The Quest for Laws and Structure

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Abstract. The purpose of this paper is to illustrate, on some concrete examples, the quest of theoretical physicists for new laws of Nature and for appropriate mathematical structures that enables them to formulate and analyze new laws in as simple terms as possible and to derive consequences therefrom. The examples are taken from thermodynamics, atomism and quantum theory.[1]

Contents

1. Introduction: Laws of Nature and Mathematical Structure

"Truth is ever to be found in the simplicity, and not in the multiplicity and confusion of things." – Isaac Newton

The editor of this book has asked us to contribute texts that can be understood by readers without much formal training in mathematics and the natural sciences. Somewhat against my natural inclinations I have therefore attempted to write an essay that does not contain very many heavy formulae or mathematical derivations that are essential for an understanding of the main message I would like to convey. Actually, the reader can understand essential elements of that message without studying the formulae. I hope that Newton was right and that this little essay is worth my efforts.

Ever since the times of Leucippus (of Miletus, 5th Century BC) and Democritus (of Abdera, Thrace, born around 460 BC) – if not already before – human beings have strived for the discovery of universal laws according to which simple natural processes evolve. Leucippus and Democritus are the originators of the following remarkable ideas about how Nature might work:

[1]One might want to add to the title: "…and for Unification" – but that would oblige us to look farther afield than we can in this essay.

(1) *Atomism* (matter consists of various species of smallest, indivisible building blocks)

(2) *Nature evolves according to eternal Laws* (processes in Nature can be described mathematically, their description being derived from laws of Nature)

(3) *The Law of Causation* (every event is the consequence of some cause)

Atomism is an idea that has only been fully confirmed, empirically, early in the 20th Century. Atomism and Quantum Theory turn out to be Siamese twins, as I will indicate in a little more detail later on. The idea that the evolution of Nature can be described by precise mathematical laws is central to all of modern science. It has been reiterated by different people in different epochs – well known are the sayings of Galileo Galilei [2] and Eugene P. Wigner [3]. The overwhelming success of this idea is quite miraculous; it will be the main theme of this essay. The law of causation has been a fundamental building block of classical physics [4]; but after the advent of quantum theory it is no longer thought to apply to the microcosm.

In modern times, the idea of *universal natural laws* appears in Newton's Law of Universal Gravitation, which says that the trajectories of soccer balls and gun bullets and the motion of the moon around Earth and of the planets around the sun all have the same cause, namely the gravitational force, that is thought to be universal and to be described in the form of a precise mathematical law, Newton's celebrated "$1/r^2$- law". The gravitational force is believed to satisfy the "equivalence principle", which says that, locally, gravitational forces can be removed by passing to an accelerated frame, (i.e., locally one cannot distinguish between the action of a gravitational force and acceleration). This principle played an important role in Einstein's intellectual journey to the General Theory of Relativity, whose 100th anniversary physicists are celebrating this year. Incidentally, the $1/r^2$-law of gravitation explains why a mechanics of point particles, which represents a concrete implementation of the idea of "atoms", is so successful in describing the motion of extended bodies, such as the planets orbiting the sun. The point is that the gravitational attraction emanating from a *spherically symmetric* distribution of matter is *identical* to the force emanating from a point source with the same total mass located at the center of gravity of that distribution. This fact is called *"Newton's theorem"*. It is reported that it took Newton a rather long time to understand and prove it. (I recommend the proof of this beautiful theorem as an exercise to the reader.) Newton's theorem also applies to systems of particles with electrostatic Coulomb interactions. In this context it has played an important role in the construction of thermodynamics for systems of nuclei and electrons presented in [1].

But rather than meditating Newton's law of universal gravitation, I propose to consider the Theory of Heat and meditate the Second Law of Thermodynamics; (see sect. 2, and [2]). This will serve to illustrate the assertion that discovering a Law of Nature is a miracle far deeper and more exciting than cooking up some shaky model that depends on

[2] "Philosophy is written in that great book which ever lies before our eyes – I mean the Universe – but we cannot understand it if we do not first learn the language and grasp the symbols, in which it is written. This book is written in the mathematical language."

[3] "The Unreasonable Effectiveness of Mathematics in the Natural Sciences," in: Communications in Pure and Applied Mathematics, vol. 13, No. I (1960).

[4] "Alle Naturwissenschaft ist auf die Voraussetzung der vollständigen kausalen Verknüpfung jeglichen Geschehens begründet." – Albert Einstein, (talk at Physical Society in Zurich, 1910)

numerous parameters and can be put on a computer, with the purpose to fit an elephant; (a rather dubious activity that has become much too fashionable). Our presentation will also illustrate the claim that discovering and formulating a law of Nature and deriving consequences therefrom can only be achieved once the right mathematical structure has been found within which that law can be formulated precisely and further analyzed. This will also be a key point of our discussion in section 4, which, however, is considerably more abstract and demanding than the one in section 2.

New theories or frameworks in physics can often be viewed as "deformations" of precursor theories/frameworks. This point of view has been proposed and developed in [3] and references given there. As an example, the framework of quantum mechanics can be understood as a deformation of the framework of Hamiltonian mechanics. The Poincaré symmetry of the special theory of relativity can be understood as a deformation of the Galilei symmetry of non-relativistic physics; (conversely, the Galilei group can be obtained as a "contraction" of the Poincaré group). Essential elements of the mathematics needed to understand how to implement such deformations have been developed in [4] and, more recently, in [5]. In section 3, we illustrate this point of view by showing that atomistic theories of matter can be obtained by deformation/quantization of theories treating matter as a continuous medium. This is a relatively recent observation made in [6] – perhaps more an amusing curiosity than a deep insight. It leads to the realization that the Hamiltonian mechanics of systems of identical point particles can be viewed as the quantization of a theory of dust described as a continuous medium (Vlasov theory).

In section 4, we sketch a novel approach (called "*ETH approach*") to the foundations of quantum mechanics. We will only treat non-relativistic quantum mechanics, which is a theory with a globally defined time. (But a relativistic incarnation of our approach appears to be feasible, too.) Most people, including grown-up professors of theoretical physics, appear to have rather confused ideas about a theory of events and experiments in quantum mechanics. Given that quantum mechanics has been created more than ninety years ago and that it may be considered to be the most basic and successful theory of physics, the confusion surrounding its interpretation may be perceived as something of an intellectual scandal. In section 4 we describe ideas that have a chance to lead to progress on the way towards a clear and logically consistent interpretation of quantum mechanics. For those readers who are able to follow our thought process, the presentation in section 4 will show, I hope convincingly, how important the quest for (or search of) an appropriate *mathematical structure* is when one attempts to formulate and then understand and use new theories in physics. It will lead us into territory where the air is rather thin and considerable abstraction cannot be avoided. Clearly, neither the mathematical, nor the physical details of this story, which is subtle and lengthy, can be explained in this essay. But I believe it is sufficiently important to warrant the sketch contained in section 4. Readers not familiar with the standard formulation of basic quantum mechanics and some functional analysis may want to stop reading this essay at the end of section 3.

2. The Second Law of Thermodynamics

"The thermal agency by which a mechanical effect may be obtained is the transference of heat from one body to another at a lower temperature." – Sadi Carnot

Nicolas Léonard Jonel Sadi Carnot was a French engineer who, after a faltering military career, developed an interest in Physics. He was born in 1796 and died young of cholera in 1832. In his only publication, *"Réflexions sur la puissance motrice du feu et sur les machines propres à développer cette puissance"*, of 1824, Carnot presented a very general law governing *heat engines* (and steam locomotives): Let T_1 denote the absolute temperature of the boiler of a steam engine with a time-periodic work cycle, and let $T_2 < T_1$ be the absolute temperature of the environment which the engine is immersed in (coupled to). Carnot argued that the "degree of efficiency", η, of the engine, namely the amount of work, W, delivered by the engine during one work cycle divided by the amount of heat energy, Q, needed during one work cycle to heat the boiler and keep it at its (constant) temperature T_1 is always smaller than or equal to $1 - (T_2/T_1)$, i.e.,

$$\eta := \frac{W}{Q} \leq 1 - \frac{T_2}{T_1}, \tag{1}$$

a quantity always smaller than 1 – so, some of the energy used to heat the boiler is apparently always "wasted", in the sense that it cannot be converted into mechanical work but is released into the environment! Carnot's law can also be read in reverse: Unless the environment, which a heat engine is immersed in, has a temperature strictly smaller than the "internal temperature" of that heat engine (i.e., the temperature of its boiler), it is *impossible* to extract any mechanical work from the engine.

Carnot's law is unbelievably simple and unbelievably interesting, because it is universally applicable and because it has spectacular consequences. For example, it says that one cannot generate mechanical work simply by cooling a heat bath, such as the Atlantic Ocean, at roughly the same temperature as that of the atmosphere. In other words, it is impossible to extract heat energy from a heat bath in thermal equilibrium and convert it into mechanical work without transmitting some part of that heat energy into a heat bath at a *lower* temperature. One says that it is impossible to construct a *"perpetuum mobile"* of the second kind. This is very sad, because if "perpetua mobilia" of the second kind existed we would never face any energy crisis, and the climate catastrophe would not threaten us.

Carnot's discovery gave birth to the theory of heat, *Thermodynamics*, and his law later led to the introduction of a quantity called *Entropy*, which I introduce and discuss below. This quantity is not only fundamental for thermodynamics and statistical mechanics, but, somewhat surprisingly, has come to play a crucial role in information theory and has applications in biology. Scientists have studied it until the present time and keep discovering new aspects and applications of entropy.

Actually, entropy was originally defined and introduced into thermodynamics by *Rudolf Julius Emanuel Clausius*, born Rudolf Gottlieb (1822 – 1888), who was one of the central figures in founding the theory of heat. He realized that the main consequences deduced from the so-called "Carnot cycle" (a mathematical description of the work cycle of a heat engine, alluded to above, leading to the law expressed in Eq. (1)) can also be derived from the following general principle: Consider two macroscopically large heat baths, one at temperature T_1 (the boiler) and the other one (the refrigerator) at temperature $T_2 < T_1$.

