Weierstrass Institute for
Applied Analysis and Stochastics

Classical many-body systems with Lennard-Jones-type potential

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Background and goals of this talk

In simple words:

- We throw N particles randomly into a box in $\mathbb{R}^d$ with volume N/ρ.
- The particles are *a priori* independent and uniformly distributed, but ...
- ... we modify their joint distribution by using an exponential pair-interaction weight with strength β that makes clumping impossible and prefers a certain positive distance between any two particles.
- Describing what we will see in the limit $N \to \infty$ is generally very difficult, but ...
- ... for small ρ and large β we will see a clear decomposition into small groups and can approximately describe the configuration with explicit formulas, and ...
- ... for fixed ρ and large β, we will see in dimension 1 that the particles approach a regular grid.

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for physicists:

- We consider a classical stable interacting many-particle system with attraction via a Lennard–Jones-type potential in continuous space.
- We study the transition between gaseous and solid phase in the thermodynamic limit.
- We obtain explicit results in two particular regimes at low temperature, $\beta \to \infty$:

$$\text{low density } \rho \downarrow 0, \qquad \text{fixed density } \rho \in (0, \infty).$$

The dilute low-temperature regime: much empty space, strong interaction

- The particles organise themselves into small groups called clusters or droplets.
- We approximate the system with a well-known ideal mixture of clusters and prove that the difference vanishes exponentially with vanishing temperature.
- The questions about a percolation phase transition and existence of Gibbs measures are naturally contained in our description.

The low-temperature regime: approximating a grid – crystallization

- We consider particular potentials in dimension one at fixed, sufficiently large density ρ.
- The particles form $\asymp N$ clusters with optimal inner and boundary structure and Gaussian approximation.

We always assume that ρ is smaller than the close-packing threshold ρ_{cp} (which is ∞ if there is no hard core).

Energy

Energy of N particles in $\mathbb{R}^d$:

$$U_N(\boldsymbol{x}) = U_N(x_1, \ldots, x_N) = \sum_{\substack{i,j=1 \\ i \neq j}}^{N} v\big(|x_i - x_j|\big), \qquad \text{for } \boldsymbol{x} = (x_1, \ldots, x_N) \in (\mathbb{R}^d)^N.$$

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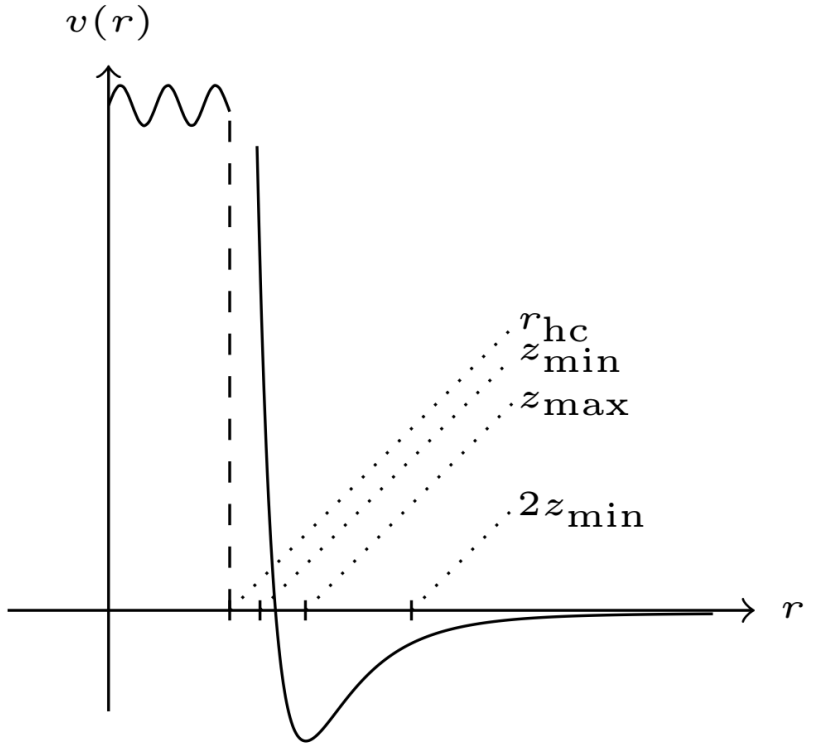

- $v(r) \to \infty$ as $r \downarrow 0$ sufficiently fast:
  short-distance repulsion (possibly hard-core) implying stability,
- strict negative minimum at some $a \in (0, \infty)$:
  preference of a certain positive distance,
- compact support:
  bounded interaction length.

v is called stable if $\inf_{N \in \mathbb{N}} \frac{1}{N} \inf_{\mathbf{x} \in (\mathbb{R}^d)^N} U(\mathbf{x}) > -\infty$.

The Gibbs measure

$$\mathbb{P}^{(N)}_{\beta,\Lambda}(\mathrm{d}\boldsymbol{x}) = \frac{1}{Z_\Lambda(\beta,N)N!}\mathrm{e}^{-\beta U_N(\boldsymbol{x})}\,\mathrm{d}\boldsymbol{x}, \qquad \boldsymbol{x}\in\Lambda^N, \beta>0,$$

with partition function

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The connectivity structure

x and y are connected if $|x-y|\le R$. Clusters (droplets) = connected components

$$N_k(\boldsymbol{x}) = \text{number of } k\text{-clusters in } \boldsymbol{x}=(x_1,\dots,x_N)$$

k-cluster density: $\rho_{k,\Lambda}(\boldsymbol{x}) = \dfrac{N_k(\boldsymbol{x})}{|\Lambda|}$,

cluster size distribution: $\boldsymbol{\rho}_\Lambda = \big(\rho_{k,\Lambda}\big)_{k\in\mathbb{N}}$.

$\boldsymbol{\rho}_\Lambda$ is an $M_{N/|\Lambda|}$-valued random variable, where

$$M_\rho := \Big\{(\rho_k)_{k\in\mathbb{N}}\in[0,\infty)^{\mathbb{N}}\,\Big|\,\sum_{k\in\mathbb{N}}k\rho_k\le\rho\Big\}, \qquad \rho\in(0,\infty).$$

Questions and answers

- Is there a formula for the limiting free energy $\lim_{N\to\infty} \frac{1}{|\Lambda_N|} \log Z_{\Lambda_N}(\beta, N)$?

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- If for $\beta = \infty$ there is crystallisation; do we have this also for large β?
  Very difficult in $d \geq 2$, recently proved in $d = 1$. $\Longrightarrow$ [JANSEN, K., SCHMIDT, THEIL 2020/21], Part (III)

Free energy and Gibbs measures (I)

Using level-three large-deviation theory, one can express the limiting free energy in terms of a variational formula. Minimisers turn out to be Gibbs measures, but phase transitions in the sense of non-uniqueness is open.

Using a Poisson point process ω_{P} and the interaction function

$$F(\omega) = \sum_{x \in \omega \cap U} \sum_{y \in \omega} v(|x-y|), \qquad U = [-\tfrac{1}{2}, \tfrac{1}{2}]^d$$

and the counting function $N_U(\omega) = \omega(U)$, we can write

$$Z_\Lambda(\beta, N) = \mathbb{E}\Big[\mathrm{e}^{-\beta|\Lambda|\langle F, R_\Lambda(\omega_{\mathrm{P}})\rangle} \mathbb{1}\{\langle N_U, R_\Lambda(\omega_{\mathrm{P}})\rangle = \rho\}\Big],$$

where

$$R_\Lambda(\omega) = \frac{1}{|\Lambda|} \int_\Lambda \mathrm{d}x \, \delta_{\theta_x(\omega)}$$

is the empirical stationary field. The latter satisfies a large-deviation principle [GEORGII/ZESSIN (1993)]

$$\lim_{N\to\infty} \frac{1}{|\Lambda_N|} \log \mathbb{P}(R_{\Lambda_N}(\omega_{\mathrm{P}}) \approx P) = -I(P)$$

where $I(P)$ is the entropy density function of ω_{P}

Then the limiting free energy can be written (under suitable assumptions on v) as

$$f(\beta,\rho) = -\frac{1}{\beta}\lim_{N\to\infty}\frac{1}{|\Lambda_N|}\log Z_{\Lambda_N}(\beta,N)$$
$$= -\frac{1}{\beta} + \inf\Big\{\frac{1}{\beta}I(P) + \langle F,P\rangle\colon P\in\mathcal{P}_\theta, \langle N_U,P\rangle = \rho\Big\}.$$

