Failure of the Ornstein–Zernike asymptotics for the pair correlation function at high temperature and small density

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Joint work with Yacine Aoun, Dmitry Ioffe and Sébastien Ott



- Introduction -

Ornstein–Zernike asymptotics for the pair correlation function

► In 1914 and 1916, Ornstein and Zernike developed a (heuristic) theory of correlations in fluids with quickly decaying interactions. In particular, they concluded that, at large distances, the density-density correlation satisfies

$$G(r) \sim r^{-(d-1)/2} e^{-\nu r}$$

where ν is the **inverse correlation length**.

- ► The OZ theory has become a major piece in the modern statistical theory of fluids and can be found in most textbooks today.
- ▶ In the 1960s, it was realized that the above prediction fails close to a critical point (where $\nu=0$). It was however generally expected to hold away from the critical point, in particular at sufficiently high temperatures and/or sufficiently small densities.





As I'll explain, the situation is actually more subtle than previously thought...

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▶ Let $h \in \mathbb{R}$ and $(J_x)_{x \in \mathbb{Z}^d} \subset [0, \infty)$ such that $J_0 = 0$ and $J_x = J_{-x}$. We also assume (except on 1 slide) that $\exists C, c > 0$ such that $J_x \leq Ce^{-c||x||}$ for all $x \in \mathbb{Z}^d$.

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- ▶ The **Hamiltonian** in $\Lambda \subseteq \mathbb{Z}^d$ is the function

$$\mathscr{H}_{\Lambda}(\sigma) = -\sum_{\{x,y\}\subset\Lambda} J_{y-x}\,\sigma_x\sigma_y - h\sum_{x\in\Lambda}\sigma_x$$

defined on configurations $\sigma = (\sigma_x)_{x \in \Lambda} \in \{\pm 1\}^{\Lambda}$.

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lacktriangle The **Gibbs measure in** Λ at inverse temperature $\beta \geq$ 0 is the probability measure

$$\mathbb{P}_{\Lambda;\beta,h}(\sigma) = \frac{\mathrm{e}^{-\beta\mathscr{H}_{\Lambda}(\sigma)}}{Z_{\Lambda;\beta,h}}.$$

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▶ We are interested in the (infinite-volume) **Gibbs measure** uniquely defined by

$$\mathbb{P}_{\beta,h} = \lim_{\Lambda \uparrow \mathbb{Z}^d} \mathbb{P}_{\Lambda;\beta,h} \quad \text{(when } h \neq 0\text{)}, \qquad \mathbb{P}_{\beta,0} = \lim_{h \downarrow 0} \mathbb{P}_{\beta,h}.$$

lacktriangle The **2-point function** is defined, for any $x\in\mathbb{Z}^d$, by

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$$u_{\beta,h}(\vec{s}) = -\lim_{n \to \infty} \frac{1}{n} \log \mathsf{G}_{\beta,h}([n\vec{s}]),$$

where $[x] \in \mathbb{Z}^d$ is the coordinatewise integer part of $x \in \mathbb{R}^d$.

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lacktriangle There exists $eta_{\rm c}=eta_{\rm c}(d)\in(0,+\infty]$ such that

$$(\beta, h) \neq (\beta_c, 0) \implies \min_{\vec{s}} \nu_{\beta, h}(\vec{s}) > 0$$

$$\forall \vec{s} \in \mathbb{S}^{d-1}, \nu_{\beta_c, 0}(\vec{s}) = 0$$

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lacktriangle When $(eta,h)
eq (eta_c,0)$, $u_{eta,h}$ can be extended to a norm on \mathbb{R}^d :

$$\nu_{\beta,h}(\mathbf{x}) = \|\mathbf{x}\| \cdot \nu_{\beta,h}(\hat{\mathbf{x}}),$$

where $\hat{x} = x/\|x\| \in \mathbb{S}^{d-1}$.

