Weierstrass Institute for
Applied Analysis and Stochastics

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The free energy of the interacting Bose gas, loops and interlacements

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SPP2265
Random Geometric Systems

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Hamilton operator for a quantum system of N particles in a box $\Lambda \subset \mathbb{R}^d$ with mutually repellent pair interaction:

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

- The kinetic energy term Δ_i acts on the i-th particle.
- The pair potential $v\colon \mathbb{R}^d \to [0, \infty)$ measurable. (Later assumed to be continuous, bounded, compactly supported and superstable.)

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We describe Bosons and introduce a symmetrisation at temperature $1/\beta$ in a centred box Λ:

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.

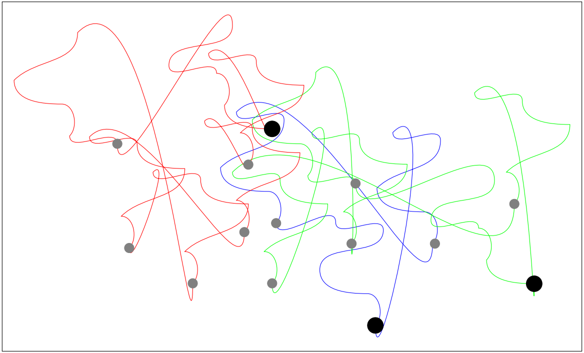
Free energy per volume in the thermodynamic limit:

$$\mathrm{f}(\beta, \rho) = \lim_{N \to \infty} \frac{1}{|\Lambda_N|} \log Z_N(\beta, \Lambda_N), \qquad |\Lambda_N| \sim N/\rho.$$

Purpose of this talk: Derive a formula for $\mathrm{f}(\beta, \rho)$, based on a path-integral representation in terms of the Brownian loop soup.

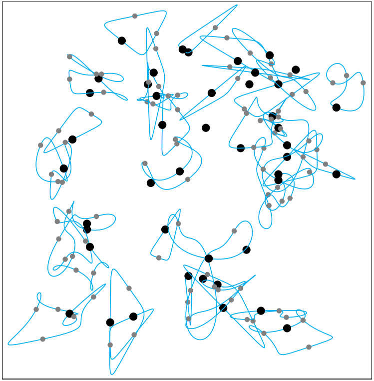
- Unterstanding the conjectured Bose–Einstein condensation phase transition is one of the great open problems in mathematical physics.
- Definition of BEC is more tricky than just non-analyticity of $\mathrm{f}(\beta, \cdot)$.
- Connection with Brownian loops goes back to a vaguely formulated idea from [Feynman 1953].
- Mathematical foundation of loop soup representations due to [Ginibre 1970]; little used in proofs yet in the analysis / mathphys literature on the Bose gas.
- Driving force (not only) for probabilists: Bose–Einstein condensate $\Longleftrightarrow$ long loops?
- Brownian loop soup was introduced also in [Lawler/Werner 2004] for studying conformal invariance in $d = 2$.
- We consider periodic boundary condition and Dirichlet zero boundary condition, but suppress this in this talk.

The Bose gas can be written as a random ensemble of Brownian cycles (bridges) $B^{(k,i)}$ of length k, $i = 1, \dots, l_k$ with $N = \sum_{k \in \mathbb{N}} k l_k$ particles.

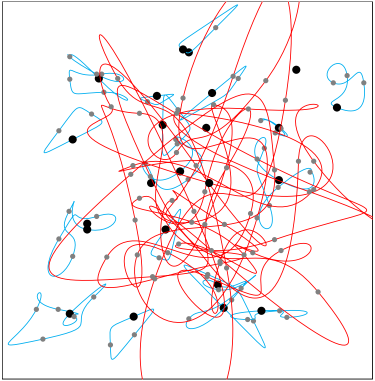


Bose gas consisting of 14 particles, organised in three Brownian cycles, assigned to three Poisson points. The red cycle contains six particles, the green and the blue each four.