[JANSEN 2016] extends this formula to the cluster-size distribution. Indeed, define

$$\rho_k(P) = \int P(\mathrm{d}\omega)\sum_{x\in\omega\cap U}\mathbb{1}\{|\mathcal{C}_\omega(x)| = k\},$$

where $\mathcal{C}_\omega(x)$ is the cluster that contains x, then

Variational formula for constrained partition function

$$f(\beta,\rho,(\rho_k)_{k\in\mathbb{N}}) = -\frac{1}{\beta}\lim_{N\to\infty}\frac{1}{|\Lambda_N|}\log\int_{\Lambda_N^N}\mathrm{d}\mathbf{x}\,\mathrm{e}^{-\beta U_N(\mathbf{x})}\mathbb{1}\{\rho_{k,\Lambda_N}(\mathbf{x}) = \rho_k\,\forall k\in\mathbb{N}\}$$
$$= -\frac{1}{\beta} + \min\Big\{\frac{1}{\beta}I(P) + \langle F,P\rangle\colon P\in\mathcal{P}_\theta, \rho_k(P) = \rho_k\,\forall k\in\mathbb{N}\Big\}.$$

Brief explanation of this concept:
For a given point cloud $(x_i)_{i\in I}$ in $\mathbb{R}^d$, a collection of interaction functionals $\{\phi(x_i,x_j)\}_{i\neq j}\cup\{f(x_i)\}_{i\in I}$ is given. For any box Λ and any boundary configuration $x_{\Lambda^{\mathrm{c}}}$ in Λ^{c}, a probability measure on configurations x_Λ in Λ is defined by

$$\mathbb{P}_{\Lambda,\mu}^{(x_{\Lambda^{\mathrm{c}}})}\big(\mathrm{d}x_\Lambda\big)=\frac{1}{Z_{\Lambda,\mu}^{(x_{\Lambda^{\mathrm{c}}})}}\,\mathrm{e}^{\sum_{i,j}\,\phi(x_i,x_j)}\,\mathrm{e}^{\mu\sum_{i\in I}\,f(x_i)}\mathbb{P}_\Lambda\big(\mathrm{d}(x_\Lambda)\big),$$

where the reference measure $\mathbb{P}_\Lambda$ is the restriction (better: projection) of a standard PPP to Λ, and $\mu\in\mathbb{R}$ is called a chemical potential.
Now a probability measure $Q\in\mathcal{P}_\theta$ is called a Gibbs measure for the interacting functionals and the chemical potential if, for any box Λ,

$$\int Q(\mathrm{d}x_{\Lambda^{\mathrm{c}}})\mathbb{P}_{\Lambda,\mu}^{(x_{\Lambda_{\mathrm{c}}})}(\mathrm{d}x_\Lambda)=Q_\Lambda(\mathrm{d}x_\Lambda),$$

In our case, $\phi(x,y)=-\beta v(|x-y|)$ and $f(x)=1$.
Rule of thumb: Existence often no problem, but uniqueness. The latter characterises a phase transition.

Recall the

Gibbs variational principle, [GEORGII 95]

$P \in \mathcal{P}_\theta$ is a (β, μ)-Gibbs measure (then we write $P \in \mathcal{G}_{\beta,\mu}$) if and only if it minimizes $\frac{1}{\beta} I(P) + \langle F, P \rangle - \mu\rho(P)$.

The parameter μ is called a chemical potential, and $\rho(P) = \sum_{k\in\mathbb{N}} k\rho_k(P)$.

Gibbs measures and minimizers, [JANSEN 2016]

$$(\rho_k)_k \text{ minimises} \quad \Longleftrightarrow \quad \exists\, P \in \mathcal{P}_\theta \cap \mathcal{G}_{\beta,\mu} \text{ for some } \mu \in \mathbb{R},$$
$$\text{satisfying } \rho(P) = \rho,\ \rho_k(P) = \rho_k\ \forall k.$$

Now note the general statement

Percolation, [JANSEN 2016]

For any $P \in \mathcal{P}_\theta$,

$$\sum_{k\in\mathbb{N}} k\rho_k(P) < \rho(P) \quad \Longleftrightarrow \quad P(\text{there is an infinite cluster}) > 0.$$

Remarks

- v is assumed to have a compact support and an attractive tail (v is negative just before the supremum of the support), furthermore superstable and integrable where it is finite. These are standard and imply, e.g., existence of Gibbs measures.
- Furthermore, $(\mathbb{R}^d)^N \ni \mathbf{x} \mapsto U(\mathbf{x})$ is assumed to have a minimizer that has positive spacing. This and the following condition is used for bounds on percolation (seee later).
- The most restrictive assumption is that this map has a minimizer with diameter $\leq O(N^{1/d})$. Criteria for this are known [THEIL (2006)] in $d = 2$, but not in $d \geq 3$.
- The variational approach is able to make a link with Gibbs measures and their percolation properties, but not (yet) with phase transitions (in the sense of non-uniqueness of Gibbs measures).
- Criteria for (non-)percolation will come later.

Regimes considered

We study the cluster-size distribution in the box $\Lambda = [0, L]^d$ in the thermodynamic limit

$$N \to \infty, \qquad L = L_N \to \infty, \qquad \text{such that } \frac{N}{L_N^d} \to \rho \in (0, \infty),$$

followed by the dilute low-temperature limit [JANSEN, K., METZGER *AAP* 2015]

$$\beta \to \infty, \rho \downarrow 0 \qquad \text{such that } -\frac{1}{\beta} \log \rho \to \nu \in (0, \infty),$$

Here we study the statistics of the sizes of the clusters in terms of a large-deviation principle.

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constrained free energy : $$f_\Lambda(\beta, \tfrac{N}{|\Lambda|}, (\rho_k)_k) := -\frac{1}{\beta|\Lambda|} \log Z_\Lambda(\beta, N, (\rho_k)_k).$$

limiting constrained free energy : $$f(\beta, \rho) := \lim_{\substack{N, L \to \infty \\ N/L^d \to \rho}} f_{[0,L]^d}(\beta, \tfrac{N}{L^d}, (\rho_k)_k).$$

[JANSEN (2016)] showed

$$\frac{1}{N!} \int_{\Lambda^N} \mathrm{e}^{-\beta U_N(\boldsymbol{x})} \mathbb{1}\Big\{(\rho_{k,\Lambda}(\boldsymbol{x}))_{k\in\mathbb{N}} \approx (\rho_k)_{k\in\mathbb{N}}\Big\} \,\mathrm{d}\boldsymbol{x} \approx \exp\Big(-\beta|\Lambda| f(\beta, \rho, (\rho_k)_{k\in\mathbb{N}})\Big),$$

Rate function

$$J_{\beta,\rho}\big((\rho_k)_{k\in\mathbb{N}}\big) = \beta\big(f(\beta,\rho,(\rho_k)_{k\in\mathbb{N}}) - f(\beta,\rho)\big).$$

An LDP without identification of the rate function:

Large deviation principle with convex rate function, [JKM15]

The distribution of $\boldsymbol{\rho}_\Lambda$ under $\mathbb{P}^{(N)}_{\beta,\Lambda}$ with $\Lambda = [0,L]^d$ satisfies a large deviation principle with speed $|\Lambda| = L^d$. The rate function $J_{\beta,\rho}\colon M_{\rho+\varepsilon} \to [0,\infty]$ is convex, and its effective domain $\{J_{\beta,\rho}(\cdot) < \infty\}$ is contained in M_ρ. In particular, $\boldsymbol{\rho}_\Lambda$ convereges weakly towards the minimizers $(\rho_k)_k$ of $J_{\beta,\rho}$ (which are the ones of $f(\beta,\rho,\cdot)$).

Let us derive a much clearer picture in the dilute low-temperature limit.