- RIGOROUS RESULTS -

1. Finite-range interactions

$$\exists R < \infty, \quad ||x|| > R \implies J_x = 0.$$

Asymptotic behavior of the 2-point function

Ornstein–Zernike asymptotic behavior holds when $\beta < \beta_c$ or $h \neq 0$:

Theorem

Assume that $\beta < \beta_{\rm c}$ or $h \neq {\rm 0}.$ Then, as $n \to \infty$,

$$\mathsf{G}_{\beta,h}([n\vec{s}\,]) = \frac{\Psi_{\beta,h}(\vec{s}\,)}{n^{(d-1)/2}}\,\mathrm{e}^{-\nu_{\beta,h}(\vec{s}\,)n}\,(1+\mathsf{o}(1))$$

Moreover, the functions $\Psi_{\beta,h}$ and $\nu_{\beta,h}$ are analytic in \vec{s} .

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Moreover, the functions $\Psi_{\beta,h}$ and $\nu_{\beta,h}$ are analytic in \vec{s} .

The above result has a long history. Some milestones are

- > Wu 1966, Wu−McCoy−Tracy−Barouch 1976:
- ⊳ Abraham–Kunz 1977, Paes-Leme 1978:
- Campanino−Ioffe−V. 2003:
- ⊳ Campanino-Ioffe-V. 2008:
- ⊳ Ott 2020:

- exact computation in d=2 when h=0
- any dimension, h=0 and $\beta\ll 1$
- any dimension, h=0 and $eta<eta_{
 m c}$
- extension to Potts models
- any dimension, $h \neq 0$ and β arbitrary

Knowledge much less complete when h=0 and $\beta>\beta_c$, but **OZ can be violated**:

Theorem

Assume that h=0 and $\beta>\beta_{\rm c}$. Then, as $n\to\infty$,

$$\mathsf{G}_{\beta,h}([\vec{ns}]) = \begin{cases} \frac{\Psi_{\beta,0}(\vec{s})}{n^2} \, \mathrm{e}^{-\nu_{\beta,0}(\vec{s})n} \, (1+\mathrm{o}(1)) & \text{in the planar case} \\ \frac{\Psi_{\beta,0}(\vec{s})}{n^{(d-1)/2}} \, \mathrm{e}^{-\nu_{\beta,0}(\vec{s})n} \, (1+\mathrm{o}(1)) & \text{when } d \geq 3, \beta \gg 1 \end{cases}$$

exact computations in the planar case

⊳ Bricmont-Fröhlich 1985:

$$d > 3$$
, $\beta \gg 1$

Remarks: 1. OZ decay expected to persist for all $\beta > \beta_c$ when $d \ge 3$.

2. OZ expected to hold when d=2 and the graph is not planar.

- RIGOROUS RESULTS -

2. Infinite-range interactions

[From now on, for simplicity, we assume that h=0 and omit it from the notations. However, many results extend to all $h\neq 0$.]

Subexponential decay of interactions

► Assume that interactions decay **strictly slower than exponentially**:

$$\forall c>0,\quad \lim_{\|x\|\to\infty}e^{c\|x\|}J_x=+\infty.$$

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▶ In fact, sharp asymptotics have been obtained:

Theorem	[Newman-Spohn 1998]
Assume that $eta < eta_{ extsf{c}}.$ Then, as $\ extsf{x}\ o \infty$,	
$G_{\beta}(x) = \beta \chi_{\beta}^2 J_{x}(1 + o(1)),$	
where $\chi_{eta} = \sum_{\mathtt{x}} G_{eta}(\mathtt{x})$ is the magnetic susceptibility.	

▶ This result was extended to Potts models by Aoun (2020).

Superexponential decay of interactions

► Assume that interactions decay **strictly faster than exponentially**:

$$\forall c \in \mathbb{R}, \quad \lim_{\|x\| \to \infty} e^{c\|x\|} J_x = 0.$$

In this case, the results obtained in the finite-range case when $\beta < \beta_{\rm c}$ extend verbatim:

In particular, OZ asymptotic behavior holds in all dimensions.

Exponential decay of interactions

Let us thus consider the "critical" case of exponentially decaying interactions:

$$J_{x}=\psi(x)e^{-\|x\|},$$

where

- $ho \ \|\cdot\|$ denotes an arbitrary norm on \mathbb{R}^d
- $hd \psi$ is subexponential

and we assume in this talk, for simplicity, that

$$\forall x \in \mathbb{R}^d, \quad \psi(x) = \psi(||x|||) > 0.$$



It is a general result that $\lim_{\beta\uparrow\beta_c} \nu_{\beta}(\vec{s}) = 0$ for all $\vec{s}\in\mathbb{S}^{d-1}$.