Imagine that the two heat baths are connected by a thermal contact (e.g., a copper wire hooked up to the boiler at one end and to the refrigerator at the other end). Then – if there isn't any heat pump connected to the system that consumes mechanical work – *heat energy always flows from the boiler to the refrigerator*. This assertion has become known as the 2^{nd} *Law of Thermodynamics* in the formulation of Clausius.
It led him to discover entropy. Once one understands what entropy is and what properties it has, one can *derive* Clausius' law – at least for sufficiently simple heat baths – in the following precise form: Let $\mathcal{P}_i(t)$ be the amount of heat energy released per second by heat bath/reservoir i at time t, with $i = 1, 2$. Then, for sufficiently simple models of heat baths, one can show that

$$\mathcal{P}_1(t) + \mathcal{P}_2(t) \to 0, \quad \text{as } t \to \infty, \tag{2}$$

and that $\mathcal{P}_1(t)$ has a limit, denoted $\mathcal{P}_\infty$, as time $t \to \infty$. (This last claim is the really difficult one to understand; see [7] and references given there.) The 2^{nd} Law of Thermodynamics in the formulation of Clausius then says that

$$\mathcal{P}_\infty \underbrace{\left(\frac{1}{T_2} - \frac{1}{T_1}\right)}_{>0} \geq 0, \tag{3}$$

i.e., after having waited for a sufficiently long time until the total system has reached a *stationary state*, heat bath 1 (the boiler) releases a *positive* amount of heat energy per second, $\mathcal{P}_\infty > 0$, while heat bath 2 (the refrigerator) absorbs/swallows an *equal* amount of heat energy.

Before I define entropy and present some remarks explaining what Carnot's Law (1) and Clausius' Law (3) have to do with entropy (-production), I would like to draw some *general lessons*. It has become somewhat fashionable among scientists not properly trained in mathematics and physics to try to export physical or chemical laws, such as Carnot's law (1), to other fields; e.g., to the social sciences. So, for example, inspired by Carnot's law, one might speculate that creative activities will be almost entirely absent in a completely just and harmonious society that is in perfect equilibrium, ($W = 0$ if all temperature differences vanish, i.e., $T_1 = T_2$). This might then be advanced as an argument *against* striving for social justice and harmony. One may go on and speculate that Carnot's law explains why the degree of efficiency of society's investment in various human endeavors, such as science, tends to be smaller than right-wing politicians would like it to be. Encouraged by such "insights", one starts to construct models describing the yield of society's investment in science that depend on hundreds of parameters and involve some "non-linear equations". Of course, these models turn out to be too complicated to be studied analytically, but are believed to describe "chaotic behavior". So they are put on a computer, which can produce misleading data if the models really describe chaotic behavior. But, after adjusting sufficiently many of those parameters, the models appear to describe reality, and they are then used to determine the allotment of funding to different groups of researchers. – And so on. Well, let me pause to warn against frivolous transplantations of concepts, such as entropy, non-linear dynamics, chaos, catastrophe theory, etc. from the context that has given rise to them, to entirely different contexts. Without the necessary caution this may lead to bad mistakes! For example, the degree of efficiency of society's investment in science and engineering has been much, much higher than one might reasonably and naïvely expect – Carnot's Law simply does *not* apply here!

I think that, in doing honest and serious science, one should be humble. Heat engines are highly complicated pieces of mechanical engineering. I admire the engineers who were able to see through the intricacies involved in designing such machines. That there is a *universal law* as simple as Carnot's Law (1) that applies to *all* of them should be viewed as a miracle. And, although this law is very, very simple, to *discover* it and *understand* why it applies to *all* heat engines, independently of their mechanical complexity, is a highly non-trivial accomplishment! Carnot's discovery was not published in *'Science'* or *'Nature'*, and his *h-index*[5] equals 1. But the impact of his discovery has been truly enormous. The point I wish to make here is that the discovery of a reliable and universal Law of Nature, even of a very simple one, such as Carnot's, is a miracle that happens only relatively rarely. Physics is concerned with the study of phenomena that are so simple that one may hope to discover precise mathematical laws governing some of these phenomena – and, yet, the discovery of such laws is a rather rare event, and it is advisable not to expect that an interesting one is found every second year.

I now turn to some remarks about *entropy* and how one of its properties enables us to understand the origin of Carnot's and Clausius' laws; (see [8] for more details).
Let us consider a boiler at temperature T_1 and a refrigerator at temperature T_2 connected by a thermal contact. The quantity

$$\mathcal{P}_1(t)/T_1 + \mathcal{P}_2(t)/T_2$$

is an expression for the amount of "entropy production" per second at time t. If entropy production per second has a limit, as $t \to \infty$, then this limit is always *non-negative*! I will try to explain this a little later in this section. If the state of the system consisting of the boiler, the refrigerator and the thermal contact approaches a *stationary state*, as $t \to \infty$[6], then the "heat flows" $\mathcal{P}_i(t), i = 1, 2,$ have limits, as t tends to ∞. Together with the simple fact (2), this implies the 2^{nd} Law in the formulation of Eq. (3)!
Next I turn to Carnot's Law (1). Let $\Delta Q_1^{\nearrow}(n)$ denote the amount of heat energy lost by the boiler of a heat engine, i.e., heat bath 1, in the n^{th} work cycle, and let $\Delta Q_2^{\swarrow}(n)$ be the amount of heat energy absorbed by the refrigerator, heat bath 2, during the n^{th} cycle. By energy conservation, the amount of mechanical work, $W(n)$, produced by the heat engine in the n^{th} cycle is then given by

$$W(n) = \Delta Q_1^{\nearrow}(n) - \Delta Q_2^{\swarrow}(n).$$

It turns out that the *"entropy production"* in the n^{th} cycle is given by

$$\sigma(n) := -\frac{\Delta Q_1^{\nearrow}(n)}{T_1} + \frac{\Delta Q_2^{\swarrow}(n)}{T_2} \tag{4}$$

If the state of the total system, consisting of the boiler 1 and the refrigerator 2 connected to one another by the heat engine, approaches a *time-periodic state*, as $n \to \infty$, then

[5] Definition of the *h-index* – for "Hirsch index": Suppose a scientist has written $n + m$ papers of which n have been quoted (by other people) at least n times, while m have been quoted less than n times. Then the *h-index* of this scientist is $h = n$.

[6] a property that tends to be very difficult to prove and is understood only for rather simple examples; see [7]

the entropy production, $\sigma(n)$, per cycle approaches a *non-negative* limit, σ_∞. Then (4) implies that

$$\eta = \frac{W}{Q} \equiv \lim_{n\to\infty} \frac{W(n)}{\Delta Q_1^{\nearrow}(n)} = \lim_{n\to\infty} \frac{\Delta Q_1^{\nearrow}(n) - \Delta Q_2^{\swarrow}(n)}{\Delta Q_1^{\nearrow}(n)} \leq 1 - \frac{T_2}{T_1} \equiv \eta_{\text{Carnot}}, \tag{5}$$

which is Carnot's law (1).

What is difficult to understand (and is only proven for simple, idealized model systems) is that, in the example considered by Clausius, the state of the total system approaches a stationary state, as time tends to ∞, while in the example of the heat engine considered by Carnot, the state of the total system approaches a time-periodic state, as the number of completed work cycles approaches ∞. In fact, these properties can only be established rigorously for infinitely extended heat baths of a very simple kind [9]; although they are expected to hold in quite general models of heat baths in the thermodynamic limit. Real heat baths are finite, but macroscopically large. Then the laws of Clausius and Carnot are only valid *typically*, i.e., in most cases observed in the lab.

Next, we attempt to explain how entropy is defined in statistical mechanics. This may serve as a first illustration of the importance of the quest for (mathematical) structure in the natural sciences. For fun, and because, in section 4, I will review a few facts about quantum mechanics, I choose to explain this within quantum statistical mechanics. However, the definitions and the reasoning are similar in classical statistical mechanics. Let S be a finitely extended physical system described quantum-mechanically. In standard quantum mechanics, states of S are described by so-called density matrices, ρ, acting on some Hilbert space $\mathcal{H}$. A density matrix ρ is a positive linear operator acting on $\mathcal{H}$ that has a finite trace, i.e.,

$$\text{tr}\,(\rho) := \sum_{n=1}^{\infty} \langle e_n, \rho e_n \rangle < \infty,$$

where $\{e_n\}_{n=1}^{\infty}$ is a complete system of mutually orthogonal unit vectors in $\mathcal{H}$, (i.e., an orthonormal basis in $\mathcal{H}$), $\langle \varphi, \psi \rangle$ is the scalar product of two vectors, φ and ψ, in the Hilbert space $\mathcal{H}$, and $\rho\,\psi$ is the mathematical expression for the vector in $\mathcal{H}$ obtained by applying the linear operator ρ to the vector $\psi \in \mathcal{H}$. In fact, for a density matrix, the trace is normalized to 1,

$$\text{tr}\,(\rho) = 1.$$

So-called *pure states* of S are described by orthogonal projections, P_ψ, onto vectors $\psi \in \mathcal{H}$. (Obviously, such projections are special cases of density matrices.)
The *von Neumann entropy*, $S(\rho)$, of a state ρ of S is defined by [7]

$$S(\rho) := -\,\text{tr}\,(\rho\, \ln\rho) \tag{6}$$

We note that $S(\rho)$ is non-negative, for all density matrices ρ, (because $0 < \rho < \mathbf{1}$), and vanishes if and only if ρ is a pure state. Moreover, it is a concave functional on the space

[7] For a strictly positive operator ρ, the operator $\ln\rho$ is well defined – one can use the so-called spectral theorem for self-adjoint operators to verify this claim.

of density matrices. (Finally, it is subadditive and "strongly subadditive" [10], a deep property with interesting applications in statistical mechanics and (quantum) information theory.) Von Neumann entropy plays an important role in statistical mechanics. However, in many applications, and, in particular, in thermodynamics, another notion of entropy is more important: *relative entropy*! This is a functional that depends on *two* states, ρ_1 and ρ_2, of S. The relative entropy of ρ_1, given ρ_2, is defined by

$$S(\rho_1 \| \rho_2) := \text{ tr } \big(\rho_1(\ln\rho_1 - \ln\rho_2)\big), \tag{7}$$

(assuming that ρ_1 vanishes on all vectors in $\mathcal{H}$ on which ρ_2 vanishes). Relative entropy has the following properties:

(i) Positivity: $S(\rho_1 \| \rho_2) \geq 0$.

(ii) Convexity: $S(\rho_1 \| \rho_2)$ is jointly convex in ρ_1 and ρ_2.