Heuristics: In the regime $\beta \to \infty$, $\rho \to 0$ such that $-\beta^{-1}\log\rho \to \nu \in (0,\infty)$,

- total entropy $\approx$ sum of the entropies of the clusters,
- excluded-volume effect between the clusters may be neglected,
- mixing entropy may be neglected.

The ground state energy, i.e., zero temperature : $$E_N := \inf_{\boldsymbol{x}\in(\mathbb{R}^d)^N} U_N(\boldsymbol{x}).$$

stability & subadditivity $\implies$ $e_\infty := \lim_{N\to\infty} \frac{E_N}{N} \in (-\infty, 0)$ exists.

Interpret $q_k = k\rho_k/\rho$ as the probability that a given particle lies in a k-cluster.

Approximate rate function: $$g_\nu\big((q_k)_k\big) := \sum_{k\in\mathbb{N}} q_k \frac{E_k - \nu}{k} + \Big(1 - \sum_{k\in\mathbb{N}} q_k\Big) e_\infty$$

on the set $$\mathcal{Q} := \Big\{(q_k)_{k\in\mathbb{N}} \in [0,1]^{\mathbb{N}} \,\Big|\, \sum_{k\in\mathbb{N}} q_k \le 1\Big\}$$

Γ-convergence of the rate function, [JKM15]

In the limit $\beta\to\infty$, $\rho\to 0$ such that $-\beta^{-1}\log\rho \to \nu$, this function Γ-converges to g_ν:

$$\mathcal{Q} \to \mathbb{R}\cup\{\infty\}, \qquad (q_k)_k \mapsto \frac{1}{\rho} f\big(\beta, \rho, (\tfrac{\rho q_k}{k})_{k\in\mathbb{N}}\big)$$

Explanation of the approximations

- We approximate $f(\beta, \rho, (\rho_k)_k)$ by an ideal gas of clusters, neglecting the "excluded volume":

$$f^{\mathrm{ideal}}(\beta, \rho, (\rho_k)_k) := \sum_{k\in\mathbb{N}} k\rho_k f_k^{\mathrm{cl}}(\beta) + \Big(\rho - \sum_{k\in\mathbb{N}} k\rho_k\Big) f_\infty^{\mathrm{cl}}(\beta) + \frac{1}{\beta}\sum_{k\in\mathbb{N}} \rho_k(\log\rho_k - 1)$$
$$= \sum_{k\in\mathbb{N}} \rho_k \log\frac{\rho_k}{Z^{\mathrm{cl}}(\beta,k)} - \frac{1}{\beta}\sum_{k\in\mathbb{N}}\rho_k + \Big(\rho - \sum_{k\in\mathbb{N}} k\rho_k\Big) f_\infty^{\mathrm{cl}}(\beta),$$

  ($f_k^{\mathrm{cl}}(\beta) = \frac{1}{k}\log Z^{\mathrm{cl}}(\beta,k)$ = free energy per particle in a cluster of size k.)
- We approximate $f^{\mathrm{ideal}}(\beta, \rho, (\frac{\rho q_k}{k})_{k\in\mathbb{N}})$ with $\rho g_\nu(q)$ using two simplifications:
  - cluster internal free energies $\approx$ ground state energies: $f_k^{\mathrm{cl}}(\beta) \approx E_k$.
  - (recall $q_k = k\rho_k/\rho$)

$$\frac{1}{\beta}\sum_{k\in\mathbb{N}} \rho_k(\log\rho_k - 1) = \sum_{k\in\mathbb{N}} \rho_k \frac{\log\rho}{\beta} + \frac{\rho}{\beta}\sum_{k\in\mathbb{N}} \frac{q_k}{k}\Big(\log\frac{q_k}{k} - 1\Big)$$
$$\approx \sum_{k\in\mathbb{N}} \rho_k \frac{\log\rho}{\beta}$$
$$\approx -\rho\sum_{k\in\mathbb{N}} q_k \frac{\nu}{k}.$$

Corollary: convergence of minimisers

Recall

$$g_\nu\big((q_k)_k\big) := \sum_{k\in\mathbb{N}} q_k \frac{E_k - \nu}{k} + \Big(1 - \sum_{k\in\mathbb{N}} q_k\Big) e_\infty .$$

Consequences of Γ-convergence, [JKM15]

In the same limit $\beta \to \infty$, $\rho \downarrow 0$ such that $-\frac{1}{\beta}\log\rho \to \nu$,

- $$\frac{1}{\rho} f(\beta,\rho) \to \min_{\mathcal{Q}} g_\nu =: \mu(\nu),$$
- if ν is not a kink point of μ, then any minimiser of $J_{\beta,\rho}$ converges to the minimiser of g_ν.

- In the temperature-density plane, we look at curves approaching the origin along lines where $\rho = \mathrm{e}^{-\nu/T}$, where $T = 1/\beta$ is the temperature.
- It is easy to see that $\nu \mapsto \mu(\nu) = \inf_{\mathcal{Q}} g_\nu$ is piecewise affine and has at least one kink point. If ν is not a kink point, then g_ν has the unique minimizer $\delta_{k(\nu)}$ (Dirac sequence) with $k(\nu)$ the unique minimizer of $k \mapsto (E_k - \nu)/k$.

Corollary: LLN for cluster sizes

We put $\nu^* = \inf_{N\in\mathbb{N}}[E_N - N\mathrm{e}_\infty] \in (0,\infty)$ ($\approx$ surface energy)

Limiting distributions of cluster sizes, [JKM15]

Let $\nu \in (0,\infty)$ be not a kink point, and fix $\varepsilon > 0$. Then, if β is sufficiently large, ρ sufficiently small and $-\frac{1}{\beta}\log\rho$ is sufficiently close to ν, for boxes Λ_N with volume N/ρ,

$$\lim_{N\to\infty} \mathbb{P}^{(N)}_{\beta,\Lambda_N}\left(\left|\frac{k(\nu)}{\rho}\rho_{k(\nu),\Lambda} - 1\right| > \varepsilon\right) = 0 \quad \text{if } \nu > \nu^*,$$

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Interpretation: In this two-step limit,

- the model has only one cluster size,
- there is at least one "phase transition", possibly much more,
- in the high-temperature phase $\nu \gg 1$, all clusters are singletons,
- in any intermediate phase, all clusters have size $k(\nu)$,
- in the low-temperature phase $\nu < \nu^*$, there are only infinite clusters.

Approximation with ideal mixture

- The approximation with g_ν is difficult to interpret physically, and g_ν has some "unphysical" properties: possibly many phase transitions of $\nu \mapsto \mu(\nu)$, and many minimisers of g_ν in the kinks. We think that just one of these phase transitions is "physical", the others correspond to cross-overs inside the gas phase.

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- These assumptions are on the compactness of the shape of the relevant configurations at positive, but low temperature:
  - The main contribution to the cluster internal energy comes from compact (d-dimensional) configurations,
  - the correction term in the convergence $f_k^{\mathrm{cl}}(\beta) \to f_\infty^{\mathrm{cl}}(\beta)$ is of surface order: $kf_k^{\mathrm{cl}}(\beta) - kf_\infty^{\mathrm{cl}}(\beta) \geq Ck^{1-1/d}$.

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- [JANSEN, K. 2012] proves rigorous bounds for the comparison of the original model with the ideal-mixture model, which are exponentially small in vanishing temperature.

Back to the Gibbs measures from [JANSEN 2016]:

Bounds on (non-)percolation, [JANSEN 2016]

- For $\nu > \nu^*$ and $\rho < \mathrm{e}^{-\beta\nu}$, for all large β, any related Gibbs measure P has no infinite cluster, and the cluster size distribution has exponentially decaying tails.
- For $\nu < \nu^*$ and $\rho > \mathrm{e}^{-\beta\nu}$, for large β, P has an infinite cluster almost surely.
- Conjecture: For some large β and small ρ, there are Gibbs measures that percolate with probability in $(0, 1)$ (known to be true in the $\mathbb{Z}^d$-case!).