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$(\beta \downarrow 0)$

▷ For superexponentially decaying interactions,

$$\lim_{eta\downarrow 0}
u_eta(ec{\mathbf{s}}) = +\infty \quad ext{ for all } ec{\mathbf{s}} \in \mathbb{S}^{d-1}.$$

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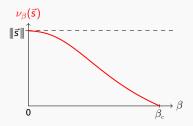
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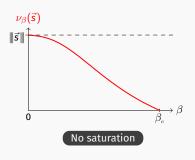
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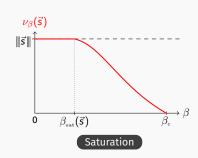
$$\lim_{\beta \downarrow 0} \nu_{\beta}(\vec{s}) = |\!|\!|\vec{s}|\!|\!| \quad \text{for all } \vec{s} \in \mathbb{S}^{d-1}.$$

► This leads to two scenarios:









- ▶ We define $\beta_{\text{sat}}(\vec{s}) = \sup\{\beta \geq 0 : \nu_{\beta}(\vec{s}) = |||\vec{s}|||\}$ and say that there is **saturation** in direction \vec{s} at inverse temperature β if $\beta < \beta_{\text{sat}}(\vec{s})$.
- $lackbox{}$ Observe that $eta_{\rm sat}(ec{{f s}})>0$ implies that $eta\mapsto
 u_{eta}(ec{{f s}})$ is not analytic on $[0,eta_{
 m c})$.

lackbox Let us introduce the generating functions (for $t \in \mathbb{R}^d$)

$$\mathbb{G}_\beta(t) = \sum_{x \in \mathbb{Z}^d} e^{t \cdot x} \, \mathsf{G}_\beta(x), \qquad \mathbb{J}(t) = \sum_{x \in \mathbb{Z}^d} e^{t \cdot x} \mathsf{J}_x.$$

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► Let us also introduce

$$\mathscr{U} = \{ x \in \mathbb{R}^d : |||x||| \le 1 \}, \quad \mathscr{W} = \{ t \in \mathbb{R}^d : \forall x \in \mathbb{R}^d, \ t \cdot x \le |||x||| \}.$$

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Easy fact: \mathcal{W} is the closure of the domain of convergence of \mathbb{J} .

 $ightharpoonup t \in \partial \mathscr{W}$ is **dual** to $\vec{s} \in \mathbb{S}^{d-1}$ if









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- Extends to many models: Potts, XY, (FK)-percolation, GFF with mass as parameter, Ising with magnetic field as parameter, etc.

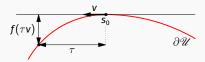
Theorem $\beta_{\text{sat}}(\vec{s}) > 0 \iff \inf_{t \in \mathscr{T}_{\vec{s}}} \mathbb{J}(t) < \infty.$

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- ► Extends to many models: Potts, XY, (FK)-percolation, GFF with mass as parameter, Ising with magnetic field as parameter, etc.
- ► Application of this criterion yields, for instance, that
 - ho If $\sum_{\ell \in \mathbb{N}} \Psi(\ell) = \infty$, then $eta_{\mathsf{sat}}(\vec{s}) = 0$ for all $\vec{s} \in \mathbb{S}^{d-1}$.

It would be useful to have a more explicit criterion in general.

A more explicit form of the criterion

▶ Local parametrization of $\partial \mathcal{U}$ at $s_0 = \vec{s} / ||\vec{s}||$:



 \blacktriangleright Assume there exist C, c > 0 and a nonnegative nondecreasing function g such that

$$C g(\tau) \ge f(\tau v) \ge c g(\tau)$$

for all small $\tau \geq 0$ and all vectors v in a supporting hyperplane to $\partial \mathscr{U}$ at s_0 .