The big conjecture is that, for $d \geq 3$ and large enough ρ, in the loop soup a macroscopic part of particles emerge in long loops, the conjectured condensate:



Subcritical (low ρ) Bose gas
without condensate



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

marked point process $\omega = \sum_{x\in\xi} \delta_{(x,f_x)} \in \mathcal{L} = \mathcal{M}_{\mathbb{N}_0}(\mathbb{R}^d \times \mathcal{C}^{(\circlearrowleft)})$

with mark space $\mathcal{C}^{(\circlearrowleft)} = \bigcup_{k\in\mathbb{N}} \mathcal{C}_k^{(\circlearrowleft)}$, where $\mathcal{C}_k = \mathcal{C}([0,\beta k] \to \mathbb{R}^d)$, and $\mathcal{C}_k^{(\circlearrowleft)} = \{f \in \mathcal{C}_k : f(\beta\ell(f)) = f(0)\}$ is the set of marks of length= particle number $\ell(f) = k$.

number of particles at points in Λ : $\quad \mathfrak{N}_\Lambda^{(\ell)}(\omega) = \sum_{x\in\Lambda\cap\xi} \ell(f_x).$

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

where

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

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

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

We pick the reference PPP $\omega_{\rm P}$ as a PPP on $\mathbb{R}^d \times \mathcal{C}^{\circlearrowleft}$ with distribution Q and intensity measure

$$\nu_\Lambda(\mathrm{d}x, \mathrm{d}f) = \sum_{k\in\mathbb{N}} \frac{1}{k} \mathrm{Leb}(\mathrm{d}x) \otimes \mu_{x,x}^{(k\beta)}(\mathrm{d}f),$$

where

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

is the Brownian bridge measure with generator Δ and time horizon $[0,\beta]$, starting from x and terminating at y. It has total mass $(4\pi\beta)^{-d/2}$. Hence,

$$\overline{q} = \frac{1}{|\Lambda_N|} \nu_\Lambda(\Lambda \times \mathcal{C}^{(\circlearrowleft)}) = (4\pi\beta)^{-d/2} \sum_{k\in\mathbb{N}} k^{-1-d/2}.$$

Here is our starting point:

PPP-representation [Adams/Collevecchio/K. 2011]

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

- Extension of state space for handling long loops.
- for simple random walk [SZNITMAN (2010]; for Brownian motions [SZNITMAN (2013)]
- prerunners for Bose gas: [AMENDARIZ, FERRARI, YUHJTMAN 2021], [VOGEL 2023]

Short definition: Homogeneous PPP on the set $\mathcal{S} = \mathcal{M}_{\mathbb{N}_0}(\mathcal{C}_\infty)$ of point measures on interlacements,

$$\mathcal{C}_\infty = \Big\{ g \in \mathcal{C}(\mathbb{R} \to \mathbb{R}^d) \colon \{ g(k\beta) \colon k \in \mathbb{Z} \} \text{ is locally finite} \Big\},$$

with Gaussian increments between the time points $\beta\mathbb{Z}$, interpolated by Brownian bridges.

Distribution: $\mathtt{R}$.

Parameters: β and $u =$ expected number of particles in $U = [-\frac{1}{2}, \frac{1}{2}]^d$.

We see the product of

$$\mathcal{L} = \mathcal{M}_{\mathbb{N}_0}(\mathbb{R}^d \times \mathcal{C}^{(\circlearrowleft)}) \qquad \text{and} \qquad \mathcal{S} = \mathcal{M}_{\mathbb{N}_0}(\mathcal{C}_\infty)$$

as the set of point processes of loops and interlacements,

$$\mathcal{L} \times \mathcal{S} = \mathcal{M}_{\mathbb{N}_0}([\mathbb{R}^d \times \mathcal{C}^{(\circlearrowleft)}] \cup \mathcal{C}_\infty).$$

For a box W, we distinguish loops according to whether they are entirely contained in W or not. In the latter case, we shred them into the pieces from entering W till exiting W, but we never cut legs.