Crystallisation: zero temperature

Recall the ground state energy and its limit:

$$E_N := \inf_{\boldsymbol{x} \in (\mathbb{R}^d)^N} U_N(\boldsymbol{x}) \qquad \text{and} \qquad e_0 := \lim_{N \to \infty} \frac{E_N}{N} \in (-\infty, 0).$$

The minimising configurations (the ground states) are shown to approach a crystal in $d = 2$ in [THEIL 2006)] in $d = 2$ (after pioneering works like [HEITMANN/RADIN 1980], [RADIN 1981] and [SÜTŐ 2005]) and in [FLATLEY/THEIL 2015] in $d = 3$, under some technical conditions.

It is widely open to describe how the finite-box configuration approaches the crystal. Most contributions to this question are made in strongly simplifying models.

Here we turn to one dimension and give detailed answers [JANSEN, K., SCHMIDT, THEIL 2020] and [JKST 2021].

The crystalline structure of the ground states for our potential have been shown in [VENTEVOGEL 1978], [GARDNER/RADIN 1979], [RADIN 1984], [RADIN/SCHULMAN 1983]. Potentials that decay at $r \to \infty$ faster than r^{-2} are known not to show crystallization at positive temperature [BLANC/LEWIN 2015].

Note that there is no phase transition in $d = 1$ (similarly to percolation).

We are using classical equilibrium statistical mechanics.

(finite-range) energy for particles $0 = x_1 < x_2 < \cdots < x_N = L$:

$$U_N^{(m)}(\mathbf{x}) = \sum_{0<i<j\le N\,:\,|j-i|\le m} v(x_j - x_i), \qquad m \in \mathbb{N} \cup \{\infty\}.$$

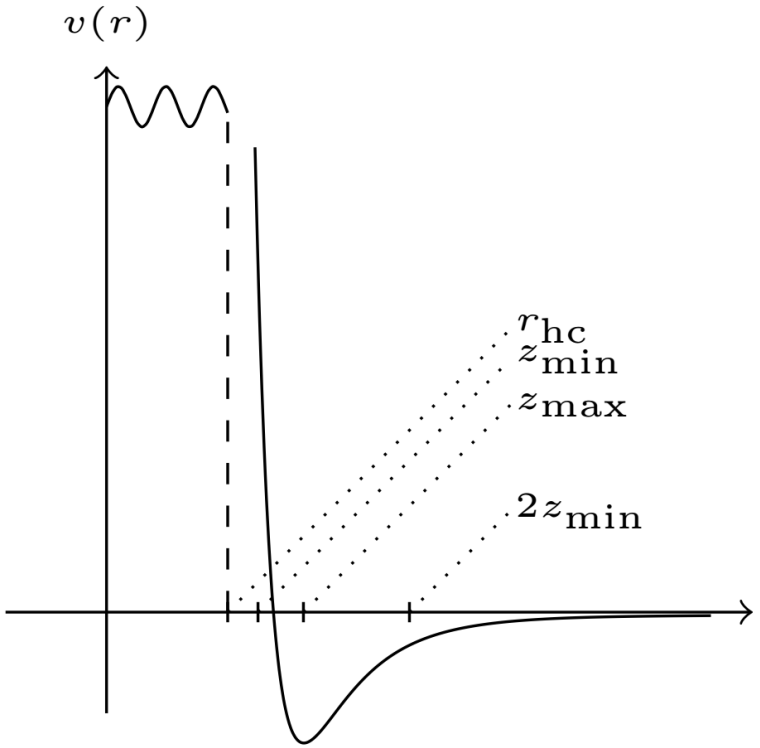
canonical partition function $Z_N^{(m)}(\beta, L)$, canonical Gibbs measure $\mathbb{P}_{N,L}^{(m,\beta)}$.

Free enery per particle:

$$f^{(m)}(\beta, \ell) = -\frac{1}{\beta} \lim_{N\to\infty} \frac{1}{N} \log Z_N^{(m)}(\beta, \ell N).$$

Pressure $p^{(m)}(\beta, \ell) = -\frac{\partial}{\partial \ell} f^{(m)}(\beta, \ell)$.

Assumptions on v



For some $\alpha_1, \alpha_2 > 0$ and $s > 2$,

- $v(z) \geq -\alpha_1 z^{-s}$ for all $z > 0$ and $v(z) + v(z_{\mathrm{max}}) - 2\alpha_1 \sum_{n=2}^{\infty} (nz)^{-s} > 0$ for $z < z_{\mathrm{min}}$.
- v'' is decreasing in $[z_{\mathrm{min}}, z_{\mathrm{max}}]$ and increasing and non-positive in $[2z_{\mathrm{min}}, \infty)$.
- $v''(z) > -\alpha_2 z^{-s-2}$ for $z > r_{\mathrm{c}}$ and $v''(z_{\mathrm{max}}) + \sum_{n=2}^{\infty} n^2 v(nz_{\mathrm{min}}) > 0$.

This is satisfied, e.g., by the Lennard–Jones potential $v(r) = r^{-12} - r^{-6}$.

Cauchy–Born density and surface energy

1. The limiting ground state energy e_0 is equal to $\min_{r>0} W(r) = W(a)$ with the Cauchy–Born density $W(r) = \sum_{k=1}^{m} v(kr)$.
2. The surface energy $e_{\mathrm{surf}} = \lim_{N\to\infty}[E_N - Ne_0] \in (0,\infty)$ exists.

Analogies for $\beta \in (0,\infty)$: With $z_j = x_j - x_{j-1}$,

$$-\frac{1}{\beta}\log\Big(\int_{[0,R]^{N-1}} \mathrm{e}^{-\beta U_N(\mathbf{z})+p\beta\sum_{j=2}^{N} z_j}\,\mathrm{d}\mathbf{z}\Big) = Ng^{(R)}(\beta,p) + g^{(R)}_{\mathrm{surf}}(\beta,p) + o(1),$$

and, for $\beta\to\infty$,

$$g^{(R)}(\beta,0) \to e_0 \qquad \text{and} \qquad g^{(R)}_{\mathrm{surf}}(\beta,0) \to e_{\mathrm{surf}}.$$

We assume that $m = 2$ and suppress it from notation.

Low-temperature asymptotics

(a) For $0 \ll \ell < a$,

$$\lim_{\beta\to\infty} f(\beta,\ell) = W(\ell) \in (a,\infty) \qquad \text{and} \qquad \lim_{\beta\to\infty} p(\beta,\ell) = -W'(\ell) \in (0,\infty).$$

(b) For $\ell \in (a,\infty)$, as $\beta \to \infty$,

$$\begin{aligned} f(\beta,\ell) &= e_0^{(R)}(\beta) - \frac{2}{\beta}\sqrt{\ell-a}\,\mathrm{e}^{-\beta e_{\mathrm{surf}}^{(R)}(\beta)/2}(1+o(1)), \\ p(\beta,\ell) &= \frac{1}{\beta\sqrt{\ell-a}}\,\mathrm{e}^{-\beta e_{\mathrm{surf}}^{(R)}(\beta)/2}(1+o(1)). \end{aligned}$$

In particular, $\lim_{\beta\to\infty} f(\beta,\ell) = W(a) = e_0$.

Cracks and clusters

With a threshold parameter $R > \sup \operatorname{supp}(v)$, we call (x_{j-1}, x_j) a crack (or gap, void, broken bond) if $z_j = x_j - x_{j-1} > R$, and we call groups of x's between cracks clusters.
Let M_N be the number of clusters. If $M_N = n$ then let $0 < i_1 < i_2 \cdots < i_n$ be the indices i such that $z_i > R$. Define

$$\nu_N = \frac{1}{M_N} \sum_{k=1}^{M_N} \delta_{i_k - i_{k-1}} \qquad \text{and} \qquad \widehat{\nu}_N = \frac{1}{M_N - 1} \sum_{j=1}^{N} \mathbb{1}\{z_j > R\} \delta_{z_j - R}.$$

Define, for $\ell > a$ and $\beta \to \infty$,

$$q_{\beta,\ell} = \frac{\mathrm{e}^{-\beta e_{\mathrm{surf}}^{(R)}(\beta)}}{\beta p(\beta, \ell)} = \sqrt{\ell - a}\, \mathrm{e}^{-\beta e_{\mathrm{surf}}^{(R)}(\beta)/2} (1 + o(1)).$$

Low-temperature behaviour of cracks and clusters

For all sufficiently large β, in the limit $N \to \infty$, in distribution under $\mathbb{P}_{N, N\ell}^{(\beta)}$,

$$\frac{M_N}{N} \to q_{\beta,\ell}, \qquad \nu_N \to \mathrm{Geo}\left(\tfrac{q_{\beta,\ell}}{1+q_{\beta,\ell}}\right), \qquad \widehat{\nu}_N \to \mathrm{Exp}(\beta p(\beta, \ell)).$$

The convergences are exponentially fast in N.