Then the following more explicit version of the criterion holds:

$$\beta_{\text{sat}}(\vec{s}) > 0 \iff \sum_{\ell \geq 1} \psi(\ell) \big(\ell g^{-1}(1/\ell)\big)^{d-1} < \infty.$$

An example

ightharpoonup Let us illustrate the previous criterion for the model on \mathbb{Z}^2 with

$$J_x = ||x||_p^\alpha e^{-||x||_p},$$

where $\|\cdot\|_p$ is the p-norm, $\alpha\in\mathbb{R}$ and we assume $p\in(2,\infty)$.

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- ▶ Let $\vec{s} \in \mathbb{S}^1$ and $s_0 = (x_0, y_0) = \vec{s} / \|\vec{s}\|_p$.
- ▶ When both x_0 and y_0 are nonzero,

$$f(\tau v) = \frac{p-1}{2} \frac{x_0^{p-2} y_0^{p-2}}{(x_0^{2p-2} + y_0^{2p-2})^{3/2}} \tau^2 + o(\tau^2).$$

(. U

We can thus choose $g(\tau) = \tau^2$. It follows that

$$eta_{\text{sat}}(\vec{s}) > 0 \iff \sum_{\ell > 1} \ell^{\alpha}(\ell\sqrt{1/\ell}) < \infty \iff \alpha < -\frac{3}{2}.$$

An example

lacktriangle In the remaining cases, that is, when $ec s\in\{\pm(1,0),\pm(0,1)\}$,

$$f(\tau v) = \frac{1}{p} \tau^p + o(\tau^p).$$

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$$\beta_{sat}(\vec{s})>0\iff \sum_{\ell\geq 1}\ell^{\alpha}\big(\ell\sqrt[p]{1/\ell}\big)<\infty\iff \alpha<\frac{1}{p}-2.$$



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We can thus choose $g(\tau) = \tau^p$. Therefore,

$$\beta_{\text{sat}}(\vec{s}) > 0 \iff \sum_{\ell \geq 1} \ell^{\alpha}(\ell \sqrt[p]{1/\ell}) < \infty \iff \alpha < \frac{1}{p} - 2.$$

- ► This shows that the positivity of $\beta_{\text{sat}}(\vec{s})$ (and a fortiori its actual value) depends on the norm. It also **depends in general on the direction**: when $-\frac{3}{2} > \alpha \geq \frac{1}{p} 2$,
 - $\, \triangleright \, \, \beta_{\text{sat}}(\vec{s}\,) = 0 \text{ for } \vec{s} \in \{\pm(1,0),\pm(0,1)\}$
 - $\triangleright \beta_{sat}(\vec{s}) > 0$ in all the other directions.

Consequences for OZ behavior

ightharpoonup When $eta_{
m sat}(ec{s})>0$, **OZ** asymptotics are known not to hold at sufficiently high temperatures for various classes of interactions. For instance:

$$\forall \psi(x) = C e^{-c \|x\|^{\alpha}} \text{ with } 0 < \alpha < 1$$

$$\forall \psi(x) = C e^{-c (\log \|x\|)^{\alpha}} \text{ for some } \alpha > 1$$

$$\forall \psi(x) = C \|x\|^{-\alpha} \text{ for some } \alpha > d$$

Theorem

[Aoun-Ioffe-Ott-V. 2021]

Assume that $\beta_{\rm sat}(\vec s)>0$ and that ψ is as above. Then, for all β small enough, there exist $c_+>c_->0$ such that, for all n,

$$c_{-}J_{[n\vec{s}]} \leq \mathsf{G}_{\beta}([n\vec{s}]) \leq c_{+}J_{[n\vec{s}]}.$$

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► Current work in progress:

- ▷ more general classes of prefactors

- ightarrow proof that OZ holds for all $eta \in (eta_{\mathsf{sat}}(ec{\mathsf{s}}), eta_{\mathsf{c}})$
- $\,\,\,\,\,\,\,\,\,$ proof that OZ usually holds at $eta_{\mathrm{sat}}(ec{s})$

— COMMENTS ON THE PROOF —

- 1. Preliminaries.
- ▶ When $\beta < \beta_c$,

$$G_{\beta}(x) = \sum_{\gamma: 0 \to x} q_{\beta}(\gamma),$$
 (1)

where γ is a self-avoiding path from 0 to x and $q_{\beta}(\gamma)$ a suitable non-negative weight.