restricted projection operator of loops in a box W:

$$\Pi_W^{(\mathcal{L})}(\omega) = \sum_{x\in\xi:\ f_x(k\beta)\in W\ \forall k\in[\ell(f_x)]} \delta_{(x,f_x)},$$

shredding operator on interlacements (there is also a loop-version $\Pi_W^{(\mathcal{S})}(\omega)$):

$$\Pi_W^{(\mathcal{S})}(\varpi) = \sum_{g\in\Gamma}\sum_{i\in\Gamma_W(g)} \delta_{g_i} \in \mathcal{S}_W = \mathcal{M}_{\mathbb{N}_0}(\mathcal{C}_W) \qquad \varpi = \sum_{g\in\Gamma}\delta_g \in \mathcal{S},$$

Joint projection operator: $\Pi_W = (\Pi_W^{(\mathcal{L})}, \Pi_W^{(\mathcal{S})})$.

boundary-shred operator

$$\partial\Pi_W^{(\mathcal{S})}(\varpi) = \sum_{g\in\Gamma}\sum_{i\in\Gamma_W(g)} \delta_{(g(k_1\beta),k_2-k_1,g(k_2\beta))} \in \mathcal{T}_W = \mathcal{M}_{\mathbb{N}_0}(W\times\mathbb{N}\times W^{\mathrm{c}}),$$

We aim at a formula of the form (with energy F and entropy I)

$$\mathrm{f}(\beta,\rho) = \overline{q} - \inf\Big\{F(P) + I(P)\colon P \in \mathcal{M}_1^{(\mathrm{s})}(\mathcal{L}\times\mathcal{S}), \langle P, \mathfrak{N}_U^{(\ell)}\rangle = \rho\Big\}.$$

Here is the entropy term.

Notation: $\mathtt{R}_W(\mu,\cdot)$ = regular version of the conditional distribution of $\Pi_W^{(\mathcal{S})}(\mathtt{R})$ given $\partial\Pi_W^{(\mathcal{S})}(\mathtt{R}) = \mu$. (There is an explicit formula; it does not depend on u.)

Joint specific relative entropy density

The following limit exists for any $P \in \mathcal{M}_1^{(\mathrm{s})}(\mathcal{L}\times\mathcal{S})$ with finite expected particle number in U (with $W = W_R = [-R,R]^d$):

$$\mathrm{h}^{(\mathcal{L},\mathcal{S})}(P \mid \mathtt{Q}\times\mathtt{R}) = \lim_{R\to\infty} \frac{1}{|W|} H_{\mathcal{L}_W\times\mathcal{S}_W}\Big(\Pi_W(P) \,\Big|\, \Pi_W^{(\mathcal{L})}(P) \otimes [\partial\Pi_W^{(\mathcal{S})}(P)\otimes \mathtt{R}_W]\Big).$$

$\mathrm{h}^{(\mathcal{L},\mathcal{S})}$ is lower semi-continuous and affine. Moreover, for any sequence $(K_R)_{R\in\mathbb{N}}$ of compact sets $K_R \subset \mathcal{T}_{W_R}$, the restricted level set is compact for any $c\in\mathbb{R}$:

$$\bigcap_{R\in\mathbb{N}} \big\{P \in \mathcal{M}_1^{(\mathrm{s})}(\mathcal{L}\times\mathcal{S})\colon \partial\Pi_{W_R}^{(\mathcal{S})}(P) \in K_R, \mathrm{h}^{(\mathcal{L},\mathcal{S})}(P \mid \mathtt{Q}\otimes\mathtt{R}) \le c\big\}.$$