We also show that the average spacing in each cluster is a.

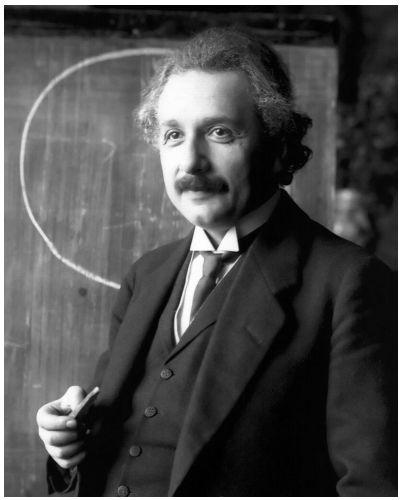
Weierstrass Institute for
Applied Analysis and Stochastics

The interacting Bose gas as a marked point process

Wolfgang König (WIAS Berlin und TU Berlin)

A prediction of 1924

- In 1924, the unknown young physicist SATYENDRA NATH BOSE asked the famous ALBERT EINSTEIN to help him publishing his latest achievement in *Zeitschrift für Physik*.
- Einstein translated the manuscript into German and had published it there for Bose.
- He stressed that the new method is suitable for explaining the quantum mechanics of the ideal gas. He extended the idea to atoms in a second paper: he predicted the existence of a previously unknown state of matter, now known as the Bose–Einstein condensate.



ALBERT EINSTEIN (1879-1955) in 1921

SATYENDRA NATH BOSE (1894-1974) in 1925

- An experimental realisation had to wait until 1995, where some ten thousands of atoms appeared in that condensate at a temperature of 10^{-9} K. $\Longrightarrow$ Nobel Prize in 2001

A quantum system of N particles in a box $\Lambda \subset \mathbb{R}^d$ with mutually repellent interaction is described by the Hamilton operator

$$\mathcal{H}_N^{(\Lambda)} = -\sum_{i=1}^{N} \Delta_i + \sum_{1 \le i < j \le N} v(x_i - x_j), \qquad x_1, \dots, x_N \in \Lambda.$$

- The kinetic energy term Δ_i acts on the i-th particle.
- The pair potential $v \colon \mathbb{R}^d \to [0, \infty)$ is symmetric and has (for simplicity) compact support.

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We concentrate on Bosons and introduce a symmetrisation. The symmetrised trace of $\exp\{-\beta \mathcal{H}_N^{(\Lambda)}\}$ at fixed temperature $1/\beta \in (0, \infty)$ in Λ is the

$$\text{partition function:} \qquad Z_N(\beta, \Lambda) = \mathrm{Tr}_+\big(\exp\{-\beta \mathcal{H}_N^{(\Lambda)}\}\big).$$

(the trace of the projection on the set of symmetric ($=$ permutation invariant) wave functions).

We will be working in the thermodynamic limit and will take a centred box Λ_N with volume N/ρ with $\rho \in (0, \infty)$ the particle density.

Abstract main strategy (1)

Our overall goal is to make the partition function $Z_N(\beta, \Lambda_N)$ amenable to a large-deviation analysis by rewriting it in a form like

$$Z_N(\beta, \Lambda_N) = \mathbb{E}\Big[\mathrm{e}^{-|\Lambda_N| F(\mathfrak{X}_N)} \mathbb{1}_{\{G(\mathfrak{X}_N)=c\}}\Big],$$

where $c \in \mathbb{R}$, and F and G are continuous and bounded functions on some nice state space $\mathcal{X}$,

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$$Z_N(\beta, \Lambda_N) = \mathbb{E}\Big[\mathrm{e}^{-|\Lambda_N| F(\mathfrak{R}_N)} \mathbb{1}_{\{G(\mathfrak{R}_N)=c\}}\Big],$$

where $c \in \mathbb{R}$, and F and G are continuous and bounded functions on some nice state space $\mathcal{X}$, and $(\mathfrak{R}_N)_{N\in\mathbb{N}}$ is an $\mathcal{X}$-valued sequence of random variables that satisfy a large-deviation principle:

$$\lim_{N\to\infty} \frac{1}{|\Lambda_N|} \log \mathbb{P}(\mathfrak{R}_N \in A) = -\inf_A I, \qquad A \subset \mathcal{X},$$

for some rate function $I\colon \mathcal{X} \to [0, \infty]$.

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Varadhan's lemma then implies that

$$\lim_{N\to\infty} \frac{1}{|\Lambda_N|} \log \mathbb{E}\Big[\mathrm{e}^{-|\Lambda_N| F(\mathfrak{R}_N)} \mathbb{1}_{\{G(\mathfrak{R}_N)=c\}}\Big]$$
$$= -\inf\Big\{F(R) + I(R)\colon R \in \mathcal{X}, G(R) = c\Big\}.$$

(If G is only lower semi-continuous, one should have '$G(R) \le c$' in the formula, and we have *a priori* only '$\le$' instead of '$=$'.)

Abstract main strategy (2)

We need four main reformulation steps:

- Feynman-Kac formula: N interacting Brownian bridges with symmetrised initial-terminal condition,
- Cycle expansion: Reorganisation in terms of the cycle lengths of the concatenated Brownian bridges,
- Marked Poisson point process: Rewrite in terms of a PPP with the cycles attached as marks.
- Stationary empirical field: Translation into the stationary empirical field.

The stationary empirical field, $\mathfrak{R}_N$, will turn out to be the above mentioned large-deviation reference process.

The first step is classic, the second well-known, and the third and fourth stem from [ADAMS, COLLEVECCHIO, K. (2011)] in this context.

A Brownian bridge B in Λ_N with generator Δ and time horizon $[0,\beta]$, starting from x and terminating at y under $\mu_{x,y}^{(\beta)}$:

$$\mu_{x,y}^{(\beta)}(A) = \mathbb{P}_x(B \in A; B_\beta \in \mathrm{d}y), \qquad A \subset \mathcal{C}([0,\beta] \to \mathbb{R}^d).$$

The operator $\mathrm{e}^{\beta\Delta}$ has density $\mu_{x,y}^{(\beta)}$ in the sense that

$$\mathrm{e}^{\beta\Delta}(f)(x,y)\text{“} = \text{”}\mu_{x,y}^{(\beta)}(\mathrm{d}f), \qquad f \in \mathcal{C}([0,\beta] \to \mathbb{R}^d).$$

The total mass of $\mu_{x,x}^{(\beta)}$ is $(4\pi\beta)^{-d/2}$.

In $\mathcal{H}_N$, we have N independent Brownian bridges $B^{(1)}, \dots, B^{(N)} \in \mathcal{C}([0,\beta] \to \mathbb{R}^d)$. The symmetrisation is expressed by a sum over all permutations σ of $1, \dots, N$ with the condition $B_\beta^{(i)} = B_0^{(\sigma(i))}$.

The pair interaction is

$$\mathcal{G}_N(\beta) = \sum_{1 \le i < j \le N} \int_0^\beta \mathrm{d}s\, v\big(|B_s^{(i)} - B_s^{(j)}|\big).$$

Feynman-Kac formula [GINIBRE (1970)]:

For $\mathrm{bc} \in \{\mathrm{Dir}, \mathrm{per}\}$, any $N \in \mathbb{N}$ and any measurable bounded set Λ,

$$Z_N^{(\mathrm{bc})}(\beta, \Lambda) = \frac{1}{N!} \sum_{\sigma \in \mathfrak{S}_N} \int_{\Lambda^N} \mathrm{d}x_1 \cdots \mathrm{d}x_N \bigotimes_{i=1}^{N} \mu_{x_i, x_{\sigma(i)}}^{(\beta, \mathrm{bc})} \Big[\mathrm{e}^{-\mathcal{G}_N(\beta)} \Big],$$

where $\mathfrak{S}_N$ is the set of permutations of $1, \ldots, N$.