(iii) Monotonicity: Let $\mathcal{T}$ be a trace-preserving, "completely positive" map on the convex set of density matrices on $\mathcal{H}$. Then

$$S\big(\rho_1 \| \rho_2\big) \geq S\big(\mathcal{T}(\rho_1) \| \mathcal{T}(\rho_2)\big).$$

See, e.g., [11] for precise definitions and a proof of property (iii). I don't think that it is important that all readers understand what is being written here. I hope those who don't may now feel motivated to learn a little more about entropy. To get them started, I include an appendix where property (i) – positivity of relative entropy – is derived. I think it is interesting to see how relative entropy and, in particular, the fact that it is *positive* can be applied to understand inequalities (1) (Carnot) and (3) (Clausius).
Let us start with (3). Let ρ_t be the true state at time t of the total system consisting of the two heat baths, 1 and 2, joined by a thermal contact; and let ρ_{eq} denote the state describing perfect thermal equilibrium of the heat baths 1 and 2 at temperatures T_1 and T_2, respectively, *before* they are coupled by a thermal contact; (the state of the thermal contact decoupled from the heat baths is unimportant in this argument). Then a rather straightforward calculation shows that

$$\frac{d}{dt} S(\rho_t \| \rho_{eq}) = \frac{\mathcal{P}_1(t)}{T_1} + \frac{\mathcal{P}_2(t)}{T_2}. \tag{8}$$

Now, if the state ρ_t of the total system approaches a stationary state, ρ_∞, as $t \to \infty$, then the right side of Eq. (8) has a limit, as t tends to ∞, and hence the time derivative, $dS(\rho_t \| \rho_{eq})/dt$, of the relative entropy $S(\rho_t \| \rho_{eq})$ has a limit, denoted σ_∞, as t tends to ∞. Since $S(\rho_t \| \rho_{eq})$ is non-negative, by property (1) above, σ_∞ must be *non-negative*; and this proves inequality (3)!
Next we turn to the proof of (1). Let ρ_n denote the state at the beginning of the n^{th} work cycle of a system consisting of the two heat baths 1 and 2 connected to one another by a heat engine that exhibits a time-periodic work cycle, and let ρ_{eq} be the state of the system with the heat engine removed (meaning that the heat engine is not connected to the heat baths and is in a state of very high temperature), which describes thermal equilibrium of

the heat baths 1 and 2 at temperatures T_1 and T_2, respectively. It is quite simple to show that

$$\sigma(n) := S(\rho_{n+1}\|\rho_{eq}) - S(\rho_n\|\rho_{eq}) = -\frac{\Delta Q_1^{\nearrow}(n)}{T_1} + \frac{\Delta Q_2^{\swarrow}(n)}{T_2}.$$

If the total system approaches a time-periodic state, as $n \to \infty$, then the right side of this equation approaches a well-defined limit, as n tends to ∞, and hence

$$\lim_{n\to\infty} \sigma(n) =: \sigma_\infty$$

exists, too. Since $S(\rho_{n+1}\|\rho_{eq})$ is non-negative, for all $n = 1, 2, 3, \ldots$, by property (1) above, σ_∞ must be non-negative, too. This proves (5)!

Note that, apparently, the difference between the degree of efficiency, η, of a heat engine and the Carnot degree, $\eta_{\text{Carnot}} = 1 - T_2/T_1$, can be expressed in terms of the amount of entropy that is produced per work cycle.

A definition and a few important properties of (relative) entropy can be found in the appendix.

To summarize the message I have intended to convey in this section, let me first repeat my claim that the discovery of precise and universally applicable laws of Nature, such as Carnot's or Clausius' laws, is a miracle that only happens quite rarely. Second, we have just learned on these examples that a deeper understanding of the origin of laws of Nature emerges only once one has found the right mathematical structure within which to formulate and analyze them. In our examples, the key structure is the one of states of physical systems and their time evolution, and of a functional defined on the space of (pairs of) states, namely relative entropy.

3. Atomism and Quantization

"The crucial step was to write down elements in terms of their atoms...I don't know how they could do chemistry beforehand, it didn't make any sense." – Sir Harry Kroto

"Hier (namely in Quantum theory) liegt der Schlüssel der Situation, der Schlüssel nicht nur zur Strahlungstheorie, sondern auch zur molekularen Konstitution der Materie." [8] – Arnold Sommerfeld

Let me recall that, almost 500 years BCE, Leucippus and Democritus proposed the idea that matter is composed of "atoms". Although their idea played an essential role in the birth of modern chemistry – brought forward by John Dalton (1766-1844) and his followers – and in the work of James Clerk Maxwell (1831-1879) on the theory of gases, the existence of atoms was only unambiguously confirmed experimentally at the beginning of the 20^{th} Century by Jean Perrin (1870-1942).[9] From the point of view of the mechanics known to scientists towards the end of the 19^{th} Century, it must have looked

[8] Quantum Theory is the key not only for the theory of radiation but also for an understanding of the atomistic constitution of matter, in: "Das Plancksche Wirkungsquantum und seine allgemeine Bedeutung für die Molekularphysik".

[9] As one finds in Wikipedia: In 1895, Perrin showed that cathode rays were negatively charged. He then determined Avogadro's number by several different methods. He also explained the source of solar energy as

appropriate to describe matter as a *continuous medium* – as originally envisaged for fluid dynamics by Daniel Bernoulli (1700-1782) and Leonhard Euler (1707-1783), the famous mathematicians and mathematical physicists from Basel. The atomistic structure of the Newtonian mechanics of point particles could have appeared as merely an artefact well adapted to Newton's $1/r^2$- law of gravitation, as already mentioned above. The most elegant and versatile formulation of classical mechanics known towards the end of the 19^{th} Century was the one discovered by William Rowan Hamilton (1805-1865). In this formulation, physical quantities pertinent to a mechanical system are described as real-valued continuous functions on a space of pure states, Γ, the so-called "phase space" of the system, thought to be what mathematicians call a "symplectic manifold". The reader does not need to know what symplectic manifolds are. It is enough to believe me that if the space of pure states of a physical system has the structure of a symplectic manifold then the physical quantities of the system (i.e., the real-valued continuous functions on Γ) determine so-called Hamiltonian vector fields, which are generators of one-parameter groups of flows on Γ. As such, they form a Lie algebra: To every pair, F and G, of real-valued, continuously differentiable functions representing two physical quantities of the system one can associate a real-valued continuous function, $\{F, G\}$, the so-called *Poisson bracket* of F and G. If $F = H$ is the Hamilton function of the system whose associated vector field generates the time evolution of the system, and if G is such that $\{H, G\} = 0$ then G is conserved under the time evolution determined by H – one says that G is a "conservation law". Furthermore G gives rise to a flow on Γ that commutes with the time evolution on Γ; i.e., the vector field associated with G generates a one-parameter group of *symmetries* of the system – *connection between symmetries and conservation laws.*
If one starts from a model of matter as a continuous medium and attempts to describe it as an instance of Hamiltonian mechanics one is necessarily led to consider infinite-dimensional Hamiltonian mechanics, or *Hamiltonian field theory*. Examples of Hamiltonian field theories are the *Vlasov theory* of material dust (such as large clusters of stars) often used in astrophysics and cosmology, Euler's description of *incompressible fluids* such as water, and *Maxwell's theory* of the electromagnetic field, including wave optics.

In 1925, *Heisenberg*[10] and, soon after, *Dirac*[11] discovered how one can pass from the classical Hamiltonian mechanics of a fairly general class of physical systems to the *quantum mechanics* of these systems. Their discoveries are paradigmatic examples of the importance of finding the *natural mathematical structure* that enables one to formulate a new law of Nature.
Heisenberg's 1925 paper on quantum-theoretical "Umdeutung" contains the revolutionary idea to associate with each physical quantity of a Hamiltonian mechanical system represented by a real-valued continuous function F on the phase space Γ of the system

thermonuclear reactions of hydrogen.
After Albert Einstein had published his explanation of Brownian motion of a "test particle" as due to collisions with atoms in a liquid, Perrin did experimental work to verify Einstein's predictions, thereby settling a century-long dispute about John Dalton's hypothesis concerning the existence of atoms.

[10] Werner Heisenberg (1901-1976): "Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen", Zeitschrift für Physik **33**(1925), 879 - 893

[11] Paul Adrien Maurice Dirac (1902-1984): "On the Theory of Quantum Mechanics", Proc. Royal Soc. (1926), 661- 677

a "symmetric matrix" (more precisely, a self-adjoint linear operator), $\widehat{F}$, representing the same physical quantity – *but in a quantum-mechanical description of the system!* Since matrix multiplication is non-commutative, two operators, $\widehat{F}$ and $\widehat{G}$, representing physical quantities of a quantum-mechanical system do generally *not* commute with one another. Dirac then recognized that one should replace the Poisson bracket, $\{F, G\}$, of two functions on phase space by $\frac{i}{\hbar}\times$ the *commutator*, $[\widehat{F}, \widehat{G}]$, of the corresponding matrices, where $\hbar$ is Planck's constant. Thus, the Heisenberg-Dirac recipe for the "quantization" of a Hamiltonian system reads as follows:

$$\begin{aligned} F \text{ (real function on } \Gamma) &\quad\mapsto\quad \widehat{F} \text{ (self-adjoint linear operator)} \\ \{F, G\} \text{ (Poisson bracket)} &\quad\mapsto\quad \frac{i}{\hbar}[\widehat{F}, \widehat{G}] \text{ (commutator)} \end{aligned} \tag{9}$$

Remarks:

- The commutator, $[A, B]$, between two matrices or linear operators A and B is defined by
$$[A, B] := A \cdot B - B \cdot A.$$
- Planck's constant $\hbar$ is sometimes replaced by another so-called "deformation parameter", such as Newton's constant G_N, or some other "coupling constant", etc.
- The operators $\widehat{F}$ are usually thought to act on a separable Hilbert space $\mathcal{H}$.

The map
$$\widehat{\ } : F \mapsto \widehat{F}$$
is *not* an algebra homomorphism, because the real-valued continuous functions on Γ form an abelian (commutative) algebra under point-wise multiplication, whereas matrix multiplication is *non-commutative*; moreover, the product, $\widehat{F} \cdot \widehat{G}$, of two self-adjoint operators, $\widehat{F}$ and $\widehat{G}$, is not a self-adjoint operator, unless the operators $\widehat{F}$ and $\widehat{G}$ commute.
Let me briefly digress into somewhat more technical territory. Readers not familiar with the notions discussed in the following paragraph are advised to pass to Eq. (13). For the purposes of a general discussion, one can always assume that the functions F on Γ are bounded and that the operators $\widehat{F}$ are bounded operators on $\mathcal{H}$. In the analysis of systems with infinitely many degrees of freedom, such as the electromagnetic field, it is actually convenient to use a more abstract formulation, interpreting the operators $\widehat{F}$ as elements of a C^*- algebra, $\mathcal{C}$, that plays the role, in quantum mechanics, that the algebra, $C(\Gamma)$, of bounded continuous functions on phase space Γ plays in classical mechanics.