- Centred box Λ_N with volume $\sim N/\rho$.
- Regular decomposition $\Lambda_N = \bigcup_{z\in Z_{N,R}} z + W_R$, with $Z_{N,R} \subset 2R\mathbb{Z}^d$.
- $\mathfrak{N}_{\Lambda_N}^{(\neg R)}$ = number of particles in loops that have particles only in one of the $z + W_R$.
- $\mathfrak{N}_{\Lambda_N}^{(R)}$ = number of particles in loops that have particles in more than one of the $z + W_R$.
- $F_U(\omega, \varpi)$ = interaction between any particle in $U = [-\frac{1}{2}, \frac{1}{2}]^d$ and all others.
- transformed probability measure

$$\mathrm{d}\widehat{\mathtt{Q}}^{(\Lambda,\mathrm{bc})} = \frac{\mathrm{e}^{-\Phi_{\Lambda,\Lambda}}}{\widehat{Z}_N^{(\mathrm{bc})}(\Lambda)}\,\mathrm{d}\mathtt{Q}^{(\Lambda,\mathrm{bc})}.$$

Constrained free energy

In the limit as $N \to \infty$, followed by $R \to \infty$, the pair $\frac{1}{|\Lambda_N|}(\mathfrak{N}_{\Lambda_N}^{(R)}, \mathfrak{N}_{\Lambda_N}^{(\neg R)})$ satisfies under the measure $\widehat{\mathtt{Q}}^{(\Lambda_N,\mathrm{bc})}$ an LDP on $\{(\rho_1,\rho_2) \in [0,\infty)^2 \colon \rho_1 + \rho_2 = \rho\}$ with continuous and convex rate function $(\rho_1,\rho_2) \mapsto \chi(\rho_1,\rho_2) - \overline{\chi}(\rho)$, where

$$\chi(\rho_1,\rho_2) = \inf\Big\{\mathrm{h}^{(\mathcal{L},\mathcal{S})}(P \mid \mathtt{Q}\otimes\mathtt{R}) + \langle F_U, P\rangle \colon P \in \mathcal{M}_1^{(\mathrm{s})}(\mathcal{L}\times\mathcal{S}),$$
$$\langle \mathfrak{N}_U^{(\ell,\mathcal{L})}, P\rangle = \rho_1, \langle \mathfrak{N}_U^{(\ell,\mathcal{S})}, P\rangle = \rho_2\Big\}.$$

- The number of particles in Λ_N in loops of lengths $\leq L$ and $> L$, respectively, are exponentially equivalent to $(\mathfrak{N}^{(R)}_{\Lambda_N}, \mathfrak{N}^{(\neg R)}_{\Lambda_N})$ in the limit $N \to \infty$, followed by $R \to \infty$, respectively $L \to \infty$.
- We assumed the interaction potential v to be continuous, bounded and compactly supported, to avoid serious technicalities. However, we needed super-stability, in order to have a sufficient mutual repellence. This implies nice compactness properties of the formula!
- In [ADAMS, COLLEVECCHIO, K. 2011], only short loops were adequately treated, and only small ρ could be handled.
- In [COLLINS, JAHNEL, K. 2023], a simplified model (boxes in stead of loops) was treated for any ρ, but no phase transition could be proved.
- In [BELLOT, DEREUDRE, MAÏDA 2024], a Gibbs measure is constructed that might be related to the minimizers of our formula (difficult to judge about yet).
- Part of the proof is an LDP for something like the empirical stationary field $\frac{1}{|\Lambda|}\int_\Lambda \mathrm{d}x\, \delta_{\theta_x(\varpi)}$ on volume-scale. However, [SZNITMAN 2023] derives some LDP on capacity-scale $|\Lambda_N|^{1-2/d}$.

A first step towards proving BEC should be to show that, for sufficiently large $\rho = \rho_1 + \rho_2$, any minimizer P for $\overline{\chi}(\rho)$ has a non-trivial interlacement-part.

In the non-interacting case $v = 0$, this is known since long with critical value

$$\rho_{\mathrm{c}} = (4\pi\beta)^{-d/2}\zeta(d/2) = \sum_{k\in\mathbb{N}} k q_k, \qquad \text{with} \qquad q_k = \frac{1}{k}(4\pi\beta k)^{-d/2}.$$