Every permutation σ with the same cycle structure gives the same contribution. Indeed, concatenate the Brownian bridges along every cycle and carry out the integrals over the corresponding $x_i \in \Lambda_N$. By the Markov property,

$$\int_{\mathbb{R}^d} \mu_{x,y}^{(\beta)}(\mathrm{d}f_1) \mu_{y,z}^{(\beta)}(\mathrm{d}f_2)\, \mathrm{d}y = \mu_{x,z}^{(2\beta)}(\mathrm{d}(f_1 \diamond f_2)), \qquad f_1, f_2 \in \mathcal{C}([0, \beta] \to \mathbb{R}^d),$$

where $f_1 \diamond f_2 \in \mathcal{C}([0, 2\beta] \to \mathbb{R}^d)$ is the concatenation of f_1 and f_2.
We obtain a random number of cycles of motions with random lengths, with total sum of lengths equal to N.

Cycle expansion:

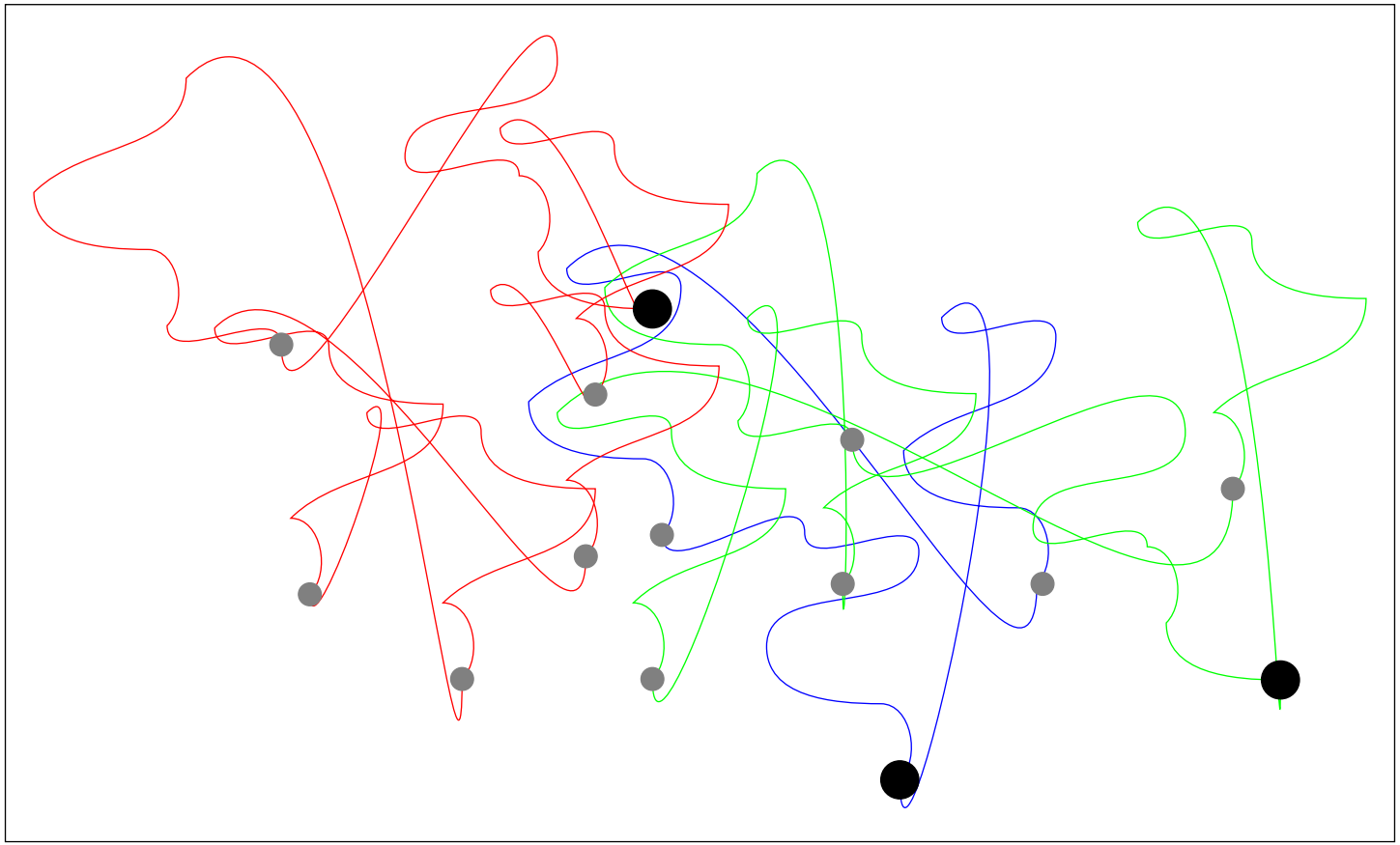
For any $N \in \mathbb{N}$ and any measurable bounded set Λ,

$$Z_N(\beta,\Lambda) = \sum_{\substack{\lambda_1,\lambda_2,\cdots\in\mathbb{N}\\ \sum_k k\lambda_k = N}} \bigotimes_{k\in\mathbb{N}} \left(\mathbb{E}_\Lambda^{(\beta k)}\right)^{\otimes\lambda_k} \left[\mathrm{e}^{-\mathcal{G}_{N,\beta}}\right] \prod_{k\in\mathbb{N}} \frac{(4\pi\beta k)^{-d\lambda_k/2}|\Lambda|^{\lambda_k}}{\lambda_k! k^{\lambda_k}},$$

where $\mathbb{E}_\Lambda^{(\beta k)} = \frac{1}{|\Lambda|}\int_\Lambda \mathrm{d}x (4\pi\beta k)^{d/2}\mu_{x,x}^{(\beta k)}$ is the (normalised) expectation w.r.t. a Brownian bridge from x to x, and x is uniformly distributed over Λ.

- λ_k is the number of cycles of length k, that is, the number of Brownian bridges with time horizon $[0,\beta k]$.
- $\mathcal{G}_N(\beta)$ summarizes all the interaction between any two different parts of any cycle(s).
- The last term summarizes the combinatorics (number of permutations with given cycle structure) and the normalisations.

Illustration



Bose gas consisting of 14 particles, organised in three Brownian cycles, assigned to three Poisson points. The red cycle contains six particles, the green and the blue each four.

We are heading towards a probabilistic, spatial description of the partition function in terms of a

$$\text{marked Poisson point process} \qquad \omega_{\mathrm{P}} = \sum_{x \in \xi_{\mathrm{P}}} \delta_{(x, B_x)}.$$

- Each Poisson point $x \in \xi_{\mathrm{P}}$ has a Brownian cycle B_x starting and ending at x as a mark.
- ω_{P} is a point process on $\mathbb{R}^d \times E$, where $E = \bigcup_{k \in \mathbb{N}} \mathcal{C}_k$ is the mark space, and $\mathcal{C}_k = \mathcal{C}([0, \beta k] \to \mathbb{R}^d)$ is the set of marks of length k.
- We choose its intensity measure as $\sum_{k \in \mathbb{N}} \frac{1}{k} \mathrm{Leb}(\mathrm{d}x) \otimes \mu_{x,x}^{(k\beta)}(\mathrm{d}f)$.

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- We choose its intensity measure as $\sum_{k \in \mathbb{N}} \frac{1}{k} \mathrm{Leb}(\mathrm{d}x) \otimes \mu_{x,x}^{(k\beta)}(\mathrm{d}f)$.

Alternatively, the intensity measure of ξ_{P} is equal to $q\mathrm{Leb}$, where

$$q = \sum_{k \in \mathbb{N}} q_k \qquad \text{where} \quad q_k = (4\pi\beta)^{-d/2} k^{-1-d/2} = \frac{1}{k} \mu_{x,x}^{(\beta k)}(\mathcal{C}_k).$$

Given ξ_{P}, the marks B_x with $x \in \xi_{\mathrm{P}}$ have length with probability q_k/q and then have the law $\mu_{x,x}^{(k\beta)}/kq_k$ on $\mathcal{C}_k$.