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where γ is a self-avoiding path from 0 to x and $q_{\beta}(\gamma)$ a suitable non-negative weight.

lacktriangle One can show that there exists $\mathcal{C}_{\beta}>0$ such that, if $\gamma=(\gamma_0,\gamma_1,\ldots,\gamma_n)$ is self-avoiding,

$$\prod_{i=1}^{n} \beta J_{\gamma_{i}-\gamma_{i-1}} \ge q_{\beta}(\gamma) \ge \prod_{i=1}^{n} C_{\beta} J_{\gamma_{i}-\gamma_{i-1}}.$$
 (2)

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where γ is a self-avoiding path from 0 to x and $q_{\beta}(\gamma)$ a suitable non-negative weight.

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$$\prod_{i=1}^{n} \beta J_{\gamma_{i}-\gamma_{i-1}} \ge q_{\beta}(\gamma) \ge \prod_{i=1}^{n} C_{\beta} J_{\gamma_{i}-\gamma_{i-1}}.$$
 (2)

lacktriangledown Recall that $\mathbb{G}_eta(t)=\sum_{x\in\mathbb{Z}} \mathrm{e}^{tx}\mathsf{G}_eta(x)$ and $\mathbb{J}(t)=\sum_{x\in\mathbb{Z}} \mathrm{e}^{tx}\ J_x\ .$

Observe that

- \triangleright the radii of convergence of \mathbb{G}_{β} and \mathbb{J} are given by $\nu_{\beta}(1)$ and ||1||, respectively;
- \triangleright (1) and (2) imply that $\nu_{\beta}(1) \leq ||1||$ (use $\gamma = \{0, x\}$ for a lower bound on \mathbb{G}_{β}).

1. Preliminaries.

▶ When $\beta < \beta_c$,

$$\mathsf{G}_{\beta}(\mathsf{x}) = \sum_{\gamma:\, 0 \to \mathsf{x}} \mathsf{q}_{\beta}(\gamma),\tag{1}$$

where γ is a self-avoiding path from 0 to x and $q_{\beta}(\gamma)$ a suitable non-negative weight.

lacktriangle One can show that there exists $\mathcal{C}_{eta}>0$ such that, if $\gamma=(\gamma_0,\gamma_1,\ldots,\gamma_n)$ is self-avoiding,

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 (2)

$$\begin{array}{l} \blacktriangleright \text{ Recall that } \mathbb{G}_{\beta}(t) = \sum_{x \in \mathbb{Z}} e^{tx} \underbrace{G_{\beta}(x)}_{\text{e}^{-\nu_{\beta}(1) \cdot |x|}} \text{and } \mathbb{J}(t) = \sum_{x \in \mathbb{Z}} e^{tx} \underbrace{J_{x}}_{\text{e}^{-\parallel 1 \parallel \cdot |x|}}.$$

Observe that

- \triangleright the radii of convergence of \mathbb{G}_{β} and \mathbb{J} are given by $\nu_{\beta}(1)$ and ||1||, respectively;
- \triangleright (1) and (2) imply that $\nu_{\beta}(1) \leq ||1||$ (use $\gamma = \{0, x\}$ for a lower bound on \mathbb{G}_{β}).

▶ Note that, using (1),

$$\mathbb{G}_{\beta}(t) = \sum_{x \in \mathbb{Z}} e^{tx} \, G_{\beta}(x)
= \sum_{x \in \mathbb{Z}} e^{tx} \sum_{\gamma: 0 \to x} q_{\beta}(\gamma)
= \sum_{x \in \mathbb{Z}} e^{tx} \sum_{n \ge 1} \sum_{\substack{y_1, \dots, y_n \\ \sum_k y_k = x}} q_{\beta}((0, y_1, y_1 + y_2, \dots, y_1 + \dots + y_n))
= \sum_{x \in \mathbb{Z}} \sum_{n \ge 1} \sum_{\substack{y_1, \dots, y_n \\ \sum_k y_k = x}} e^{t(y_1 + \dots + y_n)} q_{\beta}((0, y_1, y_1 + y_2, \dots, y_1 + \dots + y_n))
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▶ Note that, using (1),

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$$= \sum_{n \ge 1} \sum_{y_1, \dots, y_n} e^{t(y_1 + \dots + y_n)} q_{\beta}((0, y_1, y_1 + y_2, \dots, y_1 + \dots + y_n)). \tag{3}$$

▶ Let $\vec{s} = 1$. Then $\mathcal{T}_{\vec{s}} = \{ \|1\| \}$.