In classical mechanics, *states* are given by probability measures on phase space Γ. This is equivalent to saying that states are given by positive normalized linear functionals on the algebra $C(\Gamma)$ of continuous functions on Γ. This definition of states can immediately be carried over to quantum mechanics: A state of a quantum system whose physical quantities are represented by the self-adjoint operators in a C^*- algebra $\mathcal{C}$ is a positive normalized linear functional on $\mathcal{C}$.
Definition: A positive normalized linear functional, ρ, on a C^*- algebra $\mathcal{A}$ containing an

identity element $\mathbf{1}$,[12] (for example, $\mathcal{A} = C(\Gamma)$, where Γ is a compact topological space, or $\mathcal{A} = \mathcal{C}$), is a $\mathbb{C}$- linear map,

$$\rho : \mathcal{A} \ni X \mapsto \rho(X) \in \mathbb{C}, \tag{10}$$

with the properties that

$$\rho(X) \geq 0, \text{ for every positive operator } X \in \mathcal{A}, \quad \rho(\mathbf{1}) = 1. \tag{11}$$

So-called *pure states* on $\mathcal{A}$ are states that cannot be written as convex combinations of at least two distinct states. In the example where $\mathcal{A} = C(\Gamma)$, a pure state is a Dirac delta function on a point of Γ. This means that pure states of a Hamiltonian mechanical system can be identified with points in phase space Γ (and, hence, the space of pure states of such a system does usually not have any relationship to a linear space, as would be the case in standard quantum mechanics).
From a pair, $(\mathcal{A}, \rho)$, of a C^*- algebra $\mathcal{A}$ and a state ρ on $\mathcal{A}$ one can always reconstruct a Hilbert space, $\mathcal{H}_\rho$, and a representation, π_ρ, of $\mathcal{A}$ on $\mathcal{H}_\rho$. This is the contents of the so-called Gel'fand-Naimark-Segal construction. (See, e.g., [12] for definitions, basic results and proofs.)
We recall that if the operators $\widehat{F}$ and $\widehat{G}$ representing two physical quantities of some system do not commute then they cannot be measured simultaneously: If the system is prepared in a state ρ the uncertainties, $\Delta_\rho \widehat{F}$ and $\Delta_\rho \widehat{G}$, in a simultaneous measurement of the quantities represented by the operators $\widehat{F}$ and $\widehat{G}$ satisfy the celebrated Heisenberg Uncertainty Relation

$$\Delta_\rho \widehat{F} \cdot \Delta_\rho \widehat{G} \geq \frac{1}{2} |\rho([\widehat{F}, \widehat{G}])|. \tag{12}$$

As a special case we mention that if x denotes the position of a particle moving on the real line $\mathbb{R}$ and p denotes its momentum then

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}, \tag{13}$$

in an arbitrary state of the system.

The Heisenberg-Dirac recipe expressed in Eq. (9) can be applied to *Vlasov theory* [13] and *Maxwell's theory* [14] , and to many other interesting examples of Hamiltonian systems or Hamiltonian field theories. In these examples, atomism always arises as a consequence of quantization.
In the following, I propose to sketch the example of Vlasov theory. This is a theory describing the mechanics of (star) dust viewed as a continuous material medium. A state of dust at time t is described by the density, $f_t(x, v)$, of dust with velocity $v \in \mathbb{R}^3$ observed at the point x in physical space $\mathbb{E}^3$. Clearly $f_t(x, v)$ is non-negative, and

$$\int d^3x \int d^3v \; f_t(x, v) = \nu,$$

[12] this will always be assumed in what follows
[13] first proposed by *Anatoly Alexandrovich Vlasov* (1908 – 1975) in 1938.
[14] named after the eminent Scottish mathematical physicist *James Clerk Maxwell* (1831 – 1879)

where ν is the number of moles of dust. This quantity is conserved, i.e., independent of time t. The density of dust at the point $x \in \mathbb{E}^3$ at time t is given by

$$n_t(x) := \int d^3v \; f_t(x,v).$$

The equation of motion of the state f_t is given by the so-called Vlasov (collision-free Boltzmann) equation:

$$\frac{\partial}{\partial t} f_t(x,v) + v \cdot \nabla_x f_t(x,v) - \nabla V_{\text{eff}}[f_t](x) \cdot \nabla_v f_t(x,v) = 0, \tag{14}$$

where

$$V_{\text{eff}}[f_t](x) := V(x) + \int d^3y \; \phi(x-y) \; n_t(y). \tag{15}$$

In this expression, $V(x)$ is the potential of an external force acting on the dust at the point $x \in \mathbb{E}^3$, $\phi(x-y)$ is a two-body potential describing the force between dust at point x and dust at point y in physical space.

In the following, I sketch how Vlasov theory can be *quantized* by applying the Heisenberg-Dirac recipe. Since my exposition is somewhat more technical than the rest of this essay, I want to disclose what the result of this exercise is: *The quantization of Vlasov theory is nothing but the Newtonian mechanics of an arbitrary number of identical point particles moving in physical space under the influence of an external force with potential given by the function V and interacting with each other through two-body forces whose potential is given by $N^{-1}\phi$, where N^{-1} is a "deformation parameter" that plays the role of Planck's constant $\hbar$ in the Heisenberg-Dirac recipe.* – Readers not familiar with infinite-dimensional Hamiltonian systems or not very interested in mathematical considerations are encouraged to proceed to the material after Eq. (33).

Since $f_t(x,v) \geq 0$, it can be written as a product (factorized)

$$f_t(x,v) = \overline{\alpha_t(x,v)} \cdot \alpha_t(x,v), \tag{16}$$

where $\alpha_t(x,v)$ is a complex-valued function of (x,v), with

$$|\alpha_t(x,v)| = \sqrt{f_t(x,v)}.$$

Clearly, the phase, $\alpha_t/|\alpha_t|$, of α_t is *not* observable. Perhaps surprisingly, it appears to be a good idea to encode the time evolution of the density f_t into a dynamical law for α_t. Here is how this can be done: Let $\Gamma_1 := \mathbb{E}^3 \times \mathbb{R}^3$ denote the "one-particle phase space" of pairs, (x,v), of points in physical space and velocities. By $\Gamma_\infty := H^1(\Gamma_1)$ we denote the complex Sobolev space of index 1 over Γ_1. This space can be interpreted as an ∞- dimensional affine phase space. Functions $\alpha \in \Gamma_\infty$ and their complex conjugates, $\overline{\alpha}$, serve as complex coordinates for Γ_∞. The symplectic structure of Γ_∞ can be encoded into the Poisson brackets:

$$\begin{aligned} \{\alpha(x,v), \alpha(x',v')\} &= \{\overline{\alpha}(x,v), \overline{\alpha}(x',v')\} = 0, \\ \{\alpha(x,v), \overline{\alpha}(x',v')\} &= -i\delta(x-x')\delta(v-v'). \end{aligned} \tag{17}$$

We introduce a Hamilton functional on Γ_∞:

$$\mathcal{H}(\overline{\alpha},\alpha) := i\int\int d^3x d^3v\, \overline{\alpha}(x,v)[v\cdot\nabla_x - (\nabla V)(x)\cdot\nabla_v]\alpha(x,v) \tag{18}$$
$$-\frac{i}{2}\int\int d^3x d^3v\, \overline{\alpha}(x,v)\Big(\nabla_x \int\int d^3x' d^3v'\; \phi(x-x')|\alpha(x',v')|^2\Big)\cdot\nabla_v\alpha(x,v).$$

Hamilton's equations of motion are given by

$$\dot{\alpha}_t(x,v) = \{\mathcal{H},\alpha_t(x,v)\}, \quad \dot{\overline{\alpha}}_t(x,v) = \{\mathcal{H},\overline{\alpha}_t(x,v)\}. \tag{19}$$

It is a straightforward exercise [6] to show that these equations imply the Vlasov equation for the density $f_t(x,v) = |\alpha_t(x,v)|^2$.
Note that this theory has a huge group of local symmetry transformations: The "gauge transformations"

$$\alpha_t(x,v) \mapsto \alpha_t(x,v)\; e^{i\theta_t(x,v)} \tag{20}$$

where the phase $\theta_t(x,v)$ is an arbitrary real-valued, smooth function on Γ_1, are symmetries of the theory. The global gauge transformation obtained by setting $\theta_t(x,v) =: \theta \in \mathbb{R}$ form a continuous group of symmetries, $\simeq U(1)$, that gives rise to a conservation law,

$$\|\alpha_t\|_2^2 = \int d^3x \int d^3v\; f_t(x,v) = \text{ const. in time } t, \tag{21}$$

in accordance with *Noether's theorem*.

Next, we propose to quantize Vlasov theory by applying the Heisenberg-Dirac recipe (9) to the variables $\alpha,\overline{\alpha}$; i.e., we replace α and $\overline{\alpha}$ by operators,

$$\alpha \mapsto \widehat{\alpha} =: a, \qquad \overline{\alpha} \mapsto \widehat{\overline{\alpha}} =: a^*, \tag{22}$$

and trade the poisson brackets in (17) for commutators:

$$[a(x,v), a(x',v')] = [a^*(x,v), a^*(x',v')] = 0,$$

and

$$[a(x,v), a^*(x',v')] = N^{-1}\cdot\delta(x-x')\;\delta(v-v'), \tag{23}$$

where the dimensionless number $N\nu$ is proportional to the number of "atoms" present in the system; i.e., the role of Planck's constant $\hbar$ is played by N^{-1}. The creation- and annihilation operators, a^* and a, act on Fock space, $\mathcal{F}$:

$$\mathcal{F} := \oplus_{n=0}^{\infty}\mathcal{F}^n, \tag{24}$$

where

$$\mathcal{F}^0 := \mathbb{C}|0\rangle, \quad \text{with } a(x,v)|0\rangle = 0, \forall x,v,$$

and

$$\mathcal{F}^n := \Big\langle \int\cdots\int \varphi_n(x_1,v_1,...,x_n,v_n)\prod_{i=1}^{n} a^*(x_i,v_i)d^3x_i d^3v_i|0\rangle\Big\rangle, \tag{25}$$

where $\langle \cdot \rangle$ indicates that the (linear) span is taken.
The physical interpretation of the "n-particle wave functions" φ_n is that

$$f_n(x_1, v_1, ..., x_n, v_n) := |\varphi_n(x_1, v_1, ..., x_n, v_n)|^2 \tag{26}$$

is the state density on n-particle phase space

$$\Gamma_n := \Gamma_1^{\times n}$$

for n identical classical particles moving in physical space. (The state of the system is obtained by multiplying the densities f_n by the Liouville measures $\prod_{i=1}^n d^3x_i d^3v_i$.)

