Weierstrass Institute for
Applied Analysis and Stochastics

Leibniz Association

A box version of the interacting Bose gas

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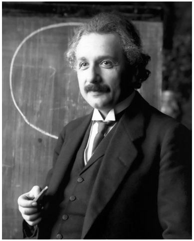
based on joint works with Adams/Collevecchio [AoP 11] and Collin/Jahnel (ongoing)

- In 1924, the unknown young physicist SATYENDRA NATH BOSE asked the famous ALBERT EINSTEIN to help him to publish 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 large quantum system of N particles in a centred box $\Lambda \subset \mathbb{R}^d$ with mutually repellent interaction, described by the Hamilton operator

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

- The kinetic energy term Δ_i acts on the i-th particle.
- The pair potential $v\colon (0,\infty) \to [0,\infty]$ decays quickly at ∞.
- We will concentrate on Bosons and introduce a symmetrisation.

Symmetrised trace of $\exp\{-\beta\mathcal{H}_N^{(\Lambda)}\}$ at fixed temperature $1/\beta \in (0,\infty)$ and fixed particle density $\rho \in (0,\infty)$:

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

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

Goal of this talk:

Try to describe the particle system in the thermodynamic limit $N \to \infty$ in a box $\Lambda_N \subset \mathbb{R}^d$ with volume N/ρ.

Long-term goal: Understand Bose–Einstein condensation (BEC).

Main quantity for the description of the interacting Bose gas:

Theorem A: Limiting free energy

The following limit exists for $|\Lambda_N| = N/\rho$:

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

- Proof by standard methods (subadditivity), see [Ruelle (1969)], e.g.
- Does not depend on boundary conditions.

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Our goals:

(1) Derive a formula for $f(\beta, \rho)$, using level-three large deviations.

(2) Derive from that the condensation phase transition.

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

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

- 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 $\sum_{k \in \mathbb{N}} \frac{1}{k} \mathrm{Leb}(\mathrm{d}x) \otimes \mu_{x,x}^{(k\beta)}(\mathrm{d}f)$, where $\mu_{x,y}^{(k\beta)}$ is the canonical measure for a Brownian bridge $x \to y$ with time interval $[0, \beta k]$.

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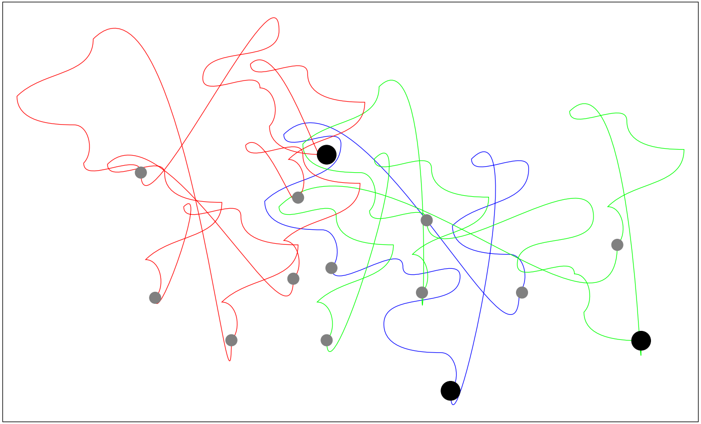
- We choose its intensity measure as $\sum_{k\in\mathbb{N}} \frac{1}{k}{\rm Leb}({\rm d}x) \otimes \mu_{x,x}^{(k\beta)}({\rm d}f)$, where $\mu_{x,y}^{(k\beta)}$ is the canonical measure for a Brownian bridge $x \to y$ with time interval $[0,\beta k]$.

Alternatively, the intensity measure of $\xi_{\rm P}$ is equal to $q{\rm Leb}$, 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 $\xi_{\rm P}$, the marks B_x with $x \in \xi_{\rm P}$ have length with probability q_k/q and then have the law $\mu_{x,x}^{(k\beta)}/kq_k$ on $\mathcal{C}_k$.



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.

Rewrite of the partition function

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 simplicity, I replace Λ by $\mathbb{R}^d$.)

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

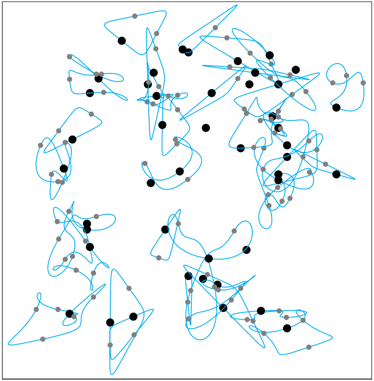
$$\mathrm{e}^{\beta\Delta}(f) = \mu_{f(0),f(\beta)}^{(\beta)}(\mathrm{d}f), \qquad f \in \mathcal{C}_1.$$

- The Feynman–Kac formula extends this formula to the operator $\mathrm{e}^{\beta(\Delta+v(x))}$; an exponential of $\int_0^\beta v(B_s)\,\mathrm{d}s$ appears.
- For $\mathcal{H}_N$, we have N Brownian bridges $B^{(1)},\dots,B^{(N)} \in \mathcal{C}_1$. The symmetrisation is a sum over all permutations σ of $1,\dots,N$ with the condition $B_\beta^{(i)} = B_0^{(\sigma(i))}$. Decompose σ into cycles, then we have Brownian cycles of various lengths.
- The Brownian bridges enjoy the Markov property:

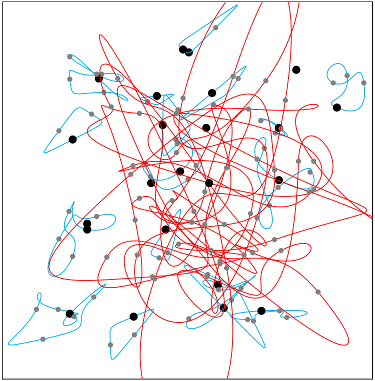
$$\int_{\mathbb{R}^d} \mu_{x,y}^{(\beta)}(\mathrm{d}f_1)\mu_{y,z}^{(\beta)}(\mathrm{d}f_2)\,\mathrm{d}y = \mu_{x,z}^{(2\beta)}(\mathrm{d}(f_1 \diamond f_2)), \qquad f_1, f_2 \in \mathcal{C}_1,$$

  where $f_1 \diamond f_2 \in \mathcal{C}_2$ is the concatenation of f_1 and f_2.
- In each cycle of length k, integrate out over all but one of the legs, and you obtain an element of $\mathcal{C}_k$ with distribution $\mu_{x,x}^{(\beta k)}$.

Illustration of condensate phase transition



Subcritical (low ρ) