_N}$. We conclude: Up to an error that is smaller than ε, uniformly in N, (3.116) is of the form

$$\big\langle P(a_N^*, a_N)\, z^{\widehat{\mathcal{N}}_N}\,\chi(\widehat{\mathcal{N}}_N/\zeta)\big\rangle\,,$$

where P is some polynomial in the rescaled creation and annihilation operators $a_N^*(x)$, $a_N(x)$.

Repeating the above argument for the right-hand side of (3.115), we find using (3.101a) that, up to an error term smaller than ε, it is of the form

$$\langle P(\overline{\alpha}, \alpha)\, z^{\mathcal{N}}\, \chi(\mathcal{N}/\zeta)\rangle\,,$$

where the polynomial P is *the same* as above.

Thus it suffices to show

$$\lim_{N\to\infty} \langle P(a_N^*, a_N)\, z^{\widehat{\mathcal{N}}_N}\, \chi(\widehat{\mathcal{N}}_N/\zeta)\rangle \;=\; \langle P(\overline{\alpha}, \alpha)\, z^{\mathcal{N}}\, \chi(\mathcal{N}/\zeta)\rangle$$

for an arbitrary monomial P. We start by *anti-Wick-ordering* $P(a_N^*, a_N)$, i.e. by using the commutation relations (3.87) to write $P(a_N^*, a_N)$ as a sum of terms in which all creation operators $a_N^*(x)$ stand to the right of the annihilation operators $a_N(x)$. In the limit $N \to \infty$ the subleading terms vanish (as they are proportional to N^{-r}, where $r \geqslant 1$ is the number of contractions arising from the ordering). What remains is the anti-Wick-ordered version of $P(a_N^*, a_N)$, which is of the form

$$a_N(x_1)\cdots a_N(x_k)a_N^*(y_1)\cdots a_N^*(y_l)\,,$$

for some $x_1, \dots, x_k, y_1, \dots, y_l \in \Lambda$. The claim thus reduces to

$$\begin{aligned}\lim_{N\to\infty} \Big\langle a_N(x_1)\cdots a_N(x_k)a_N^*(y_1)\cdots a_N^*(y_l)\, z^{\widehat{\mathcal{N}}_N}\, \chi(\widehat{\mathcal{N}}_N/\zeta)\Big\rangle \\ = \Big\langle \alpha(x_1)\cdots a(x_k)\overline{\alpha}(y_1)\cdots \overline{\alpha}(y_l)\, z^{\mathcal{N}}\, \chi(\mathcal{N}/\zeta)\Big\rangle\,. \qquad (3.117)\end{aligned}$$

By cyclicity of the trace we get

$$\begin{aligned}\Big\langle a_N(x_1)\cdots a_N(x_k)a_N^*(y_1)\cdots a_N^*(y_l)\, z^{\widehat{\mathcal{N}}_N}\, \chi(\widehat{\mathcal{N}}_N/\zeta)\Big\rangle \\ = \Big\langle a_N^*(y_1)\cdots a_N^*(y_l)\, z^{\widehat{\mathcal{N}}_N}\, \chi(\widehat{\mathcal{N}}_N/\zeta)\, a_N(x_1)\cdots a_N(x_k)\Big\rangle\,.\end{aligned}$$

By (3.109), this is equal to

$$\begin{aligned}\frac{1}{N^{|\Lambda|}\pi^{|\Lambda|}} \int_\Gamma \mathrm{d}\alpha\, \Big\langle W_\alpha\,,\, a_N^*(y_1)\cdots a_N^*(y_l)\, z^{\widehat{\mathcal{N}}_N}\, \chi(\widehat{\mathcal{N}}_N/\zeta)\, a_N(x_1)\cdots a_N(x_k)\, W_\alpha\Big\rangle \\ = \frac{1}{\pi^{|\Lambda|}} \int_\Gamma \mathrm{d}\alpha\, \Big\langle a_N(y_1)\cdots a_N(y_l) W_{\sqrt{N}\alpha}\,,\, z^{\widehat{\mathcal{N}}_N}\, \chi(\widehat{\mathcal{N}}_N/\zeta)\, a_N(x_1)\cdots a_N(x_k)\, W_{\sqrt{N}\alpha}\Big\rangle\,,\end{aligned}$$

after the variable transformation $\alpha \mapsto \alpha/\sqrt{N}$. Using (3.110) we get

$$\frac{1}{\pi^{|\Lambda|}} \int_\Gamma \mathrm{d}\alpha\; \alpha(x_1)\cdots a(x_k)\overline{\alpha}(y_1)\cdots\overline{\alpha}(y_l)\, \langle W_{\sqrt{N}\alpha}, z^{\widehat{\mathcal{N}}_N}\, \chi(\widehat{\mathcal{N}}_N/\zeta)\, W_{\sqrt{N}\alpha}\rangle\,. \qquad (3.118)$$

To conclude the proof of Theorem 3.32, we need to show (3.117), i.e.

$$\begin{aligned}\lim_{N\to\infty} \frac{1}{\pi^{|\Lambda|}} \int_\Gamma \mathrm{d}\alpha\; \alpha(x_1)\cdots a(x_k)\overline{\alpha}(y_1)\cdots\overline{\alpha}(y_l)\, \langle W_{\sqrt{N}\alpha}, z^{\widehat{\mathcal{N}}_N}\, \chi(\widehat{\mathcal{N}}_N/\zeta)\, W_{\sqrt{N}\alpha}\rangle \\ = \frac{1}{\pi^{|\Lambda|}} \int_\Gamma \mathrm{d}\alpha\; \alpha(x_1)\cdots a(x_k)\overline{\alpha}(y_1)\cdots\overline{\alpha}(y_l)\, z^{\mathcal{N}(\alpha)}\chi(\mathcal{N}(\alpha)/\zeta)\,. \qquad (3.119)\end{aligned}$$

We do this by dominated convergence. Set $f(\lambda) := z^\lambda \chi(\lambda/\zeta)$. Then, from (3.111) and (3.108) we get

$$\begin{aligned}
\big\langle W_{\sqrt{N}\alpha}\,, z^{\widehat{\mathcal{N}}_N}\,\chi(\widehat{\mathcal{N}}_N/\zeta)\,W_{\sqrt{N}\alpha}\big\rangle &= \big\langle W_{\sqrt{N}\alpha}\,, f(\widehat{\mathcal{N}}_N)\,W_{\sqrt{N}\alpha}\big\rangle \\
&= \sum_{n\in\mathbb{N}^\Lambda} \big|\big\langle B_n\,, W_{\sqrt{N}\alpha}\big\rangle\big|^2 f\big(\|n\|_1/N\big) \\
&= \mathrm{e}^{-N\|\alpha\|^2} \sum_{n\in\mathbb{N}^\Lambda}\prod_{x\in\Lambda} \frac{\big(N|\alpha(x)|^2\big)^{n(x)}}{n(x)!} f\big(\|n\|_1/N\big) \\
&= \int \Bigg(\prod_{x\in\Lambda} \mathrm{d}\mu_{N,|\alpha(x)|^2}(u(x))\Bigg)\, f(\|u\|_1)\,,
\end{aligned} \tag{3.120}$$

where the measure $\mu_{N,s}$ on $\mathbb{R}$ is defined by

$$\mu_{N,s} \;:=\; \mathrm{e}^{-Ns}\sum_{m\geqslant 0}\frac{(Ns)^m}{m!}\,\delta_{m/N}\,,$$

where $\delta_{m/N}$ is the delta mass at m/N. Clearly, $\mu_{N,s}$ is a probability measure. Moreover, a short calculation shows that its mean is s and its variance s/N. Therefore $\mu_{N,s}$ converges to δ_s in probability, and hence weakly, as $N\to\infty$. Since f is continuous and bounded, we get

$$\lim_{N\to\infty}\big\langle W_{\sqrt{N}\alpha}\,, z^{\widehat{\mathcal{N}}_N}\,\chi(\widehat{\mathcal{N}}_N/\zeta)\,W_{\sqrt{N}\alpha}\big\rangle \;=\; f(\|\alpha\|^2) \;=\; z^{\mathcal{N}(\alpha)}\chi(\mathcal{N}(\alpha)/\zeta)\,.$$

In order to find a function that dominates the integrand $I_N(\alpha)$ on the left-hand side of (3.119), we estimate

$$\begin{aligned}
I_N(\alpha) \;&:=\; \big|\alpha(x_1)\cdots a(x_k)\overline{\alpha}(y_1)\cdots\overline{\alpha}(y_l)\,\big\langle W_{\sqrt{N}\alpha}\,, z^{\widehat{\mathcal{N}}_N}\,\chi(\widehat{\mathcal{N}}_N/\zeta)\,W_{\sqrt{N}\alpha}\big\rangle\big| \\
&\leqslant\; \|\alpha\|^{k+l}\,\big\langle W_{\sqrt{N}\alpha}\,, z^{\widehat{\mathcal{N}}_N}\,W_{\sqrt{N}\alpha}\big\rangle\,.
\end{aligned}$$

From (3.120) we get

$$\begin{aligned}
\big\langle W_{\sqrt{N}\alpha}\,, z^{\widehat{\mathcal{N}}_N}\,W_{\sqrt{N}\alpha}\big\rangle \;&=\; \mathrm{e}^{-N\|\alpha\|^2}\sum_{n\in\mathbb{N}^\Lambda}\prod_{x\in\Lambda}\frac{\big(N|\alpha(x)|^2\big)^{n(x)}}{n(x)!} z^{\|n\|_1/N} \\
&=\; \prod_{x\in\Lambda}\Bigg(\mathrm{e}^{-N|\alpha(x)|^2}\sum_{m\geqslant 0}\frac{\big(N|\alpha(x)|^2\big)^m}{m!} z^{m/N}\Bigg) \\
&=\; \exp\!\big(-\|\alpha\|^2 N(1-z^{1/N})\big)\,.
\end{aligned}$$

Since

$$N(1-z^{1/N}) \;=\; -\log z + O(N^{-1})$$

for $N\to\infty$, we conclude that, for N large enough,

$$I_N(\alpha) \;\leqslant\; \|\alpha\|^{k+l} z^{\|\alpha\|^2/2}\,,$$

which is integrable over Γ. Hence the proof of Theorem 3.32 is complete.

3.4.5. A note on the thermodynamic limit. The arguments of the previous section rely crucially on the fact that Λ is finite. A cluster expansion along the lines of Section 3.3.2, combined with time evolution of observables, is difficult to control. However, if one introduces a cutoff proportional to N in the particle density, the creation and annihilation operators become bounded, and the problem essentially reduces to the spin system discussed in Section 3.3.

The obvious solution is to restrict the trace in (3.99) to the subspace $\mathcal{F}_{\zeta N}$ of $\mathcal{F}$ that contains at most ζN particles per lattice site. While this approach works, it is unsatisfactory in the sense that $\mathcal{F}_{\zeta N}$ is not invariant under time evolution.

A better approach is to use a formulation in terms of quantum spins, thus reducing the problem to a special case of the problem considered in Section 3.3. One takes a quantum spin system with spins of magnitude $s = \zeta N$ and defines $a_N(x) := \frac{1}{\sqrt{2\zeta N}} S_-(x)$. The vacuum is given by $\Omega := |-s\rangle$. It is easy to check that, on any subspace of bounded particle number, a_N and a_N^* satisfy commutations relations that go over to (3.87) as $N \to \infty$.

Chapter 4

The Mean-Field Limit of a Quantum Gas with Coulomb Interaction

This chapter is devoted to the mean-field limit in quantum mechanics. We consider a quantum gas in 3 dimensions (although our results may be trivially extended to higher dimensions), consisting of N particles. The N-particle mean-field Hamiltonian is given by

$$H_N = \sum_{i=1}^{N} h_i + \frac{1}{N} \sum_{1 \leqslant i < j \leqslant N} w(x_i - x_j) . \tag{4.1}$$

We consider interaction potentials w that exhibit at most Coulomb-type singularities $|x|^{-1}$, and one-particle Hamiltonians of the form $h = -\Delta + v$, where v is a weak external potential (which in our case means that $v \in L^3_w + L^\infty$). Here, for convenience, we choose physical units in which the mass of the particles is $1/2$.

In the case of a Bose gas, we prove that the mean-field dynamics is governed by the Hartree equation. To this end, we state and prove a Egorov-type theorem (Theorem 4.13) and discuss as an application the dynamics of coherent states (Theorem 4.15). In the case of a Fermi gas, we prove that the mean-field dynamics is governed by the Hartree-Fock equation (Theorem 4.24). We also describe how the quantum many-body theory of a Fermi gas may be viewed as the quantization of a "superhamiltonian" system, and prove a Egorov-type theorem (Theorem 4.28).

While the mean-field limit of a Fermi gas with Coulomb interaction potential has not been previously considered in the literature, the study of the mean-field limit of a Bose gas with Coulomb interaction potential has a (relatively short) history. The first result is due to Erdős and Yau [EY01]. This result was improved by Rodnianski and Schlein in [RS07] by deriving explicit bounds on the rate of convergence to the mean-field limit; their method is inspired by a semiclassical argument of Hepp [Hep74].

In this chapter we present a new, simple way of handling singular interaction potentials[1]. It yields a Egorov-type formulation of convergence to the mean-field limit, thus obviating the need to consider particular (traditionally coherent) states as initial conditions. Another, technical, advantage of our method is that it requires no regularity (traditionally H^1- or H^2-regularity) when applied to coherent states. Our proof is based on a diagrammatic expansion of the dynamics. We sketch its key ideas.

[1]This method is inspired by [FGS07], where results were obtained for the quantum Bose gas with bounded interaction potential. In [Sch07], partial results were obtained for the quantum Bose gas with Coulomb interaction potential.

(i) Use the Schwinger-Dyson expansion to construct the Heisenberg-picture dynamics of p-particle operators
$$\mathrm{e}^{\mathrm{i}tH_N}\,\widehat{\mathrm{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tH_N}$$
(in the notation of Section 4.1).

(ii) Use *Dispersive estimates* and *combinatorial estimates* (counting of graphs) to prove convergence of the Schwinger-Dyson expansion on N-particle Hilbert space, uniformly in N and for small $|t|$. Diagrams containing l loops yield a contribution of order N^{-l}.

(iii) Show that the tree diagrams ($l = 0$) converge to the Schwinger-Dyson expansion of the Hartree dynamics (in the case of a Bose gas) or the Hartree-Fock dynamics (in the case of a Fermi gas).

(iv) Extend (ii) and (iii) to arbitrary times by using unitarity and conservation laws.

This chapter is organized as follows. In section 4.1 we introduce a general formalism which is convenient when dealing with quantum gases. Section 4.2 contains an implementation of step (i) above. The convergence of the Schwinger-Dyson series for bounded interaction potentials is briefly discussed in Section 4.3. Section 4.4 implements step (ii) above. In Section 4.5, we discuss the mean-field limit of a Bose gas, and prove convergence to the Hartree dynamics as outlined in steps (iii) and (iv) above. Section 4.6 is devoted to the mean-field limit of a Fermi gas; we prove convergence to the Hartree-Fock dynamics as outlined in steps (iii) and (iv) above. Finally, Section 4.7 extends our results to more general interaction potentials as well as nonvanishing external potentials.

4.1. Quantum gases: the setup

The setup is similar to the lattice Bose gas (Section 3.4.1). We use n to denote particle number, as the variable N is reserved for the inverse parameter of the quantization associated with the mean-field limit (see Section 4.5).

We briefly review the main ingredients of many-body quantum theory, mainly in order to establish notations (see [BR02] for more details). Throughout this chapter we consider the one-particle Hilbert space
$$\mathcal{H} \;:=\; L^2(\mathbb{R}^3, \mathrm{d}x)\,.$$
The n-particle space is $\mathcal{H}_\pm^{(n)} := P_\pm \mathcal{H}^{\otimes n}$, where $P_\pm$ is the orthogonal projector onto the symmetric/antisymmetric subspace of $\mathcal{H}^{\otimes n}$. We often work on the Fock space $\mathcal{F}_\pm := \bigoplus_{n \geqslant 0} \mathcal{H}_\pm^{(n)}$, where we adopt the usual convention that $\mathcal{H}_\pm^{(0)} = \mathbb{C}$. A state $\Phi \in \mathcal{F}_\pm$ is a sequence $\Phi = (\Phi^{(n)})_{n \geqslant 0}$ with $\Phi^{(n)} \in \mathcal{H}_\pm^{(n)}$. The scalar product on $\mathcal{F}_\pm$ is given by
$$\langle \Phi\,, \Psi \rangle \;=\; \sum_{n \geqslant 0} \langle \Phi^{(n)}\,, \Psi^{(n)} \rangle\,.$$
The vector $\Omega = (1, 0, 0, \dots)$ is called the *vacuum*. By a slight abuse of notation, we denote a vector of the form $\Phi = (0, \dots, 0, \Phi^{(n)}, 0, \dots) \in \mathcal{F}_\pm$ by its non-vanishing n-particle component $\Phi^{(n)}$. Define also the subspace of vectors with a finite particle number
$$\mathcal{F}_\pm^0 \;:=\; \{\Phi \in \mathcal{F}_\pm \,:\, \Phi^{(n)} = 0 \text{ for all but finitely many } n\}\,.$$

On $\mathcal{F}_\pm$ we have the usual creation and annihilation operators, a^* and a, which map the one-particle space $\mathcal{H}$ into densely defined closable operators on $\mathcal{F}_\pm$. For $f \in \mathcal{H}$ and $\Phi \in \mathcal{F}_\pm$, they are defined by

$$\begin{aligned}
\big(a^*(f)\Phi\big)^{(n)}(x_1,\dots,x_n) &:= \frac{1}{\sqrt{n}}\sum_{i=1}^{n}(\pm 1)^{i-1}\, f(x_i)\Phi^{(n-1)}(x_1,\dots,x_{i-1},x_{i+1},\dots,x_n)\,,\\
\big(a(f)\Phi\big)^{(n)}(x_1,\dots,x_n) &:= \sqrt{n+1}\int \mathrm{d}y\;\overline{f(y)}\Phi^{(n+1)}(y,x_1,\dots,x_n)\,.
\end{aligned}$$

It is not hard to see that $a(f)$ and $a^*(f)$ are adjoints of each other. Furthermore, they satisfy the canonical (anti)commutation relations

$$\big[a(f), a^*(g)\big]_\mp \;=\; \langle f\,, g\rangle\,\mathbb{1}\,, \qquad \big[a^\#(f), a^\#(g)\big]_\mp \;=\; 0\,, \tag{4.2}$$

where $[A,B]_\mp := AB \mp BA$, and $a^\# = a^*$ or a. In order to simplify notation, we usually identify $c\mathbb{1}$ with c, where $c \in \mathbb{C}$.

For our purposes, it is more natural to work with the rescaled creation and annihilation operators

$$a_N^\# \;:=\; \frac{1}{\sqrt{N}}\,a^\#\,,$$

where $N > 0$. We also introduce the operator-valued distributions defined formally by

$$a_N^\#(x) \;:=\; a_N^\#(\delta_x)\,,$$

where δ_x is the delta function at x. The formal expression $a_N^\#(x)$ has a rigorous meaning as a densely defined sesquilinear form on $\mathcal{F}_\pm$ (see [RS75] for details). In particular one has that

$$a_N(f) \;=\; \int \mathrm{d}x\;\bar{f}(x)\,a_N(x)\,, \qquad a_N^*(f) \;=\; \int \mathrm{d}x\; f(x)\,a_N^*(x)\,.$$

Furthermore, the (anti)commutation relations (4.2) imply that

$$\big[a_N(x), a_N^*(y)\big]_\mp \;=\; \frac{1}{N}\delta(x-y)\,, \qquad \big[a_N^\#(x), a_N^\#(y)\big]_\mp \;=\; 0\,, \tag{4.3}$$

In the following a central role is played by p-particles operators, i.e. closed operators $a^{(p)}$ on $\mathcal{H}_\pm^{(p)}$. When using second-quantized notation it is convenient to use the operator kernel of $a^{(p)}$. Here is what this means (see [RS80] for details). Let $\mathcal{S}(\mathbb{R}^d)$ be the usual Schwartz space of smooth functions of rapid decrease, and $\mathcal{S}'(\mathbb{R}^d)$ its topological dual. The nuclear theorem states that to every operator A on $L^2(\mathbb{R}^d)$, such that the map $(f,g) \mapsto \langle f\,, Ag\rangle$ is separately continuous on $\mathcal{S}(\mathbb{R}^d) \times \mathcal{S}(\mathbb{R}^d)$, there belongs a tempered distribution ("kernel") $\tilde{A} \in \mathcal{S}'(\mathbb{R}^{2d})$, such that

$$\langle f\,, Ag\rangle \;=\; \tilde{A}(\bar{f} \otimes g)\,.$$

In the following we identify $\tilde{A}$ with A. In the suggestive physicist's notation we thus have

$$\langle f\,, a^{(p)} g\rangle \;=\; \int \mathrm{d}x_1\cdots\mathrm{d}x_p\,\mathrm{d}y_1\cdots\mathrm{d}y_p\;\overline{f(x_1,\dots,x_p)}\,a^{(p)}(x_1,\dots,x_p;y_1,\dots,y_p)\,g(y_1,\dots,y_p)\,,$$

where $f, g \in \mathcal{S}(\mathbb{R}^{3p})$. It will be easy to verify that all p-particle operators that appear in the following satisfy the above condition; this is for instance the case for all bounded $a^{(p)} \in \mathcal{L}(\mathcal{H}_\pm^{(p)})$.

Next, we define second quantization $\widehat{\mathrm{A}}_N$. It maps a closed operator on $\mathcal{H}_\pm^{(p)}$ to a closed operator on $\mathcal{F}_\pm$ according to the formula[2]

$$\widehat{\mathrm{A}}_N(a^{(p)}) := \int \mathrm{d}x_1 \cdots \mathrm{d}x_p \, \mathrm{d}y_1 \cdots \mathrm{d}y_p \\ a_N^*(x_p) \cdots a_N^*(x_1) \, a^{(p)}(x_1, \dots, x_p; y_1, \dots, y_p) \, a_N(y_1) \cdots a_N(y_p) \,. \tag{4.4}$$

In order to understand the action of $\widehat{\mathrm{A}}_N(a^{(p)})$ on $\mathcal{H}_\pm^{(n)}$, we write

$$\Phi^{(n)} = \frac{N^{n/2}}{\sqrt{n!}} \int \mathrm{d}z_1 \cdots \mathrm{d}z_n \; \Phi^{(n)}(z_1, \dots, z_n) \, a_N^*(z_n) \cdots a_N^*(z_1) \, \Omega$$

and apply $\widehat{\mathrm{A}}_N(a^{(p)})$ to the right-hand side. By using the (anti)commutation relations (4.3) to pull the p annihilation operators $a_N(y_i)$ through the n creation operators $a_N^*(z_i)$, and $a_N(x)\,\Omega = 0$, we get the "first quantized" expression

$$\widehat{\mathrm{A}}_N(a^{(p)})\big|_{\mathcal{H}_\pm^{(n)}} = \begin{cases} \frac{p!}{N^p} \binom{n}{p} P_\pm (a^{(p)} \otimes \mathbb{1}^{(n-p)}) P_\pm & \text{if } n \geqslant p \\ 0 \,, & \text{if } n < p \,. \end{cases} \tag{4.5}$$

This may be viewed as an alternative definition of $\widehat{\mathrm{A}}_N(a^{(p)})$.

We define $\widehat{\mathfrak{A}}$ as the linear span of $\big\{\widehat{\mathrm{A}}_N(a^{(p)}) \, : \, p \in \mathbb{N}, \, a^{(p)} \in \mathcal{L}(\mathcal{H}_\pm^{(p)})\big\}$. Then $\widehat{\mathfrak{A}}$ is a $*$-algebra of closable operators on $\mathcal{F}_\pm^0$. We list some of its important properties, whose straightforward proofs we omit.

(i) $\widehat{\mathrm{A}}_N(a^{(p)})^* = \widehat{\mathrm{A}}_N((a^{(p)})^*)$.

(ii) If $a^{(p)} \in \mathcal{L}(\mathcal{H}_\pm^{(p)})$ and $b^{(q)} \in \mathcal{L}(\mathcal{H}_\pm^{(q)})$, then

$$\widehat{\mathrm{A}}_N(a^{(p)}) \, \widehat{\mathrm{A}}_N(b^{(q)}) = \sum_{r=0}^{\min(p,q)} \binom{p}{r} \binom{q}{r} \frac{r!}{N^r} \, \widehat{\mathrm{A}}_N\big(a^{(p)} \bullet_r b^{(q)}\big) \,, \tag{4.6}$$

where

$$a^{(p)} \bullet_r b^{(q)} := P_\pm \, (a^{(p)} \otimes \mathbb{1}^{(q-r)}) \, (\mathbb{1}^{(p-r)} \otimes b^{(q)}) \, P_\pm \in \mathcal{L}(\mathcal{H}_\pm^{(p+q-r)}) \,. \tag{4.7}$$

(iii) The operator $\widehat{\mathrm{A}}(a^{(p)})$ leaves the n-particle subspaces $\mathcal{H}_\pm^{(n)}$ invariant.

(iv) If $a^{(p)} \in \mathcal{L}(\mathcal{H}_\pm^{(p)})$ and $b \in \mathcal{L}(\mathcal{H})$ is invertible, then

$$\Gamma(b^{-1}) \, \widehat{\mathrm{A}}_N(a^{(p)}) \, \Gamma(b) = \widehat{\mathrm{A}}_N\big((b^{-1})^{\otimes p} \, a^{(p)} \, b^{\otimes p}\big) \,, \tag{4.8}$$

where $\Gamma(b)$ is defined on $\mathcal{H}_\pm^{(n)}$ by $b^{\otimes n}$.

(v) If $a^{(p)} \in \mathcal{L}(\mathcal{H}_\pm^{(p)})$ then

$$\Big\| \widehat{\mathrm{A}}_N(a^{(p)})\big|_{\mathcal{H}_\pm^{(n)}} \Big\| \leqslant \left(\frac{n}{N}\right)^p \|a^{(p)}\| \,. \tag{4.9}$$

[2]Such an object is rigorously defined as a sesquilinear form on the space $\{\Phi \in \mathcal{F}_\pm^0 \, : \, \Phi^{(n)} \in \mathcal{S}(\mathbb{R}^{3n}) \; \forall n\}$, on which it is closable.

Of course, on an appropriate dense domain, (4.6) holds for unbounded operators $a^{(p)}$ and $b^{(q)}$ too. We introduce the notation

$$\big[a^{(p)}, b^{(q)}\big]_r \;:=\; a^{(p)} \bullet_r b^{(q)} - b^{(q)} \bullet_r a^{(p)} . \tag{4.10}$$

Note that $\big[a^{(p)}, b^{(q)}\big]_0 = 0$. Thus,

$$\big[\widehat{\mathrm{A}}_N(a^{(p)}), \widehat{\mathrm{A}}_N(b^{(q)})\big] \;=\; \sum_{r=1}^{\min(p,q)} \binom{p}{r}\binom{q}{r} \frac{r!}{N^r}\, \widehat{\mathrm{A}}_N\big(\big[a^{(p)}, b^{(q)}\big]_r\big) . \tag{4.11}$$

Next, we move on to discuss dynamics. Take a one-particle Hamiltonian $h^{(1)} \equiv h$ of the form $h = -\Delta + v$, where Δ is the Laplacian over $\mathbb{R}^3$ and v is some real function. We denote by V the multiplication operator $v(x)$. Two-body interactions are described by a real, even function w on $\mathbb{R}^3$. This induces a two-particle operator $W^{(2)} \equiv W$ on $\mathcal{H}^{\otimes 2}$, defined as the multiplication operator $w(x_1 - x_2)$. We define the Hamiltonian

$$\widehat{H}_N \;:=\; \widehat{\mathrm{A}}_N(h) + \frac{1}{2}\widehat{\mathrm{A}}_N(W) . \tag{4.12}$$

Under suitable assumptions on v and w that we make precise in the following sections, one shows that $\widehat{H}_N$ is a well-defined self-adjoint operator on $\mathcal{F}_\pm$. It is convenient to introduce $H_N := N\widehat{H}_N$. On $\mathcal{H}_\pm^{(n)}$ we have the "first quantized" expression

$$H_N\big|_{\mathcal{H}_\pm^{(n)}} \;=\; \sum_{i=1}^n h_i + \frac{1}{N}\sum_{1\leqslant 1<j\leqslant n} W_{ij} \;=:\; H_0 + \frac{1}{N}W , \tag{4.13}$$

in self-explanatory notation.

4.2. Schwinger-Dyson expansion and loop counting

Without loss of generality, we assume throughout the following that $t \geqslant 0$.

Let $a^{(p)} \in \mathcal{L}(\mathcal{H}_\pm^{(p)})$ and w be bounded, i.e. $w \in L^\infty(\mathbb{R}^3)$. Using the fundamental theorem of calculus and the fact that the unitary group $(\mathrm{e}^{-\mathrm{i}tH_0})_{t\in\mathbb{R}}$ is strongly differentiable one finds

$$\begin{aligned}
&\mathrm{e}^{\mathrm{i}tH_N}\, \widehat{\mathrm{A}}_N(a^{(p)})\, \mathrm{e}^{-\mathrm{i}tH_N}\, \Phi^{(n)} \\
&\quad=\; \mathrm{e}^{\mathrm{i}sH_N}\mathrm{e}^{-\mathrm{i}sH_0}\mathrm{e}^{\mathrm{i}tH_0}\, \widehat{\mathrm{A}}_N(a^{(p)})\, \mathrm{e}^{-\mathrm{i}tH_0}\mathrm{e}^{\mathrm{i}sH_0}\mathrm{e}^{-\mathrm{i}sH_N}\, \Phi^{(n)}\big|_{s=t} \\
&\quad=\; \widehat{\mathrm{A}}_N(a_t^{(p)})\, \Phi^{(n)} + \int_0^t \mathrm{d}s\; \mathrm{e}^{\mathrm{i}sH_N}\mathrm{e}^{-\mathrm{i}sH_0} \frac{\mathrm{i}N}{2}\Big[\widehat{\mathrm{A}}_N(W_s), \widehat{\mathrm{A}}_N(a_t^{(p)})\Big]\, \mathrm{e}^{\mathrm{i}sH_0}\mathrm{e}^{-\mathrm{i}sH_N}\, \Phi^{(n)} ,
\end{aligned}$$

where $(\cdot)_t := \Gamma(\mathrm{e}^{ith})(\cdot)\Gamma(\mathrm{e}^{-ith})$ denotes free time evolution. As an equation between operators defined on $\mathcal{F}_\pm^0$, this reads

$$\mathrm{e}^{\mathrm{i}tH_N}\, \widehat{\mathrm{A}}_N(a^{(p)})\, \mathrm{e}^{-\mathrm{i}tH_N} \;=\; \widehat{\mathrm{A}}_N(a_t^{(p)}) + \int_0^t \mathrm{d}s\; \mathrm{e}^{\mathrm{i}sH_N}\mathrm{e}^{-\mathrm{i}sH_0} \frac{\mathrm{i}N}{2}\Big[\widehat{\mathrm{A}}_N(W_s), \widehat{\mathrm{A}}_N(a_t^{(p)})\Big]\, \mathrm{e}^{\mathrm{i}sH_0}\mathrm{e}^{-\mathrm{i}sH_N} . \tag{4.14}$$

Iteration of (4.14) yields the formal power series

$$\sum_{k=0}^{\infty} \int_{\Delta^k(t)} \mathrm{d}\underline{t} \, \frac{(\mathrm{i}N)^k}{2^k} \Big[\widehat{\mathrm{A}}_N(W_{t_k}), \dots \Big[\widehat{\mathrm{A}}_N(W_{t_1}), \widehat{\mathrm{A}}_N(a_t^{(p)})\Big] \dots\Big] . \tag{4.15}$$

It is easy to see that, on $\mathcal{H}_{\pm}^{(n)}$, the k-th term of (4.15) is bounded in norm by

$$\frac{\big(tn^2 \|w\|_\infty / N\big)^k}{k!} \left(\frac{n}{N}\right)^p \|a^p\| . \tag{4.16}$$

Therefore, on $\mathcal{H}_{\pm}^{(n)}$, the series (4.15) converges in norm for all times. Furthermore, (4.16) implies that the rest term arising from the iteration of (4.14) vanishes for $k \to \infty$, so that (4.15) is equal to (4.14).

The mean-field limit is the limit $n = \nu N \to \infty$, where $\nu > 0$ is some constant. The above estimate is clearly inadequate to prove statements about the mean-field limit. In order to obtain estimates uniform in N, more care is needed.

To see why the above estimate is so crude, consider the commutator

$$\frac{\mathrm{i}N}{2} \Big[\widehat{\mathrm{A}}_N(W_s), \widehat{\mathrm{A}}_N(a_t^{(p)})\Big]\Big|_{\mathcal{H}_{\pm}^{(n)}} = \frac{p!}{N^p} \binom{n}{p} \frac{\mathrm{i}}{N} P_{\pm} \sum_{1 \leqslant i < j \leqslant n} \big[W_{ij,s}, a_t^{(p)} \otimes \mathbb{1}^{(n-p)}\big] P_{\pm} .$$

We see that most terms of the commutator vanish (namely, whenever $p < i < j$). Thus, for large n, the above estimates are highly wasteful. This can be remedied by more careful bookkeeping. We split the commutator into two terms: the *tree terms*, defined by $1 \leqslant i \leqslant p$ and $p+1 \leqslant j \leqslant n$, and the *loop terms*, defined by $1 \leqslant i < j \leqslant p$. All other terms vanish. This splitting can also be inferred from (4.11).

The naming originates from a diagrammatic representation (see Figure 4.1). A p-particle operator is represented as a wiggly vertical line to which are attached p horizontal branches on the left and p horizontal branches on the right. Each branch on the left represents a creation operator $a_N^*(x_i)$, and each branch on the right an annihilation operator $a_N(y_i)$. The product $\widehat{\mathrm{A}}_N(a^{(p)})\widehat{\mathrm{A}}_N(b^{(q)})$ of two operators is given by the sum over all possible pairings of the annihilation operators in $\widehat{\mathrm{A}}_N(a^{(p)})$ with the creation operators in $\widehat{\mathrm{A}}_N(b^{(q)})$. Such a contraction is graphically represented as a horizontal line joining the corresponding branches. We consider diagrams that arise in this manner from the multiplication of a finite number of operators of the form $\widehat{\mathrm{A}}_N(a^{(p)})$.

We now generalize this idea to a systematic scheme for the multiple commutators appearing in the Schwinger-Dyson expansion. To this end, we decompose the multiple commutator

$$\frac{(\mathrm{i}N)^k}{2^k} \Big[\widehat{\mathrm{A}}_N(W_{t_k}), \dots \Big[\widehat{\mathrm{A}}_N(W_{t_1}), \widehat{\mathrm{A}}_N(a_t^{(p)})\Big] \dots\Big]$$

into a sum of 2^k terms obtained by writing out each commutator. Each resulting term is a product of $k+1$ second-quantized operators, which we furthermore decompose into a sum over all possible contractions for which $r > 0$ in (4.6) (at least one contraction for each multiplication). The restriction $r > 0$ follows from $[a^{(p)}, b^{(q)}]_0 = 0$. This is equivalent to saying that all diagrams are connected.

We call the resulting terms *elementary*. The idea is to classify all elementary terms according to their number of loops l. Write

$$\frac{(\mathrm{i}N)^k}{2^k} \Big[\widehat{\mathrm{A}}_N(W_{t_k}), \dots \Big[\widehat{\mathrm{A}}_N(W_{t_1}), \widehat{\mathrm{A}}_N(a_t^{(p)})\Big] \dots\Big] = \sum_{l=0}^{k} \frac{1}{N^l} \widehat{\mathrm{A}}_N\big(F_{t,t_1,\dots,t_k}^{(k,l)}(a^{(p)})\big) , \tag{4.17}$$

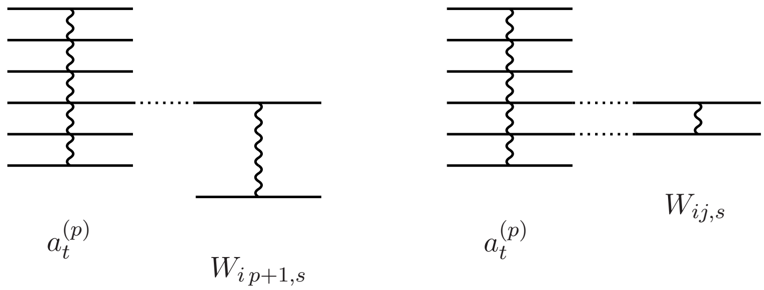


Figure 4.1: *Two terms of the product $\widehat{\mathrm{A}}_N(a_t^{(p)})\,\widehat{\mathrm{A}}_N(W_s)$, represented as labelled diagrams. A tree term (left) produces a tree diagram. A loop term (right) produces a diagram with one loop.*

where $F^{(k,l)}_{t,t_1,\dots,t_k}(a^{(p)})$ is a $(p+k-l)$-particle operator, equal to the sum of all elementary terms with l loops. It is defined through the recursion relation (on $\mathcal{H}_\pm^{(p+k-l)}$)

$$
\begin{aligned}
F^{(k,l)}_{t,t_1,\dots,t_k}(a^{(p)}) \;&=\; \mathrm{i}(p+k-l-1)\Big[W_{t_k}, F^{(k-1,l)}_{t,t_1,\dots,t_{k-1}}(a^{(p)})\Big]_1 \\
&\qquad + \mathrm{i}\binom{p+k-l}{2}\Big[W_{t_k}, F^{(k-1,l-1)}_{t,t_1,\dots,t_{k-1}}(a^{(p)})\Big]_2 \\
&=\; \mathrm{i}P_\pm \sum_{i=1}^{p+k-l-1}\Big[W_{i\,p+k-l,t_k}, F^{(k-1,l)}_{t,t_1,\dots,t_{k-1}}(a^{(p)})\otimes \mathbb{1}\Big]P_\pm \\
&\qquad + \mathrm{i}P_\pm \sum_{1\leqslant i<j\leqslant p+k-l}\Big[W_{ij,t_k}, F^{(k-1,l-1)}_{t,t_1,\dots,t_{k-1}}(a^{(p)})\Big]P_\pm\,,
\end{aligned}
\tag{4.18}
$$

as well as $F^{(0,0)}_t(a^{(p)}) := a_t^{(p)}$. If $l<0$, $l>k$, or $p+k-l>n$ then $F^{(k,l)}_{t,t_1,\dots,t_k}(a^{(p)})=0$. The interpretation of the recursion relation is simple: a (k,l)-term arises from either a $(k-1,l)$-term without adding a loop or from a $(k-1,l-1)$-term to which a loop is added. It is not hard to see, using induction on k and the definition (4.18), that (4.17) holds. It is often convenient to have an explicit formula for the decomposition into elementary terms:

$$
F^{(k,l)}_{t,t_1,\dots,t_k}(a^{(p)}) \;=\; \sum_{\alpha=1}^{c(p,k,l)} F^{(k,l)(\alpha)}_{t,t_1,\dots,t_k}(a^{(p)})\,,
$$

where $F^{(k,l)(\alpha)}_{t,t_1,\dots,t_k}(a^{(p)})$ is an elementary term, and $c(p,k,l)$ is the number of elementary terms in $F^{(k,l)}_{t,t_1,\dots,t_k}(a^{(p)})$.

In order to establish a one-to-one correspondence between elementary terms and diagrams, we introduce a labelling scheme for diagrams. Consider an elementary term arising from a choice of contractions in the multiple commutator of order k, along with its diagram. We label all vertical lines v with an index $i_v\in\mathbb{N}$ as follows. The vertical line of $a^{(p)}$ is labelled by 0. The vertical line of the first (i.e. innermost in the multiple commutator) interaction operator is labelled by 1, of the second by 2, and so on (see Figure 4.2). Conversely, every elementary term is uniquely determined by its labelled diagram. We consequently use $\alpha=1,\dots,c(p,k,l)$ to index either elementary terms or labelled diagrams.

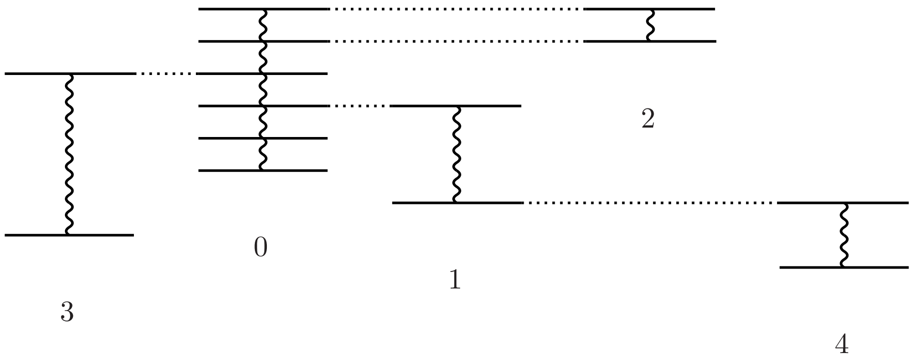


Figure 4.2: *The labelled diagram corresponding to a one-loop elementary term in the commutator of order* 4.

Use the shorthand $\underline{t} = (t_1, \ldots, t_k)$ and define

$$F_t^{(k,l)}(a^{(p)}) \;:=\; \int_{\Delta^k(t)} \mathrm{d}\underline{t}\; F_{t,\underline{t}}^{(k,l)}(a^{(p)})\,. \tag{4.19}$$

In summary, we have an expansion in terms of the number of loops l:

$$\mathrm{e}^{\mathrm{i}tH_N}\, \widehat{\mathrm{A}}_N(a^{(p)})\, \mathrm{e}^{-\mathrm{i}tH_N} \;=\; \sum_{k=0}^{\infty}\sum_{l=0}^{k} \frac{1}{N^l}\, \widehat{\mathrm{A}}_N\big(F_t^{(k,l)}(a^{(p)})\big)\,, \tag{4.20}$$

which converges in norm on $\mathcal{H}_{\pm}^{(n)}$, $n \in \mathbb{N}$, for all times t.

4.3. Convergence for bounded interaction

For a bounded interaction potential, $\|w\|_\infty < \infty$, it is now straightforward to control the mean-field limit.

Lemma 4.1. *We have the bound*

$$\Big\| F_{t,\underline{t}}^{(k,l)}(a^{(p)}) \Big\| \;\leqslant\; c(p,k,l)\|w\|_\infty^k\, \|a^{(p)}\|\,. \tag{4.21}$$

Furthermore,

$$c(p,k,l) \;\leqslant\; 2^k \binom{k}{l}\, (p+k-l)^l\, (p+k-1)\cdots p\,. \tag{4.22}$$

Proof. Assume first that $l = 0$. Then the number of labelled diagrams is clearly given by $2^k p \cdots (p+k-1)$. Now if there are l loops, we may choose to add them at any l of the k steps when computing the multiple commutator. Furthermore, each addition of a loop produces at most $p + k - l$ times more elementary terms than the addition of a tree branch. Combining these observations, we arrive at the claimed bound for $c(p,k,l)$.

Alternatively, it is a simple exercise to show the claim, with $c(p,k,l)$ replaced by the bound (4.22), by induction on k. □

LEMMA 4.2. *Let $\nu > 0$ and $t < (8\nu\|w\|_\infty)^{-1}$. Then, on $\mathcal{H}_\pm^{(\nu N)}$, the Schwinger-Dyson series (4.20) converges in norm, uniformly in N.*

PROOF. Recall that $p+k-l \leqslant n$ for nonvanishing $\widehat{\mathrm{A}}_N\big(F_{t,\underline{t}}^{(k,l)}(a^{(p)})\big)\big|_{\mathcal{H}_\pm^{(n)}}$. We find

$$
\begin{aligned}
&\sum_{k=0}^{\infty}\sum_{l=0}^{k}\frac{1}{N^l}\int_{\Delta^k(t)}\mathrm{d}\underline{t}\,\Big\|\widehat{\mathrm{A}}_N\big(F_{t,\underline{t}}^{(k,l)}(a^{(p)})\big)\big|_{\mathcal{H}_\pm^{(\nu N)}}\Big\| \\
&\qquad\leqslant \sum_{k=0}^{\infty}\sum_{l=0}^{k}\frac{(p+k-l)^l}{N^l}\,\mathbb{1}_{\{p+k-l\leqslant \nu N\}}\,\frac{1}{k!}(2\|w\|_\infty t)^k\binom{k}{l}\binom{p+k-1}{k}k!\,\nu^{p+k-l}\,\|a^{(p)}\| \\
&\qquad\leqslant \sum_{k=0}^{\infty}(8\nu\|w\|_\infty t)^k\,(2\nu)^p\,\|a^{(p)}\| \\
&\qquad= \frac{1}{1-8\nu\|w\|_\infty t}\,(2\nu)^p\,\|a^{(p)}\|\,,
\end{aligned}
$$

where we used that $\sum_{l=0}^{k}\binom{k}{l} = 2^k$, and in particular $\binom{k}{l}\leqslant 2^k$. □

In the spirit of semi-classical expansions, we can rewrite the Schwinger-Dyson series to get a "$1/N$-expansion", whereby all l-loop terms add up to an operator of order $O(N^{-l})$.

LEMMA 4.3. *Let $t < (8\nu\|w\|_\infty)^{-1}$ and $L \in \mathbb{N}$. Then we have on $\mathcal{H}_\pm^{(\nu N)}$*

$$
\mathrm{e}^{\mathrm{i}tH_N}\,\widehat{\mathrm{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tH_N} \;=\; \sum_{l=0}^{L-1}\frac{1}{N^l}\sum_{k=l}^{\infty}\widehat{\mathrm{A}}_N\big(F_t^{(k,l)}(a^{(p)})\big) + O\Big(\frac{1}{N^L}\Big),
$$

where the sum converges uniformly in N.

PROOF. Instead of the full Schwinger-Dyson expansion (4.15), we can stop the expansion whenever L loops have been generated. More precisely, we iterate (4.14) and use (4.11) at each iteration to split the commutator into tree ($r=1$) and loop ($r=2$) terms. Whenever a term obtained in this fashion has accumulated L loops, we stop expanding and put it into a remainder term. Thus all fully expanded terms are precisely those arising from diagrams containing up to $L-1$ loops, and it is not hard to show that the remainder term is of order N^{-L}.

In view of later applications, we also give a proof using the fully expanded Schwinger-Dyson series. From Lemma 4.2 we know that the sum converges on $\mathcal{H}_\pm^{(\nu N)}$ in norm, uniformly in N, and can be reordered as

$$
\mathrm{e}^{\mathrm{i}tH_N}\,\widehat{\mathrm{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tH_N} \;=\; \sum_{l=0}^{\infty}\frac{1}{N^l}\sum_{k=l}^{\infty}\int_{\Delta^k(t)}\mathrm{d}\underline{t}\;\widehat{\mathrm{A}}_N\big(F_{t,\underline{t}}^{(k,l)}(a^{(p)})\big)\,,
$$

as an identity on $\mathcal{H}_{\pm}^{(\nu N)}$. Proceeding as above we find

$$\begin{aligned}
&\sum_{l=L}^{\infty} \frac{1}{N^l} \sum_{k=l}^{\infty} \int_{\Delta^k(t)} \mathrm{d}\underline{t} \, \Big\| \widehat{\mathrm{A}}_N \big(F_{t,\underline{t}}^{(k,l)}(a^{(p)})\big)\big|_{\mathcal{H}_{\pm}^{(\nu N)}} \Big\| \\
&\quad \leqslant \frac{1}{N^L} \sum_{l=L}^{\infty} \sum_{k=l}^{\infty} \frac{(p+k-l)^l}{N^{l-L}} \mathbb{1}_{\{p+k-l \leqslant \nu N\}} \frac{1}{k!} (2\|w\|_\infty t)^k \binom{k}{l} \binom{p+k-1}{k} k! \, \nu^{p+k-l} \, \|a^{(p)}\| \\
&\quad \leqslant \frac{1}{(\nu N)^L} \sum_{l=L}^{\infty} \sum_{k=l}^{\infty} (p+k-l)^L (8\nu\|w\|_\infty t)^k \, (2\nu)^p \, \|a^{(p)}\| \\
&\quad = \frac{1}{(\nu N)^L} \sum_{l=L}^{\infty} \sum_{k=0}^{\infty} (p+k)^L (8\nu\|w\|_\infty t)^{k+l} \, (2\nu)^p \, \|a^{(p)}\| \\
&\quad \leqslant \frac{1}{(\nu N)^L} \sum_{l=L}^{\infty} (8\nu\|w\|_\infty t)^l \frac{\mathrm{e}^p \, L!}{(1-8\nu\|w\|_\infty t)^{L+1}} (2\nu)^p \, \|a^{(p)}\| \\
&\quad = \frac{1}{(\nu N)^L} \frac{\mathrm{e}^p \, L! \, (8\nu\|w\|_\infty t)^L}{(1-8\nu\|w\|_\infty t)^{L+2}} (2\nu)^p \, \|a^{(p)}\| \,,
\end{aligned}$$

where in the second last step we used the following elementary lemma. □

LEMMA 4.4. *Let* $|x| < 1$. *Then*

$$\sum_{k=0}^{\infty} (p+k)^L x^k \;\leqslant\; \frac{\mathrm{e}^p \, L!}{(1-x)^{L+1}} \,.$$

PROOF. Let first $p = 0$.

$$\begin{aligned}
\frac{L!}{(1-x)^{L+1}} \;&=\; \partial_x^L \frac{1}{1-x} \;=\; \sum_{k=L}^{\infty} k(k-1)\cdots(k-L+1) x^{k-L} \\
&=\; \sum_{k=0}^{\infty} (k+L)\cdots(k+1) x^k \;\geqslant\; \sum_{k=0}^{\infty} k^L x^k \,.
\end{aligned}$$

Thus,

$$\begin{aligned}
\sum_{k=0}^{\infty} (p+k)^L x^k \;&=\; \sum_{k=0}^{\infty} \sum_{l=0}^{L} \binom{L}{l} p^{L-l} k^l x^k \;\leqslant\; \sum_{l=0}^{L} \binom{L}{l} p^{L-l} \frac{l!}{(1-x)^{l+1}} \\
&\leqslant\; \frac{L!}{(1-x)^{L+1}} \sum_{l=0}^{L} \frac{1}{(L-l)!} p^{L-l} \;\leqslant\; \frac{\mathrm{e}^p \, L!}{(1-x)^{L+1}} \,.
\end{aligned}$$

□

4.4. Convergence for Coulomb interaction

In this section we consider an interaction potential of the form

$$w(x) \;=\; \kappa \frac{1}{|x|} \,, \tag{4.23}$$

where $\kappa \in \mathbb{R}$. We take the one-body Hamiltonian to be

$$h = -\Delta\,,$$

the nonrelativistic kinetic energy without external potentials. We assume this form of h and w throughout Sections 4.4, 4.5, and 4.6. In Section 4.7, we discuss some generalizations.

4.4.1. Kato smoothing. The non-relativistic dispersive nature of the free time evolution $\mathrm{e}^{\mathrm{i}t\Delta}$ is essential for controlling singular potentials. It embodied by the following dispersive estimate, which is sometimes referred to as Kato's smoothing estimate, as it was first derived using Kato's theory of smooth perturbations; see [RS78, Sim92]. Here we present a new, elementary proof, which yields the sharp constant and may be easily generalized to free Hamiltonians of the form $(-\Delta)^\gamma$, where $1/2 < \gamma < d/2$.

LEMMA 4.5. *For $d \geqslant 3$ and $\varphi \in L^2(\mathbb{R}^d)$ we have*

$$\int \mathrm{d}t\, \big\| |x|^{-1}\, \mathrm{e}^{\mathrm{i}t\Delta}\, \varphi \big\|^2 \;\leqslant\; \frac{\pi}{d-2} \|\varphi\|^2\,. \tag{4.24}$$

More generally, for $d \geqslant 2$ and γ satisfying $1/2 < \gamma < d/2$ we have

$$\int \mathrm{d}t\, \big\| |x|^{-\gamma}\, \mathrm{e}^{-\mathrm{i}t(-\Delta)^\gamma}\, \varphi \big\|^2 \;\leqslant\; c_{d,\gamma}\, \|\varphi\|^2\,, \tag{4.25}$$

for some constant $c_{d,\gamma} > 0$.

REMARK 4.6. *The constant in (4.24) is sharp. Indeed, (4.24) is saturated if φ is Gaussian. To show this, consider the wave function*

$$\varphi(x) \;=\; \Big(\frac{a}{\pi}\Big)^{d/4} \mathrm{e}^{-\frac{a}{2}|x|^2}\,,$$

where $a > 0$. Note that the normalization of φ is chosen so that $\|\varphi\| = 1$. By Fourier transformation we find

$$(\mathrm{e}^{\mathrm{i}t\Delta}\varphi)(x) \;=\; \Big(\frac{a}{\pi}\Big)^{d/4} \frac{1}{(1+2\mathrm{i}at)^{d/2}} \exp\Big(-\frac{a}{2(1+2\mathrm{i}at)}|x|^2\Big)\,.$$

This yields

$$\begin{aligned}
\big\| |x|^{-1}\, \mathrm{e}^{\mathrm{i}t\Delta}\, \varphi \big\|^2 \;&=\; \int \mathrm{d}x\, \frac{1}{|x|^2} \Big(\frac{a}{\pi(1+4a^2t^2)}\Big)^{d/2} \exp\Big(-\frac{a}{1+4a^2t^2}|x|^2\Big) \\
&=\; |\mathbb{S}^{d-1}| \Big(\frac{a}{\pi(1+4a^2t^2)}\Big)^{d/2} \int_0^\infty \mathrm{d}r\; r^{d-3} \exp\Big(-\frac{a}{1+4a^2t^2}\, r^2\Big)\,.
\end{aligned}$$

Here $\mathbb{S}^{d-1}$ is the unit sphere in $\mathbb{R}^d$ and $|\mathbb{S}^{d-1}| = 2\pi^{d/2}/\Gamma(d/2)$ its surface measure. After evaluating the integral we get

$$\begin{aligned}
\big\| |x|^{-1}\, \mathrm{e}^{\mathrm{i}t\Delta}\, \varphi \big\|^2 \;&=\; |\mathbb{S}^{d-1}| \Big(\frac{a}{\pi(1+4a^2t^2)}\Big)^{d/2} \frac{1}{2} \Big(\frac{1+4a^2t^2}{a}\Big)^{d/2-1} \Gamma\Big(\frac{d}{2}-1\Big) \\
&=\; \frac{|\mathbb{S}^{d-1}|}{2\pi^{d/2}} \frac{a}{1+4a^2t^2} \frac{\Gamma(d/2)}{d/2-1} \\
&=\; \frac{1}{d-2} \frac{2a}{1+4a^2t^2}\,.
\end{aligned}$$

Thus,

$$\int \mathrm{d}t \, \big\| |x|^{-1} \, \mathrm{e}^{\mathrm{i}t\Delta} \, \varphi \big\|^2 \;=\; \frac{\pi}{d-2} \, .$$

REMARK 4.7. *At the endpoint $\gamma = 1/2$ the dispersion law of the time evolution is $\omega(k) = |k|$. Thus all spatial frequency components have the same propagation speed, i.e. there is no dispersion and the smoothing effect of the time evolution (which relies on the fast propagation of high spatial frequencies) vanishes. It is therefore not surprising that the endpoint $\gamma = 1/2$ is excluded in* (4.25)*. Similarly, the claim is false at the other endpoint $\gamma = d/2$. This can be seen by noting that, for instance if φ is Gaussian, $\mathrm{e}^{-\mathrm{i}t(-\Delta)^{d/2}} \varphi$ is nonzero in a neighbourhood of* 0 *for small times. Since $|x|^{-d}$ is not locally integrable, it follows that the left-hand side of* (4.25) *is ∞.*

REMARK 4.8. *It is easy to see that our proof of* (4.25) *remains valid if the power law potential $v(x) = |x|^{-\gamma}$ is replaced with a potential v satisfying*

$$|\widehat{v^2}(k)| \;\lesssim\; \frac{1}{|k|^{d-2\gamma}} \, ,$$

where $\widehat{\cdot}$ denotes Fourier transformation.

PROOF OF LEMMA 4.5. The left-hand side of (4.24) defines a quadratic form in φ. By density, if we prove (4.24) for all $\varphi \in \mathcal{S}$, it follows that (4.24) holds for all $\varphi \in L^2$. Let us therefore assume that $\varphi \in \mathcal{S}$. By monotone convergence, we have

$$\int \mathrm{d}t \, \big\| |x|^{-1} \, \mathrm{e}^{\mathrm{i}t\Delta} \, \varphi \big\|^2 \;=\; \lim_{\eta \downarrow 0} f(\eta) \, ,$$

where

$$f(\eta) \;:=\; \int \mathrm{d}t \, \big\| |x|^{-1} \, \mathrm{e}^{\mathrm{i}t\Delta} \, \varphi \big\|^2 \, \mathrm{e}^{-\frac{\eta}{2}t^2} \;=\; \int \mathrm{d}t \, \big\langle \varphi \, , \mathrm{e}^{-\mathrm{i}t\Delta} \, |x|^{-2} \, \mathrm{e}^{\mathrm{i}t\Delta} \, \varphi \big\rangle \, \mathrm{e}^{-\frac{\eta}{2}t^2}$$

In order to write the scalar product in Fourier space, we recall (see e.g. [LL01]) that, for $0 < \alpha < d$, we have

$$\widehat{|x|^{-\alpha}}(k) \;=\; 2^{d/2-\alpha} \frac{\Gamma\big(\frac{d-\alpha}{2}\big)}{\Gamma\big(\frac{\alpha}{2}\big)} \frac{1}{|k|^{d-\alpha}} \, .$$

In particular,

$$\widehat{|x|^{-2}}(k) \;=\; \frac{(2\pi)^{d/2}}{(d-2)|\mathbb{S}^{d-1}|} \frac{1}{|k|^{d-2}} \, .$$

Thus,

$$f(\eta) \;=\; \frac{(2\pi)^{d/2}}{(2\pi)^{d/2}(d-2)|\mathbb{S}^{d-1}|} \int \mathrm{d}t \, \mathrm{e}^{-\frac{\eta}{2}t^2} \int \mathrm{d}p_1 \, \mathrm{d}p_2 \, \overline{\varphi(p_1)} \, \mathrm{e}^{\mathrm{i}tp_1^2} \, \frac{1}{|p_1 - p_2|^{d-2}} \, \mathrm{e}^{-\mathrm{i}tp_2^2} \, \varphi(p_2) \, .$$

Using Fubini's theorem we get

$$\begin{aligned}
f(\eta) \;&=\; \frac{1}{(d-2)|\mathbb{S}^{d-1}|} \int \mathrm{d}p_1 \, \mathrm{d}p_2 \, \overline{\varphi(p_1)} \, \frac{1}{|p_1 - p_2|^{d-2}} \, \varphi(p_2) \int \mathrm{d}t \, \mathrm{e}^{-\frac{\eta}{2}t^2} \, \mathrm{e}^{\mathrm{i}t(p_1^2 - p_2^2)} \\
&=\; \frac{1}{(d-2)|\mathbb{S}^{d-1}|} \int \mathrm{d}p_1 \, \mathrm{d}p_2 \, \overline{\varphi(p_1)} \, \frac{1}{|p_1 - p_2|^{d-2}} \, \varphi(p_2) \, 2\pi \frac{1}{\sqrt{2\pi\eta}} \, \mathrm{e}^{-\frac{1}{2\eta}(p_1^2 - p_2^2)^2} \\
&\leqslant\; \frac{2\pi}{(d-2)|\mathbb{S}^{d-1}|} \int \mathrm{d}p_1 \, \mathrm{d}p_2 \, |\varphi(p_1)| \, |\varphi(p_2)| \, \frac{1}{|p_1 - p_2|^{d-2}} \, \frac{1}{\sqrt{2\pi\eta}} \, \mathrm{e}^{-\frac{1}{2\eta}(p_1^2 - p_2^2)^2} \\
&\leqslant\; \frac{2\pi}{(d-2)|\mathbb{S}^{d-1}|} \int \mathrm{d}p_1 \, \mathrm{d}p_2 \, |\varphi(p_2)|^2 \, \frac{1}{|p_1 - p_2|^{d-2}} \, \frac{1}{\sqrt{2\pi\eta}} \, \mathrm{e}^{-\frac{1}{2\eta}(p_1^2 - p_2^2)^2} \, ,
\end{aligned}$$

where in the last step we used the inequality $2ab \leqslant a^2 + b^2$ and symmetry. This implies

$$f(\eta) \;\leqslant\; \frac{2\pi}{(d-2)|\mathbb{S}^{d-1}|} \, \|\varphi\|^2 \sup_{p_2} \int \mathrm{d}p_1 \, \frac{1}{|p_1 - p_2|^{d-2}} \, \frac{1}{\sqrt{2\pi\eta}} \, \mathrm{e}^{-\frac{1}{2\eta}(p_1^2 - p_2^2)^2} \,.$$

Let us write $p_2 = \lambda p$ and $k := p_1/\lambda$, where $\lambda > 0$ and $p \in \mathbb{S}^{d-1}$. Thus we get

$$f(\eta) \;\leqslant\; \frac{2\pi}{(d-2)|\mathbb{S}^{d-1}|} \, \|\varphi\|^2 \sup_{\lambda > 0,\, p \in \mathbb{S}^{d-1}} \int \mathrm{d}k \, \frac{1}{|k - p|^{d-2}} \, \frac{\lambda^2}{\sqrt{2\pi\eta}} \, \mathrm{e}^{-\frac{\lambda^4}{2\eta}(k^2 - 1)^2} \,.$$

We do the integral over k using polar coordinates:

$$k \;=\; \sqrt{v}\, e \,, \qquad \mathrm{d}k \;=\; \frac{\sqrt{v}^{\,d-2}}{2} \, \mathrm{d}v \, \mathrm{d}e \,, \qquad v \in (0, \infty) \,,\; e \in \mathbb{S}^{d-1} \,,$$

where $\mathrm{d}e$ denotes the usual surface measure on $\mathbb{S}^{d-1}$. This gives

$$\int_0^\infty \mathrm{d}v \; g(v) \, \frac{\lambda^2}{\sqrt{2\pi\eta}} \, \mathrm{e}^{-\frac{\lambda^4}{2\eta}(v-1)^2} \,,$$

where

$$g(v) \;:=\; \frac{\sqrt{v}^{\,d-2}}{2} \int_{\mathbb{S}^{d-1}} \mathrm{d}e \, \frac{1}{|\sqrt{v}\, e - p|^{d-2}} \;=\; \frac{1}{2} \int_{\mathbb{S}^{d-1}} \mathrm{d}e \, \frac{1}{|e - p/\sqrt{v}|^{d-2}} \,. \tag{4.26}$$

Next, recall Newton's theorem for spherically symmetric mass distributions (see e.g. [LL01]): If μ is a spherically symmetric, finite, complex measure on $\mathbb{R}^d$, then

$$\int \mathrm{d}\mu(y) \, \frac{1}{|x - y|^{d-2}} \;=\; \frac{1}{|x|^{d-2}} \int \mathrm{d}\mu(y) \; \mathbb{1}_{\{|y| \leqslant |x|\}} + \int \mathrm{d}\mu(y) \, \frac{1}{|y|^{d-2}} \mathbb{1}_{\{|y| > |x|\}} \,.$$

This yields

$$g(v) \;=\; \frac{1}{2} \begin{cases} \left|\mathbb{S}^{d-1}\right| \sqrt{v}^{\,d-2} & \text{if } v \leqslant 1 \\ \left|\mathbb{S}^{d-1}\right| & \text{if } v > 1 \,. \end{cases}$$

Thus, g is continuous and takes on its maximum value at 1. Since

$$\frac{\lambda^2}{\sqrt{2\pi\eta}} \, \mathrm{e}^{-\frac{\lambda^4}{2\eta}(v-1)^2}$$

is an approximate delta-function centred at 1 it follows that

$$\sup_\lambda \int_0^\infty \mathrm{d}v \; g(v) \, \frac{\lambda^2}{\sqrt{2\pi\eta}} \, \mathrm{e}^{-\frac{\lambda^4}{2\eta}(v-1)^2} \;=\; \lim_{\lambda \to \infty} \int_0^\infty \mathrm{d}v \; g(v) \, \frac{\lambda^2}{\sqrt{2\pi\eta}} \, \mathrm{e}^{-\frac{\lambda^4}{2\eta}(v-1)^2} \;=\; g(1) \,.$$

Thus,

$$f(\eta) \;\leqslant\; \frac{1}{2} \, \frac{2\pi}{(d-2)|\mathbb{S}^{d-1}|} \, \left|\mathbb{S}^{d-1}\right| \|\varphi\|^2 \;=\; \frac{\pi}{d-2} \|\varphi\|^2 \,.$$

This completes the proof of (4.24).

The proof of (4.25) follows the proof of (4.24) up to (4.26). The claim then follows from

$$\sup_{v \geqslant 0} \int_{\mathbb{S}^{d-1}} \mathrm{d}e \, \frac{1}{|e - p/\sqrt{v}|^{d-2\gamma}} \;<\; \infty \,,$$

for $p \in \mathbb{S}^{d-1}$ and $2\gamma > 1$. $\square$

In order to avoid tedious discussions of operator domains in equations such as (4.14), we introduce a cutoff to make the interaction potential bounded. For $\varepsilon \geqslant 0$ set

$$w^\varepsilon(x) \;:=\; w(x)\mathbb{1}_{\{|w(x)|\leqslant \varepsilon^{-1}\}}\,,$$

so that $\|w^\varepsilon\|_\infty \leqslant \varepsilon^{-1}$. Now the Kato smoothing estimate (4.24) implies, for $\varepsilon \geqslant 0$,

$$\int_{\mathbb{R}} \big\|w^\varepsilon\, \mathrm{e}^{\mathrm{i}t\Delta}\,\varphi\big\|^2\,\mathrm{d}t \;\leqslant\; \int_{\mathbb{R}} \big\|w\, \mathrm{e}^{\mathrm{i}t\Delta}\,\varphi\big\|^2\,\mathrm{d}t \;\leqslant\; \pi\kappa^2\,\|\varphi\|^2\,. \tag{4.27}$$

An immediate consequence is the following lemma.

LEMMA 4.9. *Let $\Phi^{(n)} \in \mathcal{H}_\pm^{(n)}$. Then*

$$\int_{\mathbb{R}} \big\|W_{ij}^\varepsilon\,\mathrm{e}^{-\mathrm{i}tH_0}\,\Phi^{(n)}\big\|^2\,\mathrm{d}t \;\leqslant\; \frac{\pi\kappa^2}{2}\|\Phi^{(n)}\|^2\,. \tag{4.28}$$

PROOF. By symmetry we may assume that $(i,j) = (1,2)$. Choose centre of mass coordinates $X := (x_1+x_2)/2$ and $\xi = x_2 - x_1$, set $\tilde{\Phi}^{(n)}(X,\xi,x_3,\dots,x_n) := \Phi^{(n)}(x_1,\dots,x_n)$, and write

$$\int_{\mathbb{R}} \big\|W_{12}^\varepsilon\,\mathrm{e}^{-\mathrm{i}tH_0}\,\Phi^{(n)}\big\|^2\,\mathrm{d}t \;=\; \int_{\mathbb{R}} \big\|w^\varepsilon(\xi)\,\mathrm{e}^{2\mathrm{i}t\Delta_\xi}\,\tilde{\Phi}^{(n)}\big\|^2\,\mathrm{d}t\,,$$

since $H_0 = -\Delta_1 - \Delta_2 = -\Delta_X/2 - 2\Delta_\xi$ and $[\Delta_X, w^\varepsilon(\xi)] = 0$. Therefore, by (4.27) and Fubini's theorem, we find

$$\begin{aligned}
\int_{\mathbb{R}} \big\|W_{12}^\varepsilon\,\mathrm{e}^{-\mathrm{i}tH_0}\,\Phi^{(n)}\big\|^2\,\mathrm{d}t \;&=\; \int \mathrm{d}X\,\mathrm{d}x_3\cdots\mathrm{d}x_n \int \mathrm{d}t\,\mathrm{d}\xi\,\big|w^\varepsilon(\xi)\,\mathrm{e}^{2\mathrm{i}t\Delta_\xi}\,\tilde{\Phi}^{(n)}(X,\xi,x_3,\dots,x_n)\big|^2\\
&\leqslant\; \frac{\pi\kappa^2}{2}\int \mathrm{d}X\,\mathrm{d}x_3\cdots\mathrm{d}x_n \int \mathrm{d}\xi\,\big|\tilde{\Phi}^{(n)}(X,\xi,x_3,\dots,x_n)\big|^2\\
&=\; \frac{\pi\kappa^2}{2}\|\Phi^{(n)}\|^2\,.
\end{aligned}$$

□

By Cauchy-Schwarz we then find that

$$\int_0^t \big\|W_{ij,s}^\varepsilon\,\Phi^{(n)}\big\|\,\mathrm{d}s \;\leqslant\; t^{1/2}\left(\int_{\mathbb{R}}\big\|W_{ij}^\varepsilon\,\mathrm{e}^{-\mathrm{i}sH_0}\,\Phi^{(n)}\big\|^2\mathrm{d}s\right)^{1/2} \;\leqslant\; \left(\frac{\pi\kappa^2 t}{2}\right)^{1/2}\|\Phi^{(n)}\|\,. \tag{4.29}$$

By iteration, this implies that, for all elementary terms α,

$$\int_0^t \mathrm{d}t_1\dots\int_0^t \mathrm{d}t_k\,\big\|F_{t,\underline{t}}^{(k,l)(\alpha),\varepsilon}(a^{(p)})\Phi^{(p+k-l)}\big\| \leqslant \left(\frac{\pi\kappa^2 t}{2}\right)^{k/2}\|a^{(p)}\|\,\|\Phi^{(p+k-l)}\|\,, \tag{4.30}$$

where the superscript ε reminds us that $F_{t,\underline{t}}^{(k,l)(\alpha),\varepsilon}(a^{(p)})$ is computed with the regularized potential w^ε. Thus one finds

$$\big\|F_t^{(k,l),\varepsilon}(a^{(p)})\big\| \;\leqslant\; c(p,k,l)\left(\frac{\pi\kappa^2 t}{2}\right)^{k/2}\|a^{(p)}\|\,,$$

for all $\varepsilon \geqslant 0$.

Unfortunately, the above procedure does not recover the factor $1/k!$ arising from the time-integration over the k-simplex $\Delta^k(t)$, which is essential for our convergence estimates. First iterating (4.28) and then using Cauchy-Schwarz yields a factor $1/\sqrt{k!}$, which is still not good enough.

A solution to this problem must circumvent the highly wasteful procedure of replacing the integral over $\Delta^k(t)$ with an integral over $[0,t]^k$. The key observation is that, in the sum over all labelled diagrams, each diagram appears of the order of $k!$ times with different labellings.

4.4.2. Graph counting. In order to make the above idea precise, we make use of graphs (related to the above diagrams) to index terms in our expansion of the multiple commutator

$$\frac{(\mathrm{i}N)^k}{2^k}\Big[\widehat{\mathrm{A}}_N(W_{t_k}),\dots\Big[\widehat{\mathrm{A}}_N(W_{t_1}),\widehat{\mathrm{A}}_N(a_t^{(p)})\Big]\dots\Big]\,. \tag{4.31}$$

The idea is to assign to each second quantized operator a vertex $v = 0,\dots,k$, and to represent each creation and annihilation with an incident edge. A pairing of an annihilation operator with a creation operator is represented by joining the corresponding edges. The vertex 0 has $2p$ edges and the vertices $1,\dots,k$ have 4 edges. We call the vertex 0 the *root*.

The edges incident to each vertex v are labelled using a pair $\lambda = (d,i)$, where $d = a,c$ is the *direction* (a stands for "annihilation" and c for "creation") and i labels edges of the same direction; $i = 1,\dots,p$ if $v = 0$ and $i = 1,2$ if $v = 1,\dots,k$. Thus, a labelled edge is of the form $\{(v_1,\lambda_1),(v_2,\lambda_2)\}$. Graphs G with such labelled edges are graphs over the vertex set $V(G) = \{(v,\lambda)\}$. We denote the set of edges of a graph G (a set of unordered pairs of vertices in $V(G)$) by $E(G)$. The degree of each (v,λ) is either 0 or 1; we call (v,λ) an *empty edge* of v if its degree is 0. We often speak of connecting two empty edges, as well as removing a nonempty edge; the definitions are self-explanatory.

We may drop the edge labelling of G to obtain a (multi)graph $\widetilde{G}$ over the vertex set $\{0,\dots,k\}$: Each edge $\{(v_1,\lambda_1),(v_2,\lambda_2)\}\in E(G)$ gives rise to the edge $\{v_1,v_2\}\in E(\widetilde{G})$. We understand a path in G to be a sequence of edges in $E(G)$ such that two consecutive edges are adjacent in the graph $\widetilde{G}$. This leads to the notions of connectedness of G and loops in G.

The *admissible graphs* – i.e. graphs indexing a choice of pairings in the multiple commutator (4.31) – are generated by the following growth process. We start with the empty graph G_0, i.e. $E(G_0) = \emptyset$. In a first step, we choose one or two empty edges of 1 of the same direction and connect each of them to an empty edge of 0 of opposite direction. Next, we choose one or two empty edges of 2 of the same direction and connect each of them to an empty edge of 0 or 1 of opposite direction. We continue in this manner for all vertices $3,\dots,k$. We summarize some key properties of admissible graphs G.

(a) G is connected.

(b) The degree of each (v,λ) is either 0 or 1

(c) The labelled edge $\{(v_1,\lambda_1),(v_2,\lambda_2)\}\in E(G)$ only if λ_1 and λ_2 have opposite directions.

Property (c) implies that each graph G has a canonical directed representative, where each edge is ordered from the a-label to the c-label. See Figure 4.3 for an example of such a graph.

We call a graph G of type (p,k,l) whenever it is admissible and it contains l loops. We denote by $\mathcal{G}(p,k,l)$ the set of graphs of type (p,k,l).

By definition of admissible graphs, each contraction in (4.31) corresponds to a unique admissible graph. A contraction consists of at least k and at most $2k$ pairings. A contraction giving rise to a graph of type (p,k,l) has $k+l$ pairings. The summand in (4.31) corresponding to any given l-loop contraction is given by an *elementary term* of the form

$$\frac{(\mathrm{i}N)^k}{2^k\,N^{k+l}}\widehat{\mathrm{A}}_N\big(b^{(p+k-l)}\big)\,, \tag{4.32}$$

where the $(p+k-l)$-particle operator $b^{(p+k-l)}$ is of the form

$$b^{(p+k-l)} \;=\; P_\pm\, W_{i_1j_1,t_{v_1}}\cdots W_{i_rj_r,t_{v_r}}\,\big(a_t^{(p)}\otimes \mathbb{1}^{(k-l)}\big)\,W_{i_{r+1}j_{r+1},t_{v_{r+1}}}\cdots W_{i_kj_k,t_{v_k}}P_\pm\,, \tag{4.33}$$

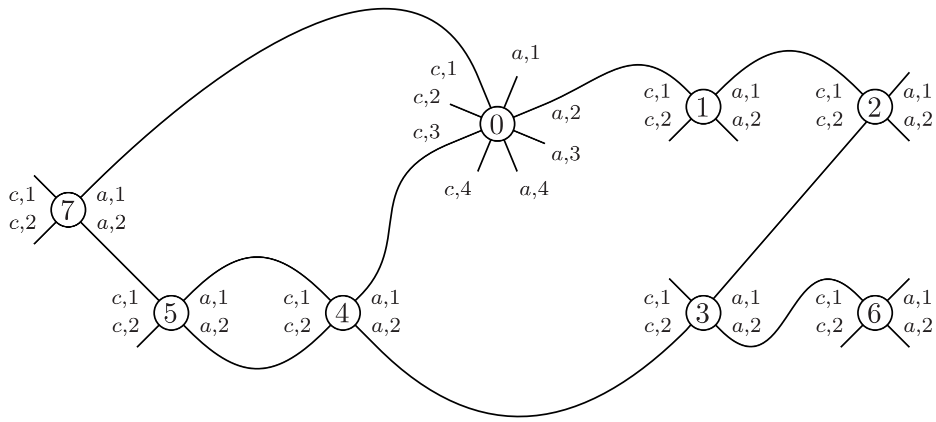


Figure 4.3: *An admissible graph of type* $(p = 4, k = 7, l = 3)$.

for some $r = 0, \dots, k$. Indeed, the (anti)commutation relations (4.3) imply that each pairing produces a factor of $1/N$. Furthermore, the creation and annihilation operators of each summand corresponding to any given contraction are (by definition) Wick ordered, and one readily sees that the associated integral kernel corresponds to an operator of the form (4.33). Thus we recover the splitting (4.17), whereby $F^{(k,l)}_{t,t_1,\dots,t_k}(a^{(p)})$ is a sum, indexed by all l-loop graphs, of elementary terms of the form (4.33).

As remarked above, we need to exploit that many graphs have the same topological structure, i.e. can be identified after some permutation of the labels $\{1, \dots, k\}$ of the vertices corresponding to interaction operators. We therefore define an equivalence relation on the set of graphs: $G \sim G'$ if and only if there exists a permutation $\sigma \in S_k$ such that $G' = R_\sigma(G)$. Here $R_\sigma(G)$ is the graph defined by

$$\{(v_1, \lambda_1), (v_2, \lambda_2)\} \in E(R_\sigma(G)) \iff \{(\sigma(v_1), \lambda_1), (\sigma(v_2), \lambda_2)\} \in E(G)\,,$$

where $\sigma(0) \equiv 0$. We call equivalence classes $[G]$ *graph structures*, and denote the set of graph structures of admissible graphs of type (p, k, l) by $\mathcal{Q}(p, k, l)$.

Note that, in general, $R_\sigma(G)$ need not be admissible if G is admissible. It is convenient to increase $\mathcal{G}(p, k, l)$ to include all $R_\sigma(G)$ where $\sigma \in S_k$ and G is admissible. In order to keep track of the admissible graphs in this larger set, we introduce the symbol i_G which is by definition 1 if $G \in \mathcal{G}(p, k, l)$ is admissible and 0 otherwise. Because $R_\sigma(G) \neq G$ if $\sigma \neq \mathrm{id}$,

$$\big|\mathcal{G}(p, k, l)\big| \;=\; k!\,\big|\mathcal{Q}(p, k, l)\big|\,. \tag{4.34}$$

Our goal is to find an upper bound on the number of graph structures of type (p, k, l), which is sharp enough to show convergence of the Schwinger-Dyson series (4.15). Let us start with tree graphs: $l = 0$. In this case the number of graph structures is equal to 2^k times the number of ordered trees[3] with $k + 1$ vertices, whose root has at most $2p$ children and whose other vertices have at most 3 children. The factor 2^k arises from the fact that each vertex $v = 1, \dots, k$ can use either of the two empty edges of compatible direction to connect to its parent. We thus need some basic facts about ordered trees, which are covered in the following (more or less standard) combinatorial digression.

[3]An ordered tree is a rooted tree in which the children of each vertex are ordered.

For $x, t \in \mathbb{R}$ and $n \in \mathbb{N}$ define

$$A_n(x,t) \;:=\; \frac{x}{x+nt}\binom{x+nt}{n} \tag{4.35}$$

as well as $A_0(x,t) := 1$. After some juggling with binomial coefficients one finds

$$\sum_{k=0}^{n} A_k(x,t) A_{n-k}(y,t) \;=\; A_n(x+y,t)\,; \tag{4.36}$$

see [Knu98] for details. Therefore

$$\sum_{n_1+\cdots+n_r=n} A_{n_1}(x_1,t)\cdots A_{n_r}(x_r,t) \;=\; A_n(x_1+\cdots+x_r,t)\,. \tag{4.37}$$

Set

$$C_n^m \;:=\; A_n(1,m) \;=\; \frac{1}{1+nm}\binom{1+nm}{n} \;=\; \frac{1}{n(m-1)+1}\binom{nm}{n}, \tag{4.38}$$

the n'th m-ary *Catalan number*. Thus we have

$$\sum_{n_1+\cdots+n_r=n} C_{n_1}^m\cdots C_{n_r}^m \;=\; \frac{r}{r+nm}\binom{r+nm}{n}. \tag{4.39}$$

In particular,

$$\sum_{n_1+\cdots+n_m=n-1} C_{n_1}^m\cdots C_{n_m}^m \;=\; C_n^m\,. \tag{4.40}$$

Define an m-tree to be an ordered tree such that each vertex has at most m children. The number of m-trees with n vertices is equal to C_n^m. This follows immediately from $C_0^m = 1$ and from (4.40), which expresses that all trees of order n are obtained by adding m (possibly empty) subtrees of combined order $n-1$ to the root.

We may now compute $|\mathcal{Q}(p,k,0)|$. Since the root of the tree has at most $2p$ children, we may express $|\mathcal{Q}(p,k,0)|$ as the number of ordered forests comprising $2p$ (possibly empty) 3-trees whose combined order is equal to k. Therefore, by (4.39),

$$|\mathcal{Q}(p,k,0)| \;=\; 2^k \sum_{n_1+\cdots+n_{2p}=k} C_{n_1}^3\cdots C_{n_{2p}}^3 \;=\; 2^k\frac{2p}{2p+3k}\binom{2p+3k}{k}. \tag{4.41}$$

Next, we extend this result to all values of l in the form of an upper bound on $|\mathcal{Q}(p,k,l)|$.

LEMMA 4.10. *Let $p, k, l \in \mathbb{N}$. Then*

$$|\mathcal{Q}(p,k,l)| \;\leqslant\; 2^k\binom{k}{l}\binom{2p+3k}{k}(p+k-l)^l\,. \tag{4.42}$$

PROOF. The idea is to remove edges from $G \in \mathcal{G}(p,k,l)$ to obtain a tree graph, and then use the special case (4.41).

In addition to the properties (a) – (c) above, we need the following property of $\mathcal{G}(p,k,l)$:

(d) If $G \in \mathcal{G}(p,k,l)$ then there exists a subset $\mathcal{V} \subset \{1,\ldots,k\}$ of size l and a choice of direction $\delta : \mathcal{V} \to \{a,c\}$ such that, for each $v \in \mathcal{V}$, both edges of v with direction $\delta(v)$ are nonempty. Denote by $\mathcal{E}(v) \subset E(G)$ the set consisting of the two above edges. We additionally require that removing one of the two edges of $\mathcal{E}(v)$ from G, for each $v \in \mathcal{V}$, yields a tree graph, with the property that, for each $v \in \mathcal{V}$, the remaining edge of $\mathcal{E}(v)$ is contained in the unique path connecting v to the root.

This is an immediate consequence of the growth process for admissible graphs. The set $\mathcal{V}$ corresponds to the set of vertices whose addition produces two edges. Note that property (d) is independent of the representative and consequently holds also for non-admissible $G \in \mathcal{G}(p,k,l)$.

Before coming to our main argument, we note that a tree graph $T \in \mathcal{G}(p,k,0)$ gives rise to a natural lexicographical order on the vertex set $\{1,\dots,k\}$. Let $v \in \{1,\dots,k\}$. There is a unique path that connects v to the root. Denote by $0 = v_1, v_2, \dots, v_q = v$ the sequence of vertices along this path. For each $j = 1,\dots,q-1$, let λ_j be the label of the edge $\{v_j, v_{j+1}\}$ at v_j. We assign to v the string $S(v) := (\lambda_1,\dots,\lambda_{q-1})$. Choose some (fixed) ordering of the sets of labels $\{\lambda\}$, for each v. Then the set of vertices $\{1,\dots,k\}$ is ordered according to the lexicographical order of the string $S(v)$.

We now start removing loops from a given graph $G \in \mathcal{G}(p,k,l)$. Define R_1 as the graph obtained from G by removing all edges in $\bigcup_{v\in\mathcal{V}} \mathcal{E}(v)$. By property (d) above, R_1 is a forest comprising l trees. Define T_1 as the connected component of R_1 containing the root. Now we claim that there is at least one $v \in \mathcal{V}$ such that both edges of $\mathcal{E}(v)$ are incident to a vertex of T_1. Indeed, were this not the case, we could choose for each $v \in \mathcal{V}$ an edge in $\mathcal{E}(v)$ that is not incident to any vertex of T_1. Call R_1' the graph obtained by adding all such edges to R_1. Now, since no vertex in $\mathcal{V}$ is in the connected component of R_1, it follows that no vertex in $\mathcal{V}$ is in the connected component R_1'. This is a contradiction to property (d) which requires that R_1' should be a (connected) tree.

Let us therefore consider the set $\tilde{\mathcal{V}}$ of all $v \in \mathcal{V}$ such that both edges of $\mathcal{E}(v)$ are incident to a vertex of T_1. We have shown that $\tilde{\mathcal{V}} \neq \emptyset$. For each choice of v and e, where $v \in \tilde{\mathcal{V}}$ and $e \in \mathcal{E}(v)$, we get a forest of $l-1$ trees by adding e to the edge set of R_1. Then v is in the same tree as the root, so that each such choice of v and e yields a string $S(v)$ as described above. We choose v_1 and $e(v_1)$ as the unique couple that yields the smallest string (note that different choices have different strings). Finally, set G_1 equal to G from which $e(v_1)$ has been removed, and $\mathcal{V}_1 := \mathcal{V} \setminus \{v\}$.

We have thus obtained an $(l-1)$-loop graph G_1 and a set $\mathcal{V}_1$ of size $l-1$, which together satisfy the property (d). We may therefore repeat the above procedure. In this manner we obtain the sequences $v_1,\dots,v_l$ and $G_1,\dots,G_l$. Note that G_l is obtained by removing the edges $e(v_1),\dots,e(v_l)$ from G, and is consequently a tree graph. Also, by construction, the sequence $v_1,\dots,v_l$ is increasing in the lexicographical order of G_l.

Next, consider the tree graph G_l. Each edge $e(v_j)$ connects the single empty edge of v_j with direction $\delta(v_j)$ with an empty edge of opposite direction of a vertex v, where v is smaller than v_j in the lexicographical order of G_l. It is easy to see that, for each j, there are at most $(p+k-l)$ such connections.

We have thus shown that we can obtain any $G \in \mathcal{G}(p,k,l)$ by choosing some tree $G_l \in \mathcal{G}(p,k,0)$, choosing l elements v_j out of $\{1,\dots,k\}$, ordering them lexicographically (according to the order of G_l) and choosing an edge out of at most $(p+k-l)$ possibilities for $v_1,\dots,v_l$. Thus,

$$\bigl|\mathcal{G}(p,k,l)\bigr| \leqslant \binom{k}{l} (p+k-l)^l \bigl|\mathcal{G}(p,k,0)\bigr| .$$

The claim then follows from (4.34) and (4.41). □

4.4.3. Proof of convergence. We are now armed with everything we need in order to estimate

$\int_{\Delta^k(t)} \mathrm{d}\underline{t}\, F_{t,\underline{t}}^{(k,l)}(a^{(p)})$. Recall that

$$F_{t,t_1,\dots,t_k}^{(k,l)}(a^{(p)}) \;=\; \frac{\mathrm{i}^k}{2^k} \sum_{G\in\mathcal{G}(p,k,l)} i_G\, F_{t,t_1,\dots,t_k}^{(k,l)(G)}(a^{(p)})\,, \tag{4.43}$$

where $F_{t,t_1,\dots,t_k}^{(k,l)(G)}(a^{(p)})$ is an elementary term of the form (4.33) indexed by the graph G. We rewrite this using graph structures. Pick some choice $\mathcal{P}:\mathcal{Q}(p,k,l)\to\mathcal{G}(p,k,l)$ of representatives. Then we get

$$\begin{aligned}
F_{t,t_1,\dots,t_k}^{(k,l)}(a^{(p)}) \;&=\; \frac{\mathrm{i}^k}{2^k} \sum_{Q\in\mathcal{Q}(p,k,l)} \sum_{G\in Q} i_G\, F_{t,t_1,\dots,t_k}^{(k,l)(G)}(a^{(p)})\\
&=\; \frac{\mathrm{i}^k}{2^k} \sum_{Q\in\mathcal{Q}(p,k,l)} \sum_{\sigma\in S_k} i_{R_\sigma(\mathcal{P}(Q))}\, F_{t,t_1,\dots,t_k}^{(k,l)(R_\sigma(\mathcal{P}(Q)))}(a^{(p)})\,.
\end{aligned} \tag{4.44}$$

Now, by definition of R_σ, we see that

$$F_{t,t_1,\dots,t_k}^{(k,l)(R_\sigma(G))}(a^{(p)}) \;=\; F_{t,t_{\sigma(1)},\dots,t_{\sigma(k)}}^{(k,l)(G)}(a^{(p)})\,.$$

Thus,

$$\begin{aligned}
\int_{\Delta^k(t)} \mathrm{d}\underline{t}\, F_{t,t_1,\dots,t_k}^{(k,l)}(a^{(p)}) \;&=\; \frac{\mathrm{i}^k}{2^k} \sum_{Q\in\mathcal{Q}(p,k,l)} \sum_{\sigma\in S_k} i_{R_\sigma(\mathcal{P}(Q))} \int_{\Delta^k(t)} \mathrm{d}\underline{t}\, F_{t,t_{\sigma(1)},\dots,t_{\sigma(k)}}^{(k,l)(\mathcal{P}(Q))}(a^{(p)})\\
&=\; \frac{\mathrm{i}^k}{2^k} \sum_{Q\in\mathcal{Q}(p,k,l)} \int_{\Delta^k_Q(t)} \mathrm{d}\underline{t}\, F_{t,t_1,\dots,t_k}^{(k,l)(\mathcal{P}(Q))}(a^{(p)})\,,
\end{aligned}$$

where

$$\Delta^k_Q(t) \;:=\; \{(t_1,\dots,t_k) \,:\, \exists\sigma\in S_k \,:\, i_{R_\sigma(\mathcal{P}(Q))}=1,\, (t_{\sigma(1)},\dots,t_{\sigma(k)})\in\Delta^k(t)\} \;\subset\; [0,t]^k$$

is a union of disjoint simplices.

Therefore, (4.29) and (4.33) imply, for any $\Phi^{(p+k-l)}\in\mathcal{H}_\pm^{(p+k-l)}$, that

$$\begin{aligned}
\left\|\int_{\Delta^k(t)} \mathrm{d}\underline{t}\, F_{t,\underline{t}}^{(k,l)}(a^{(p)})\,\Phi^{(p+k-l)}\right\| \;&\leqslant\; \frac{1}{2^k} \sum_{Q\in\mathcal{Q}(p,k,l)} \int_{\Delta^k_Q(t)} \mathrm{d}\underline{t}\, \left\|F_{t,t_1,\dots,t_k}^{(k,l)(\mathcal{P}(Q))}(a^{(p)})\,\Phi^{(p+k-l)}\right\|\\
&\leqslant\; \frac{1}{2^k} \sum_{Q\in\mathcal{Q}(p,k,l)} \int_{[0,t]^k} \mathrm{d}\underline{t}\, \left\|F_{t,t_1,\dots,t_k}^{(k,l)(\mathcal{P}(Q))}(a^{(p)})\,\Phi^{(p+k-l)}\right\|\\
&\leqslant\; \frac{1}{2^k} \sum_{Q\in\mathcal{Q}(p,k,l)} \left(\frac{\pi\kappa^2 t}{2}\right)^{k/2} \|a^{(p)}\|\|\Phi^{(p+k-l)}\|\\
&\leqslant\; \binom{2p+3k}{k}\binom{k}{l}(p+k-l)^l\left(\frac{\pi\kappa^2 t}{2}\right)^{k/2} \|a^{(p)}\|\|\Phi^{(p+k-l)}\|\,,
\end{aligned}$$

where the last inequality follows from Lemma 4.10. Of course, the above treatment remains valid for regularized potentials. We summarize:

$$\|F_t^{(k,l),\varepsilon}(a^{(p)})\| \;\leqslant\; \binom{2p+3k}{k}\binom{k}{l}(p+k-l)^l\left(\frac{\pi\kappa^2 t}{2}\right)^{k/2} \|a^{(p)}\|\,, \tag{4.45}$$

for all $\varepsilon \geqslant 0$.

Using (4.45) we may now proceed exactly as in the case of a bounded interaction potential. Let

$$\rho(\kappa, \nu) \;:=\; \frac{1}{128\pi\kappa^2\nu^2}\,. \tag{4.46}$$

The removal of the cutoff and summary of the results are contained in

Lemma 4.11. *Let $t < \rho(\kappa, \nu)$. Then we have on $\mathcal{H}_\pm^{(\nu N)}$*

$$\mathrm{e}^{\mathrm{i}tH_N}\, \widehat{\mathrm{A}}_N(a^{(p)})\, \mathrm{e}^{-\mathrm{i}tH_N} \;=\; \sum_{k=0}^{\infty}\sum_{l=0}^{k} \frac{1}{N^l}\, \widehat{\mathrm{A}}_N\big(F_t^{(k,l)}(a^{(p)})\big)\,, \tag{4.47}$$

in operator norm, uniformly in N. Furthermore, for $L \in \mathbb{N}$, we have the $1/N$-expansion

$$\mathrm{e}^{\mathrm{i}tH_N}\, \widehat{\mathrm{A}}_N(a^{(p)})\, \mathrm{e}^{-\mathrm{i}tH_N} \;=\; \sum_{l=0}^{L-1} \frac{1}{N^l} \sum_{k=l}^{\infty} \widehat{\mathrm{A}}_N\big(F_t^{(k,l)}(a^{(p)})\big) + O\Big(\frac{1}{N^L}\Big)\,, \tag{4.48}$$

where the sum converges on $\mathcal{H}_\pm^{(\nu N)}$ uniformly in N.

Proof. Using (4.45) we may repeat the proof of Lemma 4.3 to the letter to prove the statements about convergence. Thus (4.47) holds for all $\varepsilon > 0$.

What remains is the proof of (4.47) for $\varepsilon = 0$. Our strategy is to show that both sides of (4.48) with $\varepsilon > 0$ converge strongly to the same expression with $\varepsilon = 0$.

We first show the strong convergence of $F_t^{(k,l),\varepsilon}(a^{(p)})$. Let $\Phi^{(n)} \in \mathcal{H}_\pm^{(n)}$ and consider

$$\big\|(W_{ij,s}^\varepsilon - W_{ij,s})\Phi^{(n)}\big\| \;=\; \big\|\mathbb{1}_{\{|W_{ij}| > \varepsilon^{-1}\}} W_{ij} e^{-isH_0}\Phi^{(n)}\big\| \;\leqslant\; \big\|W_{ij} e^{-isH_0}\Phi^{(n)}\big\|\,.$$

Since the right-hand side is in $L^1([0,t])$, we may use dominated convergence to conclude that

$$\lim_{\varepsilon\to 0}\int_0^t \mathrm{d}s\; \big\|(W_{ij,s}^\varepsilon - W_{ij,s})\Phi^{(n)}\big\| \;=\; 0\,.$$

Now

$$\begin{aligned}
&\int_0^t \mathrm{d}s \int_0^t \mathrm{d}s'\; \big\|W_{ij,s}^\varepsilon W_{i'j',s'}^\varepsilon \Phi^{(n)} - W_{ij,s}W_{i'j',s'}\Phi^{(n)}\big\| \\
&\quad\leqslant \int_0^t \mathrm{d}s \int_0^t \mathrm{d}s'\; \big\|W_{ij,s}^\varepsilon W_{i'j',s'}^\varepsilon \Phi^{(n)} - W_{ij,s}^\varepsilon W_{i'j',s'}\Phi^{(n)}\big\| \\
&\qquad + \int_0^t \mathrm{d}s \int_0^t \mathrm{d}s'\; \big\|W_{ij,s}^\varepsilon W_{i'j',s'} \Phi^{(n)} - W_{ij,s}W_{i'j',s'}\Phi^{(n)}\big\|\,.
\end{aligned}$$

The first term is bounded by

$$\Big(\frac{\pi\kappa^2 t}{2}\Big)^{1/2} \int_0^t \mathrm{d}s'\; \big\|W_{i'j',s'}^\varepsilon \Phi^{(n)} - W_{i'j',s'}\Phi^{(n)}\big\| \;\to\; 0\,, \qquad \varepsilon \to 0\,.$$

The integrand of the second term is bounded by $2\big\|W_{ij,s}W_{i'j',s'}\Phi^{(n)}\big\| \in L^1([0,t]^2)$, so that dominated convergence implies that the second term vanishes in the limit $\varepsilon \to 0$. A straightforward generalization of this argument shows that

$$F_t^{(k,l),\varepsilon}(a^{(p)})\, \Phi^{(p+k-l)} \;\to\; F_t^{(k,l)}(a^{(p)})\, \Phi^{(p+k-l)}\,,$$

as claimed. Since the series (4.47) converges uniformly in ε, we find that

$$\sum_{k=0}^{\infty}\sum_{l=0}^{k}\frac{1}{N^l}\,\widehat{\mathrm{A}}_N\big(F_t^{(k,l),\varepsilon}(a^{(p)})\big)\,\Phi^{(n)} \;\to\; \sum_{k=0}^{\infty}\sum_{l=0}^{k}\frac{1}{N^l}\,\widehat{\mathrm{A}}_N\big(F_t^{(k,l)}(a^{(p)})\big)\,\Phi^{(n)}\,,$$

as $\varepsilon \to 0$.

Next, we show that $\mathrm{e}^{-\mathrm{i}tH_N^\varepsilon}\Phi^{(n)} \to \mathrm{e}^{-\mathrm{i}tH_N}\Phi^{(n)}$. This follows from the strong resolvent convergence of H_N^ε to H_N as $\varepsilon \to 0$, by Trotter's theorem [RS80]. Let $W^\varepsilon := \sum_{i<j} W_{ij}^\varepsilon$, and consider

$$\begin{aligned} N\left\|(H_N^\varepsilon-\mathrm{i})^{-1}\Phi^{(n)}-(H_N-\mathrm{i})^{-1}\Phi^{(n)}\right\| &= \left\|(H_N^\varepsilon-\mathrm{i})^{-1}(W-W^\varepsilon)(H_N-\mathrm{i})^{-1}\Phi^{(n)}\right\| \\ &\leqslant \left\|(W-W^\varepsilon)(H_N-\mathrm{i})^{-1}\Phi^{(n)}\right\|. \end{aligned}$$

Clearly $\Psi^{(n)} := (H_N-\mathrm{i})^{-1}\Phi^{(n)}$ is in the domain of H_N. By the Kato-Rellich theorem [RS75], $\Psi^{(n)}$ is in the domain of W_{ij} for all i, j. Therefore,

$$\left\|(W_{ij}-W_{ij}^\varepsilon)(H_N-\mathrm{i})^{-1}\Phi^{(n)}\right\| \;=\; \left\|\mathbb{1}_{\{|W_{ij}|>\varepsilon^{-1}\}}W_{ij}\Psi^{(n)}\right\| \;\to\; 0$$

as $\varepsilon \to 0$. Therefore

$$\mathrm{e}^{\mathrm{i}tH_N^\varepsilon}\,\widehat{\mathrm{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tH_N^\varepsilon}\Phi^{(n)} \;\to\; \mathrm{e}^{\mathrm{i}tH_N}\,\widehat{\mathrm{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tH_N}\Phi^{(n)}$$

as $\varepsilon \to 0$, and the proof is complete. $\square$

4.5. The mean-field limit of a Bose gas

In this section we consider a quantum Bose gas and identify its mean-field dynamics as the dynamics given by the Hartree equation.

4.5.1. The Hartree equation. The Hartree equation reads

$$\mathrm{i}\partial_t\varphi \;=\; h\varphi + (w*|\varphi|^2)\varphi\,. \tag{4.49}$$

It is the equation of motion of a classical Hamiltonian system with phase space $\Gamma := H^1(\mathbb{R}^3)$. Here $H^1(\mathbb{R}^3)$ is the usual Sobolev space of index one. In analogy to $\widehat{\mathrm{A}}_N$ we define A as the map from closed operators on $\mathcal{H}_+^{(p)}$ to functions on phase space, through

$$\begin{aligned} \mathrm{A}(a^{(p)})(\varphi) &:= \langle\varphi^{\otimes p}, a^{(p)}\,\varphi^{\otimes p}\rangle \\ &= \int \mathrm{d}x_1\cdots\mathrm{d}x_p\,\mathrm{d}y_1\cdots\mathrm{d}y_p\;\bar\varphi(x_p)\cdots\bar\varphi(x_1)\,a^{(p)}(x_1,\dots,x_p;y_1,\dots,y_p)\,\varphi(y_1)\cdots\varphi(y_p)\,. \end{aligned}$$

We define the algebra of "classical" observables $\mathfrak{A}$ as the linear hull of

$$\{A(a^{(p)})\;:\;p\in\mathbb{N},\,a^{(p)}\in\mathcal{L}(\mathcal{H}_+^{(p)})\}\,.$$

The Hamilton function is given by

$$H \;:=\; \mathrm{A}(h)+\frac{1}{2}\mathrm{A}(W)\,,$$

i.e.

$$H(\varphi) \;=\; \int \mathrm{d}x\, |\nabla\varphi|^2 + \frac{1}{2}\int \mathrm{d}x\, (w * |\varphi|^2)|\varphi|^2 \;=\; \langle \varphi, h\,\varphi\rangle + \frac{1}{2}\langle \varphi^{\otimes 2}, W\,\varphi^{\otimes 2}\rangle\,. \tag{4.50}$$

Using the Hardy-Littlewood-Sobolev and Sobolev inequalities (see e.g. [LL01]) one sees that $H(\varphi)$ is well-defined on Γ:

$$\int \mathrm{d}x\,\mathrm{d}y\, \frac{|\varphi(x)|^2\,|\varphi(y)|^2}{|x-y|} \;\lesssim\; \big\||\varphi|^2\big\|_{6/5}^2 \;=\; \|\varphi\|_{12/5}^4 \;\lesssim\; \|\varphi\|_{H^1}^4\,,$$

where the symbol $\lesssim$ means the left side is bounded by the right-hand side multiplied by a positive constant that is independent of φ.

The Hartree equation is equivalent to

$$\mathrm{i}\partial_t\varphi \;=\; \partial_{\bar\varphi} H(\varphi)\,.$$

The symplectic form on Γ is given by

$$\omega = \mathrm{i}\int \mathrm{d}x\; \mathrm{d}\bar\varphi(x)\wedge \mathrm{d}\varphi(x)\,,$$

which induces a Poisson bracket given by

$$\{\varphi(x), \bar\varphi(y)\} \;=\; \mathrm{i}\delta(x-y)\,, \qquad \{\varphi(x),\varphi(y)\} \;=\; \{\bar\varphi(x),\bar\varphi(y)\} \;=\; 0\,.$$

For $A, B \in \mathfrak{A}$ we have that

$$\{A, B\} \;=\; \mathrm{i}\int \mathrm{d}x\, \left[\frac{\delta A}{\delta\varphi(x)}\,\frac{\delta B}{\delta\overline{\varphi}(x)} - \frac{\delta B}{\delta\varphi(x)}\,\frac{\delta A}{\delta\overline{\varphi}(x)}\right].$$

The “mass” function

$$N(\varphi) \;:=\; \int \mathrm{d}x\, |\varphi|^2$$

is the generator of the gauge transformations $\varphi \mapsto \mathrm{e}^{-\mathrm{i}\theta}\varphi$. By the gauge invariance of the Hamiltonian, $\{H, N\} = 0$, we conclude, at least formally, that N is a conserved quantity. Similarly, the energy H is formally conserved.

The algebra of classical observables $\mathfrak{A}$ has the following properties.

(i) $\overline{\mathrm{A}(a^{(p)})} = \mathrm{A}\big((a^{(p)})^*\big)$.

(ii) If $a^{(p)} \in \mathcal{L}(\mathcal{H}_+^{(p)})$ and $b \in \mathcal{L}(\mathcal{H})$, then

$$\mathrm{A}(a^{(p)})(b\varphi) \;=\; \mathrm{A}\big((b^*)^{\otimes p} a^{(p)} b^{\otimes p}\big)(\varphi)\,.$$

(iii) If $a^{(p)}$ and $b^{(q)}$ are p- and q-particle operators, respectively, then

$$\big\{\mathrm{A}(a^{(p)}), \mathrm{A}(b^{(q)})\big\} \;=\; \mathrm{i}pq\mathrm{A}\big(\big[a^{(p)}, b^{(q)}\big]_1\big)\,. \tag{4.51}$$

(iv) If $a^{(p)} \in \mathcal{L}(\mathcal{H}_+^{(p)})$, then

$$|\mathrm{A}(a^{(p)})(\varphi)| \;\leqslant\; \|a^{(p)}\|\,\|\varphi\|^{2p}\,. \tag{4.52}$$

The free time evolution

$$\phi_t^0(\varphi) \;:=\; \mathrm{e}^{-\mathrm{i}th}\varphi$$

is the Hamiltonian flow corresponding to the free Hamilton function $\mathrm{A}(h)$. We abbreviate the free time evolution of observables $A \in \mathfrak{A}$ by $A_t \;:=\; A \circ \phi_t^0$. Thus, $\mathrm{A}(a^{(p)})_t = \mathrm{A}(a_t^{(p)})$.

In order to define the Hamiltonian flow on all of $L^2(\mathbb{R}^3)$, we rewrite the Hartree equation (4.49) with initial data $\varphi(0) = \varphi$ as an integral equation

$$\varphi(t) \;=\; \mathrm{e}^{-\mathrm{i}th}\varphi - \mathrm{i}\int_0^t \mathrm{d}s\, \mathrm{e}^{-\mathrm{i}(t-s)h}(w * |\varphi(s)|^2)\varphi(s)\,. \tag{4.53}$$

LEMMA 4.12. *Let $\varphi \in L^2(\mathbb{R}^3)$. Then (4.53) has a unique global solution $\varphi(\cdot) \in C(\mathbb{R}; L^2(\mathbb{R}^3))$, which depends continuously on the initial data φ. Furthermore, $\|\varphi(t)\| = \|\varphi\|$ for all t. Finally, we have a Schwinger-Dyson expansion for observables: Let $a^{(p)} \in \mathcal{L}(\mathcal{H}_+^{(p)})$, $\nu > 0$ and $t < \rho(\kappa,\nu)$. Then*

$$\begin{aligned}\mathrm{A}(a^{(p)})(\varphi(t)) \;&=\; \sum_{k=0}^{\infty} \mathrm{A}\big(F_t^{(k,0)}(a^{(p)})\big)(\varphi)\\ &=\; \sum_{k=0}^{\infty} \frac{1}{2^k}\int_{\Delta^k(t)} \mathrm{d}\underline{t}\,\big\{\mathrm{A}(W_{t_k}),\dots\big\{\mathrm{A}(W_{t_1}),\mathrm{A}(a_t^{(p)})\big\}\dots\big\}(\varphi)\,,\end{aligned} \tag{4.54}$$

uniformly in the ball $B_\nu := \{\varphi \in L^2(\mathbb{R}^3) \,:\, \|\varphi\|^2 \leqslant \nu\}$.

PROOF. The well-posedness of (4.53) is a well-known result; see for instance [CG75, Zag92]. The remaining statements follow from a "tree expansion", which also yields an existence result. We first use the Schwinger-Dyson expansion to construct an evolution on the space of observables. We then show that this evolution stems from a Hamiltonian flow that satisfies the Hartree equation (4.53).

First, we generalize our class of "observables" to functions that are not gauge invariant, i.e. that correspond to bounded operators $a^{(q,p)} \in \mathcal{L}(\mathcal{H}_+^p;\mathcal{H}_+^q)$. We set $\mathrm{A}(a^{(q,p)})(\varphi) := \langle \varphi^{\otimes q}, a^{(q,p)}\varphi^{\otimes p}\rangle$, and denote by $\widetilde{\mathfrak{A}}$ the linear hull of observables of the form $\mathrm{A}(a^{(q,p)})$ with $a^{(q,p)} \in \mathcal{L}(\mathcal{H}_+^p;\mathcal{H}_+^q)$.

It is convenient to introduce the abbreviations

$$G \;:=\; \{\mathrm{A}(h),\,\cdot\,\}\,, \qquad D \;:=\; \frac{1}{2}\{\mathrm{A}(W),\,\cdot\,\}\,.$$

Then e^{Gt} is well-defined on $\widetilde{\mathfrak{A}}$ through $(\mathrm{e}^{Gt}A)(\varphi) = A(\mathrm{e}^{-\mathrm{i}h}\varphi)$, where $A \in \widetilde{\mathfrak{A}}$. Note also that

$$D_s \;:=\; \mathrm{e}^{Gs}D\mathrm{e}^{-Gs} \;=\; \frac{1}{2}\{\mathrm{A}(W_s),\,\cdot\,\}\,.$$

Let $A \in \widetilde{\mathfrak{A}}$. We use the Schwinger-Dyson series for $\mathrm{e}^{(G+D)t}$ to define the flow $S(t)A$ through

$$\begin{aligned}S(t)A \;&:=\; \sum_{k=0}^{\infty}\int_{\Delta^k(t)} \mathrm{d}\underline{t}\; D_{t_k}\cdots D_{t_1}\,\mathrm{e}^{Gt}A\\ &=\; \sum_{k=0}^{\infty}\int_{\Delta^k(t)} \mathrm{d}\underline{t}\;\frac{1}{2^k}\big\{\mathrm{A}(W_{t_k}),\dots\big\{\mathrm{A}(W_{t_1}),A_t\big\}\dots\big\}\,.\end{aligned} \tag{4.55}$$

Our first task is to show convergence of (4.55) for small times.

Let $A = \mathrm{A}(a^{(q,p)})$. As with (4.51) one finds, after short computation, that

$$\frac{1}{2}\{\mathrm{A}(W), \mathrm{A}(a^{(q,p)})\} \;=\; \mathrm{A}\bigg(\mathrm{i}\sum_{i=1}^{q} W_{i\,q+1}(a^{(q,p)} \otimes \mathbb{1}) - \mathrm{i}\sum_{i=1}^{p}(a^{(q,p)} \otimes \mathbb{1})W_{i\,p+1}\bigg). \tag{4.56}$$

Thus we see that the nested Poisson brackets in (4.55) yield a "tree expansion" which may be described as follows. Define $T^{(k)}_{t,t_1,\dots,t_k}(a^{(q,p)})$ recursively through

$$\begin{aligned}
T^{(0)}_t(a^{(q,p)}) \;&:=\; a^{(q,p)}_t\,,\\
T^{(k)}_{t,t_1,\dots,t_k}(a^{(q,p)}) \;&:=\; \mathrm{i}P_+ \sum_{i=1}^{q+k-1} W_{i\,q+k,t_k}\Big(T^{(k-1)}_{t,t_1,\dots,t_{k-1}}(a^{(q,p)}) \otimes \mathbb{1}\Big)P_+\\
&\qquad - \mathrm{i}P_+ \sum_{i=1}^{p+k-1}\Big(T^{(k-1)}_{t,t_1,\dots,t_{k-1}}(a^{(q,p)}) \otimes \mathbb{1}\Big)W_{i\,p+k,t_k}P_+\,.
\end{aligned}$$

Note that $T^{(k)}_{t,t_1,\dots,t_k}(a^{(q,p)})$ is an operator from $\mathcal{H}^{(p+k)}_+$ to $\mathcal{H}^{(q+k)}_+$. Moreover, (4.56) implies that

$$\frac{1}{2^k}\left\{\mathrm{A}(W_{t_k}), \dots \left\{\mathrm{A}(W_{t_1}), \mathrm{A}(a^{(q,p)}_t)\right\}\dots\right\} \;=\; \mathrm{A}\Big(T^{(k)}_{t,t_1,\dots,t_k}(a^{(q,p)})\Big). \tag{4.57}$$

Also, by definition, we see that for gauge-invariant observables $a^{(p)}$ we have

$$T^{(k)}_{t,t_1,\dots,t_k}(a^{(p)}) \;=\; G^{(k,0)}_{t,t_1,\dots,t_k}(a^{(p)})\,.$$

We may use the methods of Section 4.4 to obtain the desired estimate. As shown in that section, $T^{(k)}_{t,t_1,\dots,t_k}(a^{(p)})$ is a sum of elementary terms, indexed by labelled ordered trees, whose root has degree at most $p+q$, and whose other vertices have at most 3 children. From (4.39) we find that there are

$$\frac{p+q}{p+q+3k}\binom{p+q+3k}{k}$$

unlabelled trees of this kind. Proceeding exactly as in Section 4.4 we find that

$$\int_{\Delta^k(t)} \mathrm{d}\underline{t}\, \Big\|T^{(k)}_{t,t_1,\dots,t_k}(a^{(q,p)})\Phi^{(p+k)}\Big\| \;\leqslant\; \binom{p+q+3k}{k}\left(\frac{\pi\kappa^2 t}{2}\right)^{k/2} \|a^{(q,p)}\|\|\Phi^{(p+k)}\|\,,$$

where $\Phi^{(p+k)} \in \mathcal{H}^{(p+k)}_+$. Let $\varphi \in L^2(\mathbb{R}^3)$ with $\|\varphi\|^2 \leqslant \nu$. Then $|\mathrm{A}(a^{(q,p)})(\varphi)| \leqslant \|a^{(q,p)}\|\|\varphi\|^{p+q}$ implies

$$\begin{aligned}
\int_{\Delta^k(t)} \mathrm{d}\underline{t}\, &\left|\frac{1}{2^k}\left\{\mathrm{A}(W_{t_k}), \dots \left\{\mathrm{A}(W_{t_1}), \mathrm{A}(a^{(q,p)}_t)\right\}\dots\right\}(\varphi)\right|\\
&\leqslant\; \binom{p+q+3k}{k}\left(\frac{\pi\kappa^2 t}{2}\right)^{k/2} \|a^{(q,p)}\|\,\nu^{k+(p+q)/2}\,.
\end{aligned} \tag{4.58}$$

Convergence of the Schwinger-Dyson series (4.55) for small times t follows immediately.

Thus, for small times t, the flow $S(t)$ is well-defined on $\widetilde{\mathfrak{A}}$, and it is easy to check that it satisfies the equation

$$S(t)A \;=\; \mathrm{e}^{Gt}A + \int_0^t \mathrm{d}s\; S(s)\,D\,\mathrm{e}^{G(t-s)}A\,, \tag{4.59}$$

for all $A \in \widetilde{\mathfrak{A}}$.

In order to establish a link with the Hartree equation (4.53), we consider $f \in L^2(\mathbb{R}^3)$ and define the function $F_f \in \widetilde{\mathfrak{A}}$ through $F_f(\varphi) := \langle f\,, \varphi\rangle$. Clearly, the mapping $f \mapsto (S(t)F_f)(\varphi)$ is antilinear and (4.58) implies that it is bounded. Thus there exists a unique vector $\varphi(t)$ such that

$$(S(t)F_f)(\varphi) \;=:\; \langle f\,, \varphi(t)\rangle\,.$$

We now proceed to show that $(S(t)A)(\varphi) = A(\varphi(t))$ for all $A \in \widetilde{\mathfrak{A}}$. By definition, this is true for $A = F_f$. As a first step, we show that

$$S(t)(AB) \;=\; (S(t)A)(S(t)B)\,, \tag{4.60}$$

where $A, B \in \widehat{\mathfrak{A}}$. Write

$$\begin{aligned} S(t)(AB) \;&=\; \sum_{k=0}^{\infty} \int_{\Delta^k(t)} \mathrm{d}\underline{t}\; D_{t_k} \cdots D_{t_1}\, \mathrm{e}^{Gt}(AB) \\ &=\; \sum_{k=0}^{\infty} \int_{\Delta^k(t)} \mathrm{d}\underline{t}\; D_{t_k} \cdots D_{t_1}\, (A_t B_t)\,, \end{aligned}$$

where we used $\mathrm{e}^{Gt}(AB) = (\mathrm{e}^{Gt}A)(\mathrm{e}^{Gt}B)$. We now claim that

$$\int_{\Delta^k(t)} \mathrm{d}\underline{t}\; D_{t_k} \cdots D_{t_1}(A_t B_t) \;=\; \sum_{l+m=k} \int_{\Delta^l(t)} \mathrm{d}\underline{t} \int_{\Delta^m(t)} \mathrm{d}\underline{s}\, \big(D_{t_l} \cdots D_{t_1} A_t\big)\big(D_{s_m} \cdots D_{s_1} B_t\big)\,, \tag{4.61}$$

where the sum ranges over $l, m \geqslant 0$. This follows easily by induction on k and using $D_s(AB) = A(D_s B) + (D_s A)B$. Then (4.60) follows immediately.

Next, we note that (4.60) implies that $(S(t)A)(\varphi) = A(\varphi(t))$, whenever A is of the form $A = \mathrm{A}(a^{(q,p)})$, where

$$a^{(q,p)} \;=\; \sum_j P_+ \big|f_1^j \otimes \cdots \otimes f_q^j\big\rangle\big\langle g_1^j \otimes \cdots \otimes g_p^j\big| P_+\,, \tag{4.62}$$

where the sum is finite, and $f_i^j, g_i^j \in L^2(\mathbb{R}^3)$. Now each $a^{(q,p)} \in \mathcal{L}(\mathcal{H}_+^{(p)}; \mathcal{H}_+^{(q)})$ can be written as the weak operator limit of a sequence $(a_n^{(q,p)})_{n\in\mathbb{N}}$ of operators of type (4.62). One sees immediately that

$$\lim_n \mathrm{A}(a_n^{(q,p)})(\varphi(t)) \;=\; \mathrm{A}(a^{(q,p)})(\varphi(t))\,.$$

On the other hand, uniform boundedness implies that $\sup_n \|a_n^{(q,p)}\| < \infty$, so that

$$\begin{aligned} &\Big\langle \varphi^{\otimes(q+k)}\,,\, W_{i_1 j_1, t_{v_1}} \cdots W_{i_r j_r, t_{v_r}} \big(a_n^{(q,p)} \otimes \mathbb{1}^{(k)}\big)\, W_{i_{r+1} j_{r+1}, t_{v_{r+1}}} \cdots W_{i_k j_k, t_{v_k}} \varphi^{\otimes(p+k)} \Big\rangle \\ &\qquad \leqslant\; \|a_n^{(q,p)}\| \Big\| W_{i_r j_r, t_{v_r}} \cdots W_{i_1 j_1, t_{v_1}} \varphi^{\otimes(q+k)} \Big\| \Big\| W_{i_{r+1} j_{r+1}, t_{v_{r+1}}} \cdots W_{i_k j_k, t_{v_k}} \varphi^{\otimes(p+k)} \Big\| \end{aligned}$$

justifies the use of dominated convergence in

$$\lim_n (S(t)\mathrm{A}(a_n^{(q,p)}))(\varphi) = (S(t)\mathrm{A}(a^{(q,p)}))(\varphi)\,.$$

We have thus shown that

$$(S(t)A)(\varphi) \;=\; A(\varphi(t))\,, \qquad \forall A \in \widetilde{\mathfrak{A}}\,. \tag{4.63}$$

Let us now return to (4.59). Setting $A = F_f$, we find that (4.59) implies

$$\begin{aligned}\langle f\,, \varphi(t)\rangle \;&=\; \langle f\,, \mathrm{e}^{-ih}\varphi\rangle + \int_0^t \mathrm{d}s\, \frac{1}{2}\Big(S(s)\{\mathrm{A}(W), (F_f)_{t-s}\}\Big)(\varphi) \\ &=\; \langle f\,, \mathrm{e}^{-ih}\varphi\rangle + \int_0^t \mathrm{d}s\, \big(\{\mathrm{A}(W), (F_f)_{t-s}\}\big)(\varphi(s))\,,\end{aligned}$$

where we used (4.63). Using (4.56) we thus find

$$\langle f\,, \varphi(t)\rangle \;=\; \langle f\,, \mathrm{e}^{-ih}\varphi\rangle - \mathrm{i}\int_0^t \mathrm{d}s\, \big\langle (\mathrm{e}^{\mathrm{i}h(t-s)}f)\otimes\varphi(s)\,, W\varphi(s)\otimes\varphi(s)\big\rangle\,, \tag{4.64}$$

which is exactly the Hartree equation (4.53) projected onto f. We have thus shown that $\varphi(t)$ as defined above solves the Hartree equation.

To show norm-conservation we abbreviate $F(s) := (w * |\varphi(s)|^2)\varphi(s)$ and write, using (4.53),

$$\begin{aligned}\|\varphi(t)\|^2 - \|\varphi\|^2 \;&=\; \mathrm{i}\int_0^t \mathrm{d}s\, \big[\big\langle F(s)\,, \mathrm{e}^{-\mathrm{i}sh}\varphi\big\rangle - \big\langle \mathrm{e}^{-\mathrm{i}sh}\varphi\,, F(s)\big\rangle\big] \\ &\qquad + \int_0^t \mathrm{d}s \int_0^t \mathrm{d}r\, \big\langle \mathrm{e}^{\mathrm{i}sh}F(s)\,, \mathrm{e}^{\mathrm{i}rh}F(r)\big\rangle\,.\end{aligned}$$

The last term is equal to

$$\int_0^t \mathrm{d}s \int_0^s \mathrm{d}r\, \big[\big\langle \mathrm{e}^{\mathrm{i}sh}F(s)\,, \mathrm{e}^{\mathrm{i}rh}F(r)\big\rangle + \big\langle \mathrm{e}^{\mathrm{i}rh}F(r)\,, \mathrm{e}^{\mathrm{i}sh}F(s)\big\rangle\big]\,.$$

Therefore (4.53) implies that

$$\|\varphi(t)\|^2 - \|\varphi\|^2 \;=\; \mathrm{i}\int_0^t \mathrm{d}s\, \big\langle F(s)\,, \varphi(s)\big\rangle - \mathrm{i}\int_0^t \mathrm{d}s\, \big\langle \varphi(s)\,, F(s)\big\rangle \;=\; 0\,,$$

since $\big\langle F(s), \varphi(s)\big\rangle \in \mathbb{R}$, as can be seen by explicit calculation. Thus we can iterate the above existence result for short times to obtain a global solution.

Furthermore, (4.64) implies that $\varphi(t)$ is weakly continuous in t. Since the norm of $\varphi(t)$ is conserved, $\varphi(t)$ is strongly continuous in t. Similarly, the Schwinger-Dyson expansion (4.55) implies that the map $\varphi \mapsto \varphi(t)$ is weakly continuous for small times, uniformly in $\|\varphi\|$ in compacts. Therefore, the map $\varphi \mapsto \varphi(t)$ is weakly continuous for all times t, and norm-conservation implies that it is strongly continuous. □

4.5.2. Wick quantization. In order to state our main result in a general setting, we shortly discuss how the many-body quantum mechanics of bosons can be viewed as a *quantization* of the (classical) Hartree theory. The parameter of the quantization (the analogue of $\hbar$ in the usual quantization of classical theories) is $1/N$. We define *quantization* as the linear map $\widehat{(\cdot)}_N : \mathfrak{A} \to \widehat{\mathfrak{A}}$ defined by the formal replacement $\varphi(x) \mapsto a_N(x)$ and $\bar{\varphi}(x) \mapsto a_N^*(x)$ followed by Wick ordering. In other words,

$$\widehat{(\cdot)}_N : \mathrm{A}(a^{(p)}) \;\mapsto\; \widehat{\mathrm{A}}_N(a^{(p)})\,.$$

Extending the definition of $\widehat{(\cdot)}_N$ to unbounded operators in the obvious way, we see that $\widehat{H}_N$ is the quantization of H.

Note that (4.6) and (4.51) imply, for $A, B \in \mathfrak{A}$,

$$\big[\widehat{A}_N, \widehat{B}_N\big] \;=\; \frac{N^{-1}}{\mathrm{i}}\widehat{\{A,B\}}_N + O\Big(\frac{1}{N^2}\Big)\,,$$

so that $1/N$ is indeed the parameter of $\widehat{(\cdot)}_N$.

4.5.3. The mean-field limit: a Egorov-type theorem. Let ϕ_t denote the Hamiltonian flow of the Hartree equation on $L^2(\mathbb{R}^3)$. Introduce the short-hand notation

$$\begin{aligned} \tau^t A \;&:=\; A \circ \phi_t\,, && A \in \mathfrak{A}\,,\\ \widehat{\tau}^t \mathbf{A} \;&:=\; \mathrm{e}^{\mathrm{i}tN\widehat{H}_N}\, \mathbf{A}\, \mathrm{e}^{-\mathrm{i}tN\widehat{H}_N}\,, && \mathbf{A} \in \widehat{\mathfrak{A}}\,. \end{aligned}$$

We may now state and prove our main result, which essentially says that, in the mean-field limit $n = \nu N \to \infty$, time evolution and quantization commute.

THEOREM 4.13. *Let $A \in \mathfrak{A}$ and $\nu > 0$. Then for any $\varepsilon > 0$ there exists a function $A_\varepsilon(t) \in \mathfrak{A}$ such that*

$$\sup_{t\in\mathbb{R}} \big\|\tau^t A - A_\varepsilon(t)\big\|_{L^\infty(B_\nu)} \;\leqslant\; \varepsilon\,,$$

as well as

$$\big\|\big(\widehat{\tau}^t \widehat{A}_N - \widehat{A_\varepsilon(t)}_N\big)\big|_{\mathcal{H}_+^{(\nu N)}}\big\| \;\leqslant\; \varepsilon + \frac{C(\varepsilon, t)}{N}\,.$$

REMARK 4.14. *The "intermediate function" $A(t)$ is required, since the full time evolution τ^t does not leave $\mathfrak{A}$ invariant.*

PROOF. Most of the work has already been done in the previous sections. Without loss of generality take $A = \mathrm{A}(a^{(p)})$ for some $p \in \mathbb{N}$ and $a^{(p)} \in \mathcal{L}(\mathcal{H}_\pm^{(p)})$. Assume that $t < \rho(\kappa, \nu)$. Taking $L = 1$ in (4.48) we get

$$\widehat{\tau}^t\, \widehat{\mathrm{A}}_N(a^{(p)})\Big|_{\mathcal{H}_+^{(\nu N)}} \;=\; \sum_{k=0}^{\infty} \widehat{\mathrm{A}}_N\big(G_t^{(k,0)}(a^{(p)})\big)\Big|_{\mathcal{H}_+^{(\nu N)}} + O\Big(\frac{1}{N}\Big)\,. \tag{4.65}$$

Comparing this with (4.54) immediately yields

$$\widehat{\tau}^t \widehat{\mathrm{A}}_N(a^{(p)}) \;=\; \widehat{\big[\tau^t \mathrm{A}(a^{(p)})\big]}_N + O\Big(\frac{1}{N}\Big)$$

on $\mathcal{H}_+^{(\nu N)}$, where $\widehat{\big[\tau^t \mathrm{A}(a^{(p)})\big]}_N$ is defined through its norm-convergent power series. This is the statement of the theorem for short times.

The extension to all times follows from an iteration argument. We postpone the details to the proof of Theorem 4.15 below. In its notation $A(t)$ is given by

$$A_\varepsilon(t) \;=\; \sum_{k_1=0}^{K_1-1} \cdots \sum_{k_m=0}^{K_m-1} \mathrm{A}\big(G_s^{(k_m,0)} G_s^{(k_{m-1},0)} \cdots G_s^{(k_1,0)} a^{(p)}\big)\,. \qquad \square$$

The result may also be expressed in terms of coherent states.

THEOREM 4.15. *Let $a^{(p)} \in \mathcal{L}(\mathcal{H}_+^{(p)})$, $\varphi \in L^2(\mathbb{R}^3)$ with $\|\varphi\| = 1$, and $T > 0$. Then there exist constants $C, \beta > 0$, depending only on p, T and κ, such that*

$$\Big|\Big\langle \varphi^{\otimes N}\,,\, \mathrm{e}^{\mathrm{i}tH_N}\,\widehat{\mathrm{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tH_N}\,\varphi^{\otimes N}\Big\rangle - \big\langle \varphi(t)^{\otimes p}\,, a^{(p)}\varphi(t)^{\otimes p}\big\rangle\Big| \;\leqslant\; \frac{C}{N^\beta}\,\|a^{(p)}\|\,, \qquad t \in [0,T]\,.$$

Here $\varphi(t)$ is the solution to the Hartree equation (4.53) with initial data φ.

PROOF. Introduce a cutoff $K \in \mathbb{N}$ and write (in self-explanatory notation)

$$\widehat{\tau}^s\widehat{\mathrm{A}}_N(a^{(p)}) \;=\; \sum_{k=0}^{K-1}\widehat{\mathrm{A}}_N\big(F_s^{(k,0)}(a^{(p)})\big) + \widehat{\tau}^s_{\geqslant K}\widehat{\mathrm{A}}_N(a^{(p)}) + \frac{1}{N}R_{N,s}(a^{(p)})\,, \tag{4.66}$$

$$\tau^s\mathrm{A}(a^{(p)}) \;=\; \sum_{k=0}^{K-1}\mathrm{A}\big(F_s^{(k,0)}(a^{(p)})\big) + \tau^s_{\geqslant K}\mathrm{A}(a^{(p)})\,. \tag{4.67}$$

To avoid cluttering the notation, from now on we drop the parentheses of the linear map $F_s^{(k,0)}$. We iterate (4.66) m times by applying it to its first term and get

$$\begin{aligned}(\widehat{\tau}^s)^m\widehat{\mathrm{A}}_N(a^{(p)}) \;&=\; \sum_{k_1=0}^{K_1-1}\cdots\sum_{k_m=0}^{K_m-1}\widehat{\mathrm{A}}_N\Big(F_s^{(k_m,0)}F_s^{(k_{m-1},0)}\cdots F_s^{(k_1,0)}a^{(p)}\Big)\\
&+(\widehat{\tau}^s)^{m-1}\widehat{\tau}^s_{\geqslant K_1}\widehat{\mathrm{A}}_N(a^{(p)}) + \sum_{j=1}^{m-1}\sum_{k_1=0}^{K_1-1}\cdots\sum_{k_j=0}^{K_j-1}(\widehat{\tau}^s)^{m-1-j}\widehat{\tau}^s_{\geqslant K_{j+1}}\widehat{\mathrm{A}}_N\Big(F_s^{(k_j,0)}F_s^{(k_{j-1},0)}\cdots F_s^{(k_1,0)}a^{(p)}\Big)\\
&+\frac{1}{N}(\widehat{\tau}^s)^{m-1}R_{N,s}(a^{(p)}) + \frac{1}{N}\sum_{j=1}^{m-1}\sum_{k_1=0}^{K_1-1}\cdots\sum_{k_j=0}^{K_j-1}(\widehat{\tau}^s)^{m-1-j}R_{N,s}\big(F_s^{(k_j,0)}\cdots F_s^{(k_1,0)}a^{(p)}\big)\,.\end{aligned} \tag{4.68}$$

A similar expression without the third line holds for $(\tau^s)^m\mathrm{A}(a^{(p)})$.

In order to control this somewhat unpleasant expression, we abbreviate

$$x := \sqrt{\frac{s}{\rho(\kappa,1)}}\,.$$

Assume that $x < 1$. Then (4.45) and (4.48) imply the estimates, valid on $\mathcal{H}_+^{(N)}$,

$$\begin{aligned}\big\|F_s^{(k,0)}\,a^{(p)}\big\| \;&\leqslant\; 4^p\|a^{(p)}\|\,x^k\,,\\
\big\|\widehat{\tau}^s_{\geqslant K}\widehat{\mathrm{A}}_N(a^{(p)})\big\| \;&\leqslant\; 4^p\|a^{(p)}\|\,\frac{x^K}{1-x}\,,\\
\big\|R_{N,s}(a^{(p)})\big\| \;&\leqslant\; (4\mathrm{e})^p\|a^{(p)}\|\,\frac{x}{(1-x)^3}\,.\end{aligned}$$

Furthermore, (4.54) implies that

$$\big\|\tau^s_{\geqslant K}\mathrm{A}(a^{(p)})\big\|_{L^\infty(B_1)} \;\leqslant\; 4^p\|a^{(p)}\|\,\frac{x^K}{1-x}\,.$$

We also need

$$\begin{aligned}
\left|\left\langle \varphi^{\otimes N}, \widehat{\mathrm{A}}_N(a^{(p)})\varphi^{\otimes N}\right\rangle - \mathrm{A}(a^{(p)})(\varphi)\right| \;&=\; \left|\frac{N\cdots(N-p+1)}{N^p} - 1\right|\left|\mathrm{A}(a^{(p)})(\varphi)\right| \\
&\leqslant\; \sum_{j=1}^{p-1}\left|\frac{N\cdots(N-j)}{N^{j+1}} - \frac{N\cdots(N-j+1)}{N^j}\right|\|a^{(p)}\| \\
&\leqslant\; \frac{p^2}{N}\|a^{(p)}\|\,. \qquad (4.69)
\end{aligned}$$

Armed with these estimates we may now complete the proof of Theorem 4.15. Suppose that $1/2 \leqslant x < 1$. Then

$$\begin{aligned}
\sum_{k_1=0}^{K_1-1}\cdots\sum_{k_m=0}^{K_m-1}\Big|\Big\langle \varphi^{\otimes N}\,,\, \widehat{\mathrm{A}}_N\Big(F_s^{(k_m,0)}F_s^{(k_{m-1},0)}\cdots F_s^{(k_1,0)}a^{(p)}\Big)\,\varphi^{\otimes N}\Big\rangle& \\
-\,\mathrm{A}\Big(F_s^{(k_m,0)}F_s^{(k_{m-1},0)}\cdots F_s^{(k_1,0)}a^{(p)}\Big)(\varphi)\Big|& \\
\leqslant\; \frac{1}{N}(p+K_1+\cdots+K_m)^2\,4^{m(p+K_1+\cdots+K_m)}\,\|a^{(p)}\|\,.&
\end{aligned}$$

Similarly, the second line of (4.68) on $\mathcal{H}_+^{(N)}$ and its classical equivalent on B_1 are bounded by

$$\sum_{j=1}^{m} x^{K_j}\,4^{j(p+K_1+\cdots+K_{j-1})}\,\|a^{(p)}\|\,.$$

Finally, the last line of (4.68) on $\mathcal{H}_+^{(N)}$ is bounded by

$$\frac{1}{N}\sum_{j=1}^{m}4^{(j+1)(p+K_1+\cdots+K_{j-1})}\,\|a^{(p)}\|\,.$$

Now pick m large enough that $T \leqslant ms$. Then it is easy to check that there exist $a_1,\dots,a_m$ such that setting

$$K_j \;=\; a_j\log N\,, \qquad j=1,\dots,m$$

implies that the three above expressions are all bounded by $CN^{-\beta}\|a^{(p)}\|$, for some $\beta > 0$. This remains of course true for all $m' \leqslant m$. Since any time $t \leqslant T$ can be reached by at most m iterations with $1/2 \leqslant x < 1$, the claim follows. □

We conclude with a short discussion on density matrices. First we recall some standard results; see for instance [RS80]. Let $\Gamma \in \mathcal{L}^1$, where $\mathcal{L}^1$ is the space of trace class operators on some Hilbert space. Equipped with the norm $\|\Gamma\|_1 := \mathrm{Tr}|\Gamma|$, $\mathcal{L}^1$ is a Banach space. Its dual is equal to $\mathcal{L}$, the space of bounded operators, and the dual pairing is given by

$$\langle A,\Gamma\rangle \;=\; \mathrm{Tr}(A\Gamma)\,, \qquad A\in\mathcal{L}\,,\Gamma\in\mathcal{L}^1\,.$$

Therefore,

$$\|\Gamma\|_1 \;=\; \sup_{A\in\mathcal{L},\,\|A\|\leqslant 1}|\mathrm{Tr}(A\Gamma)|\,. \qquad (4.70)$$

Consider an N-particle density matrix $0 \leqslant \Gamma_N \in \mathcal{L}^1(\mathcal{H}_+^{(N)})$ that satisfies $\operatorname{Tr} \Gamma_N = 1$ and is symmetric in the sense that $\Gamma_N P_+ = \Gamma_N$. Define the p-particle marginals

$$\Gamma_N^{(p)} \;:=\; \operatorname{Tr}_{p+1,\dots,N} \Gamma_N \,,$$

where $\operatorname{Tr}_{p+1,\dots,N}$ denotes the partial trace over the coordinates $p+1, \dots, N$. Define furthermore

$$\Gamma_N(t) \;=\; \mathrm{e}^{-\mathrm{i}tH_N} \Gamma_N \mathrm{e}^{\mathrm{i}tH_N} \,,$$

as well as the p-particle marginals $\Gamma_N^{(p)}(t)$ of $\Gamma_N(t)$.

Noting that

$$\operatorname{Tr}\Big(\widehat{\mathrm{A}}_N(a^{(p)})\,\Gamma_N(t)\Big) \;=\; \frac{p!}{N^p}\binom{N}{p} \operatorname{Tr}\big(a^{(p)}\Gamma_N^{(p)}(t)\big) \;=\; \operatorname{Tr}\big(a^{(p)}\Gamma_N^{(p)}(t)\big) + O\Big(\frac{1}{N}\Big)$$

we see that (4.70) and Theorem 4.15 imply the following result.

COROLLARY 4.16. *Let $\varphi \in \mathcal{H}$ with $\|\varphi\| = 1$, and let $\varphi(t)$ be the solution of* (4.53) *with initial data φ. Set $\Gamma_N := (|\varphi\rangle\langle\varphi|)^{\otimes N}$. Then, for any $p \in \mathbb{N}$ and $T > 0$ there exist constants $C, \beta > 0$, depending only on p, T and κ, such that*

$$\Big\|\Gamma_N^{(p)}(t) - \big(|\varphi(t)\rangle\langle\varphi(t)|\big)^{\otimes p}\Big\|_1 \;\leqslant\; \frac{C}{N^\beta}\,, \qquad t \in [0, T]\,.$$

REMARK 4.17. *Actually it is enough for Γ_N to factorize asymptotically. If $(\Gamma_N)_{N\in\mathbb{N}}$ is a sequence of symmetric density matrices satisfying*

$$\lim_{N\to\infty} \big\|\Gamma_N^{(1)} - |\varphi\rangle\langle\varphi|\big\|_1 \;=\; 0\,,$$

then one finds

$$\lim_{N\to 0} \Big\|\Gamma_N^{(1)}(t) - |\varphi(t)\rangle\langle\varphi(t)|\Big\|_1 \;=\; 0\,, \qquad t \in \mathbb{R}\,.$$

This is a straightforward corollary of the proof of Theorem 4.15. By a well-known argument (see for instance Lemmas 5.1 and 5.3 in Chapter 5), this implies that

$$\lim_{N\to 0} \Big\|\Gamma_N^{(p)}(t) - \big(|\varphi(t)\rangle\langle\varphi(t)|\big)^{\otimes p}\Big\|_1 \;=\; 0\,, \qquad t \in \mathbb{R}\,.$$

for all p.

4.6. The mean-field limit of a Fermi gas

In this section we consider a Fermi gas and show that its mean-field dynamics is governed by the Hartree-Fock equation. The Hartree-Fock equation is a fundamental tool, used throughout physics and chemistry, for describing a system consisting of a large number of fermions. Despite its importance for both conceptual and numerical applications, many questions surrounding it remain unsolved. One area in which significant progress has been made is the microscopic justification of the static Hartree-Fock equation, which is known to yield the correct asymptotic ground state energy of large atoms and molecules; see [LS77a, LS77b, Bac92, FS90, FS94, GS94]. The time-dependent Hartree-Fock equation, which is supposed to describe the dynamics of a large Fermi system, has received less attention. The only work in which this equation is derived from microscopic Hamiltonian dynamics is [BGGM03]. The Cauchy problem for the time-dependent Hartree-Fock equation has also been studied in the literature; see [BPF74, Cha76] and especially [Zag92], where the Cauchy problem is solved for singular interaction potentials.

A key assumption in [BGGM03] is that the interaction potential be bounded. In this section we extend the result of [BGGM03] to a class of singular interaction potentials, which includes the physically relevant Coulomb potential. We also describe how this mean-field result can be formulated as a Egorov-type theorem.

Let us briefly sketch the main result of this section. Consider a sequence of N orthonormal orbitals $\varphi_1, \dots, \varphi_N$, where φ_i is a one-particle wave function. This defines an N-particle fermionic state through the Slater determinant

$$\Psi_N := \varphi_1 \wedge \cdots \wedge \varphi_N .$$

Let $\Psi_N(t)$ be the solution of the Schrödinger equation

$$\mathrm{i}\partial_t \Psi_N(t) = H_N \Psi_N(t) , \qquad \Psi_N(0) = \Psi ,$$

where H_N is the mean-field Hamiltonian (4.1). In general, $\Psi_N(t)$ is no longer a Slater determinant for $t \neq 0$. However, one expects that this holds asymptotically for large N:

$$\Psi_N(t) \approx \varphi_1(t) \wedge \cdots \wedge \varphi_N(t) .$$

Here the orbitals $\varphi_1(t), \dots, \varphi_N(t)$ are supposed to solve the Hartree-Fock equation

$$\mathrm{i}\partial_t \varphi_i = h\varphi_i + \frac{1}{N}\sum_{j=1}^N (w * |\varphi_j|^2)\varphi_i - \frac{1}{N}\sum_{j=1}^N (w * (\varphi_i \bar{\varphi}_j))\, \varphi_j . \tag{4.71}$$

Our main result (Theorem 4.24 below) is a precise formulation of this asymptotic behaviour.

This result is of some physical relevance for studying the dynamics of excited states of electrons in large atoms or molecules in the Born-Oppenheimer approximation. Consider a molecule consisting of K nuclei at fixed positions $R_1, \dots, R_K \in \mathbb{R}^3$, as well as N electrons. The Hamiltonian is given (in appropriate units) by

$$\sum_{i=1}^N \left(-\Delta_i - \sum_{k=1}^K \frac{e_N^2 N z_k}{|x_i - R_k|} \right) + \sum_{1 \leqslant i < j \leqslant N} \frac{e_N^2}{|x_i - x_j|} .$$

Here, e_N is the elementary electric charge which we rescale with N. The electric charge of nucleus k is $e_N N z_k$, where $z_1, \dots, z_K$ are constants chosen so that $\sum_{k=1}^K z_k = 1$. This means that the molecule is electrically neutral. If we choose $e_N = e_0/\sqrt{N}$, for some fixed e_0, the Hamiltonian becomes

$$\sum_{i=1}^N \left(-\Delta_i - \sum_{k=1}^K \frac{e_0^2 z_k}{|x_i - R_k|} \right) + \frac{1}{N} \sum_{1 \leqslant i < j \leqslant N} \frac{e_0^2}{|x_i - x_j|} . \tag{4.72}$$

One problem in the above model, as well as in the works [LS77a, LS77b, Bac92, FS90, FS94, GS94], is that, as N becomes large, relativistic effects should be taken into account. Indeed, a simple argument shows that the average speed of the innermost electron of an atom with atomic number Z behaves like $Z\alpha$ (in units where the speed of light $c = 1$). Another problem in applying the time-dependent Hartree-Fock theory to the dynamics of excited states is that the interaction with the radiation field is neglected. This interaction is responsible for the relaxation of excited states to the ground state of the molecule.

A physical scenario that is quite different from the large atom or molecule described above is an interacting Fermi gas confined to a box of fixed size. As discussed in [NS81, EESY04], the natural scaling in this situation may be viewed as a combination of mean-field and semiclassical scalings. This problem was first studied in [NS81, Spo81]. The authors show that the limiting dynamics is governed by the Vlasov equation. These results were somewhat sharpened in [EESY04], where the authors compare the Hamiltonian dynamics with the dynamics of the Hartree equation, and derive estimates on the rate of convergence.

4.6.1. The Hartree-Fock equation. For simplicity of notation, we only consider spinless fermions in the following; the one-particle Hilbert space is $\mathcal{H} = L^2(\mathbb{R}^3)$. Merely cosmetic modifications extend our results to the case of spin-s fermions for which the one-particle Hilbert space is $L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1}$. To fix ideas, we consider the free Hamiltonian $h := -\Delta$ and a Coulomb two-body interaction potential $w(x) = \kappa|x|^{-1}$. By the generalizations in Section 4.7 below, our results remain valid for a free Hamiltonian of the form $h = -\Delta + v$ and a two-body interaction potential w, where w is even and $v, w \in L^\infty + L^3_w$ are both real. In particular, we may treat Hamiltonians of the form (4.72).

Some notation. It is convenient to state the time-dependent Hartree-Fock equation in terms of an infinite sequence of orbitals $\Psi = (\psi_i)_{i\in\mathbb{N}}$ which is an element of the Hilbert space

$$\tilde{\mathcal{H}} \;:=\; l^2(\mathbb{N}; L^2(\mathbb{R}^3)) \;=\; l^2(\mathbb{N}) \otimes L^2(\mathbb{R}^3)\,.$$

To simplify notation, we set $\alpha = (x, i)$ and write $\Psi(\alpha) = \psi_i(x)$. Furthermore, we abbreviate

$$\int \mathrm{d}\alpha \;:=\; \sum_{i\in\mathbb{N}} \int \mathrm{d}x\,, \qquad \delta(\alpha - \alpha') \;:=\; \delta_{ii'}\delta(x - x')\,.$$

The scalar product on $\tilde{\mathcal{H}}$ is then given by

$$\langle \Psi\,, \Psi' \rangle \;=\; \int \mathrm{d}\alpha \; \bar{\Psi}(\alpha)\Psi'(\alpha)\,.$$

Let $a^{(p)} \in \mathcal{L}(\mathcal{H}^{\otimes p})$ and define $\tilde{a}^{(p)} \in \mathcal{L}(\tilde{\mathcal{H}}^{\otimes p})$ through

$$\tilde{a}^{(p)} \;:=\; \mathbb{1}_{(l^2(\mathbb{N}))^{\otimes p}} \otimes a^{(p)}\,.$$

We have the identity

$$\|\tilde{a}^{(p)}\| \;=\; \|a^{(p)}\|\,. \tag{4.73}$$

Furthermore,

$$\left\langle \Psi^{\otimes p}, \tilde{a}^{(p)} \Psi^{\otimes p} \right\rangle \;=\; \sum_{i_1,\dots,i_p\in\mathbb{N}} \left\langle \psi_{i_1} \otimes \cdots \otimes \psi_{i_p}\,, a^{(p)}\, \psi_{i_1} \otimes \cdots \otimes \psi_{i_p} \right\rangle. \tag{4.74}$$

Hamiltonian formulation of the Hartree-Fock equation. The time-dependent Hartree-Fock equation for Ψ reads

$$\mathrm{i}\partial_t \psi_i \;=\; h\psi_i + \sum_{j\in\mathbb{N}} (w * |\psi_j|^2)\psi_i - \sum_{j\in\mathbb{N}} \big(w * (\psi_i \bar{\psi}_j)\big)\, \psi_j\,. \tag{4.75}$$

It is of interest to note that (4.75) is the Hamiltonian equation of motion of a classical Hamiltonian system with phase space $\Gamma := l^2(\mathbb{N}) \otimes H^1(\mathbb{R}^3)$.

Define the map $\tilde{\mathrm{A}}$ from closed operators $A^{(p)}$ on $\tilde{\mathcal{H}}_+^{(p)}$ to "polynomial" functions on phase space, through

$$\begin{aligned}\tilde{\mathrm{A}}(A^{(p)})(\Psi) &:= \left\langle \Psi^{\otimes p}, A^{(p)}\Psi^{\otimes p}\right\rangle \\ &= \int \mathrm{d}\alpha_1 \cdots \mathrm{d}\alpha_p \, \mathrm{d}\beta_1 \cdots \mathrm{d}\beta_p \; \bar{\Psi}(\alpha_p) \cdots \bar{\Psi}(\alpha_1) A^{(p)}(\alpha_1, \ldots, \alpha_p; \beta_1, \ldots, \beta_p) \, \Psi(\beta_1) \cdots \Psi(\beta_p) \,,\end{aligned}$$

where $A^{(p)}(\alpha_1, \ldots, \alpha_p; \beta_1, \ldots, \beta_p)$ is the distribution kernel of $A^{(p)}$. We denote by $\tilde{\mathfrak{A}}$ the linear hull of functions of the form $\tilde{\mathrm{A}}(A^{(p)})$, with $A^{(p)} \in \mathcal{L}(\tilde{\mathcal{H}}_+^{(p)})$.

The Hamilton function is given by

$$H \; := \; \tilde{\mathrm{A}}(\tilde{h}) + \frac{1}{2}\tilde{\mathrm{A}}(\tilde{\mathcal{W}}) \,, \tag{4.76}$$

where

$$\mathcal{W} \; := \; W(\mathbb{1} - E)$$

with $(E\Phi)(x_1, x_2) := \Phi(x_2, x_1)$ and W is the two-particle operator defined by multiplication by $w(x_1 - x_2)$. Written out in terms of components, (4.76) reads

$$H(\Psi) \; = \; \sum_{i \in \mathbb{N}} \langle \psi_i \, , h\psi_i \rangle + \frac{1}{2} \sum_{i,j \in \mathbb{N}} \big(\langle \psi_i \otimes \psi_j \, , W \, \psi_i \otimes \psi_j \rangle - \langle \psi_i \otimes \psi_j \, , W \, \psi_j \otimes \psi_i \rangle \big) \,.$$

Using Sobolev-type inequalities, one readily sees that H is well-defined on Γ.

A short calculation shows that the Hartree-Fock equation is equivalent to

$$\mathrm{i}\partial_t \Psi \; = \; \partial_{\bar{\Psi}} H(\Psi) \,.$$

The symplectic form on Γ is given by

$$\omega \; = \; \mathrm{i} \int \mathrm{d}\alpha \; \mathrm{d}\bar{\Psi}(\alpha) \wedge \mathrm{d}\Psi(\alpha) \,,$$

which induces the Poisson bracket

$$\{\Psi(\alpha), \bar{\Psi}(\beta)\} \; = \; \mathrm{i}\delta(\alpha - \beta) \,, \qquad \{\Psi(\alpha), \Psi(\beta)\} \; = \; \{\bar{\Psi}(\alpha), \bar{\Psi}(\beta)\} \; = \; 0 \,. \tag{4.77}$$

Thus, for two observables $A, B \in \tilde{\mathfrak{A}}$,

$$\{A, B\} (\Psi) \; = \; \mathrm{i} \int \mathrm{d}\alpha \; \left(\frac{\delta A}{\delta \Psi(\alpha)}(\Psi) \frac{\delta B}{\delta \bar{\Psi}(\alpha)}(\Psi) - \frac{\delta B}{\delta \Psi(\alpha)}(\Psi) \frac{\delta A}{\delta \bar{\Psi}(\alpha)}(\Psi) \right) \,.$$

The Hamiltonian equation of motion on Γ is the Hartree-Fock equation (4.75).

The conservation laws of the Hartree-Fock flow can be understood in terms of symmetries of the Hamiltonian (4.76). One immediately sees that (4.76) is invariant under the rotation $\Psi \mapsto (U \otimes \mathbb{1}_{L^2(\mathbb{R}^3)})\Psi$, where $U \in \mathcal{L}(l^2(\mathbb{N}))$ is unitary. A one-parameter group of such unitary transformations is generated by linear combinations of the functions $\mathrm{Re}\langle \psi_i \, , \psi_j \rangle$ and $\mathrm{Im}\langle \psi_i \, , \psi_j \rangle$, which Poisson-commute with the Hamiltonian (4.76). By Noether's principle, it follows that $\langle \psi_i \, , \psi_j \rangle$ is (at least formally) conserved. The energy H is of course formally conserved as well.

In order to solve the Hartree-Fock equation (4.75) with initial state Ψ, we rewrite it as an integral equation

$$\psi_i(t) \;=\; \mathrm{e}^{-\mathrm{i}th}\psi_i - \mathrm{i}\int_0^t \mathrm{d}s \sum_{j\in\mathbb{N}} \Big((w * |\psi_j(s)|^2)\psi_i(s) - \big(w * (\psi_i(s)\bar{\psi}_j(s))\big)\,\psi_j(s)\Big)\,. \tag{4.78}$$

The Cauchy-problem for (4.78) was solved in [Zag92]. We quote the relevant results:

LEMMA 4.18. *Let $\Psi \in \tilde{\mathcal{H}}$. Then* (4.78) *has a unique global solution $\Psi(\cdot) \in C(\mathbb{R}; \tilde{\mathcal{H}})$. Furthermore, the quantities $\langle \psi_i\,, \psi_j\rangle$ are conserved. In particular, $\|\Psi(t)\| = \|\Psi\|$.*

A Schwinger-Dyson expansion for the Hartree-Fock equation. Our main tool is the Schwinger-Dyson expansion for the flow of the Hartree-Fock equation. We use the notation $(\cdot)_t$ to denote free time evolution generated by the free Hamiltonian $\tilde{\mathrm{A}}(\tilde{h})$. Explicitly,

$$A_t(\psi_1, \psi_2, \dots) \;=\; A\big(\mathrm{e}^{-\mathrm{i}th}\psi_1, \mathrm{e}^{-\mathrm{i}th}\psi_2, \dots\big)\,.$$

LEMMA 4.19. *Let $A \in \tilde{\mathfrak{A}}$, $\nu > 0$, and $\Psi(t)$ be the solution of* (4.78) *with initial data Ψ. Then, for small times t,*

$$\begin{aligned} A(\Psi(t)) \;&=\; A_t(\Psi) + \int_0^t \mathrm{d}s\, \frac{1}{2}\{\tilde{\mathrm{A}}(\tilde{\mathcal{W}}), A_{t-s}\}(\Psi(s)) \\ &=\; \sum_{k=0}^{\infty} \frac{1}{2^k} \int_{\Delta^k(t)} \mathrm{d}\underline{t}\, \Big\{\tilde{\mathrm{A}}(\tilde{\mathcal{W}}_{t_k}), \dots \big\{\tilde{\mathrm{A}}(\tilde{\mathcal{W}}_{t_1}), A_t\big\}\Big\}(\Psi)\,, \end{aligned}$$

uniformly for $\Psi \in B_\nu := \{\Psi \in \tilde{\mathcal{H}} \,:\, \|\Psi\|^2 \leqslant \nu\}$.