Our formula yields a minimizer for $\overline{\chi}(\rho)$ of the form

$$P_\rho = \begin{cases} \mathtt{Q}^{(\rho)} \otimes \delta_{\underline{0}}, & \text{if } \rho < \rho_{\mathrm{c}}, \\ \mathtt{Q} \otimes \mathtt{R}^{(u_\rho,\beta)}, & \text{if } \rho \geq \rho_{\mathrm{c}}, \end{cases}$$

where $\underline{0}$ is the empty interlacement point process, and $\mathtt{Q}^{(\rho)}$ is the marked PPP with q_k replaced by $m_k^{(\rho)} = q_k \mathrm{e}^{\alpha_\rho k}$ where $\alpha_\rho \in (-\infty, 0]$ is picked such that $\sum_{k\in\mathbb{N}} k m_k^{(\rho)} = \rho$, and the density parameter u_ρ is picked in such a way that the expected number of particles of $\mathtt{R}^{(u_\rho,\beta)}$ in U is equal to $\rho - \rho_{\mathrm{c}}$. Then

$$J_W(\Pi_W(P_\rho)) = \frac{1}{|W|} H_{\mathcal{L}_W \times \mathcal{S}_W}\left(\Pi_W^{(\mathcal{L})}(\mathtt{Q}^{(\rho)}) \otimes \Pi_W^{(\mathcal{S})}(\mathtt{R}^{(u_\rho,\beta)}) \,\Big|\, \Pi_W^{(\mathcal{L})}(\mathtt{Q}^{(\rho\wedge\rho_{\mathrm{c}})}) \otimes \Pi_W^{(\mathcal{S})}(\mathtt{R}^{(u_\rho,\beta)}\right.$$

$$\to H(m^{(\rho)} \mid q) \qquad \text{as } W \uparrow \mathbb{R}^d,$$

which is positive for $\rho < \rho_{\mathrm{c}}$ and zero otherwise.

Define the empirical measure (with $W = W_R = [-R, R]^d$ and $W_z = z + W$)

$$\Xi_{N,R}^{(\omega)} = \frac{1}{\#Z_{N,R}} \sum_{z \in Z_{N,R}} \delta_{(\theta_z(\Pi_{W_z}^{(\mathcal{L})}(\omega)), \theta_z(\Pi_{W_z}^{(\mathcal{S})}(\omega)))} \in \mathcal{M}_1(\mathcal{L}_W \times \mathcal{S}_W), \qquad (1)$$

where θ_z is the shift-operator such that $\theta_z(W_z) = W$.

Strategy:

1. rewrite the partition function $\widehat{Z}_N$ in terms of an integral over $\Xi_{N,R}^{(\omega_{\mathrm{P}})}$ (dropping all interaction between different W_z's),
2. find a large deviation principle for $\Xi_{N,R}^{(\omega_{\mathrm{P}})}$ as $N \to \infty$,
3. use Varadhan's lemma to express the large-N exponential rate of the partition function as a variational formula on the space $\mathcal{M}_1(\mathcal{L}_W \times \mathcal{S}_W)$ with $W = [-R, R]^d$,
4. make $R \to \infty$ in that formula to arrive at χ.

The following LDP is taken from [PELETIER, RENGER, VENERONI 2013]; it goes back to an unpublished manuscript by C. Léonard; see [ADAMS, DIRR, PELETIER, ZIMMER 2011] for a conditional version of this LDP.

Sanov-type LDP for type-dependent independent random variables

Let $\mathcal{X}, \mathcal{Y}$ be two Polish spaces and pick $\rho \in \mathcal{M}_1(\mathcal{X})$ and let $(x_i^{(n)})_{i\in\mathbb{N}}$ be a sequence in $\mathcal{X}$ such that $\frac{1}{n}\sum_{i=1}^n \delta_{x_i^{(n)}}$ converges weakly towards ρ as $n \to \infty$. Let $\zeta\colon \mathcal{X} \times \mathcal{B}(\mathcal{Y}) \to [0,1]$ be a continuous Markov kernel from $\mathcal{X}$ to $\mathcal{Y}$, and let $(Y_i^{(n)})_{i\in[n]}$ have the distribution $\bigotimes_{i\in[n]} \zeta(x_i^{(n)}, \cdot)$. Then the empirical pair measure $\frac{1}{n}\sum_{i=1}^n \delta_{(x_i^{(n)}, Y_i^{(n)})}$ satisfies an LDP with rate function