The "Hamilton operator" generating the dynamical evolution of the states of the quantized theory is obtained by replacing the functions $\overline{\alpha}$ and α in the Hamilton functional $\mathcal{H}(\overline{\alpha}, \alpha)$ introduced in (18) by the operators a^* and a, respectively, and writing all creation operators a^* to the left of all annihilation operators a; ("Wick ordering"). The time-dependent Schrödinger equation for the evolution of vectors in $\mathcal{F}$ then implies the Liouville equations for the densities defined in (26),

$$\dot{f}_t(x_1, v_1, ..., x_n, v_n) = -\sum_{i=1}^{n} \Big(v_i \cdot \nabla_{x_i} + F(X_i) \cdot \nabla_{v_i}\Big) f_t(x_1, v_1, ...x_n, v_n), \tag{27}$$

where

$$F(x_i) := -\nabla_{x_i}\Big(V(x_i) + N^{-1}\sum_{j\neq i}\phi(x_i - x_j)\Big)$$

is the total force acting on the i^{th} particle, which is equal to the external force, $-(\nabla V)(x_i)$, plus the sum of the forces exerted on particle i by the other particles in the system; the strength of the interaction between two particles being proportional to N^{-1}. The equations (27) are equivalent to Newton's equations of motion for n identical particles with two-body interactions moving in physical space, (which are Hamiltonian equations of motion).

"Observables" of this theory are operators on Fock space $\mathcal{F}$ that are invariant under the symmetry transformations given by

$$a(x, v) \mapsto a(x, v)\, e^{i\theta_t(x,v)}, \quad a^*(x, v) \mapsto a^*(x, v)\, e^{-i\theta_t(x,v)}, \tag{28}$$

corresponding to the symmetries (20); (they are the elements of an infinite-dimensional group of local gauge transformations). These symmetries imply that the particle number operator

$$\widehat{\mathcal{N}} := \int \mathrm{d}^3x \int \mathrm{d}^3v\; a^*(x, v)\; a(x, v)$$

is conserved under the time evolution, and that (in the absence of an affine connection that gives rise to a non-trivial notion of parallel transport of "wave functions", φ_n) the observables of the theory are described by operators that are functionals of the densities $a^*(x, v)\; a(x, v)$. These operators generate an *abelian* (i.e., commutative) algebra. Together with the equations of motion (27), this means that the structure of observables and the predictions of this "quantum theory" are *classical*, in the sense that all observables can be diagonalized simultaneously and hence have objective values, and the time evolution of the system is *deterministic*. In fact, this theory is just a reformulation of the Newtonian mechanics of systems of arbitrarily many identical non-relativistic particles moving in physical space $\mathbb{E}^3$ under the influence of an external potential force and interacting with each other through two-body potential forces.

Thus, what we have sketched here is the perhaps somewhat remarkable observation (see [6], and references given there) that the classical Newtonian mechanics of the particle systems studied above, which treats matter as *atomistic*, can be viewed as the quantization of Vlasov theory, which treats matter as a *continuous medium* of dust. Conversely, Vlasov theory can be viewed as the "classical limit" of the Newtonian mechanics of systems of $\mathcal{O}(N)$ identical particles with two-body interactions of strength $\propto N^{-1}$, which is reached when $N \to \infty$. This has been shown (using different concepts) in [13]. Apparently, the parameter N^{-1} plays the role of Planck's constant $\hbar$.

To express these findings in words, it appears that a mechanics taking into account the atomistic structure of matter arises as the result of quantization of a mechanics that treats matter as a continuous medium.

Mathematical digression on "pre-quantization" of the one-particle phase space and on the passage to the quantum theory of systems of an arbitrary number of identical non-relativistic particles (bosons) with two-body interactions

Obviously the one-particle phase space Γ_1 carries a symplectic structure given by the symplectic 2-form

$$\omega := \mathrm{d}\, x \wedge \mathrm{d}\, v.$$

One-particle "wave functions", $\alpha(x, v)$, can be viewed as section of a complex line bundle over Γ_1 associated to a principal $U(1)$- bundle. We equip this bundle with a connection, $A = A_x\, \mathrm{d}x + A_v\, \mathrm{d}v$, (i.e., a gauge field, namely a mathematical object analogous to the well known vector potential in electrodynamics), whose curvature, i.e., the field tensor associated with A, is given by

$$\mathrm{d}\, A = \omega.$$

In these formulae, $\mathrm{d}x$ and $\mathrm{d}v$ are differentials, and "d" denotes exterior differentiation. The connection A introduces a notion of parallel transport on the line bundle of "wave functions" α. The symmetries (20) can then always be obeyed by replacing ordinary partial derivatives by *covariant* derivatives, i.e.,

$$(\nabla_x, \nabla_v) \mapsto (\nabla_x - iA_x, \nabla_v - iA_v),$$

and products

$$\overline{\alpha}(x, v)\, \alpha(x, v) \mapsto \overline{\alpha}(x, v) U_\gamma(A) \alpha(x', v'), \tag{29}$$

where $U_\gamma(A)$ is a complex phase factor describing parallel transport along a path γ from the point $(x', v') \in \Gamma_1$ to the point $(x, v) \in \Gamma_1$. These replacements lead us to the theory of "pre-quantization" of one-particle mechanics formulated over the one-particle phase space Γ_1. By applying the Heisenberg-Dirac recipe (22), (23) and then using the connection A to define parallel transport of creation- and annihilation operators, a^*, a, and n-particle wave functions φ_n, we arrive at what is called "pre-quantization" of the mechanics of arbitrary n-particle systems.

In principle, the introduction of a connection A on the line bundle of one-particle "wave functions" α would allow one to consider vast generalizations of Vlasov dynamics, based on using (29), and, subsequently, of the quantized theory resulting from the replacements (22), (23). Some of these generalizations could be understood as Vlasov theories on a "non-commutative phase space", namely the non-commutative phase space obtained by applying the Heisenberg-Dirac recipe (9) to the Poisson brackets

$$\{x^i, x^j\} = 0 = \{p_i, p_j\},$$

and

$$\{x^i, p_j\} = -\delta^i_j, \qquad i, j = 1, 2, 3.$$

This leads us to the question whether standard quantum mechanics of systems of arbitrarily many identical non-relativistic particles could be rediscovered by appropriately extending the ideas discussed so far. One approach to answering this question is to pass from pre-quantization, as sketched above, to genuine quantization by following the recipes of geometric quantization, à la Kostant and Souriau; see, e.g., [14]. (An alternative is to consider "deformation quantization", see [15], which, however, is usually inadequate to deal with concrete problems of physics.) We cannot go into explaining how this is done, as this would take us too far away from our main theme. Instead, we return to Vlasov theory, whose states are represented by densities $f(x, v)$ on one-particle phase space Γ_1. We propose to replace the factorization (16) of $f(x, v)$ by the Wigner factorization

$$f_\hbar(x, v) = \frac{1}{(2\pi)^3} \int e^{-iv\cdot y} \overline{\psi}(x - \frac{\hbar y}{2})\, \psi(x + \frac{\hbar y}{2})\, \mathrm{d}^3 y, \tag{30}$$

where the "Schrödinger wave function" ψ is an arbitrary function in $L^2(\mathbb{R}^3)$. Assuming that the time-dependent Schrödinger wave function ψ_t solves the so-called *Hartree equation*

$$i\hbar \partial_t \psi_t = \big(-\frac{\hbar^2}{2} \Delta + V + |\psi_t|^2 * \phi \big) \psi_t \tag{31}$$

one finds that $f_{\hbar,t}$ solves the Vlasov equation in the limit where $\hbar$ tends to 0.
To understand and prove this claim it is advisable to interpret $f_\hbar(x, v)$ as the Wigner transform of a general one-particle density matrix, ρ, i.e.,

$$f_\hbar(x, v) = \frac{1}{(2\pi)^3} \int e^{-ivy} \rho(x - \frac{\hbar y}{2}, x + \frac{\hbar y}{2})\, \mathrm{d}^3 y.$$

Expression (30) is the special case where $\rho(x, y) = \overline{\psi}(x)\psi(y)$ is the pure state corresponding to the wave function ψ. The equation of motion for the density $f_\hbar$ is derived from the Liouville-von Neumann equation of motion for the density matrix ρ,

$$\hbar \dot{\rho} = -i[H_{\text{eff}}, \rho] \tag{32}$$

corresponding to the effective Hamiltonian

$$H_{\text{eff}} := -\frac{\hbar^2}{2} \Delta + V + n * \phi, \tag{33}$$

where $n(x) = \rho(x,x) = \int f_\hbar(x,v)\,\mathrm{d}^3v$ is the particle density, and $(n * \phi)(x) := \int n(y)\phi(x-y)\,\mathrm{d}^3y$. It is then not hard to see that, formally, the Liouville-von Neumann equation of motion (32), with H_{eff} as in (33), implies the Vlasov equation for $f_\hbar$, as $\hbar$ approaches 0.

The Hartree equation (31) for the Schrödinger wave function ψ turns out to be a Hamiltonian evolution equation on an infinite-dimensional phase space $\hat{\Gamma}_\infty$ with complex coordinates given by the Schrödinger wave functions ψ and their complex conjugates $\overline{\psi}$. Applying the Heisenberg-Dirac recipe to quantize Hartree theory (with the same deformation parameter, N^{-1}, as in Vlasov theory), one arrives at the theory of gases of non-relativistic Bose atoms moving in an external potential landscape described by the potential V and with two-body interactions given by the potential $N^{-1}\phi$. This is an example of a quantum-mechanical many-body theory. In the limiting regime where $N \to \infty$, i.e., in the so-called mean-field (or classical) limit, one recovers Hartree theory. Details of this story can be found in [6].