PROOF. The proof of Lemma 4.12 applies with virtually no modifications. One uses (4.73), the identity

$$\tilde{\mathrm{A}}(\tilde{\mathcal{W}})_t \;=\; \tilde{\mathrm{A}}(\tilde{\mathcal{W}}_t) \;=\; \tilde{\mathrm{A}}\big((W_t(\mathbb{1} - E))\tilde{\ }\big)\,,$$

and $\|E\| = 1$. $\square$

4.6.2. The density matrix Hartree-Fock equation. From now on, we only work with orthogonal sequence of orbitals belonging to

$$\mathcal{K} \;:=\; \{\Psi \in \tilde{\mathcal{H}} \,:\, \langle \psi_i\,, \psi_j\rangle = 0,\, i \neq j\}\,.$$

By Lemma 4.18, $\Psi \in \mathcal{K}$ implies that $\Psi(t) \in \mathcal{K}$ for all t. To each sequence of orbitals Ψ we assign a one-particle density matrix

$$\gamma_\Psi \;:=\; \sum_{i\in\mathbb{N}} |\psi_i\rangle\langle\psi_i|\,.$$

It is easy to see that this defines a mapping from $\mathcal{K}$ onto the set of density matrices

$$\mathcal{D} \;:=\; \big\{\gamma \in \mathcal{L}^1(\mathcal{H}) \,:\, \gamma \geqslant 0\big\}\,.$$

Furthermore,

$$\|\gamma_\Psi\|_1 \;=\; \|\Psi\|^2\,.$$

Conversely, one may recover Ψ from γ_Ψ, up to ordering of the orbitals, by spectral decomposition. Furthermore, (4.74) implies that

$$\tilde{\mathrm{A}}(\tilde{a}^{(p)})(\Psi) \;=\; \mathrm{Tr}(a^{(p)}\gamma_\Psi^{\otimes p})\,. \tag{4.79}$$

Let $\Psi(t)$ be a solution of (4.75) with initial data Ψ and write

$$\gamma(t) \;=\; \gamma_{\Psi(t)}\,.$$

Then a short calculation shows that

$$\mathrm{i}\partial_t\gamma \;=\; [h,\gamma] + \mathrm{Tr}_2\,[\mathcal{W},\gamma\otimes\gamma]\;, \tag{4.80}$$

which is the Hartree-Fock equation for density matrices. As an integral equation in the interaction picture, this reads

$$\gamma(t) \;=\; \mathrm{e}^{-\mathrm{i}th}\,\gamma\,\mathrm{e}^{\mathrm{i}th} - \mathrm{i}\int_0^t \mathrm{d}s\;\mathrm{e}^{-\mathrm{i}(t-s)h}\;\mathrm{Tr}_2\,[\mathcal{W},\gamma(s)\otimes\gamma(s)]\;\mathrm{e}^{\mathrm{i}(t-s)h}\,. \tag{4.81}$$

Sometimes it is convenient to rewrite this using the shorthand

$$\tilde{\gamma}(t) \;:=\; \mathrm{e}^{\mathrm{i}th}\,\gamma(t)\,\mathrm{e}^{-\mathrm{i}th}\,. \tag{4.82}$$

Then (4.81) is equivalent to

$$\tilde{\gamma}(t) \;=\; \gamma - \mathrm{i}\int_0^t \mathrm{d}s\;\;\mathrm{Tr}_2\,[\mathcal{W}_s,\tilde{\gamma}(s)\otimes\tilde{\gamma}(s)]\;. \tag{4.83}$$

LEMMA 4.20. *Let $\Psi(t)$ be the solution of* (4.78)*. Then $\gamma_{\Psi(t)}$ solves* (4.81)*.*

PROOF. Let $a^{(1)} \equiv a \in \mathcal{L}(\mathcal{H})$. From Lemma 4.19 we get

$$\tilde{\mathrm{A}}(\tilde{a})(\Psi(t)) \;=\; \tilde{\mathrm{A}}(\tilde{a}_t)(\Psi) + \int_0^t \mathrm{d}s\;\big\{\tilde{\mathrm{A}}(\tilde{\mathcal{W}}),\tilde{\mathrm{A}}(\tilde{a}_{t-s})\big\}(\Psi(s))\,. \tag{4.84}$$

Now (4.77) and (4.79) imply

$$\begin{aligned}\big\{\tilde{\mathrm{A}}(\tilde{\mathcal{W}}),\tilde{\mathrm{A}}(\tilde{a})\big\}(\Psi) \;&=\; \mathrm{i}\tilde{\mathrm{A}}\big(\big[\tilde{\mathcal{W}},\tilde{a}\otimes\mathbb{1}\big]\big)(\Psi)\\ &=\; \mathrm{i}\,\mathrm{Tr}\big(\big[\mathcal{W},a\otimes\mathbb{1}\big]\gamma_\Psi\otimes\gamma_\Psi\big)\\ &=\; -\mathrm{i}\,\mathrm{Tr}\big((a\otimes\mathbb{1})\big[\mathcal{W},\gamma_\Psi\otimes\gamma_\Psi\big]\big)\,.\end{aligned}$$

Thus (4.84) reads

$$\begin{aligned}\mathrm{Tr}(a\,\gamma_{\Psi(t)}) \;&=\; \mathrm{Tr}(a_t\,\gamma_\Psi) - \mathrm{i}\int_0^t \mathrm{d}s\;\;\mathrm{Tr}\big((a_{t-s}\otimes\mathbb{1})\big[\mathcal{W},\gamma_{\Psi(s)}\otimes\gamma_{\Psi(s)}\big]\big)\\ &=\; \mathrm{Tr}\big(a\,\mathrm{e}^{\mathrm{i}th}\gamma_\Psi\mathrm{e}^{-\mathrm{i}th}\big) - \mathrm{i}\int_0^t \mathrm{d}s\;\;\mathrm{Tr}\Big(a\,\mathrm{e}^{-\mathrm{i}(t-s)h}\;\mathrm{Tr}_2\,\big[\mathcal{W},\gamma_{\Psi(s)}\otimes\gamma_{\Psi(s)}\big]\;\mathrm{e}^{\mathrm{i}(t-s)h}\Big)\,.\end{aligned}$$

Since $a \in \mathcal{L}(\mathcal{H})$ was arbitrary, this is equivalent to (4.81). $\square$

4.6.3. Slater determinants. The Hartree-Fock equation naturally describes the time evolution of quasi-free states [BR02]. Let ω_γ be the quasi-free state corresponding to the one-particle state $\gamma \in \mathcal{D}$. Define

$$\gamma^{(p)}(x_1, \dots, x_p; y_1, \dots, y_p) \;:=\; \omega_\gamma \left(a^*(y_p) \cdots a^*(y_1) a(x_1) \cdots a(x_p)\right) ,$$

where $a^*(x), a(x)$ are the fermionic creation and annihilation operators. The quasifreeness of ω_γ means that

$$\gamma^{(p)}(x_1, \dots, x_p; y_1, \dots, y_p) \;=\; \det \left(\gamma(x_i; y_j)\right)_{i,j} .$$

In other words, $\gamma^{(p)}$ is the operator kernel of

$$\gamma^{(p)} \;=\; \gamma^{\otimes p}\, \Sigma_-^{(p)} , \tag{4.85}$$

where

$$\Sigma_-^{(p)} \;:=\; p! P_-^{(p)} .$$

For the following calculations it is convenient to introduce the symbol $\varepsilon_{i_1 \dots i_p}^{j_1 \dots j_p}$, which is equal to $\operatorname{sgn} \sigma$ if $i_1, \dots, i_p$ are disjoint and there is a permutation $\sigma \in S_p$ such that $(i_1, \dots, i_p) = (j_{\sigma(1)}, \dots, j_{\sigma(p)})$, and equal to 0 otherwise. Also, for the remainder of this section, summation over any index appearing twice in an equation is implied.

LEMMA 4.21. *Let $\gamma \in \mathcal{D}$ with $\operatorname{Tr} \gamma = 1$. Then $\operatorname{Tr} \gamma^{(p)} \leqslant 1$.*

PROOF. There is an orthonormal basis $(\varphi_i)_{i \in \mathbb{N}}$ and a sequence of nonnegative numbers $(\lambda_i)_{i \in \mathbb{N}}$ such that $\sum_i \lambda_i = 1$ and $\gamma = \sum_i \lambda_i |\varphi_i\rangle\langle\varphi_i|$. Therefore,

$$\gamma^{(p)} \;=\; \varepsilon_{i_1 \dots i_p}^{j_1 \dots j_p} \lambda_{i_1} \cdots \lambda_{i_p} |\varphi_{i_1} \otimes \cdots \otimes \varphi_{i_p}\rangle\langle\varphi_{j_1} \otimes \cdots \otimes \varphi_{j_p}|$$

This yields

$$\begin{aligned}
\operatorname{Tr} \gamma^{(p)} \;&=\; \varepsilon_{i_1 \dots i_p}^{j_1 \dots j_p} \lambda_{i_1} \cdots \lambda_{i_p} \delta_{i_1 k_1} \cdots \delta_{i_p k_p} \delta_{j_1 k_1} \cdots \delta_{j_p k_p} \\
&=\; \sum_{i_1, \dots, i_p \text{ disjoint}} \lambda_{i_1} \cdots \lambda_{i_p} \\
&\leqslant\; \sum_{i_1, \dots, i_p} \lambda_{i_1} \cdots \lambda_{i_p} \;=\; 1 .
\end{aligned}$$

□

Next, we introduce a special class of quasi-free states, described by *Slater determinants.* Let $N \in \mathbb{N}$ and take an orthonormal sequence of orbitals $\Phi_N = (\varphi_1, \dots, \varphi_N)$. We define the Slater determinant

$$S(\Phi_N) \;:=\; \varphi_1 \wedge \cdots \wedge \varphi_N \;:=\; \sqrt{N!}\, P_-^{(N)}\, \varphi_1 \otimes \cdots \otimes \varphi_N \;\in\; \mathcal{H}_-^{(N)} .$$

Note that the normalization is chosen so that $\|S(\Phi_N)\| = 1$. The corresponding N-particle density matrix is

$$\Gamma_N \;:=\; |S(\Phi_N)\rangle\langle S(\Phi_N)| .$$

One finds for the p-particle marginals

$$\begin{aligned}
\Gamma_N^{(p)} \;&:=\; \operatorname{Tr}_{p+1 \dots N} \Gamma_N \\
&=\; \operatorname{Tr}_{p+1 \dots N} \frac{1}{N!}\, \varepsilon_{i_1 \dots i_N} \varepsilon_{j_1 \dots j_N} \left|\varphi_{i_1} \otimes \cdots \otimes \varphi_{i_N}\right\rangle\!\left\langle\varphi_{j_1} \otimes \cdots \otimes \varphi_{j_N}\right| \\
&=\; \frac{(N-p)!}{N!}\, \varepsilon_{i_1 \dots i_p}^{j_1 \dots j_p} \left|\varphi_{i_1} \otimes \cdots \otimes \varphi_{i_p}\right\rangle\!\left\langle\varphi_{j_1} \otimes \cdots \otimes \varphi_{j_p}\right| .
\end{aligned} \tag{4.86}$$

In order to relate the sequence Φ_N to the results of the previous sections, we define the normalized sequence

$$\Psi_N \;:=\; \frac{1}{\sqrt{N}}(\varphi_1, \dots, \varphi_N, 0, \dots)\,. \tag{4.87}$$

Thus, $\Psi_N \in \mathcal{K}$ and $\|\Psi_N\| = 1$. It is trivial to check that $\Psi_N(t)$ is a solution of (4.75) if and only if $\Phi_N(t)$ is a solution of (4.71). Similarly, $\Psi_N(t)$ is a solution of (4.78) if and only if $\Phi_N(t) = (\varphi_1(t), \dots, \varphi_N(t))$ is a solution of

$$\varphi_i(t) \;=\; \mathrm{e}^{-\mathrm{i}th}\varphi_i - \frac{\mathrm{i}}{N}\int_0^t \mathrm{d}s \, \sum_{j=1}^N \big((w * |\varphi_j(s)|^2)\varphi_i(s) - (w * (\varphi_i(s)\bar{\varphi}_j(s)))\, \varphi_j(s)\big)\,. \tag{4.88}$$

Next, from (4.86) we find

$$\gamma_N \;:=\; \Gamma_N^{(1)} \;=\; \frac{1}{N}\sum_{i=1}^N |\varphi_i\rangle\langle\varphi_i| \;=\; \sum_{i\in\mathbb{N}} |\psi_i\rangle\langle\psi_i| \;=\; \gamma_{\Psi_N}\,.$$

Thus (4.85) implies that

$$\gamma_N^{(p)} \;=\; \frac{1}{N^p}\,\varepsilon^{j_1\dots j_p}_{i_1\dots i_p}\,\big|\varphi_{i_1}\otimes\cdots\otimes\varphi_{i_p}\big\rangle\big\langle\varphi_{j_1}\otimes\cdots\otimes\varphi_{j_p}\big| \;=\; \frac{p!}{N^p}\binom{N}{p}\,\Gamma_N^{(p)}\,. \tag{4.89}$$

Thus, Slater determinants determine quasi-free states by their reduced p-particle marginals. The normalization $\frac{p!}{N^p}\binom{N}{p}$ differs slightly from the usual normalization 1 of quasi-free states, but in the limit $N \to \infty$ this difference vanishes.

An immediate consequence of (4.89) is

$$\big\langle S(\Phi_N)\,, \widehat{\mathrm{A}}_N(a^{(p)})\, S(\Phi_N)\big\rangle \;=\; \mathrm{Tr}(a^{(p)}\gamma_N^{(p)})\,. \tag{4.90}$$

Note also that

$$\|\gamma_N\| \;=\; \frac{1}{N}\,. \tag{4.91}$$

This is a special case of the well-known statement (see e.g. [LL01]) that $\big\|\mathrm{Tr}_{2\dots N}\,\Gamma\big\| \leqslant N^{-1}$, for any N-particle density matrix Γ [4].

4.6.4. Proof of convergence and the mean-field limit. We now turn to our main argument. We show that the Hartree-Fock time evolution is asymptotically ($N \to \infty$) given by the tree terms (i.e. the terms $l = 0$) of the Schwinger-Dyson series (4.20). This result is summarized in Lemma 4.23 below.

Let $\Psi = (\psi_i)_{i=1}^\infty \in \mathcal{K}$, and denote by $\Psi(t)$ the solution of the Hartree-Fock equation (4.78) with initial data Ψ. Let $\gamma(t) = \gamma_{\Psi(t)}$ be the associated one-particle density matrix.

By choosing $A = \tilde{\mathrm{A}}(\tilde{a}^{(p)})$, $a^{(p)} \in \mathcal{L}(\mathcal{H}_-^{(p)})$, in Lemma 4.19 and mimicking the proof of Lemma 4.20 one finds that

$$\mathrm{Tr}\big(a^{(p)}\,\gamma(t)^{\otimes p}\big) \;=\; \mathrm{Tr}\big(a_t^{(p)}\gamma^{\otimes p}\big) - \mathrm{i}\int_0^t \mathrm{d}s \sum_{i=1}^p \mathrm{Tr}\Big(a_{t-s}^{(p)}\,\mathrm{Tr}_{p+1}\big[\mathcal{W}_{i\,p+1}, \gamma(s)^{\otimes(p+1)}\big]\Big)\,. \tag{4.92}$$

[4] This can also be inferred from (4.91) by writing Γ as a linear combination of projectors.

It is convenient to use the representation $\tilde{\gamma}(t)$ defined in (4.82). Using the substitution $a^{(p)} \mapsto a^{(p)}_{-t}$ in (4.92) we get

$$\operatorname{Tr}\big(a^{(p)}\,\tilde{\gamma}(t)^{\otimes p}\big) \;=\; \operatorname{Tr}\big(a^{(p)}\gamma^{\otimes p}\big) - \mathrm{i}\int_0^t \mathrm{d}s \sum_{i=1}^p \operatorname{Tr}\Big(a^{(p)}\operatorname{Tr}_{p+1}\big[\mathcal{W}_{i\,p+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}\big]\Big)\,.$$

Recall that $\mathcal{W}_{ij} = W_{ij}(\mathbb{1} - E_{ij})$. Also, E_{ij} commutes with W_{ij} and with $\tilde{\gamma}(s)^{\otimes(p+1)}$. Thus, $\Sigma^{(p)}_- a^{(p)} = p!\,a^{(p)}$ implies

$$\tilde{\gamma}(t)^{\otimes p}\,\Sigma^{(p)}_- \;=\; \gamma^{\otimes p}\,\Sigma^{(p)}_- - \mathrm{i}\int_0^t \mathrm{d}s\; \operatorname{Tr}_{p+1}\left[\sum_{i=1}^p W_{ip+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}(\mathbb{1} - E_{ip+1})\right]\Sigma^{(p)}_-. \tag{4.93}$$

On the other hand, using

$$\Sigma^{(p+1)}_- \;=\; \left(\mathbb{1} - \sum_{j=1}^p E_{jp+1}\right)\Sigma^{(p)}_-$$

we find

$$\begin{aligned}\operatorname{Tr}_{p+1}\left[\sum_{i=1}^p W_{ip+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}\,\Sigma^{(p+1)}_-\right] \;&=\; \operatorname{Tr}_{p+1}\left[\sum_{i=1}^p W_{ip+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}\left(\mathbb{1} - \sum_{j=1}^p E_{jp+1}\right)\Sigma^{(p)}_-\right]\\ &=\; \operatorname{Tr}_{p+1}\left[\sum_{i=1}^p W_{ip+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}\left(\mathbb{1} - \sum_{j=1}^p E_{jp+1}\right)\right]\Sigma^{(p)}_-\,.\end{aligned}$$

Together with (4.93) this yields

$$\tilde{\gamma}(t)^{\otimes p}\,\Sigma^{(p)}_- \;=\; \gamma^{\otimes p}\,\Sigma^{(p)}_- - \mathrm{i}\int_0^t \mathrm{d}s\; \operatorname{Tr}_{p+1}\left[\sum_{i=1}^p W_{ip+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}\,\Sigma^{(p+1)}_-\right] + R_p(t)\,, \tag{4.94}$$

with an error term

$$R_p(t) \;:=\; -\mathrm{i}\sum_{1\leqslant i\neq j\leqslant p}\int_0^t \mathrm{d}s\; \operatorname{Tr}_{p+1}\left[W_{ip+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}E_{jp+1}\right]\Sigma^{(p)}_-. \tag{4.95}$$

The partial trace is most conveniently computed using operator kernels. We find

$$\begin{aligned}&\Big(W_{ip+1,s}\tilde{\gamma}(s)^{\otimes(p+1)}E_{jp+1}\Big)(x_1,\dots,x_{p+1};y_1,\dots,y_{p+1})\\ &= \int \mathrm{d}z_1\,\mathrm{d}z_2\left[\prod_{r\neq i,j}\tilde{\gamma}(s)(x_r;y_r)\right] W_s(x_i,x_{p+1};z_1,z_2)\,\tilde{\gamma}(s)(z_1;y_i)\,\tilde{\gamma}(s)(x_j;y_{p+1})\,\tilde{\gamma}(s)(z_2;y_j)\,,\end{aligned}$$

so that

$$\begin{aligned}&\operatorname{Tr}_{p+1}\Big(W_{ip+1,s}\tilde{\gamma}(s)^{\otimes(p+1)}E_{jp+1}\Big)(x_1,\dots,x_p;y_1,\dots,y_p)\\ &= \int \mathrm{d}z_1\,\mathrm{d}z_2\,\mathrm{d}z_3\left[\prod_{r\neq i,j}\tilde{\gamma}(s)(x_r;y_r)\right] W_s(x_i,z_3;z_1,z_2)\,\tilde{\gamma}(s)(z_1;y_i)\,\tilde{\gamma}(s)(x_j;z_3)\,\tilde{\gamma}(s)(z_2;y_j)\\ &= \big(\tilde{\gamma}_j(s)W_{ij,s}\tilde{\gamma}(s)^{\otimes p}\big)(x_1,\dots,x_p;y_1,\dots,y_p)\,.\end{aligned}$$

The second term of the commutator in (4.95) is the adjoint of the first and we get

$$\begin{aligned} R_p(t) &= -\mathrm{i} \sum_{1 \leqslant i \neq j \leqslant p} \int_0^t \mathrm{d}s \, \Big(\tilde{\gamma}_j(s) W_{ij,s} \tilde{\gamma}(s)^{\otimes p} - \tilde{\gamma}(s)^{\otimes p} W_{ij,s} \tilde{\gamma}_j(s) \Big) \Sigma_-^{(p)} \\ &= -\mathrm{i} \sum_{1 \leqslant i \neq j \leqslant p} \int_0^t \mathrm{d}s \, \Big(\tilde{\gamma}_j(s) W_{ij,s} \tilde{\gamma}(s)^{\otimes p} \Sigma_-^{(p)} - \tilde{\gamma}(s)^{\otimes p} \Sigma_-^{(p)} W_{ij,s} \tilde{\gamma}_j(s) \Big) \,. \end{aligned} \tag{4.96}$$

We proceed to show that, up to an error term, the expansion of the Hartree-Fock time-evolution is equal to the tree terms of the microscopic quantum-mechanical evolution. Let $a^{(p)} \in \mathcal{L}(\mathcal{H}_-^{(p)})$. Using (4.94) we find

$$\begin{aligned} \mathrm{Tr}\left(a^{(p)} \, \gamma(t)^{\otimes p} \, \Sigma_-^{(p)}\right) &= \mathrm{Tr}\left(a_t^{(p)} \, \tilde{\gamma}(t)^{\otimes p} \, \Sigma_-^{(p)}\right) \\ &= \mathrm{Tr}\left(a_t^{(p)} \, \gamma^{\otimes p} \, \Sigma_-^{(p)}\right) + \mathrm{i} \int_0^t \mathrm{d}s \sum_{i=1}^p \mathrm{Tr}\left(\left[W_{i\,p+1,s}, a_t^{(p)} \otimes \mathbb{1} \right] \, \tilde{\gamma}(s)^{\otimes(p+1)} \, \Sigma_-^{(p+1)} \right) \\ &\quad + \mathrm{Tr}\left(a_t^{(p)} \, R_p(t) \right) \,. \end{aligned}$$

Iterating this K times yields our main expansion

$$\begin{aligned} \mathrm{Tr}\left(a_t^{(p)} \, \tilde{\gamma}(t)^{\otimes p} \, \Sigma_-^{(p)}\right) &= \sum_{k=0}^{K-1} \int_{\Delta^k(t)} \mathrm{d}\underline{t} \; \mathrm{Tr}\left(F_{t,\underline{t}}^{(k,0)}(a^{(p)}) \, \gamma^{\otimes(p+k)} \Sigma_-^{(p+k)} \right) \\ &\quad + \int_{\Delta^K(t)} \mathrm{d}\underline{t} \; \mathrm{Tr}\left(F_{t,\underline{t}}^{(K,0)}(a^{(p)}) \, \tilde{\gamma}(t_K)^{\otimes(p+K)} \Sigma_-^{(p+K)} \right) \\ &\quad + \sum_{k=0}^{K-1} \sum_{1 \leqslant i \neq j \leqslant p+k} R_{ij}^k(t) \,, \end{aligned} \tag{4.97}$$

where

$$\begin{aligned} R_{ij}^k(t) := -\mathrm{i} \int_{\Delta^{k+1}(t)} \mathrm{d}\underline{t} \; \mathrm{Tr}\Big(& F_{t,t_1,\dots,t_k}^{(k,0)}(a^{(p)}) \, \tilde{\gamma}_j(t_{k+1}) \, W_{ij,t_{k+1}} \, \tilde{\gamma}(t_{k+1})^{\otimes(p+k)} \, \Sigma_-^{(p+k)} \\ & - W_{ij,t_{k+1}} \, \tilde{\gamma}_j(t_{k+1}) \, F_{t,t_1,\dots,t_k}^{(k,0)}(a^{(p)}) \, \tilde{\gamma}(t_{k+1})^{\otimes(p+k)} \, \Sigma_-^{(p+k)} \Big) \,. \end{aligned}$$

We now derive a bound on $R_{ij}^k(t)$. Let us concentrate on the first term, which we rewrite using the renaming $t_{k+1} \to s$ as

$$\int_{\Delta^k(t)} \mathrm{d}\underline{t} \int_0^{\wedge \underline{t}} \mathrm{d}s \; \mathrm{Tr}\left(F_{t,t_1,\dots,t_k}^{(k,0)}(a^{(p)}) \, \tilde{\gamma}_j(s) \, W_{ij,s} \, \tilde{\gamma}(s)^{\otimes(p+k)} \, \Sigma_-^{(p+k)} \right) \,, \tag{4.98}$$

where $\wedge \underline{t} := \min\{t_1, \dots, t_k\}$. The idea is to use a tree expansion on $\tilde{\gamma}(s)$.

LEMMA 4.22. *Let $a^{(p)} \in \mathcal{L}(\mathcal{H}_-^{(p)})$. For small times we have the tree expansion*

$$\mathrm{Tr}\big(a^{(p)} \tilde{\gamma}(t)^{\otimes p} \Sigma_-^{(p)}\big) = \sum_{k=0}^{\infty} \int_{\Delta^k(t)} \mathrm{d}\underline{t} \; \mathrm{Tr}\big(T_{\underline{t}}^{(k)}(a^{(p)}) \gamma^{\otimes(p+k)} \Sigma_-^{(p)} \big) \,, \tag{4.99}$$

where $T_{\underline{t}}^{(k)}$ is the linear operator defined by $T^{(0)}(a^{(p)}) := a^{(p)}$ and

$$T_{t_1 \dots t_k}^{(k)}(a^{(p)}) = \mathrm{i} \sum_{i=1}^{p+k-1} \left[\mathcal{W}_{i\,p+k,t_k}, T_{t_1 \dots t_{k-1}}^{(k-1)}(a^{(p)}) \otimes \mathbb{1} \right] \,.$$

PROOF. Lemma 4.19 applied to $A = \tilde{\mathrm{A}}(\tilde{a}^{(p)})$ yields

$$\mathrm{Tr}\big(a^{(p)}\tilde{\gamma}(t)^{\otimes p}\big) \;=\; \sum_{k=0}^{\infty}\int_{\Delta^k(t)} \mathrm{d}\underline{t}\;\mathrm{Tr}\big(T_{\underline{t}}^{(k)}(a^{(p)})\gamma^{\otimes(p+k)}\big)\,.$$

The claim then follows by noting that $\Sigma_-^{(p)}a^{(p)} = p!a^{(p)}$ and that $\sum_{i=1}^{p+k-1}\mathcal{W}_{i\,p+k,t_k}$ commutes with $\Sigma_-^{(p)}$. The convergence of the series is shown below. □

Thus (4.98) is equal to

$$\sum_{k'=0}^{\infty}\int_{\Delta^k(t)}\mathrm{d}\underline{t}\int_0^{\wedge\underline{t}}\mathrm{d}s\int_{\Delta^{k'}(s)}\mathrm{d}\underline{t}'\;\mathrm{Tr}\Big\{T_{\underline{t}'}^{(k')}\Big(F_{t,\underline{t}}^{(k,0)}(a^{(p)})\tilde{\gamma}_j(s)W_{ij,s}\Big)\gamma^{\otimes(p+k+k')}\Sigma_-^{(p+k)}\Big\}\,.$$

Next, we recall from (4.44) that $F_{t,t_1,\dots,t_k}^{(k,0)}(a^{(p)})$ can be written as a sum over tree graphs $Q\in\mathcal{Q}(p,k,0)$ of elementary terms of the form (4.33). Also, since the definition of $T_{t_1,\dots,t_k}^{(k)}(a^{(p)})$ is the same as the definition of $F_{0,t_1,\dots,t_k}^{(k,0)}(a^{(p)})$ with W replaced by $\mathcal{W}$, we immediately get that $T_{t_1,\dots,t_k}^{(k)}(a^{(p)})$ is equal to a sum over tree graphs $Q\in\mathcal{Q}(p,k,0)$ of elementary terms of the form

$$P_-\,\mathcal{W}_{i_1j_1,t_{v_1}}\cdots\mathcal{W}_{i_rj_r,t_{v_r}}\,\big(a_t^{(p)}\otimes\mathbb{1}^{(k-l)}\big)\,\mathcal{W}_{i_{r+1}j_{r+1},t_{v_{r+1}}}\cdots\mathcal{W}_{i_kj_k,t_{v_k}}P_-\,.$$

This implies that the series (4.99) converges for small times.

Applying the tree expansion to both $F_{t,t_1,\dots,t_k}^{(k,0)}(a^{(p)})$ and $\tilde{\gamma}(s)^{\otimes(p+k)}$ in (4.98), we see that (4.98) is equal to

$$\sum_{k'=0}^{\infty}\frac{\mathrm{i}^{k+k'}}{2^{k+k'}}\sum_{Q\in\mathcal{Q}(p,k,0)}\;\sum_{Q'\in\mathcal{Q}(p+k,k',0)} i_Q i_{Q'}\int_{\Delta_Q^k(t)}\mathrm{d}\underline{t}\int_0^{\wedge\underline{t}}\mathrm{d}s\int_{\Delta_{Q'}^{k'}(s)}\mathrm{d}\underline{t}'$$
$$\mathrm{Tr}\Big\{A\,a_{1\dots p,t}^{(p)}\,BP_-^{(p+k)}\tilde{\gamma}_j(s)W_{ij,s}\,C\,\gamma^{\otimes(p+k+k')}\Sigma_-^{(p+k)}\Big\}\,,$$

where A,B,C are operators that depend on $(Q,Q',k,k',\underline{t},\underline{t})$. A, B and C are each a product of operators of the form $W_{i'j',r}$, or $\mathcal{W}_{i'j',r}$, where r stands for a time variable in the set $\{t_1,\dots,t_k,t_1,\dots,t_{k'}\}$. Moreover, the product ABC contains k W's and k' $\mathcal{W}$'s. Finally, each time variable in $t_1,\dots,t_k,t_1,\dots,t_{k'}$ appears exactly once in the product ABC.

Let $\varphi\in\mathcal{H}^{\otimes(p+k+k')}$ and estimate

$$I\;:=\;\bigg\|\sum_{Q\in\mathcal{Q}(p,k,0)}\;\sum_{Q'\in\mathcal{Q}(p+k,k',0)} i_Q i_{Q'}\int_{\Delta_Q^k(t)}\mathrm{d}\underline{t}\int_0^{\wedge\underline{t}}\mathrm{d}s\int_{\Delta_{Q'}^{k'}(s)}\mathrm{d}\underline{t}'\;A\,a_{1\dots p,t}^{(p)}\,BP_-^{(p+k)}\tilde{\gamma}_j(s)W_{ij,s}\,C\,\varphi\bigg\|$$
$$\leqslant\;\sum_{Q\in\mathcal{Q}(p,k,0)}\;\sum_{Q'\in\mathcal{Q}(p+k,k',0)}\int_{[0,t]^k}\mathrm{d}\underline{t}\int_0^t\mathrm{d}s\int_{[0,t]^{k'}}\mathrm{d}\underline{t}'\;\Big\|A\,a_{1\dots p,t}^{(p)}\,BP_-^{(p+k)}\tilde{\gamma}_j(s)W_{ij,s}\,C\,\varphi\Big\|$$

We now perform all time integrations, starting from the left, and using at each step the Kato smoothing estimate (4.24) as well as

$$\int_0^t\mathrm{d}r\;\big\|\mathcal{W}_{i'j',r}\varphi\big\|\;\leqslant\;\sqrt{2\pi\kappa^2 t}\,\|\varphi\|\,,$$

which follows trivially from (4.24). Also, Lemma 4.18 implies that $\|\tilde{\gamma}(s)\| = \|\gamma\|$. Thus we find that

$$I \leqslant \sum_{Q \in \mathcal{Q}(p,k,0)} \sum_{Q' \in \mathcal{Q}(p+k,k',0)} \left(\frac{\pi\kappa^2 t}{2}\right)^{(k+1)/2} \left(2\pi\kappa^2 t\right)^{k'/2} \|a^{(p)}\| \|\gamma\| \|\varphi\|$$

Using the bound

$$|\mathcal{Q}(p,k,0)| \leqslant 4^p \, 32^k \,,$$

which can be inferred from (4.41), we find

$$\begin{aligned} I &\leqslant 4^p \, 32^k \, 4^{p+k} 32^{k'} \left(\frac{\pi\kappa^2 t}{2}\right)^{(k+1)/2} \left(2\pi\kappa^2 t\right)^{k'/2} \|a^{(p)}\| \|\gamma\| \|\varphi\| \\ &\leqslant 16^p \sqrt{2\pi\kappa^2 t} \left(64\sqrt{2\pi\kappa^2 t}\right)^k \left(32\sqrt{2\pi\kappa^2 t}\right)^{k'} \|a^{(p)}\| \|\gamma\| \|\varphi\| \,. \end{aligned}$$

Let $t < (2^{11}\pi\kappa^2)^{-1}$. Now Lemma 4.21 implies that $\|\gamma^{\otimes(p+k+k')}\Sigma_-^{(p+k)}\|_1 \leqslant 1$. Using the inequality $\mathrm{Tr}(A\Gamma) \leqslant \|A\| \|\Gamma\|_1$ we therefore find that (4.98) is bounded by

$$16^p \sum_{k'=0}^{\infty} \left(32\sqrt{2\pi\kappa^2 t}\right)^k \left(16\sqrt{2\pi\kappa^2 t}\right)^{k'} \|a^{(p)}\| \|\gamma\| = 16^p \frac{\left(32\sqrt{2\pi\kappa^2 t}\right)^k}{1 - 16\sqrt{2\pi\kappa^2 t}} \|a^{(p)}\| \|\gamma\| \,.$$

The second term of $R_{ij}^k(t)$ is equal to the complex conjugate of the first. We thus arrive at the desired bound

$$|R_{ij}^k(t)| \leqslant 2 \cdot 16^p \frac{\left(32\sqrt{2\pi\kappa^2 t}\right)^k}{1 - 16\sqrt{2\pi\kappa^2 t}} \|a^{(p)}\| \|\gamma\| \,. \tag{4.100}$$

Therefore the last line of (4.97) is bounded by

$$\begin{aligned} &2 \cdot 16^p \frac{1}{1 - 16\sqrt{2\pi\kappa^2 t}} \|a^{(p)}\| \|\gamma\| \sum_{k=0}^{\infty} (p+k)^2 \left(32\sqrt{2\pi\kappa^2 t}\right)^k \\ &\qquad \leqslant 4 \cdot 16^p \, \mathrm{e}^p \frac{1}{1 - 16\sqrt{2\pi\kappa^2 t}} \frac{1}{\left(1 - 32\sqrt{2\pi\kappa^2 t}\right)^3} \|a^{(p)}\| \|\gamma\| \,, \end{aligned}$$

where we used Lemma 4.4.

Next, we note that the second line of (4.97), i.e. the rest term, vanishes in the limit $K \to \infty$. The procedure is almost identical to (in fact easier than) the above estimation of $|R_{ij}^k(t)|$. The result is

$$\left| \int_{\Delta^K(t)} \mathrm{d}\underline{t} \; \mathrm{Tr}\left(F_{t,\underline{t}}^{(K,0)}(a^{(p)}) \, \tilde{\gamma}(t_K)^{\otimes(p+K)} \Sigma_-^{(p+K)}\right) \right| \leqslant 2 \cdot 16^p \frac{\left(32\sqrt{2\pi\kappa^2 t}\right)^K}{1 - 16\sqrt{2\pi\kappa^2 t}} \|a^{(p)}\| \longrightarrow 0 \,,$$

as $K \to \infty$.

Summarizing, we have proven:

Lemma 4.23. *Let $a^{(p)} \in \mathcal{L}(\mathcal{H}_-^{(p)})$. Then, for small times,*

$$\left| \mathrm{Tr}\left(a_t^{(p)} \, \tilde{\gamma}(t)^{\otimes p} \, \Sigma_-^{(p)}\right) - \sum_{k=0}^{\infty} \mathrm{Tr}\left(F_t^{(k,0)}(a^{(p)}) \, \gamma^{\otimes(p+k)} \Sigma_-^{(p+k)}\right) \right| \leqslant \|a^{(p)}\| \, \|\gamma\| \, C(p,\kappa,t) \,,$$

for some constant $C(p,\kappa,t)$.

4.6.5. Main result. We now have all the necessary ingredients to state and prove our main result. Take some fixed orthonormal sequence $\Phi = (\varphi_i)_{i\in\mathbb{N}}$. Denote by Φ_N the truncated sequence $\Phi_N = (\varphi_1, \dots, \varphi_N)$, and let $\Phi_N(t)$ be the solution of the Hartree-Fock equation (4.88) with initial data Φ_N. The N-particle density matrix evolved with the Hartree-Fock dynamics is

$$\tilde{\Gamma}_N(t) \;:=\; \big|S(\Phi_N(t))\big\rangle\big\langle S(\Phi_N(t))\big|\,.$$

The N-particle density matrix evolved with the microscopic dynamics is

$$\Gamma_N(t) \;:=\; \mathrm{e}^{-\mathrm{i}tH_N}\big|S(\Phi_N)\big\rangle\big\langle S(\Phi_N)\big|\mathrm{e}^{\mathrm{i}tH_N}\,.$$

The p-particle marginals are defined by

$$\Gamma_N^{(p)}(t) \;:=\; \mathrm{Tr}_{p+1\dots N}\,\Gamma_N(t)\,, \qquad \tilde{\Gamma}_N^{(p)}(t) \;:=\; \mathrm{Tr}_{p+1\dots N}\,\tilde{\Gamma}_N(t)\,.$$

The one-particle density matrix satisfying (4.81) is

$$\gamma_N(t) \;:=\; \tilde{\Gamma}_N^{(1)}(t)\,.$$

The quantities $\gamma_N^{(p)}(t) = \Sigma_-^{(p)}\gamma_N(t)^{\otimes p}$ and $\tilde{\Gamma}_N^{(p)}(t)$ are asymptotically equal: (4.89) implies that

$$\big\|\gamma_N^{(p)}(t) - \tilde{\Gamma}_N^{(p)}(t)\big\|_1 \;\leqslant\; \frac{p^2}{N}\,. \tag{4.101}$$

Next, let $a^{(p)} \in \mathcal{L}(\mathcal{H}_-^{(p)})$. Setting $L = 1$ in (4.48) yields

$$\mathrm{e}^{\mathrm{i}tH_N}\,\widehat{\mathrm{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tH_N} \;=\; \sum_{k=0}^{\infty}\widehat{\mathrm{A}}_N\big(G_t^{(k,0)}(a^{(p)})\big) + L_N(t)\,, \tag{4.102}$$

where $L_N(t)$, corresponding to the sum of all “loop terms”, satisfies the estimate

$$\|L_N(t)\| \;\lesssim\; C(p,\kappa,t)\|a^{(p)}\|N^{-1}\,, \tag{4.103}$$

for small times t. Thus (4.90) implies for small times

$$\begin{aligned}
\mathrm{Tr}\left(\widehat{\mathrm{A}}_N(a^{(p)})\,\Gamma_N(t)\right) \;&=\; \big\langle S(\Phi_N), \mathrm{e}^{\mathrm{i}tH_N}\,\widehat{\mathrm{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tH_N}\,S(\Phi_N)\big\rangle \\
&=\; \sum_{k=0}^{\infty}\big\langle S(\Phi_N), \widehat{\mathrm{A}}_N\big(F_t^{(k,0)}(a^{(p)})\big)\,S(\Phi_N)\big\rangle + \big\langle S(\Phi_N), L_N(t)\,S(\Phi_N)\big\rangle\,, \\
&=\; \sum_{k=0}^{\infty}\mathrm{Tr}\left(F_t^{(k,0)}(a^{(p)})\,\gamma_N^{(p+k)}\right) + \big\langle S(\Phi_N), L_N(t)\,S(\Phi_N)\big\rangle\,.
\end{aligned}$$

Using Lemma 4.23 and (4.91) we therefore get that, for small times,

$$\left|\mathrm{Tr}\left(a_t^{(p)}\,\tilde{\gamma}_N^{(p)}(t)\right) - \mathrm{Tr}\left(\widehat{\mathrm{A}}_N(a^{(p)})\,\Gamma_N(t)\right)\right| \;\leqslant\; \frac{C(p,\kappa,t)}{N}\,\|a^{(p)}\|\,.$$

Since the quantum-mechanical and the Hartree-Fock time-evolutions preserve the trace norm, we may iterate the above result, like in the proof of Theorem 4.15, to get: For all times $t \in \mathbb{R}$ we have that

$$\left|\mathrm{Tr}\left(a^{(p)}\,\gamma_N^{(p)}(t)\right) - \mathrm{Tr}\left(\widehat{\mathrm{A}}_N(a^{(p)})\,\Gamma_N(t)\right)\right| \;\leqslant\; C(p,\kappa,t)\,\|a^{(p)}\|\,f(N)\,,$$

with $\lim_{N\to\infty} f(N) = 0$. Thus, the duality $\mathcal{L} = (\mathcal{L}^1)^*$ implies the following result.

THEOREM 4.24. *Let $p \in \mathbb{N}$ and $t \in \mathbb{R}$. Then*

$$\big\|\tilde{\Gamma}_N^{(p)}(t) - \Gamma_N^{(p)}(t)\big\|_1 \;\longrightarrow\; 0\,, \qquad N \to \infty\,.$$

In particular, if $a^{(p)} \in \mathcal{L}(\mathcal{H}_-^{(p)})$, we have

$$\big\langle \mathrm{e}^{-\mathrm{i}tH_N} S(\Phi_N)\,, \widehat{\mathrm{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tH_N} S(\Phi_N)\big\rangle - \big\langle S(\Phi_N(t))\,, \widehat{\mathrm{A}}_N(a^{(p)})\, S(\Phi_N(t))\big\rangle \;\longrightarrow\; 0\,,$$

as $N \to \infty$.

REMARK 4.25. *The limit $N \to \infty$ of $\Gamma_N^{(p)}(t)$ does not exist in $\|\cdot\|_1$. Indeed, $\lim_{N\to\infty}\|\Gamma_N^{(p)}(t)\| = 0$ but $\operatorname{Tr}\Gamma_N^{(p)}(t) = 1$ (similarly for $\tilde{\Gamma}_N^{(p)}(t)$).*

REMARK 4.26. *As in Theorem 4.15, one can show that the function f is a power law: $f(N) \sim N^{-\beta(t)}$, with $\beta(t) > 0$ for all t. However, $\beta(t) \to 0$ as $t \to \infty$. Our bound on the rate of convergence is therefore far from the expected optimal rate $\beta(t) = 1$, which we only obtain for short times.*

REMARK 4.27. *Although the exchange term $-\frac{1}{N}\sum_{j=1}^{N}(w * (\varphi_i\bar{\varphi}_j))\,\varphi_j$ is essential for our proof, it is not clear from our analysis whether it is of leading order as $N \to \infty$. The exchange term is known to be of subleading order in the scaling of [NS81], and hence in that case it does not play a role in the limiting dynamics (see [EESY04]).*

4.6.6. A Egorov-type result for small times. In this section we describe how the many-body dynamics of fermions may be seen as the quantization of a classical "superhamiltonian" system, whose dynamics is approximately described by the Hartree-Fock equation.

A graded algebra of observables. We start by defining a Grassmann algebra of anticommuting variables over the one-particle space $\mathcal{H} = L^2(\mathbb{R}^3)$, and equip it with a suitable norm. Formally, we consider the infinite-dimensional Grassmann algebra generated by $\{\overline{\psi}(x), \psi(x)\}_{x\in\mathbb{R}^3}$. As it turns out, this algebra can be made into a Banach algebra under a natural choice of norm. This norm is most conveniently formulated by identifying elements of the Grassmann algebra with bounded operators between L^2-spaces.

Let

$$a \;=\; (a^{(p,q)})_{p,q\in\mathbb{N}}\,, \qquad a^{(p,q)} \in \mathcal{L}(\mathcal{H}_-^{(q)}; \mathcal{H}_-^{(p)}), \tag{4.104}$$

be a family of bounded operators. Such objects will play the role of observables in the following. By a slight abuse of notation we identify $a^{(p,q)}$ with the family obtained by adjoining zeroes to it.

Define

$$\mathfrak{B} \;:=\; \{a = (a^{(p,q)}) \,:\, a^{(p,q)} = 0 \text{ for all but finitely many } (p,q)\}\,.$$

We introduce a norm on $\mathfrak{B}$ through

$$\|a\|_{\mathfrak{B}} \;:=\; \sum_{p,q\in\mathbb{N}} \|a^{(p,q)}\|\,, \tag{4.105}$$

and define $\overline{\mathfrak{B}}$ as the completion of $\mathfrak{B}$.

We also introduce a multiplication on $\overline{\mathfrak{B}}$ defined by

$$(ab)^{(p,q)} \;:=\; \sum_{\substack{p_1+p_2=p\\ q_1+q_2=q}} (-1)^{p_2(p_1+q_1)}\, P_-(a^{(p_1,q_1)} \otimes b^{(p_2,q_2)})P_-\,. \tag{4.106}$$

The seemingly odd choice of sign will soon become clear. It is now easy to check that $\overline{\mathfrak{B}}$ is an associative Banach algebra with identity

$$\mathbb{1}^{(p,q)} \;=\; \delta_{p0}\,\delta_{q0}\,.$$

Note that $\overline{\mathfrak{B}}$ bears a $\mathbb{Z}$-grading, with degree map

$$\deg a^{(p,q)} \;:=\; p-q\,.$$

An observable is gauge invariant when its degree is equal to 0. One readily sees that

$$ab = (-1)^{\deg a\,\deg b} ba\,.$$

We now identify $\overline{\mathfrak{B}}$ with a Grassmann algebra of anticommuting variables. For $f \in \mathcal{H}$ define $\psi(f) \in \mathcal{L}(\mathcal{H};\mathbb{C}) \subset \overline{\mathfrak{B}}$ through

$$\psi(f)\,g \;:=\; \langle f\,,g\rangle \tag{4.107}$$

and $\overline{\psi}(f) \in \mathcal{L}(\mathbb{C};\mathcal{H}) \subset \overline{\mathfrak{B}}$ through

$$\overline{\psi}(f)z \;:=\; fz\,. \tag{4.108}$$

We may now consider arbitrary polynomials in the variables $\{\overline{\psi}(f), \psi(f) \;:\; f \in \mathcal{H}\}$. It is a simple matter to check that

$$\psi(f)\,\psi(g) + \psi(g)\,\psi(f) \;=\; \psi(f)\overline{\psi}(g) + \overline{\psi}(g)\,\psi(f) \;=\; \overline{\psi}(f)\,\overline{\psi}(g) + \overline{\psi}(g)\,\overline{\psi}(f) \;=\; 0\,,$$

for all $f, g \in \mathcal{H}$. Furthermore, we have that

$$\overline{\psi}(f_p)\cdots\overline{\psi}(f_1)\psi(g_1)\cdots\psi(g_q) \;=\; P_-^{(p)}\,|f_1\otimes\cdots\otimes f_p\rangle\langle g_1\otimes\cdots\otimes g_q|\,P_-^{(q)}\,. \tag{4.109}$$

Linear combinations of expressions of the form (4.109) are dense in $\overline{\mathfrak{B}}$ (in the strong operator topology). It is often convenient to write a family a of bounded operators using the "Grassmann generators" $\{\overline{\psi}, \psi\}$. To this end we set

$$\psi(x) \;:=\; \psi(\delta_x)\,, \qquad \overline{\psi}(x) \;:=\; \overline{\psi}(\delta_x)\,,$$

where δ_x is Dirac's delta mass at x. Expressions of the form (4.109) are now understood as densely defined quadratic forms. One immediately finds

$$\begin{aligned} a \;\equiv\; \mathrm{A}(a) \;:=\; \sum_{p,q} \int \mathrm{d}x_1 \ldots \mathrm{d}x_p\,\mathrm{d}y_1 \ldots \mathrm{d}y_q \\ \times\, \overline{\psi}(x_p)\cdots\overline{\psi}(x_1)\, a^{(p,q)}(x_1, \ldots, x_p; y_1, \ldots, y_q)\, \psi(y_1)\cdots\psi(y_q)\,. \end{aligned} \tag{4.110}$$

We use the notation $\mathrm{A}(a)$ to emphasize that the family a is represented using Grassmann generators.

A graded Poisson bracket. Next, we note that $\mathfrak{B}$ carries the graded Poisson bracket

$$\{a,b\} \;:=\; \mathrm{i}\int \mathrm{d}x \left[a\,\frac{\overleftarrow{\delta}}{\delta\overline{\psi}(x)}\,\frac{\overrightarrow{\delta}}{\delta\psi(x)}\,b + a\,\frac{\overleftarrow{\delta}}{\delta\psi(x)}\,\frac{\overrightarrow{\delta}}{\delta\overline{\psi}(x)}\,b\right], \tag{4.111}$$

where $a, b \in \mathfrak{B}$. Here we use the usual conventions for derivatives with respect to Grassmann variables (see e.g. [Sal99], Appendix B). In terms of kernels the graded Poisson bracket can be expressed as

$$\{\psi(x), \overline{\psi}(y)\} \;=\; \mathrm{i}\delta(x-y) \qquad \{\psi(x), \psi(y)\} \;=\; \{\overline{\psi}(x), \overline{\psi}(y)\} \;=\; 0\,. \tag{4.112}$$

We now list the important properties of the graded Poisson bracket.

(i) $\{a,b\} \;=\; (-1)^{1+\deg a\,\deg b}\{b,a\}\,.$

(ii) $(-1)^{\deg b\,(\deg a+\deg c)}\{a,\{b,c\}\} + \text{cyclic permutations} \;=\; 0\,.$

(iii) $\{a,bc\} \;=\; \{a,b\}c + (-1)^{\deg a\,\deg b}b\{a,c\}\,.$

Proof. Let us start with (i):

$$\begin{aligned}
\{a,b\} \;&=\; \mathrm{i}\int \mathrm{d}x \left[(-1)^{\deg a+1}\frac{\delta a}{\delta\overline{\psi}(x)}\frac{\delta b}{\delta\psi(x)} + (-1)^{\deg a+1}\frac{\delta a}{\delta\psi(x)}\frac{\delta b}{\delta\overline{\psi}(x)}\right]\\
&=\; \mathrm{i}\int \mathrm{d}x \left[(-1)^{\deg a\,\deg b+\deg b}\frac{\delta b}{\delta\psi(x)}\frac{\delta a}{\delta\overline{\psi}(x)} + (-1)^{\deg a\,\deg b+\deg b}\frac{\delta b}{\delta\overline{\psi}(x)}\frac{\delta a}{\delta\psi(x)}\right]\\
&=\; (-1)^{1+\deg a\,\deg b}\{b,a\}\,.
\end{aligned}$$

In order to show (ii), we note that the left-hand side can be written as a sum of three terms, the first of which contains second derivatives of a, the second second derivatives of b and the third second derivatives of c. Let us consider the third one. It is equal to the terms containing second derivatives of c of

$$\begin{aligned}
&(-1)^{\deg b(\deg a+\deg c)}\{a,\{b,c\}\} + (-1)^{\deg c(\deg b+\deg a)}\{b,\{c,a\}\}\\
&\qquad=\; (-1)^{\deg b(\deg a+\deg c)}\{a,\{b,c\}\} + (-1)^{\deg c(\deg b+\deg a)+1+\deg c\,\deg a}\{b,\{a,c\}\}\,,
\end{aligned}$$

where (i) was used. Define the derivation $L_a b := \{a,b\}$. Thus we need to compute the terms containing second derivatives of c of

$$(-1)^{\deg a\,\deg b+\deg b\,\deg c}L_aL_bc - (-1)^{\deg b\,\deg c}L_bL_ac\,.$$

Since we are only considering terms containing second derivatives of c, both derivations L_a and L_b must act only on c, and one finds

$$(-1)^{\deg a\,\deg b+\deg b\,\deg c}L_aL_bc - (-1)^{\deg a\,\deg b+\deg b\,\deg c}L_aL_bc \;=\; 0\,.$$

We omit the straightforward proof of (iii). $\square$

Furthermore, one finds by explicit calculation

$$\begin{aligned}
&\{\mathrm{A}(a^{(p_1,q_1)}), \mathrm{A}(b^{(p_2,q_2)})\}\\
&\qquad=\; \mathrm{i}\,(-1)^{(p_2+1)(p_1+q_1)}q_1p_2\,\mathrm{A}\Big[\big(a^{(p_1,q_1)}\otimes\mathbb{1}^{(p_2-1)}\big)\big(\mathbb{1}^{(q_1-1)}\otimes b^{(p_2,q_2)}\big)\Big]\\
&\qquad\quad-\mathrm{i}\,(-1)^{(q_1+1)(p_2+q_2)}p_1q_2\,\mathrm{A}\Big[\big(b^{(p_2,q_2)}\otimes\mathbb{1}^{(p_1-1)}\big)\big(\mathbb{1}^{(q_2-1)}\otimes a^{(p_1,q_1)}\big)\Big]\,.
\end{aligned} \tag{4.113}$$

States. With the algebra of observables $(\overline{\mathfrak{B}}, \|\cdot\|_{\mathfrak{B}})$ is associated the space of states

$$\mathfrak{R} \;:=\; \left(\overline{\mathfrak{B}}\right)^* .$$

By using the standard argument of the proof that $(l^1)^* = l^\infty$ (see e.g. [RS80]), one finds that

$$\mathfrak{R} \;=\; \left\{\rho = (\rho^{(p,q)})_{p,q\in\mathbb{N}} \,:\, \rho^{(p,q)} \in \mathcal{L}(\mathcal{H}_-^{(q)};\mathcal{H}_-^{(p)})\,,\; \|\rho\|_{\mathfrak{R}} < \infty\right\},$$

where

$$\|\rho\|_{\mathfrak{R}} \;:=\; \sup_{p,q\in\mathbb{N}} \|\rho^{(p,q)}\|_1$$

and

$$\|\rho^{(p,q)}\|_1 \;:=\; \sup\left\{\left|\operatorname{Tr}(\rho^{(p,q)}a^{(q,p)})\right| \,:\, a^{(q,p)} \in \mathcal{L}(\mathcal{H}_-^{(p)},\mathcal{H}_-^{(q)})\,,\; \|a^{(q,p)}\| \leqslant 1\right\}.$$

Note that if $p = q$ then $\|\cdot\|_1$ is the usual trace norm. The dual action is given by

$$\langle \rho\,, a\rangle \;:=\; \sum_{p,q\in\mathbb{N}} \operatorname{Tr}(\rho^{(p,q)}a^{(q,p)})\,.$$

We abbreviate $\rho^{(p,p)} \equiv \rho^{(p)}$ in the case of gauge invariant states. Next, we note that (4.109) implies that the operator kernel of $\rho^{(p,q)}$ may be expressed as

$$\rho^{(p,q)}(x_1,\dots,x_p;y_1,\dots,y_q) \;=\; \left\langle \rho, \overline{\psi}(y_q)\cdots\overline{\psi}(y_1)\psi(x_1)\cdots\psi(x_p)\right\rangle. \tag{4.114}$$

There is a particular subset of gauge invariant states that is of interest for studying the Hartree-Fock dynamics. Let $\gamma \in \mathcal{D}$ be a one-particle density matrix. Define the state ρ_γ through $\rho_\gamma^{(p,q)} = 0$ if $p \neq q$ and

$$\rho_\gamma^{(p,p)} \;:=\; \gamma^{(p)}\,, \tag{4.115}$$

where $\gamma^{(p)}$ is defined in (4.85). One immediately finds $\|\rho_\gamma\|_1 = \|\gamma\|_1$.

Hamilton function and dynamics. Let h be the one-particle Hamiltonian and w the two-body interaction potential. We define a Hamilton function on (a dense subset of) the phase space $\mathfrak{R}$ through

$$\begin{aligned} H \;&:=\; \mathrm{A}(h) + \frac{1}{2}\mathrm{A}(W) \\ &=\; \int \mathrm{d}x\,\mathrm{d}y\; \overline{\psi}(x)\,h(x;y)\,\psi(y) + \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\;\overline{\psi}(y)\overline{\psi}(x)\,w(w-y)\,\psi(x)\psi(y)\,. \end{aligned} \tag{4.116}$$

The Hamiltonian equation of motion reads

$$\dot{a} \;=\; \{H, a\}\,,$$

where $a \in \mathfrak{B}$. Instead of the "Heisenberg" evolution of a we consider the dual "Schrödinger" evolution of states:

$$\langle \rho(t)\,, a\rangle \;:=\; \langle \rho\,, a(t)\rangle\,.$$

The equation of motion for states reads

$$\begin{aligned} \mathrm{i}\partial_t\rho^{(p,q)}(x_1,\dots,x_p;y_1,\dots,y_q) \;&=\; \left(\sum_{i=1}^p h_{x_i} - \sum_{i=1}^q h_{y_i}\right)\rho^{(p,q)}(x_1,\dots,x_p;y_1,\dots,y_q) \\ &+ \int \mathrm{d}u\,\left(\sum_{i=1}^p w(u-x_i) - \sum_{i=1}^q w(u-y_i)\right)\rho^{(p+1,q+1)}(x_1,\dots,x_p,u;y_1,\dots,y_q,u)\,. \end{aligned} \tag{4.117}$$

This has the form of an infinite hierarchy, which decouples over subspaces of different degree. In order to show (4.117) we compute

$$\begin{aligned}\mathrm{i}\big\{H, \overline{\psi}(y_q)\cdots\overline{\psi}(y_1)\psi(x_1)\cdots\psi(x_p)\big\} &= \left(\sum_{i=1}^p h_{x_i} - \sum_{i=1}^q h_{y_i}\right)\overline{\psi}(y_q)\cdots\overline{\psi}(y_1)\psi(x_1)\cdots\psi(x_p)\\ &+ \int \mathrm{d}u\left(\sum_{i=1}^p w(u-x_i) - \sum_{i=1}^q w(u-y_i)\right)\overline{\psi}(u)\overline{\psi}(y_q)\cdots\overline{\psi}(y_1)\psi(x_1)\cdots\psi(x_p)\psi(u)\,.\end{aligned}$$

Then (4.117) follows from (4.114) and

$$\begin{aligned}\mathrm{i}\partial_t\rho^{(p,q)}(x_1,\dots,x_p;y_1,\dots,y_q) &= \mathrm{i}\partial_t\big\langle\rho, \overline{\psi}(y_q)\cdots\overline{\psi}(y_1)\psi(x_1)\cdots\psi(x_p)\big\rangle\\ &= \big\langle\rho, \mathrm{i}\big\{H, \overline{\psi}(y_q)\cdots\overline{\psi}(y_1)\psi(x_1)\cdots\psi(x_p)\big\}\big\rangle\,.\end{aligned}$$

Next, we outline how to solve the equation of motion (4.117). Let us first rewrite it as

$$\begin{aligned}\mathrm{i}\partial_t\rho^{(p,q)} &= \sum_{i=1}^p h_i\rho^{(p,q)} - \sum_{i=1}^q \rho^{(p,q)}h_i\\ &\quad + \sum_{i=1}^p \mathrm{Tr}_{p+1,q+1}\big(W_{i\,p+1}\rho^{(p+1,q+1)}\big) - \sum_{i=1}^q \mathrm{Tr}_{p+1,q+1}\big(\rho^{(p+1,q+1)}W_{i\,q+1}\big)\,.\end{aligned}$$

We may now proceed exactly as with the density matrix Hartree-Fock equation (4.80), i.e. express it as an integral equation in the interaction picture. This yields a tree expansion for the quantity $\mathrm{Tr}\big(\rho^{(p,q)}(t)\,a^{(q,p)}\big)$, where $\rho(0)\in\mathfrak{R}$. We omit the uninteresting details. As above, the tree expansion converges if $t<T$, where

$$T := (2^{11}\pi\kappa^2)^{-1}\,. \tag{4.118}$$

Unfortunately, the time evolution (4.117) does not preserve the norm of ρ, which means that we cannot iterate the short-time result.

From now on, we only consider gauge invariant quantities. Take some gauge invariant state $\rho = (\rho^{(p)})_{p\in\mathbb{N}}\in\mathfrak{R}$. For simplicity, we assume that the sequence ρ is finite (as is the case if ρ is defined by a Slater determinant, see below). Let us denote the Hamiltonian flow on $\mathfrak{R}$ by ϕ_t. We have seen that ϕ_t is well-defined by its tree expansion for $t<T$. The solution of (4.117) with initial data ρ, $\rho(t)=\phi_t(\rho)$, satisfies the equation

$$\tilde{\rho}^{(p)}(t) = \rho^{(p)} - \mathrm{i}\int_0^t \mathrm{d}s\,\sum_{i=1}^p \mathrm{Tr}_{p+1}\big[W_{i\,p+1,s}, \tilde{\rho}^{(p+1)}(s)\big]\,, \tag{4.119}$$

where $\tilde{\rho}^{(p)}(t) := \mathrm{e}^{\mathrm{i}\sum_i h_i t}\,\rho^{(p)}(t)\,\mathrm{e}^{-\mathrm{i}\sum_i h_i t}$. Let us take a gauge invariant observable $a^{(p,p)}\equiv a^{(p)}\in\mathfrak{A}$, where

$$\mathfrak{A} := \{a\in\mathfrak{B} : a^{(p,q)}=0 \text{ if } p\neq q\}$$

is the set of gauge invariant observables. Thus (4.113) implies

$$\{\mathrm{A}(a^{(p)}), \mathrm{A}(b^{(q)})\} = \mathrm{i}pq\mathrm{A}\big([a^{(p)}, b^{(q)}]_1\big)\,. \tag{4.120}$$

Next, we note that (4.119) implies

$$\begin{aligned}\mathrm{Tr}\big(a^{(p)}\rho^{(p)}(t)\big) &= \mathrm{Tr}\big(a_t^{(p)}\tilde{\rho}^{(p)}(t)\big)\\ &= \mathrm{Tr}\big(a_t^{(p)}\rho^{(p)}\big) + \mathrm{i}\int_0^t \mathrm{d}s\,\sum_{i=1}^p \mathrm{Tr}\Big(\Big[W_{i\,p+1,s}, a_t^{(p)}\otimes\mathbb{1}\Big]\tilde{\rho}^{(p+1)}(s)\Big)\,.\end{aligned}$$

Iteration of this identity gives

$$\operatorname{Tr}\big(a^{(p)}\rho^{(p)}(t)\big) \;=\; \sum_{k=0}^{\infty} \operatorname{Tr}\Big(F_t^{(k,0)}(a^{(p)})\,\rho^{(p+k)}\Big)\,.$$

Summarizing:

$$\begin{aligned}\big\langle a^{(p)} \circ \phi_t \,, \rho \big\rangle \;&=\; \big\langle a^{(p)} \,, \rho(t) \big\rangle \;=\; \operatorname{Tr}\big(a^{(p)}\rho^{(p)}(t)\big) \\ &=\; \sum_{k=0}^{\infty} \operatorname{Tr}\Big(F_t^{(k,0)}(a^{(p)})\,\rho^{(p+k)}\Big) \;=\; \Big\langle \sum_{k=0}^{\infty} F_t^{(k,0)}(a^{(p)}) \;,\; \rho \Big\rangle\,.\end{aligned}$$

This series converges for $t < T$, uniformly for bounded $\|a^{(p)}\|_{\mathfrak{B}}$ and $\|\rho\|_{\mathfrak{R}}$. Therefore we get the norm-convergent series

$$\mathrm{A}(a^{(p)}) \circ \phi_t \;=\; \sum_{k=0}^{\infty} \mathrm{A}\Big(F_t^{(k,0)}(a^{(p)})\Big)\,, \tag{4.121}$$

provided that $t < T$.

Finally, we discuss the relationship between the Hartree-Fock dynamics and the dynamics generated by (4.117). Take a density matrix $\gamma \in \mathcal{D}$ and consider the state $\rho = \rho_\gamma$ defined in (4.115). If one chooses a sequence γ_N such that $\|\gamma_N\| \to 0$ as $N \to \infty$ (e.g. a sequence of Slater determinants), then Lemma 4.23 implies that (4.117) and the Hartree-Fock equation describe the same dynamics for large N.

Quantization and a Egorov-type theorem. Next, we introduce a Wick quantization of the above "superhamiltonian" system and formulate the mean-field limit as a Egorov-type theorem.

We define *quantization* as the linear map $\widehat{(\cdot)}_N : \mathfrak{A} \to \widehat{\mathfrak{A}}$ defined by the formal replacement $\psi(x) \mapsto a_N(x)$ and $\bar{\psi}(x) \mapsto a_N^*(x)$ followed by Wick ordering. In other words,

$$\widehat{(\cdot)}_N \,:\, \mathrm{A}(a^{(p)}) \;\mapsto\; \widehat{\mathrm{A}}_N(a^{(p)})\,.$$

Using (4.113), it is easy to see that, for $A, B \in \mathfrak{A}$,

$$\big[\widehat{A}_N, \widehat{B}_N\big]_+ \;=\; \frac{N^{-1}}{\mathrm{i}} \widehat{\{A, B\}}_N + O(N^{-2})\,.$$

This identifies N^{-1} as the parameter of $\widehat{(\cdot)}_N$.

Extending the definition of $\widehat{(\cdot)}_N$ to unbounded operators in the obvious way, we define a Hamiltonian $\widehat{H}_N$ on $\mathcal{F}_-$ as the quantization of the Hamilton function H defined in (4.116). When restricted to $\mathcal{H}_-^{(N)}$, $N\widehat{H}_N$ is equal to the mean-field Hamiltonian (4.1).

Now (4.102), (4.103) and (4.121) yield the following Egorov-type theorem.

THEOREM 4.28. *Let $A \in \mathfrak{A}$ and $t < T$, with T defined in* (4.118). *Then*

$$\bigg\| \Big(\mathrm{e}^{\mathrm{i}tN\widehat{H}_N}\, \widehat{A}_N\, \mathrm{e}^{-\mathrm{i}tN\widehat{H}_N} - (\widehat{A \circ \phi_t})_N\Big)\Big|_{\mathcal{H}_-^{(N)}} \bigg\| \;\leqslant\; \frac{C}{N}\,,$$

for some $C > 0$.

4.6.7. A comment on the Hamiltonian formulation for density matrices. In Section 4.6.1, we chose a Hamiltonian formulation of the Hartree-Fock equation (4.75) in terms of sequences of orbitals. Alternatively, we could just as well have used a Hamiltonian formulation in terms of density matrices. To see how the density matrix Hartree-Fock equation (4.80) can be written as a Hamiltonian equation of motion of a classical Hamiltonian system, consider the Hilbert space

$$\widehat{\mathcal{H}} \;=\; \mathcal{L}^2(\mathcal{H})\,,$$

the space of Hilbert-Schmidt operators, with scalar product

$$\langle \kappa\,, \rho\rangle \;:=\; \mathrm{Tr}(\kappa^* \rho)\,.$$

We write the density matrix $\gamma \in \mathcal{D}$ as $\gamma = \kappa\kappa^*$, where $\kappa \in \widehat{\mathcal{H}}$. The classical phase space is then given by a Sobolev-type space of Hilbert-Schmidt operators

$$\widehat{\Gamma} \;:=\; \big\{\kappa \in \widehat{\mathcal{H}} \,:\, \mathrm{Tr}(\kappa^*(\mathbb{1} - \Delta)\kappa) < \infty\big\}\,.$$

We define polynomial functions on $\widehat{\Gamma}$ through

$$\mathrm{B}(a^{(p)})(\kappa) \;:=\; \big\langle \kappa^{\otimes p}\,, a^{(p)}\kappa^{\otimes p}\big\rangle\,,$$

where $a^{(p)} \in \mathcal{L}(\mathcal{H}^{\otimes p})$ is understood to act by left-multiplication.

The affine space $\widehat{\Gamma}$ carries a Symplectic form defined by

$$\omega \;=\; -\mathrm{i}\int \mathrm{d}x\,\mathrm{d}y\;\mathrm{d}\bar{\kappa}(x,y) \wedge \mathrm{d}\kappa(x,y)\,,$$

where $\kappa(x, y)$ is the operator kernel of κ. The Poisson bracket then reads

$$\begin{aligned} \Big\{\kappa^{\#}(x,y), \kappa^{\#}(x',y')\Big\} \;&=\; 0 \\ \big\{\kappa(x,y), \bar{\kappa}(x',y')\big\} \;&=\; -\mathrm{i}\delta(x-x')\delta(y-y')\,. \end{aligned}$$

The Hamilton function is defined by

$$H \;:=\; \mathrm{B}(h) + \frac{1}{2}\mathrm{B}(\mathcal{W})\,.$$

By using Sobolev-type inequalities one readily sees that H is well-defined on $\widehat{\Gamma}$. After a short computation, one finds that the Hamiltonian equation of motion,

$$\mathrm{i}\partial_t\kappa(x,y) \;=\; \frac{\delta H}{\delta\overline{\kappa}(x,y)} \;=\; \mathrm{i}\,\{H, \kappa(x,y)\}\,,$$

reads

$$\mathrm{i}\partial_t\kappa \;=\; h\kappa + \mathrm{Tr}_2\big(\mathcal{W}\,\kappa \otimes (\kappa\kappa^*)\big)\,.$$

It follows that $\gamma = \kappa\kappa^*$ satisfies (4.80).

4.7. Some generalizations

In this section we generalize all results of this chapter to a larger class of interaction potentials, and allow a weak external potential. For this we need Strichartz estimates for Lorentz spaces from Appendix B.

For a map $f : \mathbb{R} \to L^{p,q}$, where $L^{p,q}$ denotes a Lorentz space (see Appendix B), we define the space-time norm

$$\|f\|_{L^r_t L^{p,q}_x} := \left[\int \mathrm{d}t \, \|f(t)\|^r_{L^{p,q}} \right]^{1/r}.$$

Let us now invoke theorem B.6 with $\mathcal{H} = A_0 = L^2$, $A_1 = L^1$. We choose $U(t) = \mathrm{e}^{\mathrm{i}t\Delta}$ and recall the standard estimate $\|U(t)f\|_\infty \lesssim |t|^{-3/2}\|f\|_1$. Setting $\sigma = 3/2$ and $r = 2$, we therefore get from Theorems B.6, B.4, and B.5 that

$$\left\|\mathrm{e}^{\mathrm{i}t\Delta} f\right\|_{L^2 L^{6,2}} \lesssim \|f\|_{L^2}, \tag{4.122}$$

We are now set for proving a generalization of (4.24).

Lemma 4.29. *Let $w \in L^3_w + L^\infty$. Then there is a constant $C = C(w) > 0$, such that*

$$\int_0^1 \|w \, \mathrm{e}^{\mathrm{i}t\Delta} \varphi\|^2 \, \mathrm{d}t \leqslant C\|\varphi\|^2.$$

Proof. Let $w = w_1 + w_2$ with $w_1 \in L^\infty$ and $w_2 \in L^3_w$. Then

$$\left\|w \, \mathrm{e}^{\mathrm{i}t\Delta} \varphi\right\|_{L^2_t L^2_x} \leqslant \left\|w_1 \, \mathrm{e}^{\mathrm{i}t\Delta} \varphi\right\|_{L^2_t L^2_x} + \left\|w_2 \, \mathrm{e}^{\mathrm{i}t\Delta} \varphi\right\|_{L^2_t L^2_x}.$$

The first term is bounded by $\|w_1\|_{L^\infty}\|\varphi\|_{L^2}$. To bound the second we use Theorem B.1 and (4.122) to get

$$\left\|w_2 \, \mathrm{e}^{\mathrm{i}t\Delta} \varphi\right\|_{L^2_t L^2_x} \lesssim \|w_2\|_{L^{3,\infty}} \left\|\mathrm{e}^{\mathrm{i}t\Delta} \varphi\right\|_{L^2_t L^{6,2}_x} \lesssim \|w_2\|_{L^{3,\infty}}\|\varphi\|_{L^2}.$$

Therefore,

$$\left\|w \, \mathrm{e}^{\mathrm{i}t\Delta} \varphi\right\|_{L^2_t L^2_x} \leqslant \sqrt{C(w)}\, \|\varphi\|_{L^2}.$$ ☐

Now let us assume that $v, w \in L^\infty + L^3_w$. Set $H_0|_{\mathcal{H}^{(n)}_\pm} := \sum_{i=1}^n -\Delta_i$. Then the required generalization of Lemma 4.9 is

Lemma 4.30. *There exists a constant $C \equiv C(w, v)$ such that*

$$\int_0^1 \left\|W_{ij} \, \mathrm{e}^{-\mathrm{i}tH_0} \Phi^{(n)}\right\|^2 \mathrm{d}t \leqslant C\|\Phi^{(n)}\|^2,$$
$$\int_0^1 \left\|V_i \, \mathrm{e}^{-\mathrm{i}tH_0} \Phi^{(n)}\right\|^2 \mathrm{d}t \leqslant C\|\Phi^{(n)}\|^2,$$

where $\Phi^{(n)} \in \mathcal{H}^{(n)}_\pm$.

Proof. The claim for V follows immediately from Lemma 4.29. The estimate for W follows similarly by using centre of mass coordinates. ☐

Finally, we briefly discuss the changes to the combinatorics arising from an external potential. We classify the elementary terms according to the numbers (k, l, m), where k is the order of the multiple commutator, l is the number of loops, and m is the number of V-operators. Thus, instead of (4.18), we have the recursive definition

$$\begin{aligned} F^{(k,l,m)}_{t,t_1,\dots,t_k}(a^{(p)}) \;&=\; \mathrm{i}(p+k-l-m-1)\Big[W_{t_k}, F^{(k-1,l,m)}_{t,t_1,\dots,t_{k-1}}(a^{(p)})\Big]_1 \\ &\quad + \mathrm{i}\binom{p+k-l-m}{2}\Big[W_{t_k}, F^{(k-1,l-1,m)}_{t,t_1,\dots,t_{k-1}}(a^{(p)})\Big]_2 \\ &\quad + \mathrm{i}(p+k-l-m)\Big[V_{t_k}, F^{(k-1,l,m-1)}_{t,t_1,\dots,t_{k-1}}(a^{(p)})\Big]_1 \\ &= \mathrm{i}P_\pm \sum_{i=1}^{p+k-l-m-1} \big[W_{i\,p+k-l-m,t_k}, F^{(k-1,l,m)}_{t,t_1,\dots,t_{k-1}}(a^{(p)}) \otimes \mathbb{1}\big]P_\pm \\ &\quad + \mathrm{i}P_\pm \sum_{1\leqslant i<j\leqslant p+k-l-m} \big[W_{ij,t_k}, F^{(k-1,l-1,m)}_{t,t_1,\dots,t_{k-1}}(a^{(p)})\big]P_\pm \\ &\quad + \mathrm{i}P_\pm \sum_{i=1}^{p+k-l-m} \big[V_{i,t_k}, F^{(k-1,l,m-1)}_{t,t_1,\dots,t_{k-1}}(a^{(p)})\big]P_\pm\,, \end{aligned}$$

as well as $F^{(0,0,0)}_t(a^{(p)}) := a^{(p)}_t$. We also set $F^{(k,l,m)}_{t,t_1,\dots,t_k}(a^{(p)}) = 0$ unless $0 \leqslant l \leqslant k-m$. It is again an easy exercise to show by induction on k that

$$\frac{(\mathrm{i}N)^k}{2^k}\Big[\widehat{\mathrm{A}}_N(W_{t_k}),\dots\Big[\widehat{\mathrm{A}}_N(W_{t_1}),\widehat{\mathrm{A}}_N(a^{(p)}_t)\Big]\dots\Big] \;=\; \sum_{l=0}^{k}\sum_{m=0}^{k-l}\frac{1}{N^l}\,\widehat{\mathrm{A}}_N\big(F^{(k,l,m)}_{t,t_1,\dots,t_k}(a^{(p)})\big)\,.$$

Note that $F^{(k,l,m)}_{t,t_1,\dots,t_k}(a^{(p)})$ is a $p+k-l-m$ particle operator.

The graphs of Section 4.4 have to be modified: Each vertex corresponding to a V-operator has one edge for each direction $d = a, c$ (see Figure 4.4).

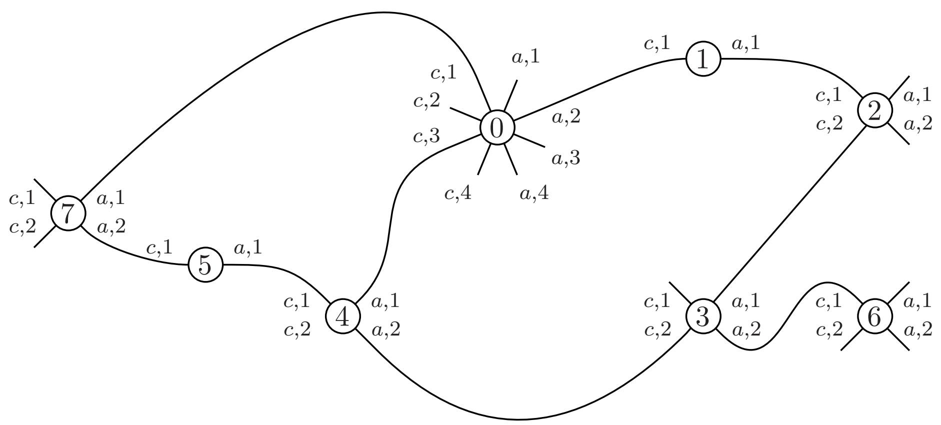


Figure 4.4: *An admissible graph of type* $(p = 4, k = 7, l = 2, m = 2)$.

Let us first consider tree graphs, $l = 0$. Take the set of trees without an external potential as in Section 4.4. By allowing each vertex $v = 1, \dots, k$ whose edges $(a, 2)$ and $(c, 2)$ are empty to stand for either an interaction potential W or an external potential V, we count all trees with an external potential. Thus, for a given m, there are at most $\binom{k}{m}|\mathcal{G}(p,k,0)|$ tree graphs contributing to $F^{(k,0,m)}_{t,t_1,\dots,t_k}(a^{(p)})$. If $l > 0$ we repeat the argument in the proof Lemma 4.10, and find that the number of graph structures contributing to $F^{(k,l,m)}_{t,t_1,\dots,t_k}(a^{(p)})$ is bounded by

$$2^k \binom{k}{m} \binom{k}{l} \binom{2p+3k}{k} (p+k-l-m)^l \,.$$

Putting all this together, we find that

$$\left\| F_t^{(k,l,m)}(a^{(p)}) \right\| \leqslant \binom{k}{m} \binom{k}{l} \binom{2p+3k}{k} (p+k-l-m)^l (Ct)^{k/2} \, \|a^{(p)}\| \,.$$

Using the condition $p+k-l-m \leqslant n$, it is then easy to see that all convergence estimates remain valid with the additional factor 2^k.

In summary, all of the results of this chapter hold if

$$v, w \in L^3_w + L^\infty \,.$$

Chapter 5

The Mean-Field Limit: Singular Potentials and Rate of Convergence

In this chapter we study the mean-field time evolution of coherent states of a Bose gas. The goal of this chapter is twofold. First, we treat a large class of external and interaction potentials. Second, we derive explicit bounds on the rate of convergence to the mean-field limit.

We consider a system of N identical bosons in d dimensions, described by a symmetric wave function $\Psi_N \in P_+ L^2(\mathbb{R}^d, \mathrm{d}x)^{\otimes N}$. The mean-field Hamiltonian is given by

$$H_N \;=\; \sum_{i=1}^{N} h_i + \frac{1}{N} \sum_{1 \leqslant i < j \leqslant N} w(x_i - x_j)\,, \tag{5.1}$$

where h_i denotes a one-particle Hamiltonian h (to be specified later) acting on the coordinate x_i, and w is an interaction potential. The time evolution of Ψ_N is governed by the N-body Schrödinger equation

$$\mathrm{i}\partial_t \Psi_N(t) \;=\; H_N \Psi_N(t)\,, \qquad \Psi_N(0) \;=\; \Psi_{N,0}\,. \tag{5.2}$$

We consider factorized[1] initial data $\Psi_{N,0} = \varphi_0^{\otimes N}$ for some $\varphi_0 \in L^2(\mathbb{R}^d)$ satisfying the normalization condition $\|\varphi_0\|_{L^2(\mathbb{R}^d)} = 1$. As discussed in Section 1.1.3, one expects that for large N the wave function $\Psi_N(t)$ is approximately factorized in the sense that[2]

$$\gamma_N^{(k)}(t) \;\approx\; \big(|\varphi(t)\rangle\langle\varphi(t)|\big)^{\otimes k} \tag{5.3}$$

for all $k \in \mathbb{N}$, where $\varphi(t)$ is a solution of the Hartree equation

$$\mathrm{i}\partial_t \varphi(t) \;=\; h\varphi(t) + \big(w * |\varphi(t)|^2\big)\varphi(t)\,, \qquad \varphi(0) \;=\; \varphi_0\,. \tag{5.4}$$

In order to make quantitative statements about the rate of convergence, we need a means of measuring the error in (5.3). There are two commonly used indicators: the projection

$$E_N^{(k)} \;:=\; 1 - \big\langle \varphi^{\otimes k}, \gamma_N^{(k)} \varphi^{\otimes k} \big\rangle$$

[1] More generally, we consider initial data that factorizes asymptotically for large N, in the sense that $\langle \varphi_0, \gamma_N^{(1)}(0)\varphi_0\rangle \to 1$ as $N \to \infty$. Here $\gamma_N^{(1)}(0)$ is the reduced 1-particle matrix of $\Psi_{N,0}$.

[2] We recall that the reduced k-particle density matrix is defined by

$$\gamma_N^{(k)}(t) \;:=\; \mathrm{Tr}_{p+1,\dots,N}\, |\Psi_N(t)\rangle\langle\Psi_N(t)|\,.$$

and the trace norm distance

$$R_N^{(k)} := \left\| \gamma_N^{(k)} - (|\varphi\rangle\langle\varphi|)^{\otimes k} \right\|_1 ,$$

where we suppress the time index t to avoid cluttering the notation. It is well known (see e.g. [LS02]) that all of these indicators are equivalent in the sense that the vanishing of either $R_N^{(k)}$ or $E_N^{(k)}$ for some k in the limit $N \to \infty$ implies that $\lim_N R_N^{(k')} = \lim_N E_N^{(k')} = 0$ for all k'. However, the rate of convergence may differ from one indicator to another. Thus, when studying rates of convergence, they are not equivalent (see Section 5.1 below for a full discussion).

In the past few years considerable progress has been made in strengthening results on the mean-field limit in mainly two directions. First, the convergence $\lim_N R_N^{(k)}(t) = 0$ for all t has been proven for a wide variety of one-particle Hamiltonians h and singular interaction potentials w. As we saw in Chapter 4, the proofs for singular interaction potentials such as the Coulomb potential are considerably more involved than for bounded interaction potentials. The first such result was the treatment of nonrelativistic bosons with Coulomb interaction potential by Erdős and Yau [EY01]. In [ES07], Elgart and Schlein extended this result to the technically more demanding case of a semirelativistic kinetic energy, $h = \sqrt{\mathbb{1} - \Delta}$ and $w(x) = \lambda |x|^{-1}$. This is a critical case in the sense that the kinetic energy has the same scaling behaviour as the Coulomb potential energy, thus requiring quite refined estimates. Another approach was adopted by Rodnianski and Schlein in [RS07]. Using methods inspired by a semiclassical argument of Hepp [Hep74] focusing on the dynamics of coherent states in Fock space, they show convergence to the mean-field limit in the case $h = -\Delta$ and $w(x) = |x|^{-1}$.

The second area of recent progress in understanding the mean-field limit is deriving estimates on the rate of convergence to the mean-field limit. Methods based on expansions, as used in [Spo80] and Chapter 4, give very weak bounds on the error $R_N^{(1)}(t)$, while weak compactness arguments, as used in [EY01] and [ES07], yield no information on the rate of convergence. From a physical point of view, where N is large but finite, it is of some interest to have tight error bounds in order to be able to address the question whether the mean-field approximation may be regarded as valid. The first reasonable estimates on the error were derived for the case $h = -\Delta$ and $w(x) = \lambda |x|^{-1}$ by Rodnianski and Schlein in their work [RS07] mentioned above. In fact they derive an explicit estimate on the error of the form

$$R_N^{(k)}(t) \leqslant \frac{C_1(k)}{\sqrt{N}} \, \mathrm{e}^{C_2(k)t}$$

for some constants $C_1(k), C_2(k) > 0$. Using a novel approach inspired by Lieb-Robinson bounds, Erdős and Schlein [ES08] further improved this estimate under the more restrictive assumption that w is bounded and its Fourier transform integrable. Their result is

$$R_N^{(k)}(t) \leqslant \frac{C_1}{N} \, \mathrm{e}^{C_2 t} \mathrm{e}^{C_3 k} ,$$

for some constants $C_1, C_2, C_3 > 0$.

In this chapter we adopt yet another approach based on a method of Pickl [Pic]. We strengthen and generalize many of the results listed above, by treating more singular interaction potentials as well as deriving estimates on the rate of convergence. Moreover, our approach allows for a large class of (possibly time-dependent) external potentials, which might for instance describe a trap confining the particles to a small volume. We also show that if the solution $\varphi(\cdot)$ of the Hartree equation satisfies a scattering condition, all of the error estimates are uniform in time.

The outline of this chapter is as follows. Section 5.1 is devoted to a short discussion of the indicators of convergence $E_N^{(k)}$ and $R_N^{(k)}$, in which we derive estimates relating them to each other. In Section 5.2 we state and prove our first main result, which concerns the mean-field limit in the case of L^2-type singularities in w; see Theorem 5.5 and Corollary 5.6. In Section 5.3 we state and prove our second main result, which allows for a larger class of singularities such as the nonrelativistic critical case $h = -\Delta$ and $w(x) = \lambda|x|^{-2}$; see Theorem 5.16. For an outline of the methods underlying our proofs, see the beginnings of Sections 5.2 and 5.3.

We adopt the following conventions throughout this chapter. Except in definitions, in statements of results and where confusion is possible, we refrain from indicating the explicit dependence of a quantity $a_N(t)$ on the time t and the particle number N. When needed, we use the notations $a(t)$ and $a|_t$ interchangeably to denote the value of the quantity a at time t. To simplify notation, we assume that $t \geqslant 0$. Integer indices on operators denote particle number: A k-particle operator A (i.e. an operator on $\mathcal{H}^{(k)}$) acting on the coordinates $x_{i_1}, \dots, x_{i_k}$, where $i_1 < \cdots < i_k$, is denoted by $A_{i_1 \dots i_k}$. Also, by a slight abuse of notation, we identify k-particle functions $f(x_1, \dots, x_k)$ with their associated multiplication operators on $\mathcal{H}^{(k)}$. The operator norm of the multiplication operator f is equal to, and will always be denoted by, $\|f\|_\infty$.

5.1. Indicators of convergence

This section is devoted to a discussion, which might also be of independent interest, of quantitative relationships between the indicators $E_N^{(k)}$ and $R_N^{(k)}$. Throughout this section we suppress the irrelevant index N.

Take a k-particle density matrix $\gamma^{(k)} \in \mathcal{L}(\mathcal{H}^{(k)})$ and a one-particle condensate wave function $\varphi \in L^2$. The following lemma gives the relationship between different elements of the sequence $E^{(1)}, E^{(2)}, \dots$, where, we recall,

$$E^{(k)} \;=\; 1 - \big\langle \varphi^{\otimes k}, \gamma^{(k)}\, \varphi^{\otimes k} \big\rangle\,. \tag{5.5}$$

Lemma 5.1. *Let $\gamma^{(k)} \in \mathcal{L}(\mathcal{H}^{(k)})$ satisfy*

$$\gamma^{(k)} \;\geqslant\; 0\,, \qquad \operatorname{Tr} \gamma^{(k)} \;=\; 1\,.$$

Let $\varphi \in L^2$ satisfy $\|\varphi\| = 1$. Then

$$E^{(k)} \;\leqslant\; k\, E^{(1)}\,. \tag{5.6}$$

Proof. Let $\big(\Phi_i^{(k)}\big)_{i \geqslant 1}$ be an orthonormal basis of $\mathcal{H}^{(k)}$ with $\Phi_1^{(k)} = \varphi^{\otimes k}$. Then

$$\begin{aligned}
\big\langle \varphi^{\otimes k}, \gamma^{(k)}\, \varphi^{\otimes k} \big\rangle \;&=\; \sum_{i \geqslant 1} \big\langle \varphi \otimes \Phi_i^{(k-1)}, \gamma^{(k)}\, \varphi \otimes \Phi_i^{(k-1)} \big\rangle - \sum_{i \geqslant 2} \big\langle \varphi \otimes \Phi_i^{(k-1)}, \gamma^{(k)}\, \varphi \otimes \Phi_i^{(k-1)} \big\rangle \\
&=\; \langle \varphi, \gamma^{(1)}\, \varphi \rangle - \sum_{i \geqslant 2} \big\langle \varphi \otimes \Phi_i^{(k-1)}, \gamma^{(k)}\, \varphi \otimes \Phi_i^{(k-1)} \big\rangle\,.
\end{aligned}$$

Therefore,

$$
\begin{aligned}
&\langle \varphi , \gamma^{(1)} \varphi \rangle - \big\langle \varphi^{\otimes k} , \gamma^{(k)} \varphi^{\otimes k} \big\rangle \\
&= \sum_{i \geqslant 2} \big\langle \varphi \otimes \Phi_i^{(k-1)} , \gamma^{(k)} \varphi \otimes \Phi_i^{(k-1)} \big\rangle \\
&\leqslant \sum_{i \geqslant 2} \sum_{j \geqslant 1} \big\langle \Phi_j^{(1)} \otimes \Phi_i^{(k-1)} , \gamma^{(k)} \Phi_j^{(1)} \otimes \Phi_i^{(k-1)} \big\rangle \\
&= \sum_{i \geqslant 1} \sum_{j \geqslant 1} \big\langle \Phi_j^{(1)} \otimes \Phi_i^{(k-1)} , \gamma^{(k)} \Phi_j^{(1)} \otimes \Phi_i^{(k-1)} \big\rangle - \sum_{j \geqslant 1} \big\langle \Phi_j^{(1)} \otimes \varphi^{\otimes (k-1)} , \gamma^{(k)} \Phi_j^{(1)} \otimes \varphi^{\otimes (k-1)} \big\rangle \\
&= 1 - \big\langle \varphi^{\otimes (k-1)} , \gamma^{(k-1)} \varphi^{\otimes (k-1)} \big\rangle \,.
\end{aligned}
$$

This yields

$$E^{(k)} \;\leqslant\; E^{(k-1)} + E^{(1)} \,,$$

and the claim follows. $\square$

REMARK 5.2. *The bound in* (5.6) *is sharp. Indeed, let us suppose that* $E^{(k)} \leqslant k\, f(k)\, E^{(1)}$ *for some function* f*. Then*

$$f(k) \;\geqslant\; \sup_{\gamma^{(k)}} \frac{E^{(k)}}{kE^{(1)}} \;\geqslant\; \sup_{0<\alpha<1} \frac{1-(1-\alpha)^k}{k\alpha} \;\geqslant\; \lim_{\alpha \to 0} \frac{1-(1-\alpha)^k}{k\alpha} \;=\; 1 \,,$$

where the second inequality follows by restricting the supremum to product states $\gamma^{(k)} = (|\psi\rangle\langle\psi|)^{\otimes k}$ *and writing* $\alpha = E^{(1)}$*.*

The next lemma describes the relationship between $E^{(k)}$ and $R^{(k)}$, where, we recall,

$$R^{(k)} \;=\; \big\| \gamma^{(k)} - (|\varphi\rangle\langle\varphi|)^{\otimes k} \big\|_1 \,.$$

LEMMA 5.3. *Let* $\gamma^{(k)} \in \mathcal{L}(\mathcal{H}^{(k)})$ *be a density matrix and* $\varphi \in L^2$ *satisfy* $\|\varphi\| = 1$*. Then*

$$E^{(k)} \;\leqslant\; R^{(k)} \,, \tag{5.7a}$$

$$R^{(k)} \;\leqslant\; \sqrt{8\, E^{(k)}} \,. \tag{5.7b}$$

PROOF. It is convenient to introduce the shorthand

$$p^{(k)} \;:=\; (|\varphi\rangle\langle\varphi|)^{\otimes k}.$$

Thus,

$$E^{(k)} \;=\; 1 - \big\langle \varphi^{\otimes k} , \gamma^{(k)} \varphi^{\otimes k} \big\rangle \;=\; \operatorname{Tr}\big(p^{(k)} - p^{(k)} \gamma^{(k)}\big) \;\leqslant\; \|p^{(k)}\| \big\| p^{(k)} - \gamma^{(k)} \big\|_1 \;=\; R^{(k)} \,,$$

which is (5.7a). In order to prove (5.7b) it is easiest to use the identity

$$\big\| p^{(k)} - \gamma^{(k)} \big\|_1 \;=\; 2 \, \big\| p^{(k)} - \gamma^{(k)} \big\| \,, \tag{5.8}$$

valid for any one-dimensional projector $p^{(k)}$ and nonnegative density matrix $\gamma^{(k)}$. This was first observed by Seiringer; see [RS07]. For the convenience of the reader we recall the proof of (5.8). Let $(\lambda_n)_{n \in \mathbb{N}}$ be the sequence of eigenvalues of the trace class operator $A := \gamma^{(k)} - p^{(k)}$. Since $p^{(k)}$ is a rank one projection, A has at most one negative eigenvalue, say λ_0. Also, $\operatorname{Tr} A = 0$ implies that $\sum_n \lambda_n = 0$. Thus, $\sum_n |\lambda_n| = 2|\lambda_0|$, which is (5.8).

Now (5.8) yields

$$R^{(k)} \;=\; \big\|p^{(k)} - \gamma^{(k)}\big\|_1 \;=\; 2\,\|p^{(k)} - \gamma^{(k)}\| \;\leqslant\; 2\sqrt{\operatorname{Tr}\big(p^{(k)} - \gamma^{(k)}\big)^2}\,.$$

Then (5.7b) follows from

$$\operatorname{Tr}\big(p^{(k)} - \gamma^{(k)}\big)^2 \;=\; 1 - 2\operatorname{Tr}\big(p^{(k)}\gamma^{(k)}\big) + \operatorname{Tr}(\gamma^{(k)})^2 \;\leqslant\; E^{(k)} - \operatorname{Tr}\big(p^{(k)}\gamma^{(k)}\big) + 1 \;=\; 2E^{(k)}\,.$$

Alternatively, one may prove (5.7b) without (5.8) by using the polar decomposition and the Cauchy-Schwarz inequality for Hilbert-Schmidt operators. □

REMARK 5.4. *Up to constant factors the bounds* (5.7) *are sharp, as the following examples show. Here we drop the irrelevant index k. Consider first*

$$\varphi \;=\; \begin{pmatrix}1\\0\end{pmatrix}, \qquad \gamma \;=\; \begin{pmatrix}1-a & 0\\ 0 & a\end{pmatrix},$$

where $0 \leqslant a \leqslant 1$. As above we set $p := |\varphi\rangle\langle\varphi|$. One finds

$$E \;=\; 1 - \langle\varphi, \gamma\,\varphi\rangle \;=\; a\,, \qquad R \;=\; \|p - \gamma\|_1 \;=\; 2a\,,$$

so that (5.7a) *is sharp up to a constant factor.*

It is not hard to see that if γ and p commute then (5.7b) *can be replaced with the stronger bound $R \lesssim E$. In order to show that in general* (5.7b) *is sharp up to a constant factor, consider*

$$\varphi \;=\; \begin{pmatrix}1\\0\end{pmatrix}, \qquad \gamma \;=\; \begin{pmatrix}1-a & \sqrt{a-a^2}\\ \sqrt{a-a^2} & a\end{pmatrix},$$

where $0 \leqslant a \leqslant 1$. One readily sees that γ is a density matrix (in fact, a one-dimensional projector). A short calculation yields

$$E \;=\; 1 - \langle\varphi, \gamma\,\varphi\rangle \;=\; a$$

as well as

$$\big\|\gamma(1-p)\big\|_1 \;=\; \sqrt{a}\,.$$

Using

$$\big\|\gamma(1-p)\big\|_1 \;=\; \big\|\gamma - p + p - \gamma p\big\|_1 \;\leqslant\; 2\,\|p - \gamma\|_1$$

we therefore find

$$R \;=\; \|p - \gamma\|_1 \;\geqslant\; \frac{\sqrt{a}}{2} \;=\; \frac{\sqrt{E}}{2}\,,$$

as desired.

5.2. Convergence for L^2-type singularities

This section is devoted to the case $w \in L^2 + L^\infty$.

5.2.1. Outline and main result. Our method relies on controlling the quantity

$$\alpha_N(t) \;:=\; E_N^{(1)}(t)\,. \tag{5.9}$$

To this end, we derive an estimate of the form

$$\dot{\alpha}_N(t) \;\leqslant\; A_N(t) + B_N(t)\,\alpha_N(t)\,, \tag{5.10}$$

which, by Grönwall's lemma (See Appendix C), implies

$$\alpha_N(t) \;\leqslant\; \alpha_N(0)\,\mathrm{e}^{\int_0^t B_N} + \int_0^t A_N(s)\,\mathrm{e}^{\int_s^t B_N}\,\mathrm{d}s\,. \tag{5.11}$$

In order to show (5.10), we differentiate $\alpha_N(t)$ and note that all terms arising from the one-particle Hamiltonian vanish. We control the remaining terms by introducing the time-dependent orthogonal projections

$$p(t) \;:=\; |\varphi(t)\rangle\langle\varphi(t)|\,, \qquad q(t) \;:=\; \mathbb{1} - p(t)\,.$$

We then partition $\mathbb{1} = p(t) + q(t)$ appropriately and use the following heuristics for controlling the terms that arise in this manner. Factors $p(t)$ are used to control singularities of w by exploiting the smoothness of the Hartree wave function $\varphi(t)$. Factors $q(t)$ are expected to yield something small, i.e. proportional to $\alpha_N(t)$, in accordance with the identity $\alpha_N(t) = \langle\Psi_N(t)\,, q_1(t)\Psi_N(t)\rangle$.

For the following it is convenient to rewrite the Hamiltonian (5.1) as

$$H_N \;=\; \sum_{i=1}^N h_i + \frac{1}{N}\sum_{1\leqslant i<j\leqslant N} W_{ij} \;=:\; H_N^0 + H_N^W\,, \tag{5.12}$$

where $W_{ij} \;:=\; w(x_i - x_j)$. We may now list our assumptions.

(A1) The one-particle Hamiltonian h is self-adjoint and bounded from below. Without loss of generality we assume that $h \geqslant 0$. We define the Hilbert space[3] $X_N \;=\; \mathcal{Q}(H_N^0)$ as the form domain of H_N^0 with norm

$$\|\Psi\|_{X_N} \;:=\; \big\|(1 + H_N^0)^{1/2}\Psi\big\|\,.$$

(A2) The Hamiltonian (5.12) is self-adjoint and bounded from below. We also assume that $\mathcal{Q}(H_N) \subset X_N$.

(A3) The interaction potential w is a real and even function satisfying $w \in L^{p_1} + L^{p_2}$, where $2 \leqslant p_1 \leqslant p_2 \leqslant \infty$.

(A4) The solution $\varphi(\cdot)$ of (5.4) satisfies

$$\varphi(\cdot) \in C(\mathbb{R}; X_1 \cap L^{q_1}) \cap C^1(\mathbb{R}; X_1^*)\,,$$

where $2 \leqslant q_2 \leqslant q_1 \leqslant \infty$ are defined through

$$\frac{1}{2} \;=\; \frac{1}{p_i} + \frac{1}{q_i}\,, \qquad i = 1, 2\,. \tag{5.13}$$

Here X_1^* denotes the dual space of X_1, i.e. the closure of L^2 under the norm $\|\varphi\|_{X_1^*} := \|(\mathbb{1} + h)^{-1/2}\varphi\|$.

[3]Note that, as a form, H_N^0 is closable (see [RS75], Theorem X.23), so that X_N is indeed a Hilbert space.

We now state our main result.

THEOREM 5.5. *Let $\Psi_{N,0} \in \mathcal{Q}(H_N)$ satisfy $\|\Psi_{N,0}\| = 1$, and $\varphi_0 \in X_1 \cap L^{q_1}$ satisfy $\|\varphi_0\| = 1$. Assume that Assumptions* (A1) – (A4) *hold. Then*

$$\alpha_N(t) \leqslant \left(\alpha_N(0) + \frac{1}{N}\right) \mathrm{e}^{\phi(t)} ,$$

where

$$\phi(t) := 32\|w\|_{L^{p_1}+L^{p_2}} \int_0^t \mathrm{d}s \, \big(\|\varphi(s)\|_{q_1} + \|\varphi(s)\|_{q_2}\big) .$$

We may combine this result with the observations of Section 5.1.

COROLLARY 5.6. *Let the sequence $\Psi_{N,0} \in \mathcal{Q}(H_N)$, $N \in \mathbb{N}$, satisfy the assumptions of Theorem 5.5 as well as*

$$E_N^{(1)}(0) \lesssim \frac{1}{N} .$$

Then we have

$$E_N^{(k)}(t) \lesssim \frac{k}{N} \mathrm{e}^{\phi(t)} , \qquad R_N^{(k)}(t) \lesssim \sqrt{\frac{k}{N}} \mathrm{e}^{\phi(t)/2} .$$

REMARK 5.7. *Corollary 5.6 implies that we can control the condensation of $k = o(N)$ particles.*

REMARK 5.8. *Assumption (A3) allows for singularities in w up to, but not including, the type $|x|^{-3/2}$ in three dimensions. In the next section we treat a larger class of interaction potentials.*

REMARK 5.9. *Assumption (A4) is typically verified by solving the Hartree equation in a Sobolev space of high index (see e.g. Section 5.2.2). Instead of requiring a global-in-time solution, it is enough to have a local-in-time solution on $[0, T)$ for some $T > 0$.*

REMARK 5.10. *If $\sup_t \phi(t) < \infty$, or in other words if $\|\varphi(t)\|_{q_1}$ and $\|\varphi(t)\|_{q_2}$ are integrable over $\mathbb{R}$, then all estimates are uniform in time. This describes a scattering regime where the time evolution is asymptotically free for large times. Such an integrability condition requires large exponents q_i, which translates to small exponents p_i, i.e. an interaction potential with strong decay.*

REMARK 5.11. *The result easily extends to time-dependent one-particle Hamiltonians $h \equiv h(t)$. Replace Assumptions (A1) and (A2) with*

(A1') The Hamiltonian $h(t)$ is self-adjoint and bounded from below. We assume that there is an operator $h_0 \geqslant 0$ that such that $0 \leqslant h(t) \leqslant h_0$ for all t. Define the Hilbert space $X_N = \mathcal{Q}\big(\sum_i (h_0)_i\big)$ as in (A1).

(A2') The Hamiltonian $H_N(t)$ is self-adjoint and bounded from below. We assume that the form-domain $\mathcal{Q}(H_N(t)) \subset X_N$ for all t. We also assume that the N-body propagator $U_N(t,s)$, defined by

$$\mathrm{i}\partial_t U_N(t,s) = H_N(t) U_N(t,s) , \qquad U_N(s,s) = \mathbb{1} ,$$

exists and satisfies $U_N(t,0)\Psi_{N,0} \in \mathcal{Q}(H_N(t))$ for all t.

It is then straightforward that Theorem 5.5 holds with the same proof.

REMARK 5.12. *In some cases (see e.g. Section 5.2.2 below) it is convenient to modify the assumptions as follows. Replace Assumptions (A3) and (A4) with*

(A3') The interaction potential w is a real and even function satisfying

$$\left\| w^2 * |\varphi|^2 \right\|_\infty \leqslant K \|\varphi\|_{X_1}^2 \tag{5.14}$$

for some constant $K > 0$. Without loss of generality we assume that $K \geqslant 1$.

(A4') The solution $\varphi(\cdot)$ of (5.4) *satisfies*

$$\varphi(\cdot) \in C(\mathbb{R}; X_1) \cap C^1(\mathbb{R}; X_1^*) .$$

Then Theorem 5.5 and Corollary 5.6 hold with

$$\phi(t) = 32K \int_0^t \mathrm{d}s \, \|\varphi(s)\|_{X_1}^2 .$$

The proof remains virtually unchanged. One replaces (5.33) *with* (5.14)*, as well as* (5.29) *with*

$$\left\| w * |\varphi|^2 \right\|_\infty \leqslant 2K \|\varphi\|_{X_1}^2 ,$$

which is an easy consequence of (5.14)*.*

5.2.2. Examples. We list two examples of systems satisfying the assumptions of Theorem 5.5.

Particles in a trap. Consider nonrelativistic particles in $\mathbb{R}^3$ confined by a strong trapping potential. The particles interact by means of the Coulomb potential: $w(x) = \lambda |x|^{-1}$, where $\lambda \in \mathbb{R}$. The one-particle Hamiltonian is of the form $h = -\Delta + v$, where v is a measurable function on $\mathbb{R}^3$. Decompose v into its positive and negative parts: $v = v_+ - v_-$, where $v_+, v_- \geqslant 0$. We assume that $v_+ \in L^1_{\mathrm{loc}}$ and that v_- is $-\Delta$-form bounded with relative bound less than one, i.e. there are constants $0 \leqslant a < 1$ and $0 \leqslant b < \infty$ such that

$$\langle \varphi , v_- \varphi \rangle \leqslant a \langle \varphi , -\Delta \varphi \rangle + b \langle \varphi , \varphi \rangle . \tag{5.15}$$

Thus $h + b\mathbb{1}$ is positive. Moreover, we claim that h is essentially self-adjoint on $C_c^\infty(\mathbb{R}^3)$. This follows by density and the fact that the equation $(h + (b+1)\mathbb{1})\varphi = f$ has a unique solution $\varphi \in \{\varphi \in L^2 : h\varphi \in L^2\}$ for each $f \in L^2$. In order to show this, define the Hilbert space $\mathcal{H}_h := \mathcal{D}\big((h + (b+1)\mathbb{1})^{1/2}\big)$ with scalar product $\langle f , g \rangle_h := \langle f , (h + (b+1)\mathbb{1}) g \rangle$; see Theorem X.23 in [RS75]. Then the map $g \mapsto \langle f , g \rangle$ is in $\mathcal{H}_h^*$, so that Riesz's representation theorem implies there is a unique $\varphi \in \mathcal{H}_h$ such that $\langle g , f \rangle = \langle g , \varphi \rangle_h$ for all $g \in \mathcal{H}_h$. The claim now follows from the density of $\mathcal{H}_h$ in L^2.

It is now easy to see that Assumptions (A1) and (A2) hold with the one-particle Hamiltonian $h + c\mathbb{1}$ for some $c > 0$. Let us assume without loss of generality that $c = 0$. Next, we verify Assumptions (A3') and (A4') (see Remark 5.12). We find

$$\left\| w^2 * |\varphi|^2 \right\|_\infty = \sup_x \left| \int \mathrm{d}y \, \frac{\lambda^2}{|x-y|^2} |\varphi(y)|^2 \right| \lesssim \langle \varphi , -\Delta \varphi \rangle \lesssim \langle \varphi , h\varphi \rangle + \langle \varphi , \varphi \rangle = \|\varphi\|_{X_1}^2 ,$$

where the second step follows from Hardy's inequality and translation invariance of Δ, and the third step is a simple consequence of (5.15). This proves Assumption (A3').

Next, take $\varphi_0 \in X_1$. By standard methods (see e.g. the presentation of [Len07]) one finds that Assumption (A4') holds. Moreover, the mass $\|\varphi(t)\|^2$ and the energy

$$E^\varphi(t) \;=\; \left[\langle \varphi , h\varphi\rangle + \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\; w(x-y)|\varphi(x)|^2|\varphi(y)|^2\right]\Bigg|_t$$

are conserved under time evolution. Using the identity $|x|^{-1} \leqslant \mathbb{1}_{\{|x|\leqslant\varepsilon\}}\varepsilon|x|^{-2} + \mathbb{1}_{\{|x|>\varepsilon\}}\varepsilon^{-1}$ and Hardy's inequality one sees that

$$\|\varphi(t)\|_{X_1}^2 \;\lesssim\; E^\varphi(t) + \|\varphi(t)\|^2\,,$$

and therefore $\|\varphi(t)\|_{X_1} \leqslant C$ for all t. We conclude: Theorem 5.5 holds with $\phi(t) = Ct$. This example generalizes the results of [EY01], [RS07], and Chapter 4.

More generally, the preceding discussion holds for interaction potentials $w \in L^3_w + L^\infty$. This follows from the following lemma by setting $f = w^2$.

LEMMA 5.13. *For $d = 3$ we have that*

$$\int \mathrm{d}x\; |f(x)||\varphi(x)|^2 \;\leqslant\; C\,\|f\|_{3/2,w}\,\langle \varphi , -\Delta\varphi\rangle\,.$$

PROOF. Let f^* be the symmetric-decreasing rearrangement of f, defined by

$$f^*(x) \;:=\; \int_0^\infty \mathrm{d}t\; \mathbb{1}_{\{|x|<R_t\}}\,,$$

where R_t is defined through $\Omega_d\, R_t^d := \big|\{x \,:\, |f(x)| > t\}\big|$ and Ω_d is the volume of the unit ball in d dimensions. See [LL01] for more details. First, we claim that

$$f^*(x) \;\leqslant\; C\frac{\|f\|_{p,w}}{|x|^{d/p}}\,. \tag{5.16}$$

Indeed, by definition of the weak L^p-norm, we have

$$\Omega_d\, R_t^d \;=\; \big|\{x \,:\, |f(x)| > t\}\big| \;\leqslant\; \frac{\|f\|_{p,w}^p}{t^p}\,,$$

from which we get

$$f^*(x) \;=\; \int_0^\infty \mathrm{d}t\; \mathbb{1}_{\{|x|<R_t\}} \;\leqslant\; \int_0^\infty \mathrm{d}t\; \mathbb{1}_{\left\{|x|<\|f\|_{p,w}^{p/d}\Omega_d^{-1/d}t^{-p/d}\right\}} \;\leqslant\; \Omega_d^{1/p}\frac{\|f\|_{p,w}}{|x|^{d/p}}\,,$$

as claimed.

Thus, using Theorem 3.4 and Remark 3.3(v) in [LL01], we find

$$\begin{aligned}\int \mathrm{d}x\; |f(x)||\varphi(x)|^2 \;&\leqslant\; \int \mathrm{d}x\; f^*(x)(|\varphi|^2)^*(x) \;=\; \int \mathrm{d}x\; f^*(x)(\varphi^*(x))^2\\ &\leqslant\; C\|f\|_{3/2,w}\int \mathrm{d}x\frac{(\varphi^*(x))^2}{|x|^2} \;\leqslant\; C\|f\|_{3/2,w}\langle \varphi^* , -\Delta\varphi^*\rangle \;\leqslant\; C\|f\|_{3/2,w}\langle \varphi , -\Delta\varphi\rangle\,,\end{aligned}$$

where we used (5.16) with $d = 3$ and $p = 3/2$, Hardy's inequality, and the fact that rearrangement decreases kinetic energy (Lemma 7.17 in [LL01]). □

A boson star. Consider semirelativistic particles in $\mathbb{R}^3$ whose one-particle Hamiltonian is given by $h = \sqrt{\mathbb{1} - \Delta}$. The particles interact by means of a Coulomb potential: $w(x) = \lambda |x|^{-1}$. We impose the condition $\lambda > -4/\pi$. This condition is necessary for both the stability of the N-body problem (i.e. Assumption (A2)) and the global well-posedness of the Hartree equation. See [LY87, Len07] for details. It is well known that Assumptions (A1) and (A2) hold in this case.

In order to show Assumption (A4) we need some regularity of $\varphi(\cdot)$. To this end, let $s > 1$ and take $\varphi_0 \in H^s$. Theorem 3 of [Len07] implies that (5.4) has a unique global solution in H^s. Therefore Sobolev's inequality implies that Assumption (A4) holds with

$$\frac{1}{q_1} \;=\; \frac{1}{2} - \frac{s}{3}\,.$$

Thus $q_1 > 6$, and Assumption (A3) holds with appropriately chosen values of p_1, p_2. We conclude: Theorem 5.5 holds for some continuous function $\phi(t)$. This example generalizes the result of [ES07].

On may in fact derive an explicit upper bound on $\phi(t)$ as follows. Assume that $s < 3/2$. In order to get an estimate on $\|\varphi(t)\|_{q_1}$, we note that Lemma 3 of [Len07] yields the bound

$$\|\varphi(t)\|_{H^s} \;\leqslant\; \|\varphi_0\|_{H^s} + \int_0^t \mathrm{d}s\, \|\varphi(s)\|_{H^{1/2}}^2\, \|\varphi(s)\|_{H^s}\,.$$

As in the previous example, conservation of energy implies that $\|\varphi(s)\|_{H^{1/2}}^2 \leqslant C$. Thus Grönwall's lemma yields

$$\|\varphi(t)\|_{H^s} \;\leqslant\; \|\varphi_0\|_{H^s}\, \mathrm{e}^{Ct}\,.$$

Therefore Sobolev's inequality and interpolation imply that Theorem 5.5 holds with $\phi(t) = C_1 \mathrm{e}^{C_2 t}$. The obtained bound is far from optimal. This deficiency is a manifestation of the fact that it is in general very hard to derive sharp estimates on the growth of high Sobolev norms of solutions of nonlinear Schrödinger equations.

5.2.3. Proof of Theorem 5.5, part I: a family of projectors. Define the time-dependent projectors

$$p(t) \;:=\; |\varphi(t)\rangle\langle\varphi(t)|\,, \qquad q(t) \;:=\; \mathbb{1} - p(t)\,.$$

Write

$$\mathbb{1} \;=\; (p_1 + q_1) \cdots (p_N + q_N) \tag{5.17}$$

and define P_k, for $k = 0, \dots, N$, as the term obtained by multiplying out (5.17) and selecting all summands containing k factors q. In other words,

$$P_k \;=\; \sum_{\substack{a \in \{0,1\}^N :\\ \sum_i a_i = k}} \prod_{i=1}^N p_i^{1-a_i} q_i^{a_i}\,. \tag{5.18}$$

If $k \neq \{0, \dots, N\}$ we set $P_k \;=\; 0$. It is easy to see that the following properties hold:

(i) P_k is an orthogonal projector,

(ii) $P_k P_l \;=\; \delta_{kl} P_k$,

(iii) $\sum_k P_k \;=\; \mathbb{1}$.

Next, for any function $f : \{0, \ldots, N\} \to \mathbb{C}$ we define the operator

$$\widehat{f} := \sum_k f(k) P_k \,. \tag{5.19}$$

It follows immediately that

$$\widehat{f}\widehat{g} = \widehat{fg}\,,$$

and that $\widehat{f}$ commutes with p_i and P_k. We shall often make use of the functions

$$m(k) := \frac{k}{N}\,, \qquad n(k) := \sqrt{\frac{k}{N}}\,.$$

We have the relation

$$\frac{1}{N}\sum_i q_i = \frac{1}{N}\sum_k \sum_i q_i P_k = \frac{1}{N}\sum_k k P_k = \widehat{m}\,. \tag{5.20}$$

Thus, by symmetry of Ψ, we get

$$\alpha = \langle \Psi\,, q_1\,\Psi \rangle = \langle \Psi\,, \widehat{m}\,\Psi \rangle\,. \tag{5.21}$$

The correspondence $q_1 \sim \widehat{m}$ of (5.20) yields the following useful bounds.

LEMMA 5.14. *For any nonnegative function $f : \{0, \ldots, N\} \to [0, \infty)$ we have*

$$\big\langle \Psi\,, \widehat{f} q_1 \Psi \big\rangle = \big\langle \Psi\,, \widehat{f}\,\widehat{m} \Psi \big\rangle\,, \tag{5.22}$$

$$\big\langle \Psi\,, \widehat{f} q_1 q_2 \Psi \big\rangle \leqslant \frac{N}{N-1}\big\langle \Psi\,, \widehat{f}\,\widehat{m}^2 \Psi \big\rangle\,. \tag{5.23}$$

PROOF. The proof of (5.22) is an immediate consequence of (5.20). In order to prove (5.23) we write, using symmetry of Ψ as well as (5.20),

$$\begin{aligned}\big\langle \Psi\,, \widehat{f}\, q_1 q_2 \Psi \big\rangle &= \frac{1}{N(N-1)}\sum_{i \neq j}\big\langle \Psi\,, \widehat{f}\, q_i q_j \Psi \big\rangle \\ &\leqslant \frac{1}{N(N-1)}\sum_{i,j}\big\langle \Psi\,, \widehat{f}\, q_i q_j \Psi \big\rangle = \frac{N}{N-1}\big\langle \Psi\,, \widehat{f}\,\widehat{m}^2 \Psi \big\rangle\,,\end{aligned}$$

which is the claim. □

Next, we introduce the shift operation τ_n, $n \in \mathbb{Z}$, defined on functions f through

$$(\tau_n f)(k) := f(k+n)\,. \tag{5.24}$$

Its usefulness for our purposes is encapsulated by the following lemma.

LEMMA 5.15. *Let $r \geqslant 1$ and A be an operator on $\mathcal{H}^{(r)}$. Let Q_i, $i = 1, 2$, be two projectors of the form*

$$Q_i = \#_1 \cdots \#_r\,,$$

where each $\#$ stands for either p or q. Then

$$Q_1 A_{1 \ldots r} \widehat{f} Q_2 = Q_1 \widehat{\tau_n f} A_{1 \ldots r} Q_2\,,$$

where $n = n_2 - n_1$ and n_i is the number of factors q in Q_i.

PROOF. Define

$$P_k^r \;:=\; \sum_{\substack{a\in\{0,1\}^{N-r}\\ \sum_i a_i=k}} \prod_{i=r+1}^{N} p_i^{1-a_i} q_i^{a_i}\,.$$

Then,

$$Q_i\widehat{f} \;=\; \sum_k f(k)\,Q_iP_k \;=\; \sum_k f(k)\,Q_iP^r_{k-n_i} \;=\; \sum_k f(k+n_i)\,Q_iP^r_k\,.$$

The claim follows from the fact that P_k^r commutes with $A_{1\dots r}$. □

5.2.4. Proof of Theorem 5.5, part II: a bound on $\dot\alpha$. Let us abbreviate

$$W^\varphi \;:=\; w*|\varphi|^2\,.$$

From Assumptions (A3) and (A4) we find $W^\varphi \in L^\infty$ (see (5.29) below). Then $\mathrm{i}\partial_t\varphi = (h+W^\varphi)\varphi$, where $h+W^\varphi\in\mathcal{L}(X_1;X_1^*)$. Thus, for any $\psi\in X_1$ independent of t we have

$$\mathrm{i}\partial_t\langle\psi\,,p\,\psi\rangle \;=\; \langle\psi\,,[h+W^\varphi\,,p]\psi\rangle\,.$$

On the other hand, it is easy to see from Assumptions (A3) and (A4) that $\widehat{m}\Psi\in\mathcal{Q}(H)$. Combining these observations, and noting that $\Psi\in\mathcal{Q}(H)\subset X$ by Assumption (A2), we see that α is differentiable in t with derivative

$$\dot\alpha \;=\; \mathrm{i}\big\langle\Psi\,,\big[H-H^\varphi\,,\widehat{m}\big]\Psi\big\rangle\,,$$

where $H^\varphi := \sum_i(h_i+W_i^\varphi)$. Thus,

$$\dot\alpha \;=\; \mathrm{i}\left\langle\Psi\;,\;\left[\frac{1}{N}\sum_{i<j}W_{ij}-\sum_i W_i^\varphi\;,\;\widehat{m}\right]\Psi\right\rangle.$$

By symmetry of Ψ and $\widehat{m}$ we get

$$\dot\alpha \;=\; \frac{\mathrm{i}}{2}\big\langle\Psi\,,\big[(N-1)W_{12}-NW_1^\varphi-NW_2^\varphi\,,\widehat{m}\big]\Psi\big\rangle\,. \tag{5.25}$$

In order to estimate the right-hand side, we introduce

$$\mathbb{1} \;=\; (p_1+q_1)(p_2+q_2)$$

on both sides of the commutator in (5.25). Of the sixteen resulting terms only three different types survive:

$$\frac{\mathrm{i}}{2}\big\langle\Psi\,,p_1p_2\big[(N-1)W_{12}-NW_1^\varphi-NW_2^\varphi\,,\widehat{m}\big]q_1p_2\Psi\big\rangle \qquad \text{(I)}$$
$$\frac{\mathrm{i}}{2}\big\langle\Psi\,,q_1p_2\big[(N-1)W_{12}-NW_1^\varphi-NW_2^\varphi\,,\widehat{m}\big]q_1q_2\Psi\big\rangle \qquad \text{(II)}$$
$$\frac{\mathrm{i}}{2}\big\langle\Psi\,,p_1p_2\big[(N-1)W_{12}-NW_1^\varphi-NW_2^\varphi\,,\widehat{m}\big]q_1q_2\Psi\big\rangle \qquad \text{(III)}\,.$$

Indeed, Lemma 5.15 implies that terms with the same number of factors q on the left and on the right vanish. What remains is

$$\dot\alpha \;=\; 2\text{(I)}+2\text{(II)}+\text{(III)}+\text{ complex conjugate}\,.$$

The remainder of the proof consists in estimating each term.

Term (I). First, we remark that

$$p_2 W_{12} p_2 \;=\; p_2 W_1^{\varphi}\,. \tag{5.26}$$

This is easiest to see using operator kernels (we drop the trivial indices $x_3, y_3, \dots, x_N, y_N$):

$$\begin{aligned}(p_2 W_{12} p_2)(x_1, x_2; y_1, y_2) \;&=\; \int \mathrm{d}z\; \varphi(x_2)\,\overline{\varphi}(z)\, w(x_1 - z)\, \delta(x_1 - y_1)\, \varphi(z)\, \overline{\varphi}(y_2)\\ &=\; \varphi(x_2)\,\overline{\varphi}(y_2)\, \delta(x_1 - y_1)\, (w * |\varphi|^2)(x_1)\,.\end{aligned}$$

Therefore,

$$(\mathrm{I}) \;=\; \frac{\mathrm{i}}{2}\big\langle \Psi\,, p_1 p_2 \big[(N-1)W_1^{\varphi} - N W_1^{\varphi}\,, \widehat{m}\big] q_1 p_2 \Psi\big\rangle \;=\; \frac{-\mathrm{i}}{2}\big\langle \Psi\,, p_1 p_2 \big[W_1^{\varphi}\,, \widehat{m}\big] q_1 p_2 \Psi\big\rangle\,.$$

Using Lemma 5.15 we find

$$(\mathrm{I}) \;=\; \frac{-\mathrm{i}}{2}\big\langle \Psi\,, p_1 p_2 W_1^{\varphi}\big(\widehat{m} - \widehat{\tau_{-1} m}\big) q_1 p_2 \Psi\big\rangle \;=\; \frac{-\mathrm{i}}{2N}\big\langle \Psi\,, p_1 p_2 W_1^{\varphi} q_1 p_2 \Psi\big\rangle\,.$$

This gives

$$\big|(\mathrm{I})\big| \;\leqslant\; \frac{1}{2N}\,\|W^{\varphi}\|_\infty \;=\; \frac{1}{2N}\big\|w * |\varphi|^2\big\|_\infty\,.$$

By Assumption (A3), we may write

$$w \;=\; w^{(1)} + w^{(2)}\,, \qquad w^{(i)} \;\in\; L^{p_i}\,. \tag{5.27}$$

By Young's inequality,

$$\big\|w^{(i)} * |\varphi|^2\big\|_\infty \;\leqslant\; \|w^{(i)}\|_{p_i} \|\varphi\|_{r_i}^2\,,$$

where r_1, r_2 are defined through

$$1 \;=\; \frac{1}{p_i} + \frac{2}{r_i}\,. \tag{5.28}$$

Therefore,

$$\big\|w * |\varphi|^2\big\|_\infty \;\leqslant\; \|w^{(1)}\|_{p_1}\|\varphi\|_{r_1}^2 + \|w^{(1)}\|_{p_2}\|\varphi\|_{r_2}^2 \;\leqslant\; \big(\|w^{(1)}\|_{p_1} + \|w^{(2)}\|_{p_2}\big)\big(\|\varphi\|_{r_1} + \|\varphi\|_{r_2}\big)^2\,.$$

Taking the infimum over all decompositions (5.27) yields

$$\|W^{\varphi}\|_\infty \;=\; \big\|w * |\varphi|^2\big\|_\infty \;\leqslant\; \|w\|_{L^{p_1} + L^{p_2}}\big(\|\varphi\|_{r_1} + \|\varphi\|_{r_2}\big)^2\,. \tag{5.29}$$

Note that Assumptions (A3) and (A4) imply

$$2 \;\leqslant\; r_i \;\leqslant\; q_1\,, \tag{5.30}$$

so that the right-hand side of (5.29) is finite. Summarizing,

$$\big|(\mathrm{I})\big| \;\leqslant\; \frac{1}{2N}\|w\|_{L^{p_1} + L^{p_2}}\big(\|\varphi\|_{r_1} + \|\varphi\|_{r_2}\big)^2\,. \tag{5.31}$$

Term (II). Applying Lemma 5.15 to (II) yields

$$\begin{aligned}(\mathrm{II}) \;&=\; \frac{\mathrm{i}}{2}\big\langle \Psi\,, q_1 p_2 \big((N-1)W_{12} - N W_2^{\varphi}\big)\big(\widehat{m} - \widehat{\tau_{-1} m}\big) q_1 q_2 \Psi\big\rangle\\ &=\; \frac{\mathrm{i}}{2}\bigg\langle \Psi\;,\; q_1 p_2 \bigg(\frac{N-1}{N} W_{12} - W_2^{\varphi}\bigg) q_1 q_2 \Psi\bigg\rangle\,,\end{aligned}$$

so that

$$\big|(\mathrm{II})\big| \;\leqslant\; \frac{1}{2}\big|\big\langle \Psi\,, q_1 p_2 W_{12} q_1 q_2 \Psi\big\rangle\big| + \frac{1}{2}\big|\big\langle \Psi\,, q_1 p_2 W_2^{\varphi} q_1 q_2 \Psi\big\rangle\big|\,. \tag{5.32}$$

The second term of (5.32) is bounded by

$$\frac{1}{2}\|W^{\varphi}\|_{\infty}\,\|q_1\Psi\|^2 \;\leqslant\; \frac{1}{2}\|w\|_{L^{p_1}+L^{p_2}}\big(\|\varphi\|_{r_1}+\|\varphi\|_{r_2}\big)^2\,\alpha\,,$$

where we used the bound (5.29) as well as (5.21).

The first term of (5.32) is bounded using Cauchy-Schwarz by

$$\frac{1}{2}\sqrt{\big\langle \Psi\,, q_1 p_2 W_{12}^2 p_2 q_1 \Psi\big\rangle}\sqrt{\langle \Psi\,, q_1 q_2 \Psi\rangle} \;=\; \frac{1}{2}\sqrt{\big\langle \Psi\,, q_1 p_2 \big(w^2 * |\varphi|^2\big)_1 p_2 q_1 \Psi\big\rangle}\sqrt{\langle \Psi\,, q_1 q_2 \Psi\rangle}\,.$$

This follows by applying (5.26) to W^2. Thus we get the bound

$$\frac{1}{2}\|q_1\Psi\|^2\sqrt{\big\|w^2 * |\varphi|^2\big\|_{\infty}} \;=\; \frac{1}{2}\alpha\sqrt{\big\|w^2 * |\varphi|^2\big\|_{\infty}}\,.$$

We now proceed as above. Using the decomposition (5.27) we get

$$\big\|w^2 * |\varphi|^2\big\|_{\infty} \;\leqslant\; 2\big\|(w^{(1)})^2 * |\varphi|^2\big\|_{\infty} + 2\big\|(w^{(2)})^2 * |\varphi|^2\big\|_{\infty}\,.$$

Then Young's inequality gives

$$\big\|(w^{(i)})^2 * |\varphi|^2\big\|_{\infty} \;\leqslant\; \big\|w^{(i)}\big\|_{p_i}^2\|\varphi\|_{q_i}^2\,,$$

which implies that

$$\big\|w^2 * |\varphi|^2\big\|_{\infty} \;\leqslant\; 2\|w\|_{L^{p_1}+L^{p_2}}^2\big(\|\varphi\|_{q_1}+\|\varphi\|_{q_2}\big)^2\,. \tag{5.33}$$

Putting all of this together we get

$$\big|(\mathrm{II})\big| \;\leqslant\; \frac{1}{2}\|w\|_{L^{p_1}+L^{p_2}}\Big[\sqrt{2}\big(\|\varphi\|_{q_1}+\|\varphi\|_{q_2}\big) + \big(\|\varphi\|_{r_1}+\|\varphi\|_{r_2}\big)^2\Big]\,\alpha\,.$$

Term (III). The final term (III) is equal to

$$\begin{aligned}\frac{\mathrm{i}}{2}\big\langle \Psi\,, p_1 p_2\big[(N-1)W_{12}\,, \widehat{m}\big] q_1 q_2 \Psi\big\rangle \;&=\; \frac{\mathrm{i}}{2}\big\langle \Psi\,, p_1 p_2 (N-1) W_{12}\big(\widehat{m} - \widehat{\tau_{-2} m}\big) q_1 q_2 \Psi\big\rangle \\ &=\; \mathrm{i}\frac{N-1}{N}\big\langle \Psi\,, p_1 p_2 W_{12} q_1 q_2 \Psi\big\rangle\,,\end{aligned}$$

where we used Lemma 5.15. Next, we note that, on the range of q_1, the operator $\widehat{n}^{-1}$ is well-defined and bounded. Thus (III) is equal to

$$\mathrm{i}\frac{N-1}{N}\big\langle \Psi\,, p_1 p_2 W_{12}\,\widehat{n}\,\widehat{n}^{-1} q_1 q_2 \Psi\big\rangle \;=\; \mathrm{i}\frac{N-1}{N}\big\langle \Psi\,, p_1 p_2\,\widehat{\tau_2 n}\,W_{12}\,\widehat{n}^{-1} q_1 q_2 \Psi\big\rangle\,,$$

where we used Lemma 5.15 again. We now use Cauchy-Schwarz to get

$$\begin{aligned}
\big|(\mathrm{III})\big| &\leqslant \sqrt{\big\langle \Psi\,, p_1p_2\, \widehat{\tau_2 n}\, W_{12}^2\, \widehat{\tau_2 n}\, p_1p_2\Psi\big\rangle}\sqrt{\big\langle \Psi\,, \widehat{n}^{-2} q_1q_2\Psi\big\rangle}\\
&= \sqrt{\big\langle \Psi\,, p_1p_2\, \widehat{\tau_2 n}\, \big(w^2 * |\varphi|^2\big)_1\, \widehat{\tau_2 n}\, p_1p_2\Psi\big\rangle}\sqrt{\big\langle \Psi\,, \widehat{m}^{-1} q_1q_2\Psi\big\rangle}\\
&\leqslant \sqrt{\big\|w^2 * |\varphi|^2\big\|_\infty}\, \|\widehat{\tau_2 n}\Psi\| \sqrt{\frac{N}{N-1}}\sqrt{\langle \Psi\,, \widehat{m}\Psi\rangle}\\
&= \sqrt{\big\|w^2 * |\varphi|^2\big\|_\infty}\sqrt{\frac{N}{N-1}}\sqrt{\big\langle \Psi\,, \widehat{\tau_2 m}\Psi\big\rangle}\sqrt{\alpha}\\
&= \sqrt{\big\|w^2 * |\varphi|^2\big\|_\infty}\sqrt{\frac{N}{N-1}}\sqrt{\big\langle \Psi\,, \widehat{m}\Psi\big\rangle + \frac{2}{N}}\,\sqrt{\alpha}\\
&\leqslant \sqrt{\big\|w^2 * |\varphi|^2\big\|_\infty}\sqrt{\frac{N}{N-1}}\left(\alpha + \sqrt{\frac{2\alpha}{N}}\right)\\
&\leqslant \sqrt{\big\|w^2 * |\varphi|^2\big\|_\infty}\sqrt{\frac{N}{N-1}}\,2\left(\alpha + \frac{1}{N}\right).
\end{aligned}$$

Using the estimate (5.33) we get finally

$$\big|(\mathrm{III})\big| \leqslant 2\sqrt{2}\|w\|_{L^{p_1}+L^{p_2}}\big(\|\varphi\|_{q_1} + \|\varphi\|_{q_2}\big)\sqrt{\frac{N}{N-1}}\left(\alpha + \frac{1}{N}\right).$$

Conclusion of the proof. We have shown that the estimate (5.10) holds with

$$\begin{aligned}
B_N(t) &= 2\|w\|_{L^{p_1}+L^{p_2}}\Big[\big(\|\varphi(t)\|_{r_1} + \|\varphi(t)\|_{r_2}\big)^2 + 6\big(\|\varphi(t)\|_{q_1} + \|\varphi(t)\|_{q_2}\big)\Big],\\
A_N(t) &= \frac{B_N(t)}{N}.
\end{aligned}$$

Using L^2-norm conservation $\|\varphi(t)\| = 1$ and interpolation we find $\|\varphi(t)\|_{r_i}^2 \leqslant \|\varphi(t)\|_{q_i}$. Thus,

$$B_N(t) \leqslant 16\|w\|_{L^{p_1}+L^{p_2}}\big(\|\varphi(t)\|_{q_1} + \|\varphi(t)\|_{q_2}\big).$$

The claim now follows from the Grönwall estimate (5.11).

5.3. Convergence for stronger singularities

In this section we extend the results of the Section 5.2 to more singular interaction potentials. We consider the case $w \in L^{p_0} + L^\infty$, where

$$\frac{1}{p_0} = \frac{1}{2} + \frac{1}{d}. \tag{5.34}$$

For example in three dimensions $p_0 = 6/5$, which corresponds to singularities up to, but not including, the type $|x|^{-5/2}$. Of course, there are other restrictions on the interaction potential which ensure the stability of the N-body Hamiltonian and the well-posedness of the Hartree equation. In practice, it is often these latter restrictions that determine the class of allowed singularities.

In the words of [RS75] (p. 169), it is "venerable physical folklore" that an N-body Hamiltonian of the form (5.12), with $h = -\Delta$ and $w(x) = |x|^{-\zeta}$ for $\zeta < 2$, produces reasonable quantum dynamics in three dimensions. Mathematically, this means that such a Hamiltonian is self-adjoint; this is a well-known result (see e.g. [RS75]). The corresponding Hartree equation is known to be globally well-posed (see [GV80]). This section answers (affirmatively) the question whether, in the case of such singular interaction potentials, the mean-field limit of the N-body dynamics is governed by the Hartree equation.

5.3.1. Outline and main result. As in Section 5.2, we need to control expressions of the form $\|w^2 * |\varphi|^2\|_\infty$. The situation is considerably more involved when w^2 is not locally integrable. An important step in dealing with such potentials in our proof is to express w as the divergence of a vector field $\xi \in L^2$. This approach requires the control of not only $\alpha = \|q_1\Psi\|^2$ but also $\|\nabla_1 q_1 \Psi\|^2$, which arises from integrating by parts in expressions containing the factor $\nabla \cdot \xi$. As it turns out, β, defined through

$$\beta_N(t) \;:=\; \langle \Psi_N \,, \widehat{n}\, \Psi_N \rangle\big|_t \,, \tag{5.35}$$

does the trick. This follows from an estimate exploiting conservation of energy (see Lemma 5.21 below). The inequality $m \leqslant n$ and the representation (5.21) yield

$$\alpha \;\leqslant\; \beta \,. \tag{5.36}$$

We consider a Hamiltonian of the form (5.12) and make the following assumptions.

(B1) The one-particle Hamiltonian h is self-adjoint and bounded from below. Without loss of generality we assume that $h \geqslant 0$. We also assume that there are constants $\kappa_1, \kappa_2 > 0$ such that

$$-\Delta \;\leqslant\; \kappa_1 \, h + \kappa_2 \,,$$

as an inequality of forms on $\mathcal{H}^{(1)}$.

(B2) The Hamiltonian (5.12) is self-adjoint and bounded from below. We also assume that $\mathcal{Q}(H_N) \subset X_N$, where X_N is defined as in Assumption (A1).

(B3) There is a constant $\kappa_3 \in (0,1)$ such that

$$0 \;\leqslant\; (1-\kappa_3)(h_1 + h_2) + W_{12} \,,$$

as an inequality of forms on $\mathcal{H}^{(2)}$.

(B4) The interaction potential w is a real and even function satisfying $w \in L^p + L^\infty$, where $p_0 < p \leqslant 2$.

(B5) The solution $\varphi(\cdot)$ of (1.26) satisfies

$$\varphi(\cdot) \;\in\; C(\mathbb{R}; X_1^2 \cap L^\infty) \cap C^1(\mathbb{R}; L^2) \,,$$

where $X_1^2 \;:=\; \mathcal{Q}(h^2) \subset L^2$ is equipped with the norm

$$\|\varphi\|_{X_1^2} \;:=\; \big\|(1+h^2)^{1/2}\varphi\big\| \,.$$

Next, define the microscopic energy per particle as

$$E_N^\Psi(t) \;:=\; \frac{1}{N}\langle \Psi_N\,, H_N\,\Psi_N\rangle\big|_t\,,$$

as well as the Hartree energy

$$E^\varphi(t) \;:=\; \left[\langle\varphi\,, h\,\varphi\rangle + \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\; w(x-y)|\varphi(x)|^2|\varphi(y)|^2\right]\Bigg|_t\,.$$

By spectral calculus, $E_N^\Psi(t)$ is independent of t. Also, invoking Assumption (B5) to differentiate $E^\varphi(t)$ with respect to t shows that $E^\varphi(t)$ is conserved as well. Summarizing,

$$E_N^\Psi(t) \;=\; E_N^\Psi(0)\,, \qquad E^\varphi(t) \;=\; E^\varphi(0)\,, \qquad t\in\mathbb{R}\,.$$

We may now state the main result of this section.

THEOREM 5.16. *Let $\Psi_{N,0}\in\mathcal{Q}(H_N)$ and assume that Assumptions (B1) – (B5) hold. Then there is a constant K, depending only on d, h, w and p, such that*

$$\beta_N(t) \;\leqslant\; \left(\beta_N(0) + E_N^\Psi - E^\varphi + \frac{1}{N^\eta}\right)\mathrm{e}^{K\phi(t)}\,,$$

where

$$\eta \;:=\; \frac{p/p_0 - 1}{2p/p_0 - p/2 - 1} \tag{5.37}$$

and

$$\phi(t) \;:=\; \int_0^t \mathrm{d}s\,\left(1 + \|\varphi(s)\|^3_{X_1^2\cap L^\infty}\right).$$

REMARK 5.17. *We have convergence to the mean-field limit whenever $\lim_N E_N^\Psi = E^\varphi$ and $\lim_N \beta_N(0) = 0$. For instance if we start in a fully factorized state, $\Psi_{N,0} = \varphi_0^{\otimes N}$, then $\beta_N(0) = 0$ and*

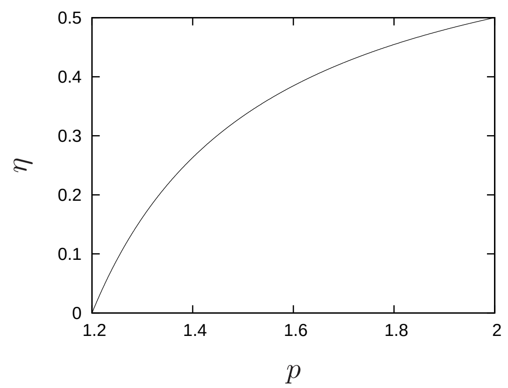
$$E_N^\Psi - E^\varphi \;=\; \frac{1}{N}\langle\varphi_0\otimes\varphi_0\,, W_{12}\,\varphi_0\otimes\varphi_0\rangle\,,$$

so that the Theorem 5.16 yields

$$E_N^{(1)}(t) \;\leqslant\; \beta_N(t) \;\lesssim\; \frac{1}{N^\eta}\mathrm{e}^{K\phi(t)}\,,$$

and the analogue of Corollary 5.6 holds.

REMARK 5.18. *The following graph shows the dependence of η on p for $d = 3$, i.e. $p_0 = 6/5$.*



REMARK 5.19. *Theorem 5.16 remains valid for a large class of time-dependent one-particle Hamiltonians $h(t)$. See Section 5.3.5 below for a full discussion.*

REMARK 5.20. *In three dimensions Assumption (B1) and Sobolev's inequality imply that $\|\varphi\|_\infty \lesssim \|\varphi\|_{X_1^2}$, so that Assumption (B5) is equivalent to $\varphi \in C(\mathbb{R}; X_1^2) \cap C^1(\mathbb{R}; L^2)$.*

5.3.2. Example: nonrelativistic particles with interaction potential of critical type. Consider nonrelativistic particles in $\mathbb{R}^3$ with one-particle Hamiltonian $h = -\Delta$. The interaction potential is given by $w(x) = \lambda|x|^{-2}$. This corresponds to a critical interaction potential in the sense that the kinetic and potential energies have the same scaling behaviour. We require that $\lambda > -1/2$, which ensures that the N-body Hamiltonian is stable and the Hartree equation has global solutions. To see this, recall Hardy's inequality in three dimensions,

$$\langle \varphi, |x|^{-2}\varphi\rangle \;\leqslant\; 4\langle \varphi, -\Delta\varphi\rangle\,. \tag{5.38}$$

Using (5.38), one easily infers that Assumptions (B1) – (B3) hold. Moreover, Assumption (B4) holds for any $p < 3/2$.

In order to verify Assumption (B5) we refer to [GV80], where local well-posedness is proven. Global existence follows by standard methods using conservation of the mass $\|\varphi\|^2$, conservation of the energy E^φ, and Hardy's inequality (5.38). Together they yield an a-priori bound on $\|\varphi\|_{X_1}$, from which an a-priori bound for $\|\varphi\|_{X_1^2}$ may be inferred; see [GV80] for details.

We conclude: For any $\eta < 1/3$ there is a continuous function $\phi(t)$ such that Theorem 5.16 holds.

5.3.3. Proof of Theorem 5.16, part I: an energy estimate. In the first step of our proof we exploit conservation of energy to derive an estimate on $\|\nabla_1 q_1 \Psi\|$.

LEMMA 5.21. *Assume that Assumptions (B1) – (B5) hold. Then*

$$\|\nabla_1 q_1 \Psi\|^2 \;\lesssim\; E^\Psi - E^\varphi + \big(1 + \|\varphi\|^2_{X_1^2 \cap L^\infty}\big)\bigg(\beta + \frac{1}{\sqrt{N}}\bigg)\,.$$

PROOF. Write

$$E^\varphi \;=\; \langle \varphi, h\varphi\rangle + \frac{1}{2}\langle \varphi, W^\varphi \varphi\rangle\,, \tag{5.39}$$

as well as

$$E^\Psi \;=\; \langle \Psi, h_1 \Psi\rangle + \frac{N-1}{2N}\langle \Psi, W_{12}\Psi\rangle\,. \tag{5.40}$$

Inserting

$$\mathbb{1} \;=\; p_1p_2 + (\mathbb{1} - p_1p_2)$$

in front of every Ψ in (5.40) and multiplying everything out yields

$$\begin{aligned}
&\big\langle \Psi, (\mathbb{1} - p_1p_2)h_1(\mathbb{1} - p_1p_2)\Psi\big\rangle \\
&\quad= E^\Psi - \langle \Psi, p_1p_2h_1p_1p_2\Psi\rangle \\
&\qquad - \frac{N-1}{2N}\langle \Psi, p_1p_2W_{12}p_1p_2\Psi\rangle \\
&\qquad - \big\langle \Psi, (\mathbb{1} - p_1p_2)h_1p_1p_2\Psi\big\rangle - \big\langle \Psi, p_1p_2h_1(\mathbb{1} - p_1p_2)\Psi\big\rangle \\
&\qquad - \frac{N-1}{2N}\big\langle \Psi, (\mathbb{1} - p_1p_2)W_{12}p_1p_2\Psi\big\rangle - \frac{N-1}{2N}\big\langle \Psi, p_1p_2W_{12}(\mathbb{1} - p_1p_2)\Psi\big\rangle \\
&\qquad - \frac{N-1}{2N}\big\langle \Psi, (\mathbb{1} - p_1p_2)W_{12}(\mathbb{1} - p_1p_2)\Psi\big\rangle\,.
\end{aligned}$$

We want to find an upper bound for the left-hand side. In order to control the last term on the right-hand side for negative interaction potentials, we need to use some of the kinetic energy on the left-hand side. To this end, we split the left-hand side by multiplying it with $1 = \kappa_3 + (1 - \kappa_3)$. Thus, using (5.39), we get

$$\begin{aligned}
&\kappa_3\big\langle\Psi\,,(\mathbb{1}-p_1p_2)h_1(\mathbb{1}-p_1p_2)\Psi\big\rangle\\
&\quad= E^\Psi - E^\varphi\\
&\qquad - \langle\Psi\,,p_1p_2h_1p_1p_2\Psi\rangle + \langle\varphi\,,h\varphi\rangle\\
&\qquad - \frac{N-1}{2N}\langle\Psi\,,p_1p_2W_{12}p_1p_2\Psi\rangle + \frac{1}{2}\langle\varphi\,,W^\varphi\varphi\rangle\\
&\qquad - \big\langle\Psi\,,(\mathbb{1}-p_1p_2)h_1p_1p_2\Psi\big\rangle - \big\langle\Psi\,,p_1p_2h_1(\mathbb{1}-p_1p_2)\Psi\big\rangle\\
&\qquad - \frac{N-1}{2N}\big\langle\Psi\,,(\mathbb{1}-p_1p_2)W_{12}p_1p_2\Psi\big\rangle - \frac{N-1}{2N}\big\langle\Psi\,,p_1p_2W_{12}(\mathbb{1}-p_1p_2)\Psi\big\rangle\\
&\qquad - \frac{N-1}{2N}\big\langle\Psi\,,(\mathbb{1}-p_1p_2)W_{12}(\mathbb{1}-p_1p_2)\Psi\big\rangle - (1-\kappa_3)\big\langle\Psi\,,(\mathbb{1}-p_1p_2)h_1(\mathbb{1}-p_1p_2)\Psi\big\rangle\,. \qquad (5.41)
\end{aligned}$$

The rest of the proof consists in estimating each line on the right-hand side of (5.41) separately. There is nothing to be done with the first line.

Line 6. The last line of (5.41) is equal to

$$\begin{aligned}
&-\frac{N-1}{2N}\Big\langle\Psi\,,\,(\mathbb{1}-p_1p_2)W_{12}(\mathbb{1}-p_1p_2)\Psi\Big\rangle - \frac{1}{2}(1-\kappa_3)\big\langle\Psi\,,(\mathbb{1}-p_1p_2)(h_1+h_2)(\mathbb{1}-p_1p_2)\Psi\big\rangle\\
&\qquad\leqslant -\frac{N-1}{2N}\Big\langle\Psi\,,\,(\mathbb{1}-p_1p_2)\big[(1-\kappa_3)(h_1+h_2)+W_{12}\big](\mathbb{1}-p_1p_2)\Psi\Big\rangle \;\leqslant\; 0\,,
\end{aligned}$$

where in the last step we used Assumption (B3).

Line 2. The second line on the right-hand side of (5.41) is bounded in absolute value by

$$\begin{aligned}
\big|\langle\varphi\,,h\varphi\rangle - \langle\Psi\,,p_1p_2h_1p_1p_2\Psi\rangle\big| &= \langle\varphi\,,h\varphi\rangle\big|\langle\Psi\,,(\mathbb{1}-p_1p_2)\Psi\rangle\big|\\
&= \langle\varphi\,,h\varphi\rangle\big|\langle\Psi\,,(q_1p_2+p_1q_2+q_1q_2)\Psi\rangle\big|\\
&\leqslant 3\,\alpha\,\langle\varphi\,,h\varphi\rangle\\
&\leqslant 3\,\beta\,\langle\varphi\,,h\varphi\rangle\,,
\end{aligned}$$

where in the last step we used (5.36).

Line 3. The third line on the right-hand side of (5.41) is bounded in absolute value by

$$\begin{aligned}
\left|\frac{1}{2}\langle\varphi\,,W^\varphi\varphi\rangle - \frac{N-1}{2N}\langle\Psi\,,p_1p_2W_{12}p_1p_2\Psi\rangle\right| &= \frac{1}{2}\big|\langle\varphi\,,W^\varphi\varphi\rangle\big|\left|1 - \frac{N-1}{N}\langle\Psi\,,p_1p_2\Psi\rangle\right|\\
&\leqslant \frac{1}{2}\|W^\varphi\|_\infty\left|\big\langle\Psi\,,(q_1p_2+p_1q_2+q_1q_2)\Psi\big\rangle + \frac{1}{N}\langle\Psi\,,p_1p_2\Psi\rangle\right|\\
&\leqslant \frac{3}{2}\|W^\varphi\|_\infty\left(\alpha + \frac{1}{N}\right)\\
&\leqslant \frac{3}{2}\|W^\varphi\|_\infty\left(\beta + \frac{1}{N}\right).
\end{aligned}$$

As in (5.29), one finds that

$$\|W^\varphi\|_\infty \;\leqslant\; \|w\|_{L^1+L^\infty}\|\varphi\|^2_{L^2\cap L^\infty}\,.$$

Line 4. The fourth line on the right-hand side of (5.41) is bounded in absolute value by

$$\begin{aligned}\bigl|\bigl\langle\Psi\,,(\mathbb{1}-p_1p_2)h_1p_1p_2\Psi\bigr\rangle\bigr| \;&=\; \bigl|\bigl\langle\Psi\,,(q_1p_2+p_1q_2+q_1q_2)h_1p_1p_2\Psi\bigr\rangle\bigr|\\ &=\; \bigl|\bigl\langle\Psi\,,q_1h_1p_1p_2\Psi\bigr\rangle\bigr|\\ &=\; \bigl|\bigl\langle\Psi\,,q_1\,\widehat{n}^{-1/2}\,\widehat{n}^{1/2}\,h_1p_1p_2\Psi\bigr\rangle\bigr|\\ &=\; \bigl|\bigl\langle\Psi\,,q_1\,\widehat{n}^{-1/2}\,h_1\,\widehat{\tau_1 n}^{1/2}\,p_1p_2\Psi\bigr\rangle\bigr|\,,\end{aligned}$$

where in the last step we used Lemma 5.15. Using Cauchy-Schwarz, we thus get

$$\begin{aligned}\bigl|\bigl\langle\Psi\,,(\mathbb{1}-p_1p_2)h_1p_1p_2\Psi\bigr\rangle\bigr| \;&\leqslant\; \sqrt{\bigl\langle\Psi\,,q_1\widehat{n}^{-1}\Psi\bigr\rangle}\,\sqrt{\bigl\langle\Psi\,,p_1p_2\,\widehat{\tau_1 n}^{1/2}\,h_1^2\,\widehat{\tau_1 n}^{1/2}\,p_1p_2\Psi\bigr\rangle}\\ &=\; \sqrt{\langle\Psi\,,\widehat{n}\,\Psi\rangle}\sqrt{\langle\varphi\,,h^2\varphi\rangle}\sqrt{\bigl\langle\Psi\,,\widehat{\tau_1 n}\,p_1p_2\Psi\bigr\rangle}\,,\end{aligned}$$

where in the second step we used Lemma 5.14. Using

$$(\tau_1 n)(k) \;=\; \sqrt{\frac{k+1}{N}} \;\leqslant\; n(k)+\frac{1}{\sqrt{N}}$$

we find

$$\begin{aligned}\bigl|\bigl\langle\Psi\,,(\mathbb{1}-p_1p_2)h_1p_1p_2\Psi\bigr\rangle\bigr| \;&\leqslant\; \sqrt{\beta}\sqrt{\langle\varphi\,,h^2\varphi\rangle}\sqrt{\langle\Psi\,,\widehat{n}\,\Psi\rangle+\frac{1}{\sqrt{N}}}\\ &=\; \sqrt{\langle\varphi\,,h^2\varphi\rangle}\sqrt{\beta}\biggl(\sqrt{\beta}+\frac{1}{N^{1/4}}\biggr)\\ &\leqslant\; 2\sqrt{\langle\varphi\,,h^2\varphi\rangle}\biggl(\beta+\frac{1}{\sqrt{N}}\biggr)\,.\end{aligned}$$

Line 5. Finally, we turn our attention to the fifth line on the right-hand side of (5.41), which is bounded in absolute value by

$$\bigl|\bigl\langle\Psi\,,p_1p_2W_{12}(\mathbb{1}-p_1p_2)\Psi\bigr\rangle\bigr| \;=\; \bigl|\bigl\langle\Psi\,,p_1p_2W_{12}(p_1q_2+q_1p_2+q_1q_2\Psi\bigr\rangle\bigr| \;\leqslant\; 2(\mathrm{a})+(\mathrm{b})\,,$$

where

$$(\mathrm{a}) \;:=\; \bigl|\bigl\langle\Psi\,,p_1p_2W_{12}q_1p_2\Psi\bigr\rangle\bigr|\,,\qquad (\mathrm{b}) \;:=\; \bigl|\bigl\langle\Psi\,,p_1p_2W_{12}q_1q_2\Psi\bigr\rangle\bigr|\,.$$

One finds, using (5.26), Lemma 5.15 and Lemma 5.14,

$$\begin{aligned}(\mathrm{a}) \;&=\; \bigl|\bigl\langle\Psi\,,p_1p_2W_1^\varphi q_1\Psi\bigr\rangle\bigr|\\ &=\; \bigl|\bigl\langle\Psi\,,p_1p_2W_1^\varphi\,\widehat{n}^{1/2}\,\widehat{n}^{-1/2}\,q_1\Psi\bigr\rangle\bigr|\\ &=\; \bigl|\bigl\langle\Psi\,,p_1p_2\,\widehat{\tau_1 n}^{1/2}\,W_1^\varphi\,\widehat{n}^{-1/2}\,q_1\Psi\bigr\rangle\bigr|\\ &\leqslant\; \|W^\varphi\|_\infty\sqrt{\bigl\langle\Psi\,,\widehat{\tau_1 n}\,\Psi\bigr\rangle}\sqrt{\bigl\langle\Psi\,,\widehat{n}^{-1}\,q_1\Psi\bigr\rangle}\\ &\leqslant\; \|W^\varphi\|_\infty\sqrt{\bigl\langle\Psi\,,\widehat{n}\,\Psi\bigr\rangle+\frac{1}{\sqrt{N}}}\,\sqrt{\bigl\langle\Psi\,,\widehat{n}\,\Psi\bigr\rangle}\\ &\leqslant\; 2\|W^\varphi\|_\infty\biggl(\beta+\frac{1}{\sqrt{N}}\biggr)\,.\end{aligned}$$

The estimation of (b) requires a little more effort. We start by splitting

$$w \;=\; w^{(p)} + w^{(\infty)}\,, \qquad w^{(p)} \in L^p\,,\; w^{(\infty)} \in L^\infty\,.$$

This yields (b) $\leqslant$ (b)$^{(p)}$+(b)$^{(\infty)}$ in self-explanatory notation. Let us first concentrate on (b)$^{(\infty)}$:

$$\begin{aligned}
(\mathrm{b})^{(\infty)} \;&=\; \big|\big\langle \Psi\,, p_1p_2 W_{12}^{(\infty)} q_1q_2\Psi\big\rangle\big| \\
&=\; \big|\big\langle \Psi\,, p_1p_2 W_{12}^{(\infty)}\, \widehat{n}\,\widehat{n}^{-1}\, q_1q_2\Psi\big\rangle\big| \\
&=\; \big|\big\langle \Psi\,, p_1p_2\, \widehat{\tau_2 n}\, W_{12}^{(\infty)}\, \widehat{n}^{-1}\, q_1q_2\Psi\big\rangle\big| \\
&\leqslant\; \|W^{(\infty)}\|_\infty \sqrt{\big\langle \Psi\,, \widehat{\tau_2 n}^2\Psi\big\rangle}\,\sqrt{\big\langle \Psi\,, \widehat{n}^{-2}\, q_1q_2\Psi\big\rangle} \\
&\leqslant\; \|w^{(\infty)}\|_\infty \sqrt{\alpha+\frac{2}{N}}\,\sqrt{\alpha} \\
&\leqslant\; 2\|w^{(\infty)}\|_\infty \left(\beta+\frac{2}{N}\right).
\end{aligned}$$

Let us now consider (b)$^{(p)}$. In order to deal with the singularities in $w^{(p)}$, we write it as the divergence of a vector field ξ,

$$w^{(p)} \;=\; \nabla\cdot\xi\,. \tag{5.42}$$

This is nothing but a problem of electrostatics, which is solved by

$$\xi \;=\; C\,\frac{x}{|x|^d} * w^{(p)}\,,$$

with some constant C depending on d. By the Hardy-Littlewood-Sobolev inequality, we find

$$\|\xi\|_q \;\lesssim\; \big\|w^{(p)}\big\|_p\,, \qquad \frac{1}{q} \;=\; \frac{1}{p}-\frac{1}{d}\,. \tag{5.43}$$

Thus if $p\geqslant p_0$ then $q\geqslant 2$. Denote by X_{12} multiplication by $\xi(x_1-x_2)$. For the following it is convenient to write $\nabla\cdot\xi = \nabla^\rho\xi^\rho$, where a summation over $\rho=1,\dots,d$ is implied.

Recalling Lemma 5.15, we therefore get

$$\begin{aligned}
(\mathrm{b})^{(p)} \;&=\; \big|\big\langle \Psi\,, p_1p_2 W_{12}^{(p)}\, \widehat{n}\,\widehat{n}^{-1} q_1q_2\Psi\big\rangle\big| \\
&=\; \big|\big\langle \Psi\,, p_1p_2\, \widehat{\tau_2 n}\, W_{12}^{(p)}\, \widehat{n}^{-1} q_1q_2\Psi\big\rangle\big| \\
&=\; \big|\big\langle \Psi\,, p_1p_2\, \widehat{\tau_2 n}\, (\nabla_1^\rho X^\rho)_{12}\, \widehat{n}^{-1} q_1q_2\Psi\big\rangle\big|\,.
\end{aligned}$$

Integrating by parts yields

$$(\mathrm{b})^{(p)} \;\leqslant\; \big|\big\langle \nabla_1^\rho\widehat{\tau_2 n}\, p_1p_2\Psi\,, X_{12}^\rho\, \widehat{n}^{-1} q_1q_2\Psi\big\rangle\big| + \big|\big\langle \widehat{\tau_2 n}\, p_1p_2\Psi\,, X_{12}^\rho\nabla_1^\rho\, \widehat{n}^{-1} q_1q_2\Psi\big\rangle\big|\,. \tag{5.44}$$

Let us begin by estimating the first term. Recalling that $p=|\varphi\rangle\langle\varphi|$, we find that the first term on the right-hand side of (5.44) is equal to

$$\begin{aligned}
\big|\big\langle X_{12}^\rho\, p_2(\nabla^\rho p)_1 \widehat{\tau_2 n}\,\Psi\,, \widehat{n}^{-1} q_1q_2\Psi\big\rangle\big| \;&\leqslant\; \sqrt{\big\langle (\nabla^\rho p)_1\widehat{\tau_2 n}\,\Psi\,, p_2 X_{12}^\rho X_{12}^\sigma\, p_2(\nabla^\sigma p)_1\widehat{\tau_2 n}\,\Psi\big\rangle}\,\big\|\widehat{n}^{-1} q_1q_2\Psi\big\| \\
&\leqslant\; \sqrt{\big\||\varphi|^2 * \xi^2\big\|_\infty}\,\|\nabla\varphi\|\,\big\|\widehat{\tau_2 n}\,\Psi\big\|\,\big\|\widehat{n}^{-1} q_1q_2\Psi\big\| \\
&\lesssim\; \|\xi\|_q\,\|\varphi\|_{L^2\cap L^\infty}\,\|\varphi\|_{X_1}\sqrt{\alpha+\frac{2}{N}}\,\sqrt{\alpha}\,,
\end{aligned}$$

where we used Young's inequality, Assumption (B1), and Lemma 5.14. Recalling that $\beta \leqslant \alpha$, we conclude that the first term on the right-hand side of (5.44) is bounded by

$$C\,\|\varphi\|^2_{X_1\cap L^\infty}\left(\beta + \frac{1}{N}\right).$$

Next, we estimate the second term on the right-hand side of (5.44). It is equal to

$$\begin{aligned}
\big|\big\langle X^\rho_{12}\, p_1p_2\, \widehat{\tau_2 n}\,\Psi\,,\nabla^\rho_1\,\widehat{n}^{-1}q_1q_2\Psi\big\rangle\big| &\leqslant \sqrt{\big\langle \widehat{\tau_2 n}\,\Psi\,, p_1p_2X^2_{12}p_1p_2\,\widehat{\tau_2 n}\,\Psi\big\rangle}\,\big\|\nabla_1\,\widehat{n}^{-1}\,q_1q_2\Psi\big\| \\
&\leqslant \sqrt{\big\||\varphi|^2 * \xi^2\big\|_\infty}\,\|\widehat{\tau_2 n}\,\Psi\|\,\big\|\nabla_1\,\widehat{n}^{-1}\,q_1q_2\Psi\big\| \\
&\leqslant \|\xi\|_q\,\|\varphi\|_{L^2\cap L^\infty}\sqrt{\alpha + \frac{2}{N}}\,\big\|\nabla_1\,\widehat{n}^{-1}\,q_1q_2\Psi\big\|\,.
\end{aligned}$$

We estimate $\big\|\nabla_1\,\widehat{n}^{-1}\,q_1q_2\Psi\big\|$ by introducing $\mathbb{1} = p_1 + q_1$ on the left. The term arising from p_1 is bounded by

$$\begin{aligned}
\big\|p_1\nabla_1\,\widehat{n}^{-1}\,q_1q_2\Psi\big\| &= \big\|p_1q_2\,\widehat{\tau_1 n}^{-1}\,\nabla_1q_1\Psi\big\| \\
&\leqslant \sqrt{\big\langle\nabla_1q_1\Psi\,, q_2\,\widehat{\tau_1 n}^{-2}\,\nabla_1q_1\Psi\big\rangle} \\
&= \sqrt{\left\langle\nabla_1q_1\Psi\;,\;\frac{1}{N-1}\sum_{i=2}^N q_i\,\widehat{\tau_1 n}^{-2}\,\nabla_1q_1\Psi\right\rangle} \\
&\leqslant \sqrt{\left\langle\nabla_1q_1\Psi\;,\;\frac{1}{N}\sum_{i=1}^N q_i\,\widehat{\tau_1 n}^{-2}\,\nabla_1q_1\Psi\right\rangle} \\
&= \sqrt{\big\langle\nabla_1q_1\Psi\,, \widehat{n}^2\,\widehat{\tau_1 n}^{-2}\,\nabla_1q_1\Psi\big\rangle} \\
&\leqslant \|\nabla_1q_1\Psi\|\,.
\end{aligned}$$

The term arising from q_1 in the above splitting is dealt with in exactly the same way. Thus we have proven that the second term on the right-hand side of (5.44) is bounded by

$$C\|\varphi\|_{L^2\cap L^\infty}\sqrt{\beta + \frac{1}{N}}\,\|\nabla_1q_1\Psi\|\,.$$

Summarizing, we have

$$(\mathrm{b})^{(p)} \lesssim \|\varphi\|^2_{X_1\cap L^\infty}\left(\beta + \frac{1}{N}\right) + \|\varphi\|_{L^2\cap L^\infty}\sqrt{\beta + \frac{1}{N}}\,\|\nabla_1q_1\Psi\|\,.$$

Conclusion of the proof. Putting all the estimates of the right-hand side of (5.41) together, we find

$$\begin{aligned}
&\big\langle\Psi\,,(\mathbb{1} - p_1p_2)h_1(\mathbb{1} - p_1p_2)\Psi\big\rangle \\
&\qquad\lesssim E^\Psi - E^\varphi + \big(1 + \|\varphi\|^2_{X^2_1\cap L^\infty}\big)\left(\beta + \frac{1}{\sqrt{N}}\right) + \|\varphi\|_{L^2\cap L^\infty}\sqrt{\beta + \frac{1}{N}}\,\|\nabla_1q_1\Psi\|\,. \qquad (5.45)
\end{aligned}$$

Next, from $\mathbb{1} - p_1p_2 = p_1q_2 + q_1$ we deduce

$$\|\sqrt{h_1}q_1\Psi\| \;=\; \big\|\sqrt{h_1}(\mathbb{1} - p_1p_2)\Psi - \sqrt{h_1}p_1q_2\Psi\big\| \;\leqslant\; \big\|\sqrt{h_1}(\mathbb{1} - p_1p_2)\Psi\big\| + \|\sqrt{h_1}p_1q_2\Psi\|\,.$$

Now, recalling that $p = |\varphi\rangle\langle\varphi|$, we find

$$\|\sqrt{h_1}p_1q_2\Psi\| \;\leqslant\; \|\sqrt{h_1}p_1\|\|q_2\Psi\| \;\leqslant\; \|\varphi\|_{X_1}\sqrt{\beta}\,.$$

Therefore,

$$\|\sqrt{h_1}q_1\Psi\|^2 \;\lesssim\; \big\|\sqrt{h_1}(\mathbb{1} - p_1p_2)\Psi\big\|^2 + \|\varphi\|^2_{X_1}\beta\,.$$

Plugging in (5.45) yields

$$\big\|\sqrt{h_1}q_1\Psi\big\|^2 \;\lesssim\; E^\Psi - E^\varphi + \big(1 + \|\varphi\|^2_{X_1^2\cap L^\infty}\big)\bigg(\beta + \frac{1}{\sqrt{N}}\bigg) + \|\varphi\|_{L^2\cap L^\infty}\sqrt{\beta + \frac{1}{N}}\,\|\nabla_1 q_1\Psi\|\,.$$

Next, we observe that Assumption (B1) implies

$$\|\nabla_1 q_1\Psi\| \;\lesssim\; \big\|\sqrt{h_1}q_1\Psi\big\| + \sqrt{\beta}\,,$$

so that we get

$$\big\|\sqrt{h_1}q_1\Psi\big\|^2 \;\lesssim\; E^\Psi - E^\varphi + \big(1 + \|\varphi\|^2_{X_1^2\cap L^\infty}\big)\bigg(\beta + \frac{1}{\sqrt{N}}\bigg) + \|\varphi\|_{L^2\cap L^\infty}\sqrt{\beta + \frac{1}{N}}\,\|\sqrt{h_1}q_1\Psi\|\,.$$

Now we claim that

$$\big\|\sqrt{h_1}q_1\Psi\big\|^2 \;\lesssim\; E^\Psi - E^\varphi + \big(1 + \|\varphi\|^2_{X_1^2\cap L^\infty}\big)\bigg(\beta + \frac{1}{\sqrt{N}}\bigg)\,. \tag{5.46}$$

This follows from the general estimate

$$x^2 \;\leqslant\; C(R + ax) \quad\Longrightarrow\quad x^2 \;\leqslant\; 2CR + C^2a^2\,,$$

which itself follows from the elementary inequality

$$C(R + ax) \;\leqslant\; CR + \frac{1}{2}C^2a^2 + \frac{1}{2}x^2\,.$$

The claim of the Lemma now follows from (5.46) by using Assumption (B1). $\square$

5.3.4. Proof of Theorem 5.16, part II: a bound on $\dot\beta$. We start exactly as in Section 5.2. Assumptions (B1) – (B5) imply that β is differentiable in t with derivative

$$\begin{aligned}\dot\beta \;&=\; \frac{\mathrm{i}}{2}\big\langle\Psi\,, \big[(N-1)W_{12} - NW_1^\varphi - NW_2^\varphi\,, \widehat{n}\big]\,\Psi\big\rangle \\ &=\; 2(\mathrm{I}) + 2(\mathrm{II}) + (\mathrm{III}) + \text{ complex conjugate}\,,\end{aligned} \tag{5.47}$$

where

$$\begin{aligned}(\mathrm{I}) \;&:=\; \frac{\mathrm{i}}{2}\big\langle\Psi\,, p_1p_2\big[(N-1)W_{12} - NW_1^\varphi - NW_2^\varphi\,, \widehat{n}\big]q_1p_2\Psi\big\rangle\,,\\ (\mathrm{II}) \;&:=\; \frac{\mathrm{i}}{2}\big\langle\Psi\,, q_1p_2\big[(N-1)W_{12} - NW_1^\varphi - NW_2^\varphi\,, \widehat{n}\big]q_1q_2\Psi\big\rangle\,,\\ (\mathrm{III}) \;&:=\; \frac{\mathrm{i}}{2}\big\langle\Psi\,, p_1p_2\big[(N-1)W_{12} - NW_1^\varphi - NW_2^\varphi\,, \widehat{n}\big]q_1q_2\Psi\big\rangle\,.\end{aligned}$$

Term (I). Using (5.26) we find

$$\begin{aligned} 2\big|(\mathrm{I})\big| &= \big|\big\langle \Psi\,, p_1p_2\big[(N-1)W_{12} - NW_1^\varphi - NW_2^\varphi\,, \widehat{n}\big]q_1p_2\Psi\big\rangle\big| \\ &= \big|\big\langle \Psi\,, p_1p_2\big[W_1^\varphi\,, \widehat{n}\big]q_1p_2\Psi\big\rangle\big| \\ &= \big|\big\langle \Psi\,, p_1p_2W_1^\varphi\big(\widehat{n} - \widehat{\tau_{-1}n}\big)q_1p_2\Psi\big\rangle\big|\,, \end{aligned}$$

where we used Lemma 5.15. Define

$$\mu(k) \;:=\; N\big(n(k) - (\tau_{-1}n)(k)\big) \;=\; \frac{\sqrt{N}}{\sqrt{k}+\sqrt{k-1}} \;\leqslant\; n^{-1}(k)\,, \qquad k = 1,\dots,N\,. \tag{5.48}$$

Thus,

$$\begin{aligned} \big|(\mathrm{I})\big| &= \frac{1}{N}\big|\big\langle \Psi\,, p_1p_2W_1^\varphi\,\widehat{\mu}\,q_1p_2\Psi\big\rangle\big| \\ &\leqslant \frac{1}{N}\|W^\varphi\|_\infty\sqrt{\big\langle \Psi\,, \widehat{\mu}^2\,q_1\Psi\big\rangle} \\ &\leqslant \frac{1}{N}\|W^\varphi\|_\infty\sqrt{\big\langle \Psi\,, \widehat{n}^{-2}\,q_1\Psi\big\rangle} \\ &\lesssim \frac{1}{N}\|\varphi\|_{L^2\cap L^\infty}^2\,, \end{aligned}$$

by (5.22).

Term (II). Using Lemma 5.15 we find

$$\begin{aligned} 2|(\mathrm{II})| &= \big|\big\langle \Psi\,, q_1p_2\big[(N-1)W_{12} - NW_2^\varphi\,, \widehat{n}\big]q_1q_2\Psi\big\rangle\big| &(5.49)\\ &= \left|\left\langle \Psi\;,\; q_1p_2\left(\frac{N-1}{N}W_{12} - W_2^\varphi\right)\widehat{\mu}\,q_1q_2\Psi\right\rangle\right| &(5.50)\\ &\leqslant \underbrace{\big|\big\langle \Psi\,, q_1p_2W_{12}\,\widehat{\mu}\,q_1q_2\Psi\big\rangle\big|}_{=:\,(\mathrm{a})} + \underbrace{\big|\big\langle \Psi\,, q_1p_2W_2^\varphi\,\widehat{\mu}\,q_1q_2\Psi\big\rangle\big|}_{=:\,(\mathrm{b})}\,. &(5.51) \end{aligned}$$

One immediately finds

$$(\mathrm{b}) \;\leqslant\; \|W^\varphi\|_\infty\,\|q_1\Psi\|\sqrt{\langle\Psi\,, \widehat{\mu}^2q_1q_2\Psi\rangle} \;\lesssim\; \|\varphi\|_{L^2\cap L^\infty}^2\beta\,.$$

In (a) we split

$$w \;=\; w^{(p)} + w^{(\infty)}\,, \qquad w^{(p)} \in L^p\,,\; w^{(\infty)} \in L^\infty\,,$$

with a resulting splitting $(\mathrm{a}) \leqslant (\mathrm{a})^{(p)} + (\mathrm{a})^{(\infty)}$. The easy part is

$$(\mathrm{a})^{(\infty)} \;\leqslant\; \|w^{(\infty)}\|_\infty\,\|q_1\Psi\|^2 \;\lesssim\; \beta\,.$$

In order to deal with $(\mathrm{a})^{(p)}$ we write $w^{(p)} = \nabla\cdot\xi$ as the divergence of a vector field ξ, exactly as in the proof of Lemma 5.21; see (5.42) and the remarks after it. We integrate by parts to find

$$\begin{aligned} (\mathrm{a})^{(p)} &= \big|\big\langle \Psi\,, q_1p_2(\nabla_1^\rho X^\rho)_{12}\,\widehat{\mu}\,q_1q_2\Psi\big\rangle\big| \\ &\leqslant \big|\big\langle \nabla_1^\rho q_1p_2\Psi\,, X_{12}^\rho\,\widehat{\mu}\,q_1q_2\Psi\big\rangle\big| + \big|\big\langle q_1p_2\Psi\,, X_{12}^\rho\nabla_1^\rho\,\widehat{\mu}\,q_1q_2\Psi\big\rangle\big|\,. \end{aligned} \tag{5.52}$$

The first term of (5.52) is equal to

$$
\begin{aligned}
\big|\big\langle X^{\rho}_{12}p_2\nabla^{\rho}_1 q_1\Psi\,,\widehat{\mu}\,q_1q_2\Psi\big\rangle\big| \;&\leqslant\; \sqrt{\big\langle \nabla^{\rho}_1 q_1\Psi\,, p_2X^{\rho}_{12}X^{\sigma}_{12}p_2\nabla^{\sigma}_1 q_1\Psi\big\rangle}\,\sqrt{\big\langle \Psi\,,\widehat{\mu}^2\,q_1q_2\Psi\big\rangle}\\
&\lesssim\; \sqrt{\|\xi^2 * |\varphi|^2\|_\infty}\,\|\nabla_1 q_1\Psi\|\,\sqrt{\big\langle\Psi\,,\widehat{n}^{-2}\,q_1q_2\Psi\big\rangle}\\
&\leqslant\; \sqrt{\|\xi^2 * |\varphi|^2\|_\infty}\,\|\nabla_1 q_1\Psi\|\,\sqrt{\frac{N}{N-1}\big\langle\Psi\,,\widehat{n}^2\Psi\big\rangle}\\
&\lesssim\; \|\xi\|_q\,\|\varphi\|_{L^2\cap L^\infty}\,\|\nabla_1 q_1\Psi\|\,\sqrt{\beta}\\
&\lesssim\; \|\nabla_1 q_1\Psi\|^2\,\|\varphi\|_{L^2\cap L^\infty} + \beta\,\|\varphi\|_{L^2\cap L^\infty}\,,
\end{aligned}
$$

where in the second step we used (5.48), in the third Lemma 5.14, and in the last (5.36), Young's inequality, and (5.43). The second term of (5.52) is equal to

$$
\begin{aligned}
&\big|\big\langle q_1p_2\Psi\,, X^{\rho}_{12}(p_1+q_1)\nabla^{\rho}_1\,\widehat{\mu}\,q_1q_2\Psi\big\rangle\big|\\
&\qquad\leqslant\; \big|\big\langle q_1p_2\Psi\,, X^{\rho}_{12}p_1\,\widehat{\tau_1\mu}\,\nabla^{\rho}_1 q_1q_2\Psi\big\rangle\big| + \big|\big\langle q_1p_2\Psi\,, X^{\rho}_{12}q_1\,\widehat{\mu}\,\nabla^{\rho}_1 q_1q_2\Psi\big\rangle\big|\,, \qquad (5.53)
\end{aligned}
$$

where we used Lemma 5.15. We estimate the first term of (5.53). The second term is dealt with in exactly the same way. We find

$$
\begin{aligned}
\big|\big\langle p_1X^{\rho}_{12}q_1p_2\Psi\,,\widehat{\tau_1\mu}\,\nabla^{\rho}_1 q_1q_2\Psi\big\rangle\big| \;&\leqslant\; \sqrt{\big\langle\Psi\,, q_1p_2X^2_{12}p_2q_1\Psi\big\rangle}\,\sqrt{\big\langle\nabla_1 q_1\Psi\,, q_2\,\widehat{\tau_1\mu}^2\,q_2\nabla_1 q_1\Psi\big\rangle}\\
&\leqslant\; \sqrt{\|\xi^2 * |\varphi|^2\|_\infty}\,\|q_1\Psi\|\,\sqrt{\big\langle\nabla_1 q_1\Psi\,,\widehat{n}^{-2}\,q_2\nabla_1 q_1\Psi\big\rangle}\\
&\lesssim \|\xi\|_q\,\|\varphi\|_{L^2\cap L^\infty}\,\sqrt{\alpha}\,\sqrt{\frac{1}{N-1}\sum_{i=2}^N\big\langle\nabla_1 q_1\Psi\,,\widehat{n}^{-2}\,q_i\nabla_1 q_1\Psi\big\rangle}\\
&\lesssim\; \|\varphi\|_{L^2\cap L^\infty}\sqrt{\beta}\sqrt{\frac{1}{N-1}\sum_{i=1}^N\big\langle\nabla_1 q_1\Psi\,,\widehat{n}^{-2}\,q_i\nabla_1 q_1\Psi\big\rangle}\\
&=\; \|\varphi\|_{L^2\cap L^\infty}\sqrt{\beta}\sqrt{\frac{N}{N-1}\big\langle\nabla_1 q_1\Psi\,,\widehat{n}^{-2}\,\widehat{n}^2\,\nabla_1 q_1\Psi\big\rangle}\\
&\lesssim\; \|\varphi\|_{L^2\cap L^\infty}\sqrt{\beta}\,\|\nabla_1 q_1\Psi\|\\
&\leqslant\; \beta\,\|\varphi\|_{L^2\cap L^\infty} + \|\nabla_1 q_1\Psi\|^2\,\|\varphi\|_{L^2\cap L^\infty}\,.
\end{aligned}
$$

In summary, we have proven that

$$
\big|(\mathrm{II})\big| \;\lesssim\; \beta\,\|\varphi\|_{L^2\cap L^\infty} + \|\nabla_1 q_1\Psi\|^2\,\|\varphi\|_{L^2\cap L^\infty}\,.
$$

Term (III). Using Lemma 5.15 we find

$$
2|(\mathrm{III})| \;=\; (N-1)\big|\big\langle\Psi\,, p_1p_2\big[W_{12}\,,\widehat{n}\big]q_1q_2\Psi\big\rangle\big| \;=\; (N-1)\big|\big\langle\Psi\,, p_1p_2W_{12}\big(\widehat{n}-\widehat{\tau_{-2}n}\big)q_1q_2\Psi\big\rangle\big|\,.
$$

Defining

$$
\nu(k) \;:=\; N\big(n(k)-(\tau_{-2}n)(k)\big) \;=\; \frac{\sqrt{N}}{\sqrt{k}+\sqrt{k-2}} \;\leqslant\; n^{-1}(k)\,, \qquad k = 2,\dots,N\,, \qquad (5.54)
$$

we have

$$
2\big|(\mathrm{III})\big| \;\leqslant\; \big|\big\langle\Psi\,, p_1p_2W_{12}\,\widehat{\nu}\,q_1q_2\Psi\big\rangle\big|
$$

As usual we start by splitting

$$w \;=\; w^{(p)} + w^{(\infty)}\,, \qquad w^{(p)} \in L^p\,,\; w^{(\infty)} \in L^\infty\,,$$

with the induced splitting (III) $=$ (III)$^{(p)}$ $+$ (III)$^{(\infty)}$. Thus, using Lemma 5.15, we find

$$\begin{aligned}
2\big|(\mathrm{III})^{(\infty)}\big| \;&=\; \big|\big\langle \Psi\,, p_1p_2W_{12}^{(\infty)}\,\widehat{n}^{1/2}\,\widehat{n}^{-1/2}\,\widehat{\nu}\,q_1q_2\Psi\big\rangle\big| \\
&=\; \big|\big\langle \Psi\,, p_1p_2\,\widehat{\tau_2 n}^{1/2}\,W_{12}^{(\infty)}\,\widehat{n}^{-1/2}\,\widehat{\nu}\,q_1q_2\Psi\big\rangle\big| \\
&\leqslant\; \|w^{(\infty)}\|_\infty \sqrt{\big\langle \Psi\,, \widehat{\tau_2 n}\,\Psi\big\rangle}\,\sqrt{\big\langle \Psi\,, \widehat{n}^{-1}\,\widehat{\nu}^2\,q_1q_2\Psi\big\rangle} \\
&\lesssim \sqrt{\beta + \sqrt{\frac{2}{N}}}\,\sqrt{\big\langle \Psi\,, \widehat{n}^{-3}\,q_1q_2\Psi\big\rangle} \\
&\leqslant\; \sqrt{\beta + \sqrt{\frac{2}{N}}}\,\sqrt{\frac{N}{N-1}\beta} \\
&\lesssim \beta + \frac{1}{\sqrt{N}}\,,
\end{aligned}$$

where in the fifth step we used Lemma 5.14.

In order to estimate (III)$^{(p)}$ we introduce a splitting of $w^{(p)}$ into "singular" and "regular" parts,

$$w^{(p)} \;=\; w^{(p,1)} + w^{(p,2)} \;:=\; w^{(p)}\,\mathbb{1}_{\{|w^{(p)}|>a\}} + w^{(p)}\,\mathbb{1}_{\{|w^{(p)}|\leqslant a\}}\,, \tag{5.55}$$

where a is a positive (N-dependent) constant we choose later. For future reference we record the estimates

$$\|w^{(p,1)}\|_{p_0} \;\leqslant\; a^{1-p/p_0}\,\|w^{(p)}\|_p^{p/p_0}\,, \tag{5.56a}$$

$$\|w^{(p,2)}\|_2 \;\leqslant\; a^{1-p/2}\,\|w^{(p)}\|_p^{p/2}\,. \tag{5.56b}$$

The proof of (5.56) is elementary; for instance (5.56a) follows from

$$\begin{aligned}
\|w^{(p,1)}\|_{p_0}^{p_0} \;&=\; \int \mathrm{d}x\,\big|w^{(p)}\big|^p\,\big|w^{(p)}\big|^{p_0-p}\,\mathbb{1}_{\{|w^{(p)}|>a\}} \\
&\qquad\qquad\leqslant\; a^{p_0-p}\int \mathrm{d}x\,\big|w^{(p)}\big|^p\,\mathbb{1}_{\{|w^{(p)}|>a\}} \;\leqslant\; a^{p_0-p}\int \mathrm{d}x\,\big|w^{(p)}\big|^p\,.
\end{aligned}$$

Let us start with (III)$^{(p,1)}$. As in (5.42), we use the representation

$$w^{(p,1)} \;=\; \nabla\cdot\xi\,.$$

Then (5.43) and (5.56a) imply that

$$\|\xi\|_2 \;\lesssim\; \|w^{(p,1)}\|_{p_0} \;\lesssim\; a^{1-p/p_0}\,. \tag{5.57}$$

Integrating by parts, we find

$$\begin{aligned}
2\big|(\mathrm{III})^{(p,1)}\big| \;&=\; \big|\big\langle \Psi\,, p_1p_2W_{12}^{(p,1)}\,\widehat{\nu}\,q_1q_2\Psi\big\rangle\big| \\
&=\; \big|\big\langle \Psi\,, p_1p_2(\nabla_1^\rho X_{12}^\rho)\,\widehat{\nu}\,q_1q_2\Psi\big\rangle\big| \\
&\leqslant\; \big|\big\langle \nabla_1^\rho p_1p_2\Psi\,, X_{12}^\rho\,\widehat{\nu}\,q_1q_2\Psi\big\rangle\big| + \big|\big\langle p_1p_2\Psi\,, X_{12}^\rho\nabla_1^\rho\,\widehat{\nu}\,q_1q_2\Psi\big\rangle\big|\,.
\end{aligned} \tag{5.58}$$

Using $\|\nabla p\| = \|\nabla \varphi\|$ and Lemma 5.14 we find that the first term of (5.58) is bounded by

$$\begin{aligned}\sqrt{\langle \nabla_1^\rho p_1 \Psi , p_2 X_{12}^\rho X_{12}^\sigma p_2 \nabla_1^\sigma p_1 \Psi\rangle}\sqrt{\langle \Psi , \widehat{\nu}^2 q_1 q_2 \Psi\rangle} &\lesssim \|\nabla p\| \, \|\varphi\|_\infty \|\xi\|_2 \sqrt{\alpha} \\ &\leqslant \|\nabla \varphi\| \, \|\varphi\|_\infty \, a^{1-p/p_0} \sqrt{\beta} \\ &\leqslant \|\nabla \varphi\| \, \|\varphi\|_\infty \big(\beta + a^{2-2p/p_0}\big) \,,\end{aligned}$$

where in the second step we used the estimate (5.57). Next, using Lemma 5.15, we find that the second term of (5.58) is equal to

$$\begin{aligned}&\big|\langle p_1 p_2 \Psi , X_{12}^\rho (p_1 + q_1) \nabla_1^\rho \, \widehat{\nu} \, q_1 q_2 \Psi\rangle\big| \\ &\qquad \leqslant \big|\langle p_1 p_2 \Psi , X_{12}^\rho p_1 \, \widehat{\tau_1 \nu} \, \nabla_1^\rho q_1 q_2 \Psi\rangle\big| + \big|\langle p_1 p_2 \Psi , X_{12}^\rho q_1 \, \widehat{\nu} \, \nabla_1^\rho q_1 q_2 \Psi\rangle\big| \,.\end{aligned}$$

We estimate the first term (the second is dealt with in exactly the same way):

$$\begin{aligned}\big|\langle p_1 p_2 \Psi , X_{12}^\rho p_1 \, \widehat{\tau_1 \nu} \, \nabla_1^\rho q_1 q_2 \Psi\rangle\big| &\leqslant \sqrt{\langle \Psi , p_1 p_2 X_{12}^2 p_1 p_2 \Psi\rangle}\sqrt{\langle \nabla_1 q_1 \Psi , \widehat{\tau_1 \nu}^2 \, q_2 \nabla_1 q_1 \Psi\rangle} \\ &\leqslant \sqrt{\|p_2 X_{12}^2 p_2\|}\sqrt{\frac{1}{N-1}\sum_{i=2}^N \langle \nabla_1 q_1 \Psi , \widehat{n}^{-2} \, q_i \nabla_1 q_1 \Psi\rangle} \\ &\leqslant \|\xi\|_2 \, \|\varphi\|_\infty \sqrt{\frac{1}{N-1}\sum_{i=1}^N \langle \nabla_1 q_1 \Psi , \widehat{n}^{-2} \, q_i \nabla_1 q_1 \Psi\rangle} \\ &\lesssim a^{1-p/p_0} \|\varphi\|_\infty \sqrt{\frac{N}{N-1} \, \langle \nabla_1 q_1 \Psi , \nabla_1 q_1 \Psi\rangle} \\ &\leqslant \|\varphi\|_\infty \big(a^{2-2p/p_0} + \|\nabla_1 q_1 \Psi\|^2\big) \,.\end{aligned}$$

Summarizing,

$$\big|(\mathrm{III})^{(p,1)}\big| \lesssim \|\varphi\|_\infty \Big(\beta \|\varphi\|_{X_1} + \|\nabla_1 q_1 \Psi\|^2 + a^{2-2p/p_0} \|\varphi\|_{X_1}\Big) \,.$$

Finally, we estimate

$$(\mathrm{III})^{(p,2)} = \big|\langle \Psi , p_1 p_2 W_{12}^{(p,2)} \, \widehat{\nu} \, q_1 q_2 \Psi\rangle\big| = \big|\langle \Psi , p_1 p_2 W_{12}^{(p,2)} \, \widehat{\nu} \, (\widehat{\chi^{(1)}} + \widehat{\chi^{(2)}}) q_1 q_2 \Psi\rangle\big| \,, \tag{5.59}$$

where

$$1 = \chi^{(1)} + \chi^{(2)} \,, \qquad \chi^{(1)}, \chi^{(2)} \in \{0,1\}^{\{0,\dots,N\}} \,,$$

is some partition of the unity to be chosen later. The need for this partitioning will soon become clear. In order to bound the term with $\chi^{(1)}$, we note that the operator norm of $p_1 p_2 W_{12}^{(p,2)} q_1 q_2$ on the full space $L^2(\mathbb{R}^{dN})$ is much larger than on its symmetric subspace. Thus, as a first step, we symmetrize the operator $p_1 p_2 W_{12}^{(p,2)} q_1 q_2$ in coordinate 2. We get the bound

$$\begin{aligned}\big|\langle \Psi , p_1 p_2 W_{12}^{(p,2)} \, \widehat{\nu} \, \widehat{\chi^{(1)}} \, q_1 q_2 \Psi\rangle\big| &= \frac{1}{N-1}\left|\left\langle \Psi , \sum_{i=2}^N p_1 p_i W_{1i}^{(p,2)} \, q_i q_1 \, \widehat{\chi^{(1)}} \, \widehat{\nu} \, q_1 \Psi \right\rangle\right| \\ &\leqslant \frac{1}{N-1} \, \big\|\widehat{\nu} \, q_1 \Psi\big\| \sqrt{\sum_{i,j=2}^N \langle \Psi , p_1 p_i W_{1i}^{(p,2)} q_1 q_i \, \widehat{\chi^{(1)}} \, q_1 q_j W_{1j}^{(p-2)} p_j p_1 \Psi\rangle} \,.\end{aligned}$$

Using

$$\big\|\widehat{\nu}\, q_1\Psi\big\| \;\leqslant\; \|\widehat{n}^{-1}q_1\Psi\| \;\leqslant\; 1$$

we find

$$\big|\big\langle\Psi\,, p_1p_2W_{12}^{(p,2)}\,\widehat{\nu}\,\widehat{\chi^{(1)}}\,q_1q_2\Psi\big\rangle\big| \;\leqslant\; \frac{1}{N-1}\sqrt{A+B}\,, \tag{5.60}$$

where

$$\begin{aligned}
A \;&:=\; \sum_{2\leqslant i\neq j\leqslant N}\big\langle\Psi\,, p_1p_iW_{1i}^{(p,2)}q_1q_i\,\widehat{\chi^{(1)}}\,q_jW_{1j}^{(p,2)}p_jp_1\Psi\big\rangle\,,\\
B \;&:=\; \sum_{i=2}^{N}\big\langle\Psi\,, p_1p_iW_{1i}^{(p,2)}q_1q_i\,\widehat{\chi^{(1)}}\,W_{1i}^{(p,2)}p_ip_1\Psi\big\rangle\,.
\end{aligned}$$

The easy part is

$$\begin{aligned}
B \;&\leqslant\; \sum_{i=2}^{N}\big\langle\Psi\,, p_1p_i\big(W_{1i}^{(p,2)}\big)^2p_ip_1\Psi\big\rangle\\
&\leqslant\; \sum_{i=2}^{N}\big\|\big(w^{(p,2)}\big)^2*|\varphi|^2\big\|_\infty\langle\Psi\,, p_1p_i\Psi\rangle\\
&\leqslant\; (N-1)\|\varphi\|_\infty^2\|w^{(p,2)}\|_2^2\\
&\lesssim\; N\,a^{2-p}\,\|\varphi\|_\infty^2\,.
\end{aligned}$$

Let us therefore concentrate on

$$\begin{aligned}
A \;&=\; \sum_{2\leqslant i\neq j\leqslant N}\big\langle\Psi\,, p_1p_iW_{1i}^{(p,2)}q_1q_i\,\widehat{\chi^{(1)}}\,\widehat{\chi^{(1)}}\,q_jW_{1j}^{(p,2)}p_jp_1\Psi\big\rangle\\
&=\; \sum_{2\leqslant i\neq j\leqslant N}\big\langle\Psi\,, p_1p_iq_j\,\widehat{\tau_2\chi^{(1)}}\,W_{1i}^{(p,2)}q_1W_{1j}^{(p,2)}\,\widehat{\tau_2\chi^{(1)}}\,q_ip_jp_1\Psi\big\rangle\\
&=\; A_1+A_2\,,
\end{aligned}$$

with $A=A_1+A_2$ arising from the splitting $q_1=\mathbb{1}-p_1$. We start with

$$\begin{aligned}
|A_1| \;&\leqslant\; \sum_{2\leqslant i\neq j\leqslant N}\big|\big\langle\Psi\,, p_1p_iq_j\,\widehat{\tau_2\chi^{(1)}}\,W_{1i}^{(p,2)}W_{1j}^{(p,2)}\,\widehat{\tau_2\chi^{(1)}}\,q_ip_jp_1\Psi\big\rangle\big|\\
&=\; \sum_{2\leqslant i\neq j\leqslant N}\big|\big\langle\Psi\,, p_1p_iq_j\,\widehat{\tau_2\chi^{(1)}}\,\sqrt{W_{1i}^{(p,2)}}\sqrt{W_{1j}^{(p,2)}}\sqrt{W_{1i}^{(p,2)}}\sqrt{W_{1j}^{(p,2)}}\,\widehat{\tau_2\chi^{(1)}}\,q_ip_jp_1\Psi\big\rangle\big|\\
&\leqslant\; \sum_{2\leqslant i\neq j\leqslant N}\big\langle\Psi\,,\widehat{\tau_2\chi^{(1)}}\,q_jp_1p_i\big|W_{1i}^{(p,2)}\big|\big|W_{1j}^{(p,2)}\big|p_1p_iq_j\,\widehat{\tau_2\chi^{(1)}}\,\Psi\big\rangle\,,
\end{aligned}$$

by Cauchy-Schwarz and symmetry of Ψ. Here $\sqrt{\cdot}$ is any complex square root.

In order to estimate this we claim that, for $i\neq j$,

$$\Big\|p_1p_i\big|W_{1i}^{(p,2)}\big|\big|W_{1j}^{(p,2)}\big|p_1p_i\Big\| \;\leqslant\; \big\|\big|w^{(p,2)}\big|*|\varphi|^2\big\|_\infty^2\,. \tag{5.61}$$

Indeed, by (5.26), we have

$$p_1p_i\big|W_{1i}^{(p,2)}\big|\big|W_{1j}^{(p,2)}\big|p_1p_i \;=\; p_1p_i\big|W_{1i}^{(p,2)}\big|p_i\big|W_{1j}^{(p,2)}\big|p_1 \;=\; p_1p_i\big(\big|w^{(p,2)}\big|*|\varphi|^2\big)_1\big|W_{1j}^{(p,2)}\big|p_1\,.$$

The operator $p_1\big(\big|w^{(p,2)}\big| * |\varphi|^2\big)_1\big|W_{1j}^{(p,2)}\big|p_1$ is equal to $f_j\, p_1$, where

$$f(x_j) \;=\; \int \mathrm{d}x_1\, \overline{\varphi(x_1)}\big(\big|w^{(p,2)}\big| * |\varphi|^2\big)(x_1)\big|w^{(p,2)}(x_1 - x_j)\big|\varphi(x_1)\,.$$

Thus,

$$\|f\|_\infty \;\leqslant\; \big\|\big|w^{(p,2)}\big| * |\varphi|^2\big\|_\infty^2\,,$$

from which (5.61) follows immediately.

Using (5.61), we get

$$\begin{aligned}
|A_1| \;&\leqslant\; \sum_{2\leqslant i\neq j\leqslant N} \big\|\big|w^{(p,2)}\big| * |\varphi|^2\big\|_\infty^2 \big\|\widehat{\tau_2\chi^{(1)}} q_1 \Psi\big\|^2 \\
&\leqslant\; N^2 \|w^{(p)}\|_p^2\, \|\varphi\|_{L^2\cap L^\infty}^4 \,\big\langle \Psi\,, \widehat{\tau_2\chi^{(1)}}\, q_1 \Psi\big\rangle \\
&\lesssim\; N^2\, \|\varphi\|_{L^2\cap L^\infty}^4 \,\big\langle \Psi\,, \widehat{\tau_2\chi^{(1)}}\, \widehat{n}^2\, \Psi\big\rangle\,.
\end{aligned}$$

Now let us choose

$$\chi^{(1)}(k) \;:=\; \mathbb{1}_{\{k\leqslant N^{1-\delta}\}} \tag{5.62}$$

for some $\delta \in (0,1)$. Then

$$(\tau_2\chi^{(1)})\, n^2 \;\leqslant\; N^{-\delta}$$

implies

$$|A_1| \;\lesssim\; \|\varphi\|_{L^2\cap L^\infty}^4\, N^{2-\delta}\,.$$

Similarly, we find

$$\begin{aligned}
|A_2| \;&\leqslant\; \sum_{2\leqslant i\neq j\leqslant N} \big|\big\langle \Psi\,, q_j\, \widehat{\tau_2\chi^{(1)}}\, p_i p_1 W_{1i}^{(p,2)} p_1 W_{1j}^{(p,2)} p_1 p_j\, \widehat{\tau_2\chi^{(1)}}\, q_i \Psi\big\rangle\big| \\
&\leqslant\; \sum_{2\leqslant i\neq j\leqslant N} \big\|w^{(p,2)} * |\varphi|^2\big\|_\infty^2 \langle \Psi\,, \widehat{\tau_2\chi^{(1)}}\, q_1 \Psi\rangle \\
&\lesssim\; N^2 \|\varphi\|_{L^2\cap L^\infty}^4 N^{-\delta} \\
&=\; \|\varphi\|_{L^2\cap L^\infty}^4 N^{2-\delta}\,.
\end{aligned}$$

Thus we have proven

$$|A| \;\lesssim\; \|\varphi\|_{L^2\cap L^\infty}^4 N^{2-\delta}\,.$$

Going back to (5.60), we see that

$$\big|\big\langle \Psi\,, p_1 p_2 W_{12}^{(p,2)}\, \widehat{\nu}\, \widehat{\chi^{(1)}}\, q_1 q_2 \Psi\big\rangle\big| \;\lesssim\; \|\varphi\|_{L^2\cap L^\infty}^2 N^{-\delta/2} + \|\varphi\|_\infty N^{-1/2}\, a^{1-p/2}\,.$$

What remains is to estimate is the term of $(\mathrm{III})^{(p,2)}$ containing $\chi^{(2)}$,

$$\begin{aligned}
\big|\big\langle \Psi\,, p_1 p_2 W_{12}^{(p,2)}\, \widehat{\nu}\, \widehat{\chi^{(2)}}\, q_1 q_2 \Psi\big\rangle\big| \;&=\; \frac{1}{N-1}\bigg|\bigg\langle \Psi\;,\; \sum_{i=2}^N p_1 p_i W_{1i}^{(p,2)}\, q_i q_1\, \widehat{\chi^{(2)}}\, \widehat{\nu}^{1/2}\, \widehat{\nu}^{1/2}\, q_1 \Psi\bigg\rangle\bigg| \\
&\leqslant\; \frac{1}{N-1}\, \big\|\widehat{\nu}^{1/2}\, q_1 \Psi\big\| \sqrt{\sum_{i,j=2}^N \big\langle \Psi\,, p_1 p_i W_{1i}^{(p,2)} q_1 q_i\, \widehat{\chi^{(2)}}\, \widehat{\nu}\, q_1 q_j W_{1j}^{(p-2)} p_j p_1 \Psi\big\rangle}\,.
\end{aligned}$$

Using

$$\big\|\widehat{\nu}^{1/2}\, q_1\Psi\big\| \;\leqslant\; \sqrt{\langle\Psi\,, \widehat{n}^{-1}\,\widehat{n}^2\,\Psi\rangle} \;=\; \sqrt{\beta}$$

we find

$$\big|\big\langle\Psi\,, p_1p_2W_{12}^{(p,2)}\,\widehat{\nu}\,\widehat{\chi^{(2)}}\,q_1q_2\Psi\big\rangle\big| \;\leqslant\; \frac{\sqrt{\beta}}{N-1}\sqrt{A+B}\,, \tag{5.63}$$

where

$$\begin{aligned} A \;&:=\; \sum_{2\leqslant i\neq j\leqslant N}\big\langle\Psi\,, p_1p_iW_{1i}^{(p,2)}q_1q_i\,\widehat{\chi^{(2)}}\,\widehat{\nu}\,q_jW_{1j}^{(p,2)}p_jp_1\Psi\big\rangle\,,\\ B \;&:=\; \sum_{i=2}^{N}\big\langle\Psi\,, p_1p_iW_{1i}^{(p,2)}q_1q_i\,\widehat{\chi^{(2)}}\,\widehat{\nu}\,W_{1i}^{(p,2)}p_ip_1\Psi\big\rangle\,. \end{aligned}$$

Since

$$\chi^{(2)}(k) \;=\; \mathbb{1}_{\{k>N^{1-\delta}\}}$$

we find

$$\chi^{(2)}\,\nu \;\leqslant\; \chi^{(2)}\,n^{-1} \;\leqslant\; N^{\delta/2}\,.$$

Thus, $\|q_1q_i\,\widehat{\chi^{(2)}}\,\widehat{\nu}\| \;\leqslant\; N^{\delta/2}$ and we get

$$\begin{aligned} B \;\leqslant\; N^{\delta/2}\sum_{i=2}^{N}\big\langle\Psi\,, p_1p_i\big(W_{1i}^{(p,2)}\big)^2p_ip_1\Psi\big\rangle \;&\leqslant\; N^{1+\delta/2}\,\big\|\big(w^{(p,2)}\big)^2 * |\varphi|^2\big\|_\infty\\ &\leqslant\; N^{1+\delta/2}\,\|w^{(p,2)}\|_2^2\,\|\varphi\|_\infty^2 \;\lesssim\; N^{1+\delta/2}\,a^{2-p}\,\|\varphi\|_\infty^2\,, \end{aligned}$$

by (5.56b).

Next, using Lemma 5.15, we find

$$\begin{aligned} A \;&=\; \sum_{2\leqslant i\neq j\leqslant N}\big\langle\Psi\,, p_1p_iq_jW_{1i}^{(p,2)}\,\widehat{\chi^{(2)}}\,\widehat{\nu}^{1/2}\,q_1\,\widehat{\chi^{(2)}}\,\widehat{\nu}^{1/2}\,W_{1j}^{(p,2)}q_ip_jp_1\Psi\big\rangle\\ &=\; \sum_{2\leqslant i\neq j\leqslant N}\big\langle\Psi\,, p_1p_iq_j\,\widehat{\tau_2\chi^{(2)}}\,\widehat{\tau_2\nu}^{1/2}\,W_{1i}^{(p,2)}q_1W_{1j}^{(p,2)}\,\widehat{\tau_2\chi^{(2)}}\,\widehat{\tau_2\nu}^{1/2}\,q_ip_jp_1\Psi\big\rangle\\ &=\; A_1+A_2\,, \end{aligned}$$

where, as above, the splitting $A = A_1 + A_2$ arises from writing $q_1 = \mathbb{1} - p_1$. Thus,

$$\begin{aligned} |A_1| \;&\leqslant\; \sum_{2\leqslant i\neq j\leqslant N}\big|\big\langle\Psi\,, p_1p_iq_j\,\widehat{\tau_2\chi^{(2)}}\,\widehat{\tau_2\nu}^{1/2}\,W_{1i}^{(p,2)}W_{1j}^{(p,2)}\,\widehat{\tau_2\chi^{(2)}}\,\widehat{\tau_2\nu}^{1/2}\,q_ip_jp_1\Psi\big\rangle\big|\\ &=\; \sum_{2\leqslant i\neq j\leqslant N}\big|\big\langle\Psi\,, p_1p_iq_j\,\widehat{\tau_2\chi^{(2)}}\,\widehat{\tau_2\nu}^{1/2}\,\sqrt{W_{1i}^{(p,2)}}\sqrt{W_{1j}^{(p,2)}}\sqrt{W_{1i}^{(p,2)}}\sqrt{W_{1j}^{(p,2)}}\,\widehat{\tau_2\chi^{(2)}}\,\widehat{\tau_2\nu}^{1/2}\,q_ip_jp_1\Psi\big\rangle\big|\\ &\leqslant\; \sum_{2\leqslant i\neq j\leqslant N}\big\langle\Psi\,, q_j\,\widehat{\tau_2\chi^{(2)}}\,\widehat{\tau_2\nu}^{1/2}\,p_1p_i\big|W_{1i}^{(p,2)}\big|\big|W_{1j}^{(p,2)}\big|p_ip_1\,\widehat{\tau_2\chi^{(2)}}\,\widehat{\tau_2\nu}^{1/2}\,q_j\Psi\big\rangle\,, \end{aligned}$$

by Cauchy-Schwarz and symmetry of Ψ. Using (5.61) we get

$$\begin{aligned} |A_1| \;&\leqslant\; N^2\,\big\|\big|w^{(p,2)}\big| * |\varphi|^2\big\|_\infty^2\,\big\langle\Psi\,, \widehat{\tau_2\nu}\,q_1\Psi\big\rangle\\ &\leqslant\; N^2\|w^{(p,2)}\|_p^2\,\|\varphi\|_{L^2\cap L^\infty}^4\,\langle\Psi\,, \widehat{n}\,\Psi\rangle\\ &\lesssim\; N^2\,\|\varphi\|_{L^2\cap L^\infty}^4\beta\,. \end{aligned}$$

Similarly,

$$
\begin{aligned}
|A_2| &\leqslant \sum_{2\leqslant i\neq j\leqslant N} \big|\big\langle \Psi\,, p_i q_j\, \widehat{\tau_2\chi^{(2)}}\, \widehat{\tau_2\nu}^{1/2}\, p_1 W^{(p,2)}_{1i} p_1 W^{(p,2)}_{1j} p_1\, \widehat{\tau_2\chi^{(2)}}\, \widehat{\tau_2\nu}^{1/2}\, q_i p_j \Psi\big\rangle\big| \\
&\leqslant \sum_{2\leqslant i\neq j\leqslant N} \big\|w^{(p,2)} * |\varphi|^2\big\|_\infty^2 \big\langle \Psi\,, \widehat{\tau_2\nu}\, q_1\Psi\big\rangle \\
&\leqslant N^2 \|w^{(p)}\|_p^2\, \|\varphi\|^4_{L^2\cap L^\infty}\, \langle \Psi\,, \widehat{n}\,\Psi\rangle \\
&\lesssim N^2\, \|\varphi\|^4_{L^2\cap L^\infty}\, \beta\,.
\end{aligned}
$$

Plugging all this back into (5.63), we find that

$$
\big|\big\langle \Psi\,, p_1p_2 W^{(p,2)}_{12}\, \widehat{\nu}\, \widehat{\chi^{(2)}}\, q_1q_2\Psi\big\rangle\big| \;\lesssim\; \beta\big(\|\varphi\|^2_{L^2\cap L^\infty} + \|\varphi\|_\infty\big) + \|\varphi\|_\infty a^{2-p} N^{\delta/2-1}
$$

Summarizing:

$$
\big|(\mathrm{III})^{(p,2)}\big| \;\lesssim\; \big(1+\|\varphi\|^2_{L^2\cap L^\infty}\big)\Big(\beta + a^{2-p}\, N^{\delta/2-1} + N^{-\delta/2} + N^{-1/2} a^{1-p/2}\Big)\,,
$$

from which we deduce

$$
\begin{aligned}
\big|(\mathrm{III})^{(p)}\big| \;\lesssim\;& \|\varphi\|_\infty \|\nabla_1 q_1\Psi\|^2 \\
&+ \big(1+\|\varphi\|_{X_1\cap L^\infty}\big)\Big(\beta + a^{2-p}\, N^{\delta/2-1} + N^{-\delta/2} + N^{-1/2} a^{1-p/2} + a^{2-2p/p_0}\Big)\,.
\end{aligned}
$$

Let us set $a \equiv a_N = N^\zeta$ and optimize in δ and ζ. This yields the relations

$$
\zeta(2-p) + \delta \;=\; 1\,, \qquad -\frac{\delta}{2} \;=\; 2\zeta\Big(1-\frac{p}{p_0}\Big)\,,
$$

which imply

$$
\frac{\delta}{2} \;=\; \frac{p/p_0 - 1}{2p/p_0 - p/2 - 1}\,,
$$

with $\delta \leqslant 1$. Thus,

$$
\big|(\mathrm{III})^{(p)}\big| \;\lesssim\; \|\varphi\|_\infty \|\nabla_1 q_1\Psi\|^2 + \big(1+\|\varphi\|_{X_1\cap L^\infty}\big)\Big(\beta + N^{-\eta}\Big)\,,
$$

where $\eta = \delta/2$ satisfies (5.37).