The criterion thus reduces to: $\beta_{\text{sat}}(1) > 0 \iff \mathbb{J}(\|1\|) < \infty$

- 2. Proof that $\mathbb{J}(||1||) < \infty \implies \beta_{\text{sat}}(1) > 0$.
- ▶ By (3) and the upper bound in (2),

$$\mathbb{G}_{\beta}(t) \leq \sum_{n \geq 1} \sum_{y_1, \dots, y_n} \prod_{k=1}^n e^{ty_k} \beta J_{y_k} = \sum_{n \geq 1} \bigl(\beta \mathbb{J}(t)\bigr)^n.$$

Therefore,

$$\mathbb{J}(t)<\infty ext{ and } eta<rac{1}{\mathbb{J}(t)} \quad \Longrightarrow \quad \mathbb{G}_{eta}(t)<\infty.$$

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Therefore,

$$\mathbb{J}(t)<\infty \text{ and } \beta<\frac{1}{\mathbb{J}(t)} \quad \Longrightarrow \quad \mathbb{G}_{\beta}(t)<\infty.$$

▶ In particular, with t = ||1||,

$$\mathbb{J}(||\!|1|\!|\!|)<\infty\implies \mathbb{G}_{\beta}(|\!|\!|1|\!|\!|)<\infty\implies |\!|\!|\!|1|\!|\!|\!|\leq \nu_{\beta}(1)\implies |\!|\!|\!|1|\!|\!|\!|=\nu_{\beta}(1),$$

for all $\beta < 1/\mathbb{J}(||1||)$. This show that $\beta_{sat}(1) > 0$.

3. Proof that $\mathbb{J}(||1||) = \infty \implies \beta_{sat}(1) = 0$.

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- ightharpoonup Let eta>0. By Fatou, there exists $\epsilon>0$ such that

$$\mathbb{J}((1-\epsilon)|\!|\!|1|\!|\!|)\geq \frac{2}{C_{\beta}}.$$

- 3. Proof that $\mathbb{J}(\|1\|) = \infty \implies \beta_{\text{sat}}(1) = 0$.
- ▶ Let β > 0. By Fatou, there exists ϵ > 0 such that

$$\mathbb{J}((1-\epsilon)|\!|\!|1|\!|\!|)\geq \frac{2}{\mathsf{C}_\beta}.$$

▶ Let $t = (1 - \epsilon) \|1\|$. Using (3) and the lower bound in (2), we obtain

$$\mathbb{G}_{\beta}(t) \geq \sum_{n\geq 1} \sum_{y_1\geq 1} \cdots \sum_{y_n\geq 1} \prod_{k=1}^n C_{\beta} J_{y_k} e^{ty_k}$$

$$= \sum_{n\geq 1} \left(C_{\beta} \sum_{y\geq 1} J_y e^{ty} \right)^n$$

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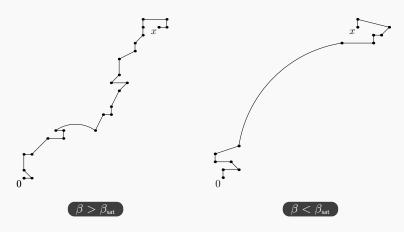
$$= +\infty.$$

- ▶ This implies that $(1 \epsilon) \|1\| \ge \nu_{\beta}(1)$ and thus $\|1\| > \nu_{\beta}(1)$.
- ▶ We conclude that $\beta_{sat}(1) \leq \beta$. Since $\beta > 0$ was arbitrary, $\beta_{sat}(1) = 0$.

— ONE FINAL REMARK —

An associated condensation phenomenon

lacktriangle Sketches of typical paths γ contributing to $G_{\beta}(x) = \sum_{\gamma: 0 \to x} q_{\beta}(\gamma)$:



► Reminiscent of the condensation phenomenon for large deviations of the sum of independent random variables, depending on the fatness of their tail.



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