For configurations $\omega = \sum_{x\in\xi} \delta_{(x,f_x)} \in \Omega$,

$$N_\Lambda^{(\ell)}(\omega) = \sum_{x\in\Lambda\cap\xi} \ell(f_x) = \text{number of particles at points in } \Lambda,$$

where $\ell(f_x)$ is the length (= particle number) of the cycle f_x. The interaction is expressed as

$$\Phi_{\Lambda,\Lambda'}(\omega) = \sum_{x\in\xi\cap\Lambda, y\in\xi\cap\Lambda'} T_{x,y}(f_x, f_y),$$

where

$$T_{x,y}(f_x, f_y) = \frac{1}{2} \sum_{i=1}^{\ell(f_x)} \sum_{j=1}^{\ell(f_y)} V(f_{x,i}, f_{y,j}), \qquad x, y \in \xi,\ f_x, f_y \in \mathcal{C},$$

and $f_{x,i}(\cdot) = f_x((i-1)\beta + \cdot)|_{[0,\beta]}$ is the i-th *leg* of a function $f_x \in \mathcal{C}$, and

$$V(f,g) = \int_0^\beta v(|f(s) - g(s)|)\,\mathrm{d}s.$$

Lemma [ADAMS/COLLEVECCHIO/K. 2011]

$$Z_N(\beta,\Lambda) = \mathrm{e}^{|\Lambda|q}\, \mathbb{E}\big[\mathrm{e}^{-\Phi_{\Lambda,\Lambda}(\omega_{\mathrm{P}})} \mathbb{1}\{N_\Lambda^{(\ell)}(\omega_{\mathrm{P}}) = N\}\big].$$

For a configuration $\omega \in \Omega$, let $\omega^{(N)}$ be the Λ_N-periodic continuation of the restriction of ω to Λ_N. The stationary empirical field is defined as

$$\mathfrak{R}_N = \frac{1}{|\Lambda_N|} \int_{\Lambda_N} \mathrm{d}y \, \delta_{\theta_y \omega_{\mathrm{P}}^{(N)}} \qquad (\text{with } \theta_y = \text{shift operator.})$$

Then $\mathfrak{R}_N$ is a random element of the set $\mathcal{P}_\theta$ of stationary marked random point fields.

Theorem. [GEORGII/ZESSIN (1994)]

$(\mathfrak{R}_N)_{N\in\mathbb{N}}$ satisfies a large-deviation principle with rate function

$$I(P) = \lim_{N\to\infty} \frac{1}{|\Lambda_N|} H\big(P_{\Lambda_N} \,\big|\, \omega_{\mathrm{P}}|_{\Lambda_N}\big).$$

I is affine, lower semicontinuous and has compact level sets.

Introduce $U = [\frac{1}{2}, \frac{1}{2}]^d$ and, for configurations $\omega = \sum_{x\in\xi} \delta_{(x,f_x)}$,

$$N_U(\omega) = |U \cap \xi| \qquad \text{and} \qquad N_U^{(\ell)}(\omega) = \sum_{x\in U\cap\xi} \ell(f_x),$$

where $\ell(f_x)$ is the length (= time horizon) of the cycle f_x. The interaction is expressed as

$$\Phi(\omega) = \frac{1}{2} \sum_{x\in U\cap\xi} \sum_{y\in\xi} \sum_{i=0}^{\ell(f_x)-1} \sum_{j=0}^{\ell(f_y)-1} \mathbb{1}_{\{(x,i)\neq(y,j)\}} \int_0^\beta \mathrm{d}s\, v\big(|f_x(i\beta+s)+x-f_y(j\beta+s)-y|\big).$$

Lemma.

$$Z_N(\beta,\Lambda_N) = \mathrm{e}^{|\Lambda_N|q} \mathbb{E}\Big[\mathrm{e}^{-|\Lambda_N|\langle \mathfrak{K}_N, \Phi\rangle} \mathbb{1}_{\{\langle \mathfrak{K}_N, N_U^{(\ell)}\rangle = \rho\}}\Big].$$

- One of the two sums over $x, y \in \Lambda_N$ goes into the definition of $\mathfrak{K}_N$, hence the x-sum in $\Phi(\omega)$ is only over U.
- The condition $\langle \mathfrak{K}_N, N_U^{(\ell)}\rangle = \rho$ says that the total length of all cycles starting in U is equal to N.

Assume that $\int v(|x|)\,\mathrm{d}x < \infty$ and that $\limsup_{r\to\infty} v(r)r^h < \infty$ for some $h > d$.

Theorem B:

For any $\beta, \rho \in (0,\infty)$,

$$\limsup_{N\to\infty} \frac{1}{|\Lambda_N|} \log Z_N(\beta,\Lambda_N) \le q - \inf\Big\{I(P) + \langle P,\Phi\rangle \colon P \in \mathcal{P}_\theta, \langle P, N_U^{(\ell)}\rangle \le \rho\Big\},$$

$$\liminf_{N\to\infty} \frac{1}{|\Lambda_N|} \log Z_N(\beta,\Lambda_N) \ge q - \inf\Big\{I(P) + \langle P,\Phi\rangle \colon P \in \mathcal{P}_\theta, \langle P, N_U^{(\ell)}\rangle = \rho\Big\}.$$

- The equality $\langle \mathfrak{R}_N, N_U^{(\ell)}\rangle = \rho$ is turned into an inequality $\langle P, N_U^{(\ell)}\rangle \le \rho$ in the limit superior (in accordance with Fatou's lemma), but not in the limit inferior.
- P stands for a stationary marked random point field $\sum_{x\in\xi} \delta_{(x,f_x)}$. Its mark f_x at x is a random continuous function $[0,\beta\ell(f_x)] \to \mathbb{R}^d$, starting at ending at x.
- The expected total length $\langle P, N_U^{(\ell)}\rangle$ of all the points in the unit box U is not larger than ρ (this is the only dependence on the particle density).
- $\langle P,\Phi\rangle$ is the expected interaction in the configuration.
- $I(P)$ measures how probable P is by comparison to the above marked Poisson process as a reference process.

In the phase

$$\mathcal{D}_v = \left\{(\beta,\rho) \in (0,\infty)^2 \colon (4\pi\beta)^{-d/2} \geq \rho \mathrm{e}^{\beta\rho \int v(|x|)\,\mathrm{d}x}\right\}$$

we find additional estimates to identify the limit:

Lemma.

For any $N \in \mathbb{N}$ and any measurable bounded Λ,

$$\frac{Z_{N+1}(\beta,\Lambda)}{Z_N(\beta,\Lambda)} \geq (4\pi\beta)^{-d/2} \frac{|\Lambda|}{N+1} \mathrm{e}^{-N\beta \int v(|x|)\,\mathrm{d}x/|\Lambda|}.$$

This yields an upper bound for the free energy ...

Corollary 1.

For any $\beta, \rho \in (0,\infty)$,

$$f(\beta,\rho) \leq \frac{\rho}{\beta} \log\left(\rho(4\pi\beta)^{d/2}\right) + \rho^2 \int v(|x|)\,\mathrm{d}x.$$

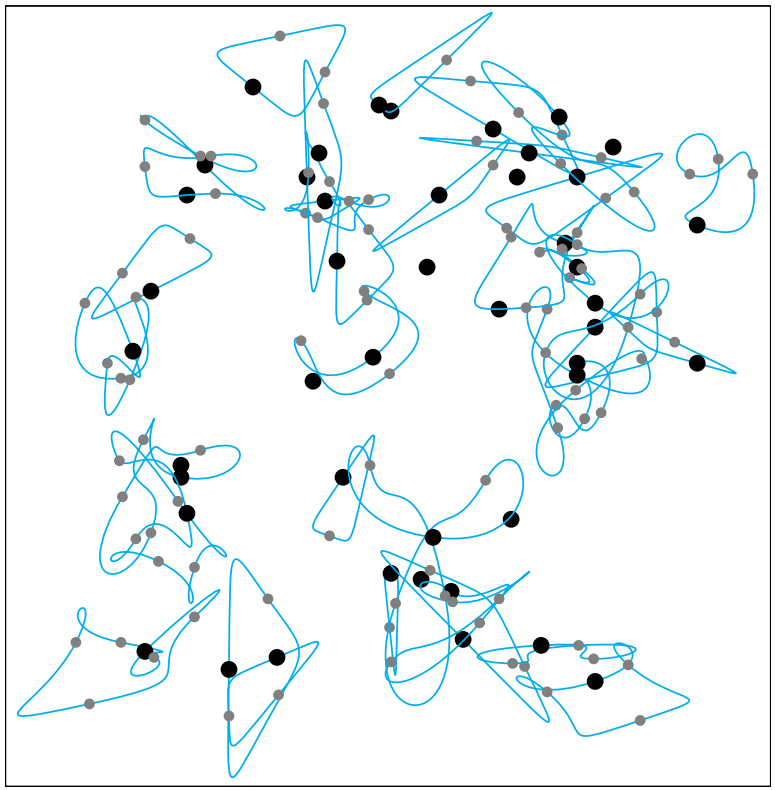
... and enables us to close the gap in Theorem B:

Corollary 2.