Vlasov theory has many interesting applications in cosmology and in plasma physics. As an example I mention the rather subtle analysis of Landau damping in plasmas presented in [16]. Hartree theory is often used to describe Bose gases in the limiting regime of high density and very weak two-body interactions, corresponding to $N \to \infty$. Another, somewhat more subtle limiting regime (low density, strong interactions of very short range) is the Gross-Pitaevskii limit considered in [17]. Hartree theory with smooth, attractive two-body interactions of short range features solitary-wave solutions. In a regime where the two-body interactions are strong, the dynamics of multi-soliton configurations is well approximated by the Newtonian mechanics of point particles of varying mass moving in an external potential V and with two-body interactions $\propto \phi$. However, whenever the motion of the solitons is not inertial they experience friction. This has been discussed in some detail in [18]. This observation may have interesting application in cosmology, as first suggested in [19].

To conclude this section, we mention that the atomistic nature of the electromagnetic field, which becomes manifest in the quanta of light or photons, can be understood by applying the Heisenberg-Dirac recipe to Maxwell's classical theory of the electromagnetic field (the deformation parameter being Planck's constant $\hbar$). Historically, this was the first example of a quantum theory. Its contours became visible in Planck's law of black-body radiation and Einstein's discovery of the quanta of radiation, the photons.

4. The structure of Quantum Theory

"... Thus, the fixed pressure of natural causality disappears and there remains, irrespective of the validity of the natural laws, space for autonomous and causally absolutely independent decisions; I consider the elementary quanta of matter to be the place of these 'decisions'." – Hermann Weyl, 1920.

In section 3, we have seen that the *atomistic constitution* of matter may be understood as resulting from Heisenberg-Dirac *quantization* of a "classical" Hamiltonian theory that treats matter as a *continuous medium*, such as Vlasov theory. In the following, we propose to sketch some fundamental features of quantum mechanics proper. It turns out that the deeply puzzling features of quantum mechanics arise from the *non-commutativity* of the algebra generated by the linear operators that represent physical quantities/properties characterizing a physical system. This non-commutativity turns out to be intimately related to the atomistic constitution of matter! In a sense, Hartree theory *is* a quantum theory – Planck's constant $\hbar$ appears explicitly in the Hartree equation that describes the time evolution of physical quantities of the theory. Hartree theory describes matter (more precisely interacting quantum gases) as a continuous medium. As a result, the algebra of physical quantities of this theory is *abelian* (commutative). When it is quantized according to the Heisenberg-Dirac recipe– as indicated in section 3 – one arrives at a theory (namely non-relativistic quantum-mechanical many-body theory) providing an atomistic description of matter, and the algebra of operators representing physical quantities becomes *non-commutative*.

The purpose of this section is to sketch some general features of *non-relativistic quantum mechanics* related to its probabilistic nature and its fundamental irreversibility. Our analysis is intended to apply to a large class of physical systems; and it is based on the assumption that the linear operators providing a quantum-mechanical description of physical quantities and events of a typical physical system, S, generate a *non-abelian* (non-commutative) algebra. An example of an important consequence of this assumption is the phenomenon of *entanglement* (see below), which does *not* appear in classical physics.

In classical physics, the operators representing physical quantities always generate an *abelian* (commutative) algebra, $\mathcal{E}^c$, over the complex numbers invariant under taking the adjoint of operators and closed in the operator norm. By a theorem due to I. M. Gel'fand (see, e.g., [12]), such an algebra is isomorphic to the algebra of complex-valued continuous functions over a compact topological (Hausdorff) space, Γ,[15] i.e.,

$$\mathcal{E}^c \simeq C(\Gamma). \tag{34}$$

The operator norm, $\|F\|$, of an element $F \in \mathcal{E}^c$ is the sup norm of the function on Γ corresponding to F, which we also denote by F. The physical quantities of the system are described by the *real-valued* continuous functions on Γ, which are the self-adjoint elements of $\mathcal{E}^c$. *States* of the system are given by probability measures on Γ; *pure* states correspond to atomic measures, i.e., Dirac δ- functions, supported on points, ξ, of Γ. Thus, the pure states are "characters" of the algebra $\mathcal{E}^c$, i.e., positive, normalized linear functionals, δ_ξ, with the property that

$$\delta_\xi(F \cdot G) = \delta_\xi(F) \cdot \delta_\xi(G).$$

Passing to a subsystem of the system described by the algebra $\mathcal{E}^c$ amounts to selecting some *subalgebra*, $\mathcal{E}^c_0$, of the algebra $\mathcal{E}^c$ invariant under taking adjoints and closed in the operator norm. Characters of $\mathcal{E}^c$ obviously determine characters of $\mathcal{E}^c_0$; i.e., *pure states of the system remain pure when one passes to a subsystem.* This implies that the phenomenon of entanglement is completely absent in classical physics.

[15] of course, Γ is usually *not* a symplectic manifold – it is symplectic, i.e., a "phase space", only if the system is Hamiltonian

Time evolution of physical quantities from time s to time t is described by *automorphisms, $\tau_{t,s}$, of $\mathcal{E}^c$, which form a one-parameter groupoid. This may sound curiously abstract. But it turns out that any such groupoid is described by flow maps,

$$\gamma_{t,s} : \Gamma \to \Gamma, \qquad \Gamma \ni \xi(s) \mapsto \xi(t) = \gamma_{t,s}(\xi(s)) \in \Gamma.$$

Under fairly general hypotheses on the properties of the maps $\gamma_{t,s}$ they are generated by (generally time-dependent) vector fields, X_t, on Γ; i.e., the trajectory $\xi(t) := \gamma_{t,s}(\xi)$ of a point $\xi \in \Gamma$ is the solution of a differential equation,

$$\dot{\xi}(t) = X_t\big(\xi(t)\big), \qquad \text{with } \xi(s) = \xi \in \Gamma.$$

These properties of time evolution are preserved when one passes from the description of a physical system to the one of a subsystem. Since all this may sound too abstract and quite incomprehensible, I summarize the main features of classical physics in words:

(A) The physical quantities of a classical system are represented by self-adjoint operators that all commute with one another. They correspond to the bounded, real-valued, continuous functions on a "state space" Γ.

(B) Pure states of the system can be identified with points in its state space Γ.

(C) *All* physical quantities have objective and unique values in every pure state of the system. Conversely, the values of all physical quantities of a system usually determine its state uniquely. Thus, pure states have an "ontological meaning": They contain complete information on all properties of the system at a given instant of time.

(D) Mixed states are given by probability measures on Γ. Probabilities associated with such mixed states are expressions of ignorance, i.e., of a lack of complete knowledge of the true state of the system at a given instant of time.[16]

(E) Time evolution of physical quantities and states is completely determined by flow maps, $\gamma_{t,s}$, from the state space Γ to itself specifying which pure states, $\xi(t)$, at time t correspond to initial states, $\xi(s)$, chosen at time s. Thus, the "Law of Causation" holds (as formulated originally by Leucippus and Democritus), and there is perfect determinism; (disregarding from the possibly huge problems of computation of dynamics for chaotic systems).

(F) All these properties of a classical description of physical systems are preserved upon passing to the description of a subsystem (that may interact strongly with its complement).

[16]One should add that, pragmatically, mixed states play an enormously important role in that they often enable us to make concrete predictions on quantities that are defined as time-averages along trajectories of true states of which one expects that they are identical to ensemble averages. Often, only the ensemble averages are accessible to concrete calculations, using measures describing certain mixed states, such as thermal equilibrium states, while time-averages along trajectories of true states remain inaccessible to quantitative evaluation.

Well, for better of worse, *these wonderful features of classical physics all disappear when one passes to a quantum-mechanical description of reality*! One of the first problems one encounters when one analyzes general features of a quantum-mechanical description of reality is that one does not know how to describe the time evolution of physical quantities of a system unless that system has interactions with the rest of the universe that are so tiny that they can be neglected over long stretches of time. Such a system is called "*isolated*". In this section, we limit our discussion to isolated systems; (but see, e.g., [20, 21].)

Here is a *pedestrian definition of an isolated physical system* – according to quantum mechanics:
Let S be an isolated physical system that we wish to describe quantum-mechanically.

(1) The physical quantities/properties of S are represented by bounded self-adjoint operators. They generate a C^*- algebra $\mathcal{E}$, i.e., an algebra of operators invariant under taking adjoints and closed in an operator norm with certain properties; (see, e.g., [12]). For simplicity, we suppose that the spectra of all the operators corresponding to physical quantities of S are finite point spectra. Then every such operator $A = A^*$ has a spectral decomposition,

$$A = \sum_{\alpha \in \sigma(A)} \alpha \, \Pi_\alpha, \tag{35}$$

where $\sigma(A)$ is the spectrum of A, i.e., the set of all its eigenvalues, and Π_α is the spectral projection of A corresponding to the eigenvalue α, (i.e., the orthogonal projection onto the eigenspace of A associated with the eigenvalue α, in case A is made to act on a Hilbert space).

(2) An *event* possibly detectable in S corresponds to an orthogonal projection $\Pi = \Pi^*$ in the algebra $\mathcal{E}$. But *not* all orthogonal projections in $\mathcal{E}$ represent events. Typically, a projection Π corresponding to an event possibly detectable in S is a spectral projection of an operator in $\mathcal{E}$ that represents a physical quantity of S.

(3) So far, *time* has not appeared in our characterization of physical systems, yet. Time is considered to be a real parameter, $t \in \mathbb{R}$. All physical quantities of S possibly observable during the interval $[s,t] \subset \mathbb{R}$ of times generate an algebra denoted by $\mathcal{E}_{[s,t]}$.[17] It is natural to assume that if $[s',t'] \subset [s,t]$ $(s \leq s', t \geq t')$

$$\mathcal{E}_{[s',t']} \subseteq \mathcal{E}_{[s,t]} \subseteq \mathcal{E}. \tag{36}$$

Events possibly detectable during the time interval $[s,t]$ are represented by certain self-adjoint (orthogonal) projections in the algebra $\mathcal{E}_{[s,t]}$.

(4) *Instruments*: An "instrument", $\mathcal{I}_S[s,t]$, serving to detect certain events in S during the time interval $[s,t]$ is given by a family of mutually orthogonal (commuting) projections, $\{\Pi_\alpha\}_{\alpha \in I_S[s,t]} \subset \mathcal{E}_{[s,t]}$. Typically, these projections will be spectral

[17] Technically speaking, this algebra is taken to be a von Neumann algebra, which has the advantage that, with an operator $A \in \mathcal{E}_{[s,t]}$, all its spectral projections also belong to $\mathcal{E}_{[s,t]}$.

projections of commuting self-adjoint operators representing certain physical quantities of S that may be observable/measurable in the time interval $[s,t]$. For the quantum mechanics describing a physical system S to make concrete predictions it is necessary to specify its list of instruments $\{\mathcal{I}_S^{(i)}[s_i,t_i]\}_{i\in\mathcal{L}_S}$, where $\mathcal{L}_S$ labels all instruments of S. It should be noted that instruments located in different intervals of time may be related to each other by the time evolution of S. (Thus, for autonomous systems, it suffices to specify all instruments $\mathcal{I}_S^{(i)}[0,\infty), i = 1,2,3,\dots$ All other instruments of S are conjugated to the ones in this list by time translation. Luckily, we do not need to go into all these details here.) We emphasize that the operators belonging to *different* instruments all of which are located in the same interval of times do, in general *not* commute with each other. For example, one instrument may measure the position of a particle at some time belonging to an interval $I \in \mathbb{R}$, while another instrument may measure its momentum at some time in I.
Remark: For most quantum systems, the set of instruments tends to be very sparse. There are many very interesting examples of idealized mesoscopic systems for which the set of instruments serving to detect events at time t consists of the spectral projections of a single self-adjoint operator $X(t)$, with

$$X(t) = U_S(s,t)X(s)U_S(t,s),$$

where $U_S(t,s)$ is the unitary propagator of the system S describing time translations of operators representing physical properties of S observable at time s to operators representing the same physical quantities at time t; (we use the Heisenberg picture – as one should always do).
The notion of an "instrument" is not intrinsic to the theory and may depend on the "observer", but *only* in the sense that the amount of information available on a given physical system depends on our abilities to *retrieve* information about it, (which may change with time). The situation is similar to the one encountered in a description of the time evolution of systems in terms of stochastic processes.

Definition. We define the algebras

$$\mathcal{E}_{\geq t} := \overline{\bigvee_{t':t<t'<\infty} \mathcal{E}_{[t,t']}}, \qquad \text{for } t \in \mathbb{R}, \tag{37}$$

where $\overline{(\cdot)}$ represents completion in the operator norm of $\mathcal{E}$. The algebra $\mathcal{E}_{\geq t}$ is the algebra of all events possibly detectable at times $\geq t$, i.e., happening in the future of time t. [18] By property (36) we have that

$$\mathcal{E} \supseteq \mathcal{E}_{\geq t} \supseteq \mathcal{E}_{\geq t'} \supseteq \mathcal{E}_{[t',t'']}, \tag{38}$$

whenever $t < t' \leq t''$.

[18] Since we are interested in projections representing events possibly detectable at times $\geq t$, it may be advantageous to assume that the algebras $\mathcal{E}_{\geq t}$ are actually von Neumann algebras; see, e.g., [12].

Next, we describe the *key idea* underlying our approach to quantum mechanics:
A necessary condition for a physical system S to feature events that may be detectable around or after some time t' (= the present), using suitable instruments $\mathcal{I}_S[t', \infty)$, is that

$$\boxed{\mathcal{E}_{\geq t} \underset{\neq}{\supset} \mathcal{E}_{\geq t'}, \quad \text{for some past time } \ t < t'.} \tag{39}$$

Property (39) expresses a fundamental *loss of access to information* concerning the past (in (39): before time t', but after time t) that occurs in systems featuring detectable events. A property similar to (39), but appropriate for local relativistic quantum theory, has been established for quantum electrodynamics (QED), formulated in the language of algebraic quantum field theory, by Detlev Buchholz and the late John Roberts in [22]. It is a consequence of Huygens' Principle [19] for theories with massless modes or particles, such as the photons of QED. It should be emphasized that a property perfectly analogous to (39) can also be derived for *classical* relativistic field theories obeying Huygens' Principle. Simple models of non-autonomous systems for which property (39) can be proven for certain (discrete) times t' have been discussed in [23].
We must ask why property (39) may actually represent a fundamental property (an "axiom", if you will) of the quantum theory of events and experiments. Our explanation is based on exploiting the phenomenon of entanglement. Suppose that the system S has been prepared in a state ρ at some time t_0. (How a system can be prepared in a specific state at approximately a fixed time is a question that we cannot answer in this essay; but see [24], where it is discussed at length.) The state ρ may be a pure state on the algebra $\mathcal{E}$.
We define a state ρ_t on the algebra $\mathcal{E}_{\geq t}$ by setting

$$\rho_t := \rho|_{\mathcal{E}_{\geq t}}, \qquad \rho_t(A) = \rho(A), \forall A \in \mathcal{E}_{\geq t}. \tag{40}$$

Because of Eq. (39), the state ρ_t may be a *mixed* state on the algebra $\mathcal{E}_{\geq t}$ *even* if it is a *pure* state on the algebra $\mathcal{E}$, assuming that these algebras are non-commutative. This is what *entanglement* is all about! Furthermore, because of loss of access to information as expressed in (39), the states ρ_t "evolve" in time. This means that, at certain times (which one can predict), one may be able to use an "instrument", in the sense of item 4 above, to detect an event, in the sense of item 2 above, of which there were no signs at earlier times. Indeed, it is precisely the fundamental property of "loss of access to information", as expressed in (39), that makes it possible to *gain* information about a system by detecting events happening in it! One may want to call this fact the "*Second Law of quantum measurement theory*". Here is a rough indication of how to understand these things somewhat more precisely:

Given that a system S has been prepared in a state ρ at some time t_0, it may happen that, around some later time t, the state ρ_t is an incoherent superposition of eigenstates of a family of commuting self-adjoint projections belonging to the algebra $\mathcal{E}_{\geq t}$ and representing *events detectable at time t* or later; see item (2), above. These projections may be those of an instrument $\mathcal{I}_S[t, \infty)$, in the sense of item (4) above. Mathematically, this

[19] after the celebrated scientist Christiaan Huygens (1629-1695), who explained many phenomena related to the wave properties of light with the help of the idea of light spheres emanating from all points in physical space already reached by light

means that

$$\rho_t(A) = \sum_{\alpha \in I_S[t,\infty)} \rho(\Pi_\alpha\, A\, \Pi_\alpha) + \rho(\Pi^\perp\, A\, \Pi^\perp), \qquad \sum_{\alpha \in I_S[t,\infty)} \Pi_\alpha = \mathbf{1} - \Pi^\perp, \tag{41}$$

where $\{\Pi_\alpha\}_{\alpha \in I_S[t,\infty)} = \mathcal{I}_S[t,\infty) \in \mathcal{E}_{\geq t}$ is an instrument, and $\Pi^\perp$ projects on whatever is *not* identifiable by this instrument.
Well, things are a little more subtle than that, as we will explain presently. Given a (C^*- or von Neumann) algebra $\mathcal{M}$ and a state ρ on $\mathcal{M}$, we define the adjoint action of an operator $A \in \mathcal{M}$ on the state ρ to be given by a bounded linear functional, $ad_A(\rho)$, defined as follows:

$$ad_A(\rho)(B) := \rho([A, B]), \quad \forall B \in \mathcal{M}. \tag{42}$$

We define the "centralizer" of the state ρ to be the subalgebra

$$\mathcal{C}_\rho := \{A \in \mathcal{M} : ad_A(\rho) = 0\} \tag{43}$$

of the algebra $\mathcal{M}$.[20] Furthermore, let $\mathcal{Z}_\rho$ denote the center of $\mathcal{C}_\rho$.[21]
Given a state ρ on the algebra $\mathcal{E}$, we define $\mathcal{C}_{\rho_t}$ to be the centralizer of the state ρ_t on the algebra $\mathcal{E}_{\geq t}$, and we denote the center of $\mathcal{C}_{\rho_t}$ by $\mathcal{Z}_{\rho_t}$.
We are now prepared to say what it means, *quantum-mechanically*, that an event detectable by an instrument $\mathcal{I}_S[t,\infty)$ happens at a certain time, given that we know the state the system has been prepared in.

Axiom concerning events in quantum mechanics:

(I) Given that the system has been prepared in state ρ, the first event after the preparation of the system, detectable by some instrument, $\mathcal{I}_S[t,\infty)$, of S, happens as soon as equation (41) holds true, provided all the projections $\Pi_\alpha \in \mathcal{I}_S[t,\infty)$ *and* the projection $\Pi^\perp$ belong to the center $\mathcal{Z}_{\rho_t}$ of the centralizer $\mathcal{C}_{\rho_t}$ of the state ρ_t.

(II) The *probability* to detect the event $\Pi_\alpha \in \mathcal{I}_S[t,\infty)$, is given by *Born's Rule*:

$$\text{Prob}\{\Pi_\alpha \text{ happens}\} = \rho(\Pi_\alpha) \tag{44}$$

and $\rho(\Pi^\perp)$ is the probability that the instrument does not detect anything it can identify.

(III) If the event corresponding to the projection Π_α is detected then the state to be used for predictions after time t must be taken to be

$$\rho_{t,\alpha}(A) := \frac{\rho(\Pi_\alpha A \Pi_\alpha)}{\rho(\Pi_\alpha)}, \quad \forall A \in \mathcal{E}_{\geq t} \tag{45}$$

[20] It is an easy exercise that I recommend to the reader to show that $\mathcal{C}_\rho$ is an algebra contained in $\mathcal{M}$ and that ρ is a trace on $\mathcal{C}_\rho$

[21] The center, $\mathcal{Z}$, of an algebra $\mathcal{N}$ consists of *all* operators in $\mathcal{N}$ that commute with *all* operators in $\mathcal{N}$. Note that $\mathcal{Z}$ is an abelian subalgebra of $\mathcal{N}$.

and if the instrument does not detect anything it can identify then the state

$$\rho_t^{\perp}(A) := \frac{\rho(\Pi^{\perp} A \Pi^{\perp})}{\rho(\Pi^{\perp})}, \quad \forall A \in \mathcal{E}_{\geq t} \tag{46}$$

must be used.

Item (III) of the axiom is sometimes called the *"collapse of the wave function"*, a terrible expression, because the "collapse" involved here is not a physical process, but the passage to a conditional expectation.

The formulation of the basic "Axiom concerning events" given above lacks certain elements of precision that cannot be provided here, because they involve concepts – such as conditional expectations defined on non-abelian algebras, etc. – and mathematical subtleties that one cannot explain on a page or two; (see, however, [25]). A precise formulation of this axiom shows that the approximate time ($\approx s_{i_0}$) at which the first event is detected after the preparation of the state of the system [22] and the instrument, $\mathcal{I}_S^{(i_0)}[s_{i_0}, t_{i_0}]$, for some $i_0 \in \mathcal{L}_S$, that detects this first event can be predicted if one knows the state the system has been prepared in; see [25].