$$\mathcal{M}_1(\mathcal{X} \times \mathcal{Y}) \ni q \mapsto \begin{cases} H_{\mathcal{X}\times\mathcal{Y}}(q \,|\, \rho \otimes \zeta) & \text{if } \pi_1(q) = \rho, \\ +\infty & \text{otherwise,} \end{cases}$$

where π_1 is the canonical projection $\mathcal{X} \times \mathcal{Y} \to \mathcal{X}$, and $\pi_1(q)$ is the corresponding image measure.

Using this LDP (and finding and employing compactness arguments), we can show that, as $N \to \infty$,

$$\frac{1}{|\Lambda_N|} \log \mathtt{Q}(\Xi_{N,R} \approx \xi) \approx -J_{W_R}(\xi) + o_R(1),$$

where J_W is the entropy term that appears in the definition of $\mathrm{h}^{(\mathcal{L},\mathcal{S})}$,

$$J_W(\xi) = \frac{1}{|W|} H_{\mathcal{L}_W \times \mathcal{S}_W}\big(\xi \,\big|\, \Pi_W^{(\mathcal{L})}(\mathtt{Q}) \otimes [\partial \Pi_W^{(\mathcal{S})}(\xi) \otimes \mathtt{R}_W]\big).$$

Using LDP-arguments, we derive:

Monotonicity of entropy in space

For $P \in \mathcal{M}_1^{(\mathrm{s})}(\mathcal{L} \times \mathcal{S})$,

$$J_{W_R}(\Pi_{W_R}(P)) \le J_{W_{mR}}(\Pi_{W_{mR}}(P)) + o_{mR}(1), \qquad m \to \infty.$$

This replaces the usual super-additivity arguments in the proof of the existence of $\mathrm{h}^{(\mathcal{L},\mathcal{S})}$!

Then adaptations of standard arguments are sufficient to derive existence and properties of $\mathrm{h}^{(\mathcal{L},\mathcal{S})}$

Here, the goal is to prove something like

$$\lim_{R\to\infty} \inf \Big\{ \frac{1}{|W_R|}\langle \xi, F_{W_R,W_R}\rangle + J_{W_R}(\xi) \colon \xi \in \mathcal{M}_1(\mathcal{L}_{W_R} \times \mathcal{S}_{W_R}), \partial\Pi^{(\mathcal{S})}_{W_R}(\xi) \in K,$$
$$\Big\langle \xi, \frac{1}{|W_R|}\mathfrak{N}^{(\ell,\mathcal{L})}_{W_R} \Big\rangle = \rho_1, \Big\langle \xi, \frac{1}{|W_R|}\mathfrak{N}^{(\ell,\mathcal{S})}_{W_R} \Big\rangle = \rho_2 \Big\}$$
$$= \inf \Big\{ \langle P, F_U\rangle + \mathrm{h}^{(\mathcal{L},\mathcal{S})}(P \mid \mathtt{Q} \otimes \mathtt{R}) \colon P \in \mathcal{M}^{(\mathrm{s})}_1(\mathcal{L} \times \mathcal{S}),$$
$$\langle P, \mathfrak{N}^{(\ell,\mathcal{L})}_U \rangle = \rho_1, \langle P, \mathfrak{N}^{(\ell,\mathcal{S})}_U \rangle = \rho_2 \Big\},$$

with some sufficiently large compact set K.

- For proving the upper bound, find intricate extension properties of ξ and compactness to construct some extension $P \in \mathcal{M}^{(\mathrm{s})}_1(\mathcal{L} \times \mathcal{S})$ of ξ in the limit $R \to \infty$. Then prove (something like) continuity of the expected particle number and lower semi-continuity of the energy and the entropy terms.
- For proving the lower bound, pick some P, approximate it with some ergodic $\widetilde{P}$, and restrict the infimum to $\xi = \Pi_W(\widetilde{P})$.