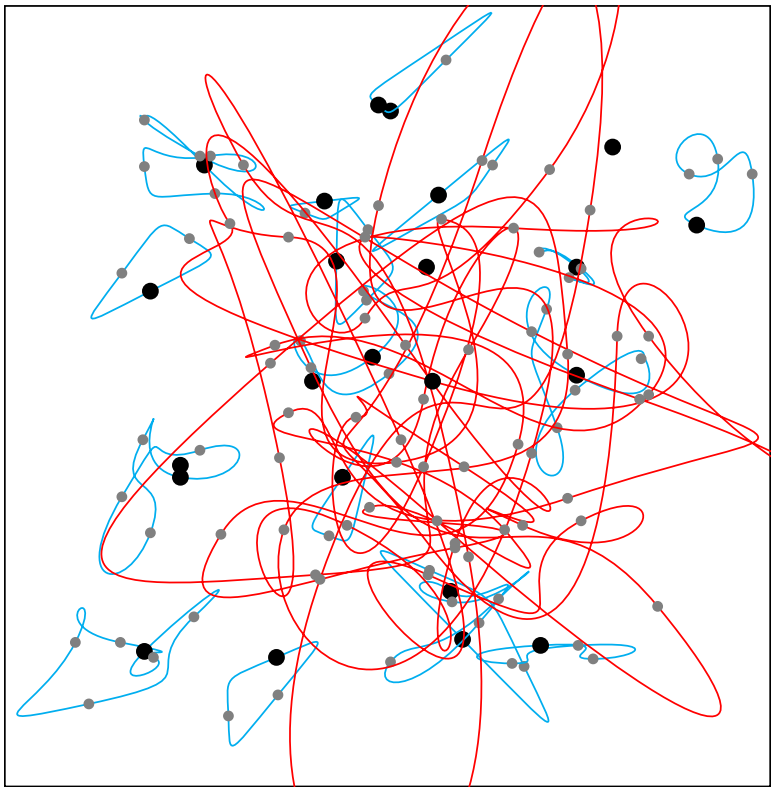
If $(\beta,\rho) \in \mathcal{D}_v$, then

$$\liminf_{N\to\infty} \frac{1}{|\Lambda_N|} \log Z_N(\beta,\Lambda_N) \geq q - \inf\left\{I(P) + \langle P, \Phi\rangle \colon P \in \mathcal{P}_\theta, \langle P, N_U^{(\ell)}\rangle \leq \rho\right\}.$$

Illustration of condensate phase transition



Subcritical (low ρ) Bose gas
without condensate



Supercritical (large ρ) Bose gas
with additional condensate (red)

The free case $v \equiv 0$ is much simpler. No space, no point processes, only cycle lengths:

$$\chi^{(v=0)}(\beta,\rho) = \inf\Big\{H(m|q)\colon m \in [0,\infty)^{\mathbb{N}}, \sum_{k\in\mathbb{N}} k m_k = \rho\Big\},$$

where $H(m|q) = \sum_k (q_k - m_k + m_k \log \frac{m_k}{q_k})$ is the relative entropy of the sequence $m = (m_k)_{k\in\mathbb{N}}$ with respect to $q = (q_k)_{k\in\mathbb{N}}$.

- m_k = effective density of points with cycles of length k,
- q_k = *a priori* k-cycle density (i.e., in the reference measure).

Euler–Lagrange equation: $m_k = q_k \mathrm{e}^{\alpha k}$ for $k \in \mathbb{N}$ with $\alpha \in \mathbb{R}$ the Lagrange multiplier.

$$\sum_k k m_k = \rho \qquad \Longrightarrow \qquad \alpha \le 0$$

Largest achievable value of ρ is

$$\rho_{\mathrm{c}}(\beta) = \sum_{k\in\mathbb{N}} k q_k = (4\pi\beta)^{-d/2}\zeta(d/2) \begin{cases} = \infty & \text{if } d \le 2, \\ < \infty & \text{if } d \ge 3. \end{cases}$$

Open conjectures

1. '$=$' holds true for any ρ.
2. Existence of minimizer P $\quad\Longleftrightarrow\quad$ absence of condensate.
3. There is a critical density $\rho_{\mathrm{c}} > 0$ (finite if and only if $d \geq 3$) such that a minimizer P exists for $\rho < \rho_{\mathrm{c}}$ and does not exist for $\rho > \rho_{\mathrm{c}}$.
4. That is,
$$\rho_{\mathrm{c}} = \sup\big\{\rho \in (0,\infty) \colon \chi(\beta,\rho) \text{ has a minimizer } P\big\}.$$
5. There is a variational formula on an extended space that describes also the condensate.

A great part of this (namely, (1) and (5)) has recently been proved for a simplified model (deterministic boxes instead of random bridges) in [COLLIN/JAHNEL/K. (2022)].

Functional analytic definition of BEC: Fix x_1 and x_2 and consider the two-point density matrix

$$\gamma_N(x_1, x_2) = \frac{1}{Z_N(\beta, \Lambda_N)} \frac{1}{N!} \sum_{\sigma \in \mathfrak{S}_N} \int_{\Lambda^N} \mathrm{d}x_3 \cdots \mathrm{d}x_N \bigotimes_{i=1}^{N} \mu^{(\beta)}_{x_i, x_{\sigma(i)}} \left[\mathrm{e}^{-\mathcal{G}_N(\beta)} \right].$$

Let K_N be the integral operator with kernel γ_N. Then

BEC holds $\quad :\Longleftrightarrow \quad$ K_N has an eigenvalue $\asymp N$.

Conjecture

BEC holds $\quad \Longleftrightarrow \quad$ Macroscopic cycles matter.

True for some mean-field models, see [Sütő (1993)], [Sütő (2002)], but disproved in some example [Ueltschi (2006)]

Literature remarks

- Vast literature in physics and mathematics, many different ansatzes
- Many results for simplified models, mostly existence of phase transition
- LIEB, SEIRINGER, SOLOVEJ, YNGVASSON (1999-2005) zero temperature, dilute-limit approximation with Gross–Pitaevski formula
- BENFATTO, CASSANDRO, MEROLA, PRESUTTI (2005): various combinatorics for free gas
- BETZ, UELTSCHI, ZEINDLER, ... (2008-2012): random geometric permutations: dropping interaction between cycles, varying q_k and type of interaction.
- BETZ, QUITMANN, TAGGI,... (2014 –): various models of random loop ensembles, reflection positivity (a correlation inequality)
- FRÖHLICH, KNOWLES, SCHLEIN, SOHINGER, DEUCHERT, SEIRINGER... (2017 –): various rescalings of box sizes, interaction lengths etc. (e.g., semi-classical limit with HARTREE approximation)
- FICHTNER, ZAGREBNOV ,...: point process approaches
- POGHOSYAN/ZESSIN, PhD students of Zessin (2013 –): construction of marked Gibbs measures
- ARMENDARIZ, PABLO FERRARI, YUHJTMAN (2019), VOGEL (2021): Brownian interlacement approach