Loss of access to information, as formulated in property (39), together with items (II) and (III) of the basic Axiom are fundamental expressions of the *probabilistic nature of quantum mechanics* (i.e., of its **indeterminism**) and of its *fundamental irreversibility*.

Whenever an event happens, in the sense of item (I) of the basic Axiom, then we should pass to the corresponding conditional state given in Eq. (45) to make predictions of the future evolution of the system, whereas if the instrument does *not* detect any event it can identify then the state in Eq. (46) must be used to predict the future. The passage from the state ρ_t to one of the states in (45) and (46) is obviously *not* a linear process and *cannot* be derived from the solution of any Schrödinger equation. The statements that the time evolution of states in quantum mechanics is described by a Schrödinger equation and that the Heisenberg picture and the Schrödinger picture are equivalent are *not* tenable when one studies physical systems featuring events – and, ultimately, only such systems are interesting for physics.

"I leave to several futures (not to all) my garden of forking paths" – Jorge Luis Borges[23]

To summarize our findings, one may say that the time evolution of states of physical systems featuring events is described, in quantum mechanics, by a generalized *"branching process"*. At every fork of the process, an event detectable by some instrument of the system happens, or an event not identifiable by that instrument happens – as formulated in the basic Axiom. The probabilities of the different outcomes are given by *Born's Rule*. If one takes notice of the particular event happening at the fork one is advised to use the corresponding state, as given in (45) and (46), for improved predictions of the future. This is a new initial state, and one then studies whether the system will feature another event in the future, in the sense of the basic Axiom, when prepared in this new initial state, etc. The

[22] i.e., the approximate time at which "a detector clicks"

[23] in: "El jardín de senderos que se bifurcan," Editorial Sur, 1941– I thank P. F. Rodriguez for having drawn my attention to this story.

different possibilities form a tree-like structure (a little like the different descendants of a parent in population dynamics – but with the difference that, in quantum mechanics, only *one* “descendant”, among all possible “descendants”, is real), and the *actual trajectory* of the system corresponds to a path on this tree-like structure, called a *“history”*. This has motivated me to call our approach to quantum mechanics the *“ETH approach”* – for “Events”, “Trees”, and “Histories”. In quantum mechanics, the **“ontology”** of a system S lies in its possible “histories”, (the probabilities or “frequencies”[24] of which are predicted by the theory).
It should be emphasized that, in quantum mechanics, the notion of “conserved quantities”, such as energy, momentum and angular momentum, becomes somewhat fuzzy in systems featuring events, because such quantities are actually not strictly conserved along “histories”: If the instrument involved in the detection of an event does not commute with the operator corresponding to a conserved quantity this quantity is not conserved when the event is detected. This follows from the “collapse rules” (45) and (46).

I conclude this essay by drawing an analogy between quantum mechanics and the standard theory of stochastic (or branching) processes: The filtration of algebras $\{\mathcal{E}_{\geq t}\}_{t\in\mathbb{R}}$ in quantum mechanics is the analogue of a filtration of abelian algebras, $\{\mathcal{E}^c_{\geq t}\}_{t\in\mathbb{R}}$, of functions defined on the path space Ξ of a stochastic process with state space X, where the functions belonging to $\mathcal{E}^c_{\geq t}$ only depend on the part $\xi_{\geq t}(\cdot) := \{\xi(t') \in X : t' > t\}$ of the trajectory $\xi(\cdot) \in \Xi$ of the process at times t or later. Quantum-mechanical events are somewhat analogous to events featured by a stochastic process, (for example the event that a trajectory $\xi(\cdot)$ of a stochastic process visits a certain measurable subset Ω of Ξ whose definition only depends on the part $\xi_{\geq t}$ of the trajectory). In the case of standard stochastic processes, all possible events generate an *abelian* algebra, and one can therefore assume that the “true” state of the system at time t corresponds to a point $\xi(t) \in X$, for all times t. In quantum mechanics, this is *not* the case! It tends to be rare that an “event” detectable by some “instrument” happens. This is a consequence of the non-commutativity of the algebras $\mathcal{E}_{\geq t}, t \in \mathbb{R}$.
In contrast to the situation in classical theories, the state of a system does *not* have an ontological significance in quantum mechanics; (the word “state” may therefore be considered to be a misnomer). It merely enables us to make plausible bets on possible events that may (or may not) happen in the future. In quantum mechanics, the “ontology” lies in the *“histories of events”* of a system, (every event giving rise to a new initial state in the range of the projection that corresponds to the event, as expressed in item (III) – the “collapse postulate” – of the basic Axiom).

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[24] a notion due to Jacob Bernoulli (1655-1705), a member of the famous Bernoulli family of Basel

and I warmly thank my colleague and friend Thomas C. Spencer for generous hospitality at the Institute and many very enjoyable discussions.

5. Appendix on Entropy

In this appendix I recall the definition of the von Neumann entropy of a density matrix and the definition of relative entropy for a pair of density matrices. I then state the most important properties of relative entropy and derive its positivity from an inequality due to O. Klein.

The von Neumann entropy of a density matrix ρ is defined by

$$S(\rho) := -\operatorname{tr}(\rho \ln\rho) \tag{47}$$

It is obviously non-negative and vanishes only if ρ is a pure state. It has various important properties among which one should mention that it is *concave, subadditive* and *strongly subadditive*; see [11].

More important for our considerations in section 2 is another functional, called *"relative entropy"*, defined on pairs of density matrices: Let ρ and σ be density matrices on $\mathcal{H}$; the relative entropy of ρ given σ is introduced as follows:

$$S(\rho\|\sigma) := \operatorname{tr}\big(\rho(\ln\rho - \ln\sigma)\big), \tag{48}$$

and it is assumed that $\ker(\sigma) \subseteq \ker(\rho)$. Important properties of relative entropy are:

- Positivity:
$$S(\rho\|\sigma) \geq 0, \quad \text{with } " = " \text{ iff } \rho = \sigma \text{ on } \ker(\rho)^{\perp}. \tag{49}$$
- Convexity: $S(\rho\|\sigma)$ is jointly convex in ρ and in σ.

For the material in section 2, positivity and joint convexity of relative entropy are the crucial properties.

Next, we state and prove a general inequality, due to O. Klein,[25] which turns out to imply the positivity of relative entropy. Let f be a real-valued, strictly convex function on the real line, and let A and B be self-adjoint operators on $\mathcal{H}$. Then

$$\operatorname{tr}(f(B)) \geq \operatorname{tr}(f(A)) + \operatorname{tr}(f'(A)\cdot(B-A)), \tag{50}$$

with "=" only if $A = B$.

Proof of inequality (50):

Let $\{\psi_j\}_{j=0}^{\infty}$ be a complete orthonormal system (CONS) of eigenvectors of B corresponding to eigenvalues β_j, $j = 0, 1, 2, \dots$ Let ψ be a unit vector in $\mathcal{H}$, and $c_j := \langle\psi_j, \psi\rangle$. Then

$$\langle\psi, f(B)\psi\rangle = \sum_j |c_j|^2 f(\beta_j) \geq f(\sum_j |c_j|^2\beta_j) = f(\langle\psi, B\psi\rangle), \tag{51}$$

[25] Oskar Benjamin Klein (1894-1977) was an eminent Swedish theorist. For example, independently of Kaluza, he invented the Kaluza-Klein unification of gravitation and electromagnetism involving a compact fifth dimension of spacee-time, and, in 1938, he was first to propose a non-abelian gauge theory of weak interactions

by convexity of f; which, moreover, also implies that

$$f(\langle\psi, B\psi\rangle) \geq f(\langle\psi, A\psi\rangle) + f'(\langle\psi, A\psi\rangle) \cdot \langle\psi, (B-A)\psi\rangle.$$

If ψ is an eigenvector of A then the R.S. is

$$= \langle\psi, [f(A) + f'(A) \cdot (B-A)]\psi\rangle. \tag{52}$$

Eq. (50) follows by summing Eqs. (51) and (52) over a CONS of eigenvectors of A. $\Box$

As an application we set $f(x) = x \ln(x)$. Then

$$f'(x) = \ln(x) + 1, \text{ and } f''(x) = \frac{1}{x} > 0, \text{ for } x > 0,$$

i.e., f is convex on $\mathbb{R}_+$. We set $A := \sigma$ and $B := \rho$. Then A and B are positive operators and hence, by the convexity of f on $\mathbb{R}_+$, Klein's inequality (50) implies that

$$\begin{aligned} \text{tr}\,(\rho \ln(\rho)) &= \text{tr}\,(f(B)) \\ &\geq \text{tr}\,(f(A)) + \text{tr}\,(f'(A) \cdot (B-A)) \\ &= \text{tr}\,(\sigma \ln(\sigma)) + \text{tr}\,([\ln(\sigma) + 1](\rho - \sigma)) \\ &= \text{tr}\,(\rho \ln(\sigma)), \end{aligned} \tag{53}$$

and we have used the fact that tr $(\rho) =$ tr (σ) $(= 1)$, and the cyclicity of the trace. This proves the positivity of relative entropy.

$\Box$

The joint convexity of the relative entropy $S(\rho\|\sigma)$ in ρ and σ is a fairly deep property that we do not prove here. Instead, we show that the von Neumann entropy $S(\rho)$ is a *concave* functional of ρ. Let $\rho = p\rho_1 + (1-p)\rho_2$. We apply Klein's inequality (50) twice, with the following choices:

- $B_1 := \rho_1, A := \rho$
- $B_2 := \rho_2, A := \rho$

Taking a convex combination of the two resulting inequalities, we find that

$$\begin{aligned} p\,\text{tr}\,(\rho_1 \ln(\rho_1)) &+ (1-p)\,\text{tr}\,(\rho_2 \ln(\rho_2)) \\ &\geq \text{tr}\,(\rho \ln(\rho)) + p(1-p)\,\text{tr}\,\big((\rho_1 - \rho_2)[\ln(\rho) + 1]\big) \\ &+ (1-p)p\,\text{tr}\,\big((\rho_2 - \rho_1)[\ln(\rho) + 1]\big) \\ &= \text{tr}\,(\rho \ln(\rho)), \end{aligned} \tag{54}$$

which completes the proof of concavity of $S(\rho) = -\text{tr}\,(\rho \ln(\rho))$.

$\Box$

For deep and sophisticated entropy inequalities we refer the reader to [10, 11].

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