Conclusion of the proof. We have shown that

$$
\dot\beta \;\lesssim\; \|\varphi\|_{L^2\cap L^\infty} \|\nabla_1 q_1\Psi\|^2 + \big(1+\|\varphi\|_{X_1\cap L^\infty}\big)\big(\beta + N^{-\eta}\big)\,.
$$

Using Lemma 5.21 we find

$$
\dot\beta \;\lesssim\; \Big(1+\|\varphi\|^3_{X_1^2\cap L^\infty}\Big)\Big(\beta + E^\Psi - E^\varphi + \frac{1}{N^\eta}\Big)\,. \tag{5.64}
$$

The claim then follows from the Grönwall estimate (5.11).

5.3.5. A remark on time-dependent external potentials. Theorem 5.16 can be extended to time-dependent external potentials $h(t)$ without too much sweat. The only complication is that energy is no longer conserved. We overcome this problem by observing that, while the energies $E^\Psi(t)$ and $E^\varphi(t)$ exhibit large variations in t, their difference remains small. In the following we estimate the quantity $E^\Psi(t) - E^\varphi(t)$ by controlling its time derivative.

We need the following assumptions, which replace Assumptions (B1) – (B3).

(B1') The Hamiltonian $h(t)$ is self-adjoint and bounded from below. We assume that there is an operator $h_0 \geqslant 0$ that such that $0 \leqslant h(t) \leqslant h_0$ for all t. We define the Hilbert space $X_N = \mathcal{Q}\big(\sum_i (h_0)_i\big)$ as in (A1), and the space $X_1^2 = \mathcal{Q}(h_0^2)$ as in (B5) using h_0. We also assume that there are time-independent constants $\kappa_1, \kappa_2 > 0$ such that

$$-\Delta \;\leqslant\; \kappa_1\, h(t) + \kappa_2$$

for all t.

We make the following assumptions on the differentiability of $h(t)$. The map $t \mapsto \langle \psi\,, h(t)\psi\rangle$ is continuously differentiable for all $\psi \in X_1$, with derivative $\langle \psi\,, \dot{h}(t)\psi\rangle$ for some self-adjoint operator $\dot{h}(t)$. Moreover, we assume that the quantities

$$\langle \varphi(t)\,, \dot{h}(t)^2 \varphi(t)\rangle\,, \qquad \big\|(\mathbb{1} + h(t))^{-1/2}\, \dot{h}(t)\, (\mathbb{1} + h(t))^{-1/2}\big\|$$

are continuous and finite for all t.

(B2') The Hamiltonian $H_N(t)$ is self-adjoint and bounded from below. We assume that $\mathcal{Q}(H_N(t)) \subset X_N$ for all t. We also assume that the N-body propagator $U_N(t,s)$, defined by

$$\mathrm{i}\partial_t U_N(t,s) = H_N(t) U_N(t,s)\,, \qquad U_N(s,s) = \mathbb{1}\,,$$

exists and satisfies $U_N(t,0)\Psi_{N,0} \in \mathcal{Q}(H_N(t))$ for all t.

(B3') There is a time-independent constant $\kappa_3 \in (0,1)$ such that

$$0 \;\leqslant\; (1-\kappa_3)(h_1(t) + h_2(t)) + W_{12}$$

for all t.

THEOREM 5.22. *Assume that Assumptions (B1') – (B3'), (B4), and (B5) hold. Then there is a continuous nonnegative function ϕ, independent of N and $\Psi_{N,0}$, such that*

$$\beta_N(t) \;\leqslant\; \phi(t)\bigg(\beta_N(0) + E_N^\Psi(0) - E^\varphi(0) + \frac{1}{N^\eta}\bigg)\,,$$

with η defined in (5.37)*.*

PROOF. We start by deriving an upper bound on the energy difference $\mathcal{E}(t) := E^\Psi(t) - E^\varphi(t)$. Assumptions (B1') and (B2') and the fundamental theorem of calculus imply

$$\mathcal{E}(t) \;=\; \mathcal{E}(0) + \int_0^t \mathrm{d}s\, \Big(\underbrace{\langle \Psi(s)\,, \dot{h}_1(s)\Psi(s)\rangle - \langle \varphi(s)\,, \dot{h}(s)\varphi(s)\rangle}_{=:\, G(s)}\Big)\,.$$

By inserting $\mathbb{1} = p_1(s) + q_1(s)$ on both sides of $\dot{h}_1(s)$ we get (omitting the time argument s)

$$G \;=\; \langle \Psi\,, p_1 \dot{h}_1 p_1 \Psi\rangle - \langle \varphi\,, \dot{h}\varphi\rangle + 2\,\mathrm{Re}\langle \Psi\,, p_1 \dot{h}_1 q_1 \Psi\rangle + \langle \Psi\,, q_1 \dot{h}_1 q_1 \Psi\rangle\,. \tag{5.65}$$

The first two terms of (5.65) are equal to

$$\big(\langle\Psi\,,p_1\Psi\rangle - 1\big)\langle\varphi\,,\dot{h}\varphi\rangle \;=\; \alpha\langle\varphi\,,\dot{h}\varphi\rangle \;\leqslant\; \beta|\langle\varphi\,,\dot{h}\varphi\rangle|\,.$$

The third term of (5.65) is bounded, using Lemmas 5.14 and 5.15, by

$$\begin{aligned}
2\big|\big\langle\Psi\,,p_1\dot{h}_1\,\widehat{n}^{1/2}\,\widehat{n}^{-1/2}\,q_1\Psi\big\rangle\big| \;&=\; 2\big|\big\langle\dot{h}_1p_1\,\widehat{\tau_1 n}^{1/2}\,\Psi\,,\widehat{n}^{-1/2}\,q_1\Psi\big\rangle\big| \\
&\leqslant\; \sqrt{\big\langle\widehat{\tau_1 n}^{1/2}\,\Psi\,,p_1\dot{h}_1^2p_1\,\widehat{\tau_1 n}^{1/2}\,\Psi\big\rangle}\,\big\|\widehat{n}^{-1/2}\,q_1\Psi\big\| \\
&\leqslant\; \sqrt{|\langle\varphi\,,\dot{h}^2\varphi\rangle|}\,\sqrt{\big\langle\Psi\,,\widehat{\tau_1 n}\,\Psi\big\rangle}\,\sqrt{\big\langle\Psi\,,\widehat{n}^{-1}\,q_1\Psi\big\rangle} \\
&\leqslant\; \sqrt{|\langle\varphi\,,\dot{h}^2\varphi\rangle|}\sqrt{\beta+\frac{1}{\sqrt{N}}}\sqrt{\beta}\,, \\
&\lesssim\; \sqrt{|\langle\varphi\,,\dot{h}^2\varphi\rangle|}\bigg(\beta+\frac{1}{\sqrt{N}}\bigg)\,.
\end{aligned}$$

The last term of (5.65) is equal to

$$\begin{aligned}
&\big\langle\Psi\,,q_1(\mathbb{1}+h_1)^{1/2}(\mathbb{1}+h)^{-1/2}\dot{h}_1(\mathbb{1}+h_1)^{-1/2}(\mathbb{1}+h)^{1/2}q_1\Psi\big\rangle \\
&\qquad\qquad\leqslant\; \big\|(\mathbb{1}+h)^{-1/2}\dot{h}(\mathbb{1}+h)^{-1/2}\big\|\,\big\|(\mathbb{1}+h_1)^{1/2}q_1\Psi\big\|^2\,.
\end{aligned}$$

Thus, using Assumption (B1') we conclude that

$$G(t) \;\leqslant\; C(t)\bigg(\beta(t)+\frac{1}{\sqrt{N}}+\big\|h_1(t)^{1/2}q_1(t)\Psi(t)\big\|^2\bigg) \tag{5.66}$$

for all t. Here, and in the following, $C(t)$ denotes some continuous nonnegative function that does not depend on N.

Next, we observe that, under Assumptions (B1') – (B3'), the proof of Lemma 5.21 remains valid for time-dependent one-particle Hamiltonians. Thus, (5.46) implies

$$\big\|h_1(t)^{1/2}q_1(t)\Psi(t)\big\|^2 \;\lesssim\; \mathcal{E}(t)+\big(1+\|\varphi(t)\|^2_{X_1^2\cap L^\infty}\big)\bigg(\beta(t)+\frac{1}{\sqrt{N}}\bigg)\,.$$

Plugging this into (5.66) yields

$$G(t) \;\leqslant\; C(t)\bigg(\beta(t)+\frac{1}{\sqrt{N}}+\mathcal{E}(t)\bigg)\,.$$

Therefore,

$$\mathcal{E}(t) \;\leqslant\; \mathcal{E}(0)+\int_0^t \mathrm{d}s\,C(s)\bigg(\beta(s)+\mathcal{E}(s)+\frac{1}{\sqrt{N}}\bigg)\,, \tag{5.67}$$

Next, we observe that, under Assumptions (B1') – (B3'), the derivation of the estimate (5.64) in the proof of Theorem 5.16 remains valid for time-dependent one-particle Hamiltonians. Therefore,

$$\beta(t) \;\leqslant\; \beta(0)+\int_0^t \mathrm{d}s\,C(s)\bigg(\beta(s)+\mathcal{E}(s)+\frac{1}{N^\eta}\bigg)\,. \tag{5.68}$$

Applying Grönwall's lemma (See Appendix C) to the sum of (5.67) and (5.68) yields

$$\beta(t)+\mathcal{E}(t) \;\leqslant\; \big(\beta(0)+\mathcal{E}(0)\big)\,\mathrm{e}^{\int_0^t C}+\frac{1}{N^\eta}\int_0^t \mathrm{d}s\,C(s)\,\mathrm{e}^{\int_0^t C}\,.$$

Plugging this back into (5.68) yields

$$\beta(t) \leqslant C(t)\left(\beta(0) + \mathcal{E}(0) + \frac{1}{N^\eta}\right),$$

which is the claim. □

Appendix A

A Short Review of Cluster Expansions

In this appendix we give a summary of cluster expansions. We first give an overview of the algebraic setting underlying cluster expansions, and, in a second part, deal with the convergence of cluster expansions. In this appendix only we use lowercase letters $x, y, \dots$ instead of the usual uppercase letters $X, Y, \dots$ to denote polymers. Uppercase letters $X, Y, \dots$ are reserved for sets of polymers.

Some definitions. Let X be a finite set and denote by $\mathscr{P}(X)$ the set of partitions of X; a partition of X is a set of nonempty disjoint subsets of X whose union is equal to X. We use the symbol $\uplus$ to denote disjoint union. We abbreviate $\mathbb{N}_n := \{1, \dots, n\}$.

A *graph* G is a pair $(V(G), E(G))$. Here $V(G)$ is a finite set of vertices; $E(G)$, the set of edges, is a set of unordered pairs of vertices $\{x, y\}$, where $x, y \in V(G)$. An edge $e \in E(G)$ is *incident* to a vertex $x \in V(G)$ if $x \in e$. Two edges $e, e' \in E(G)$ are *adjacent* if $e \cap e' \neq \emptyset$. A graph G is *connected* if, for any two points $x, y \in V(G)$, there exists a sequence of edges $e_1, \dots, e_n$ such that e_1 is incident to x, e_n is incident to y, and e_i and e_{i+1} are adjacent for $i = 1, \dots, n-1$. Denote by $\mathcal{G}(X)$ the set of graphs on the set of vertices $V(G) = X$. Denote by $\mathcal{G}_c(X) \subset \mathcal{G}(X)$ the subset of connected graphs.

A.1. The algebra of cluster expansions

In this section we describe the algebra of cluster expansions, without worrying about convergence of formal power series.

A.1.1. The connected part of an n-point function. Let $\mathbb{X}$ be an arbitrary set of polymers whose elements we denote by x. Let $X \mapsto f(X)$ be a function of the finite nonempty subsets $X \subset \mathbb{X}$. Thus, f can also be viewed as a symmetric function of a collection of polymers: $f(x_1, \dots, x_n) = f(X)$ for $X = \{x_1, \dots, x_n\}$. To each function f we assign the *connected part of f*, denoted by f_c. It is defined recursively through

$$f(X) \;=\; \sum_{P \in \mathscr{P}(X)} \prod_{Y \in P} f_c(Y)\,.$$

For example,

$$f_c(x) \;=\; f(x)\,, \qquad f_c(x, y) \;=\; f(x, y) - f(x) f(y)\,.$$

In order to get an explicit formula for f_c, we extend the definition of f by setting $f(\emptyset) := 0$. Next, introduce the multiplication

$$(f_1 * f_2)(X) \;:=\; \sum_{X_1 \uplus X_2 = X} f_1(X_1) f_2(X_2)\,.$$

It is easy to see that the set of functions $f(X)$ is an associative, commutative algebra with multiplication $*$. It has a unity $\mathbb{1}$ defined by

$$\mathbb{1}(X) := \begin{cases} 1 & \text{if } X = \emptyset\,, \\ 0 & \text{otherwise}\,. \end{cases}$$

Since $f_c(\emptyset) = 0$, the formal power series $\exp_* f_c$ is well-defined, and we find

$$\begin{aligned} (\exp_* f_c)(X) &= \mathbb{1}(X) + \sum_{k \geqslant 1} \frac{1}{k!} f_c^{*k}(X) \\ &= \mathbb{1}(X) + \sum_{k \geqslant 1} \frac{1}{k!} \sum_{X_1 \uplus \cdots \uplus X_k = X} f_c(X_1) \cdots f_c(X_k) \\ &= \mathbb{1}(X) + \sum_{k \geqslant 1} \sum_{P \in \mathscr{P} \,:\, |P| = k} \prod_{Y \in P} f_c(Y) \\ &= \mathbb{1}(X) + f(X)\,. \end{aligned}$$

By inversion of formal power series, we get the explicit ("Möbius inversion") formula

$$\begin{aligned} f_c(X) &= \log_*(\mathbb{1} + f)(X) \\ &= \sum_{k \geqslant 1} \frac{(-1)^{k-1}}{k} f^{*k}(X) \\ &= \sum_{k \geqslant 1} (-1)^{k-1} (k-1)! \frac{1}{k!} \sum_{X_1 \uplus \cdots \uplus X_k = X} f(X_1) \cdots f(X_k) \\ &= \sum_{P \in \mathscr{P}(X)} (-1)^{|P|-1} (|P| - 1)! \prod_{Y \in P} f(Y)\,. \end{aligned}$$

For example,

$$f_c(x,y,z) = f(x,y,z) - f(x,y)f(z) - f(y,z)f(x) - f(z,x)f(y) + 2f(x)f(y)f(z)\,.$$

A.1.2. The graph expansion. Let us now assume that f is generated by graphs, i.e.

$$f(X) = \sum_{G \in \mathcal{G}(X)} z(G)\,,$$

for some weight function z satisfying $z(G_1 \cup G_2) = z(G_1) z(G_2)$ whenever $V(G_1) \cap V(G_2) = \emptyset$. Here $G_1 \cup G_2$ denotes the graph whose set of vertices is $G_1 \cup G_2$ and set of edges $E(G_1) \cup E(G_2)$.

For instance we may take

$$f(X) = \sum_{G \in \mathcal{G}(X)} \prod_{x \in X} w(x) \prod_{\{x,y\} \in E(G)} \zeta(x,y)\,,$$

for some complex functions $w(x)$ and $\zeta(x,y) = \zeta(y,x)$.

Now we claim that

$$f_c(X) = \sum_{G \in \mathcal{G}_c(X)} z(G)\,.$$

Indeed, let us verify the definition of f_c:

$$\sum_{P\in\mathscr{P}(X)}\prod_{Y\in P} f_c(Y) \;=\; \sum_{P\in\mathscr{P}(X)}\prod_{Y\in P}\sum_{G\in\mathcal{G}_c(Y)} z(G) \;=\; \sum_{G\in\mathcal{G}(X)} z(G)\,,$$

where the last step follows by decomposing $G \in \mathcal{G}(X)$ into its connected components, as well as the factorization property of z.

A.1.3. Moments, cumulants, and generating functions. Let $\lambda = (\lambda_x)_{x\in\mathbb{X}}$ and consider a generating function $\chi(\lambda)$ defined on the set

$$\{\lambda : \lambda_x = 0 \text{ for all by finitely many } x \in \mathbb{X}\}\,.$$

The generating function $\chi(\lambda)$ defines a function ("moment") $f_\chi(X)$ through

$$f_\chi(X) \;:=\; \Bigg(\prod_{x\in X}\frac{\partial}{\partial\lambda_x}\Bigg)\chi(\lambda)\bigg|_{\lambda=0}\,.$$

We use the natural convention $f_\chi(\emptyset) = \chi(0)$.

Next, let us take two generating functions, χ_1 and χ_2. The moment corresponding to their product is given by

$$\begin{aligned}
f_{\chi_1\chi_2}(X) \;&=\; \Bigg(\prod_{x\in X}\frac{\partial}{\partial\lambda_x}\Bigg)\chi_1(\lambda)\chi_2(\lambda)\bigg|_{\lambda=0}\\
&=\; \sum_{X_1\uplus X_2=X}\Bigg[\Bigg(\prod_{x\in X_1}\frac{\partial}{\partial\lambda_x}\Bigg)\chi_1(\lambda)\Bigg]\Bigg[\Bigg(\prod_{x\in X_2}\frac{\partial}{\partial\lambda_x}\Bigg)\chi_2(\lambda)\Bigg]\bigg|_{\lambda=0}\\
&=\; \sum_{X_1\uplus X_2=X} f_{\chi_1}(X_1)f_{\chi_2}(X_2)\\
&=\; (f_{\chi_1} * f_{\chi_2})(X)\,.
\end{aligned}$$

Therefore the mapping $\chi \mapsto f_\chi$ is a homomorphism of associative commutative algebras. In particular, if $\chi(0) = 0$ and hence $f_\chi(\emptyset) = 0$, we find

$$f_{\exp\chi} \;=\; \exp_* f_\chi\,.$$

Also, $f_1 = \mathbb{1}$. This implies that

$$\exp_* f_\chi \;=\; \mathbb{1} + f_{\exp\chi-1}\,,$$

from which we deduce

$$f_\chi \;=\; (f_{\exp\chi-1})_c\,.$$

We may rewrite this as

$$(f_\chi)_c \;=\; f_{\log(1+\chi)}\,.$$

Here is a typical example. Let $(F_x)_{x\in\mathbb{X}}$ be a family of random variables and set

$$\chi(\lambda) \;:=\; \mathbb{E}\Big[\mathrm{e}^{\sum_{x\in\mathbb{X}}\lambda_x F_x}\Big] - 1\,.$$

Thus, χ generates the moments

$$f_\chi(X) \;=\; \mathbb{E}\left[\prod_{x\in X} F_x\right],$$

and

$$\chi_c(\lambda) \;:=\; \log \mathbb{E}\left[\mathrm{e}^{\sum_{x\in\mathbb{X}} \lambda_x F_x}\right]$$

generates the corresponding cumulants $(f_\chi)_c$.

A.1.4. The cluster expansion. Now let us assume that the set $\mathbb{X}$ is a measure space $(\mathbb{X}, \mathcal{F}, \mu)$, with some complex measure μ. Let $f(X)$ be a function on the finite subsets of $\mathbb{X}$. Consider the *partition function*

$$Z \;:=\; 1 + \sum_{n\geqslant 1} \frac{1}{n!} \int \mathrm{d}\mu(x_1)\cdots\mathrm{d}\mu(x_n)\, f(x_1,\ldots,x_n)\,,$$

understood as a formal power series[1]. We assume that all integrals are absolutely convergent. For $I \subset \mathbb{N}$ finite denote by x_I the set $\{x_i \,:\, i \in I\}$. Then we find

$$\begin{aligned}
Z \;&=\; 1 + \sum_{n\geqslant 1} \frac{1}{n!} \sum_{P\in\mathscr{P}(\mathbb{N}_n)} \int \mathrm{d}\mu(x_1)\cdots\mathrm{d}\mu(x_n) \prod_{I\in P} f_c(x_I) \\
&=\; 1 + \sum_{n\geqslant 1} \frac{1}{n!} \sum_{k\geqslant 1} \sum_{\substack{P\in\mathscr{P}(\mathbb{N}_n):\\ |P|=k}} \int \mathrm{d}\mu(x_1)\cdots\mathrm{d}\mu(x_n) \prod_{I\in P} f_c(x_I) \\
&=\; 1 + \sum_{n\geqslant 1} \frac{1}{n!} \sum_{k\geqslant 1} \frac{1}{k!} \sum_{\substack{I_1\uplus\cdots\uplus I_k=\mathbb{N}_n:\\ I_\ell\neq\emptyset\,\forall\ell}} \int \mathrm{d}\mu(x_1)\cdots\mathrm{d}\mu(x_n) \prod_{\ell=1}^{k} f_c(x_{I_\ell}) \\
&=\; 1 + \sum_{n\geqslant 1} \frac{1}{n!} \sum_{k\geqslant 1} \frac{1}{k!} \sum_{\substack{m_1+\cdots+m_k=n:\\ m_\ell\geqslant 1\,\forall\ell}} \frac{n!}{m_1!\cdots m_k!} \prod_{\ell=1}^{k} \int \mathrm{d}\mu(x_1)\cdots\mathrm{d}\mu(x_{m_\ell}) f_c(x_1,\ldots,x_{m_\ell}) \\
&=\; 1 + \sum_{k\geqslant 1} \frac{1}{k!} \left(\sum_{m\geqslant 1} \frac{1}{m!} \int \mathrm{d}\mu(x_1)\cdots\mathrm{d}\mu(x_m) f_c(x_1,\ldots,x_m)\right)^{k} \\
&=\; \exp\left(\sum_{m\geqslant 1} \frac{1}{m!} \int \mathrm{d}\mu(x_1)\cdots\mathrm{d}\mu(x_m) f_c(x_1,\ldots,x_m)\right).
\end{aligned}$$

Thus we obtain a formal power series expansion for $\log Z$.

A.2. Convergence of cluster expansions

We now prove a general estimate that implies the absolute convergence of the cluster expansion, and can also be used to easily prove the existence of the thermodynamic limits of the pressure and correlation functions, as well as exponential decay of correlations in various lattice models.

[1]For simplicity of notation, the parameter of the formal power series is absorbed into μ.

Let $\zeta(x, y)$ be a complex function that is symmetric in its arguments. We also assume that

$$|1 + \zeta(x, y)| \leqslant 1 .$$

Let us choose f of the form

$$f(x_1, \ldots, x_n) = \prod_{1 \leqslant i < j \leqslant n} (1 + \zeta(x_i, x_j))$$

so that

$$Z = 1 + \sum_{n \geqslant 1} \frac{1}{n!} \int \mathrm{d}\mu(x_1) \cdots \mathrm{d}\mu(x_n) \sum_{G \in \mathcal{G}(\mathbb{N}_n)} \prod_{\{i,j\} \in E(G)} \zeta(x_i, x_j) .$$

We have proven that

$$\log Z = \sum_{n \geqslant 1} \frac{1}{n!} \int \mathrm{d}\mu(x_1) \cdots \mathrm{d}\mu(x_n) \sum_{G \in \mathcal{G}_c(\mathbb{N}_n)} \prod_{\{i,j\} \in E(G)} \zeta(x_i, x_j)$$

as a formal power series. We often use the shorthand

$$\varphi(x_1, \ldots, x_n) := \sum_{G \in \mathcal{G}_c(\mathbb{N}_n)} \prod_{\{i,j\} \in E(G)} \zeta(x_i, x_j) .$$

A very convenient way to show the convergence of the cluster expansion is the *Kotecký-Preiss* criterion. Assume that there exists a nonnegative function a on $\mathbb{X}$, such that

$$\int \mathrm{d}|\mu|(y) \, |\zeta(x, y)| \, \mathrm{e}^{a(y)} \leqslant a(x) . \tag{A.1}$$

For lattice polymer models, where polymers x are subsets of some lattice L, one usually takes $a(x) = a|x|$ for some $a > 0$, where $|x|$ denotes the cardinality of the set x. What follows is a heuristic argument justifying this choice as essentially the only possible one. The measure μ is given by a weighted counting measure:

$$\int \mathrm{d}\mu(x) \, \phi(x) = \sum_x w(x) \phi(x) ,$$

for some weights $w(x) \in \mathbb{C}$. The function ζ is a “hard-core” repulsion of polymers, given by

$$\zeta(x, y) = \begin{cases} -1 & \text{if } x \cap y \neq \emptyset \\ 0 & \text{otherwise} . \end{cases}$$

We use the shorthand $x \nsim y$ to denote $x \cap y \neq \emptyset$. The Kotecký-Preiss condition reads

$$\sum_{y \nsim x} |w(y)| \, \mathrm{e}^{a(y)} \leqslant a(x) .$$

The rough idea of the argument is

$$\sum_{y \nsim x} |w(y)| \, \mathrm{e}^{a(y)} \approx \sum_{\ell \in x} \sum_{y \ni \ell} |w(y)| \, \mathrm{e}^{a(y)} = C|x| ,$$

where $\ell \in L$ denotes a lattice point. Here, and throughout the argument, we assume translation invariance. Let us be a little more precise:

$$\sum_{y \nsim x} |w(y)| \, \mathrm{e}^{a(y)} \;\geqslant\; \sum_{\ell \in x} |w(\{\ell\})| \mathrm{e}^{a(\{\ell\})} \;=\; C|x| \,,$$

which shows that $a(x) \geqslant C|x|$. On the other hand, one typically has $|w(x)| \approx \mathrm{e}^{-C|x|}$. Thus, if

$$\sum_{y \nsim x} |w(y)| \, \mathrm{e}^{a(y)} \;\approx\; \sum_{y \nsim x} \mathrm{e}^{-C|y|} \, \mathrm{e}^{a(y)}$$

is to be finite, we have to have $a(x) \leqslant C|x|$.

Next, we address the convergence of the cluster expansion. The following theorem gives a bound sufficient for all practical purposes.

THEOREM A.1 (CONVERGENCE OF THE CLUSTER EXPANSION). *Assume that* (A.1) *holds. Then we have*

$$1 + \sum_{n \geqslant 2} \frac{1}{(n-1)!} \int \mathrm{d}|\mu|(x_2) \cdots \mathrm{d}|\mu|(x_n) \, |\varphi(x_1, \dots, x_n)| \;\leqslant\; \mathrm{e}^{a(x_1)} \,.$$

PROOF. We follow the clever and elegant proof of [Uel04]. Let $N \in \mathbb{N}$ and define

$$K_N(x_1) \;:=\; 1 + \sum_{n=2}^{N} \frac{1}{(n-1)!} \int \mathrm{d}|\mu|(x_2) \cdots \mathrm{d}|\mu|(x_n) \, |\varphi(x_1, \dots, x_n)| \,, \tag{A.2}$$

Clearly, it is enough to show that $K_N(x_1) \leqslant \mathrm{e}^{a(x_1)}$ for all N and x_1. We show this by induction on N. Note first that, assuming $K_N(x_1) \leqslant \mathrm{e}^{a(x_1)}$, we get for all x

$$\begin{aligned}
&\sum_{n=1}^{N} \frac{1}{n!} \int \mathrm{d}|\mu|(x_1) \cdots \mathrm{d}|\mu|(x_n) \, \sum_{i=1}^{n} |\zeta(x, x_i)| \, |\varphi(x_1, \dots, x_n)| \\
&= \sum_{n=1}^{N} \frac{1}{(n-1)!} \int \mathrm{d}|\mu|(x_1) \cdots \mathrm{d}|\mu|(x_n) \, |\zeta(x, x_1)| \, |\varphi(x_1, \dots, x_n)| \\
&= \int \mathrm{d}|\mu|(x_1) \, |\zeta(x, x_1)| \, K_N(x_1) \\
&\leqslant \int \mathrm{d}|\mu|(x_1) \, |\zeta(x, x_1)| \, \mathrm{e}^{a(x_1)} \\
&\leqslant a(x) \,,
\end{aligned} \tag{A.3}$$

by the Kotecký-Preiss criterion (A.1).

Clearly, the claim is correct for $N = 1$. The idea of the induction step is as follows. Recall that φ is a sum over connected graphs G. We remove the vertex 1 from each graph G. What remains is a graph that is in general no longer connected. We decompose this graph into its connected components, and apply the induction hypothesis on each connected component.

Let us focus on the sum over connected graphs G in

$$K_N(x_1) \;=\; 1 + \sum_{n=2}^{N} \frac{1}{(n-1)!} \int \mathrm{d}|\mu|(x_2) \cdots \mathrm{d}|\mu|(x_n) \left| \sum_{G \in \mathcal{G}_c(\mathbb{N}_n)} \prod_{\{i,j\} \in E(G)} \zeta(x_i, x_j) \right| . \tag{A.4}$$

Call G' the graph obtained from G by removing the vertex 1. Decomposing G' into its connected components yields a partition $\{2,\dots,n\} = I_1 \uplus \dots \uplus I_k$, as well as a set of connected graphs $G_1,\dots,G_k$ satisfying $G_l \in \mathcal{G}_c(I_l)$ for $l=1,\dots,k$ and $G' = G_1 \cup \dots \cup G_k$.

The sum over connected graphs G can thus be rewritten as a sum over partitions $I_1 \uplus \dots \uplus I_k = \{2,\dots,n\}$, followed by a sum over connected subgraphs $G_l \in \mathcal{G}_c(I_l)$ within each partition I_l, followed by a sum, for each $l=1,\dots,k$, over nonempty subsets $J_l \subset I_l$ of vertices connected to 1. This gives

$$\sum_{G\in\mathcal{G}_c(\mathbb{N}_n)} \prod_{\{i,j\}\in E(G)} \zeta(x_i,x_j)$$

$$= \sum_{k\geqslant 1} \frac{1}{k!} \sum_{I_1\uplus\dots\uplus I_k=\{2,\dots,n\}} \prod_{l=1}^{k} \Biggl(\sum_{G_l\in\mathcal{G}_c(I_l)} \sum_{\emptyset\neq J_l\subset I_l} \prod_{\{i,j\}\in E(G_l)} \zeta(x_i,x_j) \prod_{i\in J_l} \zeta(x_1,x_i) \Biggr) .$$

Next, note that

$$\sum_{\emptyset\neq J_l\subset I_l} \prod_{i\in J_l} \zeta(x_1,x_i) \;=\; \prod_{i\in I_l} (1+\zeta(x_1,x_i)) - 1 .$$

A repeated application of

$$\prod_{i=1}^{n} (1+\alpha_i) - 1 \;=\; \Biggl(\prod_{i=1}^{n-1} (1+\alpha_i) - 1 \Biggr) (1+\alpha_n) + \alpha_n ,$$

combined with the estimate $|1+\zeta(x_i,x_j)| \leqslant 1$, yields

$$\Biggl| \sum_{\emptyset\neq J_l\subset I_l} \prod_{i\in J_l} \zeta(x_1,x_i) \Biggr| \;\leqslant\; \sum_{i\in I_l} |\zeta(x_1,x_i)| .$$

Therefore,

$$\Biggl| \sum_{G\in\mathcal{G}_c(\mathbb{N}_n)} \prod_{\{i,j\}\in E(G)} \zeta(x_i,x_j) \Biggr|$$

$$\leqslant \sum_{k\geqslant 1} \frac{1}{k!} \sum_{I_1\uplus\dots\uplus I_k=\{2,\dots,n\}} \prod_{l=1}^{k} \Biggl(\Biggl| \sum_{G_l\in\mathcal{G}_c(I_l)} \prod_{\{i,j\}\in E(G_l)} \zeta(x_i,x_j) \Biggr| \sum_{i\in I_l} |\zeta(x_1,x_i)| \Biggr) .$$

$$= \sum_{k\geqslant 1} \frac{1}{k!} \sum_{I_1\uplus\dots\uplus I_k=\{2,\dots,n\}} \prod_{l=1}^{k} \Biggl(\bigl| \varphi((x_i)_{i\in I_l}) \bigr| \sum_{i\in I_l} |\zeta(x_1,x_i)| \Biggr) .$$

Next, recall that there are $\frac{(n-1)!}{m_1!\cdots m_k!}$ partitions $I_1 \uplus \dots \uplus I_k = \{2,\dots,n\}$ such that $|I_l| = m_l$ for $l = 1,\dots k$. Inserting all this into (A.4) and changing variable names yields

$$K_N(x_1) \;\leqslant\; 1 + \sum_{n=2}^{N} \sum_{k\geqslant 1} \frac{1}{k!} \sum_{\substack{m_1,\dots,m_k\geqslant 1 \\ m_1+\dots+m_k=n-1}}$$

$$\times \prod_{l=1}^{k} \Biggl(\frac{1}{m_l!} \int \mathrm{d}|\mu|(y_1)\cdots \mathrm{d}|\mu|(y_{m_l}) \; \bigl|\varphi(y_1,\dots,y_{m_l})\bigr| \sum_{i=1}^{m_l} |\zeta(x_1,y_i)| \Biggr) .$$

Relaxing the constraint on $m_1 + \cdots + m_k \leqslant N-1$ to $m_l \leqslant N-1$ for $l = 1, \ldots, k$ yields

$$\begin{aligned} K_N(x_1) &\leqslant 1 + \sum_{k \geqslant 1} \frac{1}{k!} \prod_{l=1}^{k} \left(\sum_{m=1}^{N-1} \frac{1}{m!} \int \mathrm{d}|\mu|(y_1) \cdots \mathrm{d}|\mu|(y_m) \, \big|\varphi(y_1, \ldots, y_m)\big| \sum_{i=1}^{m} |\zeta(x_1, y_i)| \right) \\ &\leqslant \mathrm{e}^{a(x_1)}, \end{aligned}$$

where in the last step we used the induction assumption $K_{N-1}(x_1) \leqslant \mathrm{e}^{a(x_1)}$ as well as (A.3).

□

Appendix B

Tools from Harmonic Analysis

B.1. Common L^p-inequalities on $\mathbb{R}^d$

Name	Conditions	Statement
Hölder	$0 < p, q, r \leqslant \infty$ $\dfrac{1}{r} = \dfrac{1}{p} + \dfrac{1}{q}$	$\|fg\|_r \leqslant \|f\|_p \|g\|_q$
Interpolation (or log-convexity) of L^p-norms	$0 < p, q, r \leqslant \infty$ $\dfrac{1}{r} = \dfrac{\theta}{p} + \dfrac{1-\theta}{q}, \quad 0 \leqslant \theta \leqslant 1$	$\|f\|_r \leqslant \|f\|_p^\theta \|f\|_q^{1-\theta}$
Young	$1 \leqslant p, q, r \leqslant \infty$ $1 + \dfrac{1}{r} = \dfrac{1}{p} + \dfrac{1}{q}$	$\|f * g\|_r \leqslant \|f\|_p \|g\|_q$
Generalized Young	$1 < p, q, r < \infty$ $1 + \dfrac{1}{r} = \dfrac{1}{p} + \dfrac{1}{q}$	$\|f * g\|_r \leqslant C_{p,q} \|f\|_p \|g\|_{q,w}$
Weak Young	$1 < p, q, r < \infty$ $1 + \dfrac{1}{r} = \dfrac{1}{p} + \dfrac{1}{q}$	$\|f * g\|_{r,w} \leqslant C_{p,q} \|f\|_{p,w} \|g\|_{q,w}$
Hardy-Littlewood-Sobolev	$1 < p, q < \infty, \quad 0 < \lambda < d$ $2 = \dfrac{1}{p} + \dfrac{1}{q} + \dfrac{\lambda}{d}$	$\displaystyle\int \mathrm{d}x\,\mathrm{d}y\, \frac{\|f(x)\|\|g(y)\|}{\|x-y\|^\lambda} \leqslant C_{p,q,d} \|f\|_p \|g\|_q$
Generalized Hardy	$0 \leqslant s < \dfrac{d}{2}$	$\langle f\,, \|x\|^{-2s} f\rangle \leqslant C_{s,d} \langle f\,, (-\Delta)^s f\rangle$

Sobolev embedding	$1 < p < \infty\,, \quad 0 \leqslant s < \dfrac{d}{p}$ $\dfrac{1}{p^*} = \dfrac{1}{p} - \dfrac{s}{d}$	$\|f\|_{p^*} \leqslant C_{p,s,d} \||\nabla|^s f\|_p$

Remarks.

(i) Any condition in the above table that is expressed by an equality is clearly necessary, as can be seen by considering the scaling $f \mapsto R_\lambda f$, where $(R_\lambda f)(x) := f(\lambda x)$.

(ii) Sharp constants are known for many of listed inequalities; see [LL01] for more details. Of particular interest is the sharp constant for the generalized Hardy inequality [Her77],

$$C_{s,d} \;=\; \left(\frac{\Gamma\big((d-2s)/4\big)}{2^s \Gamma\big((d+2s)/4\big)}\right)^2 . \tag{B.1}$$

(iii) The weak L^p space, denoted by L^p_w, is defined for $0 < p < \infty$ as the space of functions f satisfying

$$\|f\|_{p,w}^p \;:=\; \sup_{t>0} t^p |\{|f| > t\}| \;<\; \infty\,, \tag{B.2}$$

where $|\{|f| > t\}|$ denotes the Lebesgue measure of the set of $x \in \mathbb{R}^d$ satisfying $|f(x)| > t$. Note that $\|\cdot\|_{p,w}$ is not a norm (however, as we shall soon see, if $1 < p < \infty$ then $\|\cdot\|_{p,w}$ is equivalent to a norm). The definition of $\|\cdot\|_{p,w}$ implies that $\|R_\lambda f\|_{p,w} = \lambda^{-d/p} \|f\|_{p,w}$, so that $\|\cdot\|_{p,w}$ and $\|\cdot\|_p$ have the same scaling behaviour. The space L^p_w consists of functions whose L^p-norm diverges at most logarithmically. This follows from the "layer cake representation" (a direct consequence of Fubini's theorem)

$$\|f\|_p^p \;=\; \int_0^\infty \mathrm{d}t\; p t^{p-1} |\{|f| > t\}|\,. \tag{B.3}$$

Generally, one has

$$\|f\|_p \;\geqslant\; \|f\|_{p,w}\,,$$

i.e. $L^p \subset L^p_w$. This follows by taking the supremum over t in

$$\|f\|_p^p \;\geqslant\; \int \mathrm{d}x\; |f|^p\, \mathbb{1}_{\{|f|>t\}} \;\geqslant\; t^p\, |\{|f| > t\}|\,.$$

The standard example for $f \in L^p_w \setminus L^p$ is $f(x) = |x|^{-d/p}$.

(iv) The Hardy-Littlewood-Sobolev inequality is an immediate consequence of the generalized Young inequality and the Hölder inequality. Similarly, the Sobolev embedding may be easily derived from the generalized Young inequality. Indeed, note that for $0 < s < d$ we have

$$|\nabla|^{-s} f \;=\; \frac{C_{d,s}}{|x|^{d-s}} * f\,,$$

as the Fourier transform of $|k|^{-s}$ is $C_{d,s}|x|^{s-d}$. The generalized Young inequality yields therefore

$$\||\nabla|^{-s} f\|_{p^*} \;\leqslant\; C_{p,s,d} \|f\|_p\,,$$

with p, p^*, s and d satisfying the conditions of the Sobolev embedding.

(v) An immediate consequence of the log-convexity of L^p-norms and the Sobolev embedding is the *Gagliardo-Nirenberg inequality*. Assume that

$$1 < p \leqslant q < \infty \quad \text{and} \quad 0 \leqslant s < \frac{d}{p}\,.$$

Choose $\theta \in [0,1]$ such that

$$\frac{1}{q} = \frac{1}{p} - \frac{\theta s}{d}\,.$$

Then

$$\|f\|_q \leqslant C_{p,s,d}\,\|f\|_p^{1-\theta}\,\||\nabla|^s f\|_p^\theta \leqslant C_{p,s,d}\left(\|f\|_p + \||\nabla|^s f\|_p\right).$$

In particular, $W^{s,p} \subset L^q$ with continuous injection for all $q \in [p,p^*]$.

B.2. Lorentz spaces and real interpolation

Lorentz spaces are Banach spaces that interpolate between L^p and L^p_w. We refer to [BL76] for a thorough discussion. Recall first from (B.3) that

$$\|f\|_p = p^{1/p}\left(\int_0^\infty \frac{\mathrm{d}t}{t}\,t^p\,|\{|f|>t\}|\right)^{1/p} = p^{1/p}\,\big\|t\,\big|\{|f|>t\}\big|^{1/p}\big\|_{L^p(\mathbb{R}_+,\mathrm{d}t/t)}\,.$$

Similarly, we get from (B.2) that

$$\|f\|_{p,w} = \big\|t\,\big|\{|f|>t\}\big|^{1/p}\big\|_{L^\infty(\mathbb{R}_+,\mathrm{d}t/t)}\,.$$

This motivates the following definition. For $0<p<\infty$ and $0<q\leqslant\infty$ define the *Lorentz space* $L^{p,q}(\mathbb{R}^d,\mathrm{d}x) \equiv L^{p,q}$ through

$$\|f\|_{p,q} := p^{1/q}\,\big\|t\,\big|\{|f|>t\}\big|^{1/p}\big\|_{L^q(\mathbb{R}_+,\mathrm{d}t/t)}\,. \tag{B.4}$$

By definition we have

$$L^{p,p} = L^p\,, \qquad L^{p,\infty} = L^p_w\,. \tag{B.5}$$

Although $\|\cdot\|_{p,q}$ is in general only a quasi-norm (the triangle inequality fails), for $p>1$ it is equivalent to a norm; see Theorem B.2.

Several important properties of L^p-spaces have counterparts for $L^{p,q}$-spaces. In the following we denote by p' the conjugate exponent of p, defined by $1/p' + 1/p = 1$.

Theorem B.1 (Hölder's inequality for Lorentz spaces). *Let $0 < p, p_1, p_2 < \infty$ and $0 < q, q_1, q_2 \leqslant \infty$ satisfy*

$$\frac{1}{p} = \frac{1}{p_1} + \frac{1}{p_2}\,, \qquad \frac{1}{q} = \frac{1}{q_1} + \frac{1}{q_2}\,.$$

Then we have

$$\|fg\|_{p,q} \leqslant C_{p_1,p_2,q_1,q_2}\,\|f\|_{p_1,q_1}\|g\|_{p_2,q_2}\,.$$

Proof. See [O'N63]. ∎

THEOREM B.2 (DUAL CHARACTERIZATION OF $L^{p,q}$). *Let $1 < p < \infty$ and $1 \leqslant q \leqslant \infty$. Then there exist constants $C_1, C_2 > 0$ such that*

$$C_1 \|f\|_{p,q} \leqslant \sup\left\{\left|\int \mathrm{d}x\, fg\right| : \|g\|_{p',q'} \leqslant 1\right\} \leqslant C_2 \|f\|_{p,q}\,.$$

PROOF. See [Tao06]. ☐

In particular, $L^{p,q}$ is a normed space for $1 < p < \infty$. Thus the weak L^p-space is a normed space if $p > 1$.

In order to discuss further results related to the Lorentz spaces, it is useful to introduce the real interpolation method (see [BL76] for details). For $1 \leqslant q \leqslant \infty$ and $0 < \theta < 1$ we define the real interpolation functor $(\cdot,\cdot)_{\theta,q}$ as follows. Let A_0 and A_1 be two Banach spaces contained in some larger topological vector space A. Define the real interpolation norm

$$\|a\|_{(A_0,A_1)_{\theta,q}} := \left\|t^{-\theta} K(t,a)\right\|_{L^q(\mathbb{R}_+,\mathrm{d}t/t)}\,,$$

where

$$K(t,a) := \inf_{a=a_0+a_1} \bigl(\|a_0\|_{A_0} + t\|a_1\|_{A_1}\bigr)\,.$$

Define $(A_0,A_1)_{\theta,q}$ as the space of $a \in A$ such that $\|a\|_{(A_0,A_1)_{\theta,q}} < \infty$. Then $(A_0,A_1)_{\theta,q}$ is a Banach space.

THEOREM B.3 (THE DUAL OF AN INTERPOLATION SPACE). *Let $A_0 \cap A_1$ be dense in A_0 and A_1. Assume that $1 \leqslant q < \infty$ and $0 < \theta < 1$. Then*

$$\bigl(A_0, A_1\bigr)^*_{\theta,q} = \bigl(A_0^*, A_1^*\bigr)_{\theta,q'}\,.$$

PROOF. See [BL76]. ☐

THEOREM B.4 (INTERPOLATION OF LORENTZ SPACES). *Let $0 < p_0, p_1, q_0, q_1, q \leqslant \infty$ and $p_0 \neq p_1$. Write $1/p = (1-\theta)/p_0 + \theta/p_1$, where $0 < \theta < 1$. Then*

$$\bigl(L^{p_0,q_0}, L^{p_1,q_1}\bigr)_{\theta,q} = L^{p,q}\,.$$

PROOF. See [BL76]. ☐

In particular, we get the alternative definition of Lorentz spaces by interpolation:

$$L^{p,q} = (L^{p_0}, L^{p_1})_{\theta,q}\,,$$

where $0 < p_0, p_1 \leqslant \infty$, $p_0 \neq p_1$, and $1/p = (1-\theta)/p_0 + \theta/p_1$ for $0 < \theta < 1$.

THEOREM B.5 (DUAL OF $L^{p,q}$). *Let $1 < p < \infty$ and $1 \leqslant q < \infty$. Then*

$$\bigl(L^{p,q}\bigr)^* = L^{p',q'}\,.$$

PROOF. A simple application of Theorems B.3 and B.4. ☐

Strichartz estimates yield bounds on space-time norms by exploiting the dispersive nature of time evolution. A version suitable for our needs is the following theorem. For $f : \mathbb{R} \to A$, where A is a Banach space, introduce the space-time norm

$$\|f\|_{L^pA} := \bigl\|\|f(t)\|_A\bigr\|_{L^p(\mathbb{R},\mathrm{d}t)}\,.$$

THEOREM B.6. *Let $\sigma > 0$, $\mathcal{H}$ be a Hilbert space and A_0, A_1 be Banach spaces. Suppose that for each time t we have an operator $U(t) : \mathcal{H} \to A_0^*$ satisfying*

$$\begin{aligned} \|U(t)\|_{\mathcal{L}(\mathcal{H};A_0^*)} &\lesssim 1\,, \\ \|U(t)U(s)^*\|_{\mathcal{L}(A_1;A_1^*)} &\lesssim |t-s|^{-\sigma}\,. \end{aligned}$$

Denote by A_θ the interpolation space $(A_0, A_1)_{\theta,2}$, where $0 \leqslant \theta \leqslant 1$. Assume that $2 \leqslant r = \frac{2}{\theta\sigma}$ and $(r, \theta, \sigma) \neq (2, 1, 1)$. Then we have

$$\|U(t)f\|_{L^r A_\theta^*} \lesssim \|f\|_{\mathcal{H}}\,.$$

PROOF. See [KT98]. $\square$

Appendix C

Grönwall-Type Inequalities

In this appendix we collect some Grönwall-type inequalities, which are useful in various situations where one needs to control time-dependent quantities.

Theorem C.1. *Let $\beta(t) \geqslant 0$. If*

$$u(t) \ \leqslant \ \alpha(t) + \int_0^t \beta(s) u(s) \, \mathrm{d}s$$

then

$$u(t) \ \leqslant \ \alpha(t) + \int_0^t \alpha(s)\beta(s) \mathrm{e}^{\int_s^t \beta} \, \mathrm{d}s \ = \ \alpha(0)\, \mathrm{e}^{\int_0^t \beta} + \int_0^t \dot{\alpha}(s)\, \mathrm{e}^{\int_s^t \beta} \, \mathrm{d}s \, .$$

Moreover, if

$$\dot{u}(t) \ \leqslant \ \alpha(t) + \beta(t)\, u(t)$$

then

$$u(t) \ \leqslant \ u(0)\, \mathrm{e}^{\int_0^t \beta} + \int_0^t \alpha(s)\, \mathrm{e}^{\int_s^t \beta} \, \mathrm{d}s \, .$$

Proof. Define

$$v(t) \ := \ \mathrm{e}^{-\int_0^t \beta} \int_0^t \beta(s) u(s) \, \mathrm{d}s \, .$$

Thus

$$\dot{v}(t) \ \leqslant \ \mathrm{e}^{-\int_0^t \beta} \alpha(t) \beta(t) \, .$$

The first claim follows by integration. The rest follows by integration by parts. □

The second statement is a special case of a more general principle.

Theorem C.2. *Let $X \in C^1(\mathbb{R}^2; \mathbb{R})$. Assume that $u(t)$ satisfies*

$$\dot{u}(t) \ \leqslant \ X(u(t), t) \, .$$

Denote by v the solution of

$$\dot{v}(t) \ = \ X(v(t), t) \, , \qquad v(0) = u(0) \, .$$

Then $u(t) \leqslant v(t)$ for t in the common domain of u and v.

PROOF. Note that the assumption on X guarantees that $\dot{v} = X(v,t)$ has a unique local solution. Denote by ϕ^t the solution map on $\mathbb{R}$. Let $a(u,t)$ be defined through $\phi^t(a(u,t)) = u$. By the standard theory of ordinary differential equations, $a \in C^1(\mathbb{R}^2;\mathbb{R})$. Thus, differentiating $a(v(t),t) = v(0)$ yields

$$\partial_u a(v,t)X(v,t) + \partial_t a(v,t) = 0\,.$$

Combining this with the assumption on u, we get

$$\frac{\mathrm{d}}{\mathrm{d}t} a(u(t),t) \;\leqslant\; 0\,,$$

which implies $a(u(t),t) \leqslant a(u(0),0) = a(v(t),t)$. Since the map $u \mapsto a(u,t)$ is clearly monotone increasing (the solutions of an ordinary differential equation do not cross), the claim follows. □

Sometimes the assumption of the previous theorem is too strong. An important example is the differential inequality

$$\dot{u} \;\leqslant\; \sqrt{u}\,, \qquad u(0) \;=\; 0\,. \tag{C.1}$$

One would therefore like to have a Grönwall-type estimate for situations where the local uniqueness of solutions to the corresponding differential equation breaks down. For example, the following theorem yields: (C.1) implies $u(t) \leqslant t^2/4$.

THEOREM C.3. *Let $u \mapsto f_s(u)$ be a continuous, positive, increasing function for each s. If u satisfies*

$$u(t) \;\leqslant\; \alpha(t) + \int_0^t f_s(u(s))\,\mathrm{d}s\,,$$

then

$$u(t) \;\leqslant\; x(t)\,,$$

where $x(t)$ is the largest solution of the equation

$$x(t) \;=\; \alpha(t) + \int_0^t f_s(x(s))\,\mathrm{d}s\,.$$

PROOF. Define the map $u \mapsto \Phi[u]$ through

$$\Phi[u](t) \;:=\; \alpha(t) + \int_0^t f_s(u(s))\,\mathrm{d}s\,.$$

Thus, $u \leqslant \Phi[u]$ and, since f is increasing,

$$\Phi[u](t) \;\leqslant\; \alpha(t) + \int_0^t f_s(\Phi[u](s))\,\mathrm{d}s\,,$$

Thus, the sequence $\Phi^n[u]$ is increasing and hence has a pointwise limit $u_* = \lim_n \Phi^n[u]$ with values in $[0,\infty]$. Also, monotone convergence implies that

$$\Phi[u_*] \;=\; \Phi\Big[\lim_{n\to\infty} \Phi^n[u]\Big] \;=\; \lim_{n\to\infty} \Phi^n\big[\Phi[u]\big] \;=\; u_*\,,$$

i.e. u_* satisfies

$$u_*(t) \;=\; \alpha(t) + \int_0^t f_s(u_*(s))\,\mathrm{d}s\,.$$

The claim follows. □

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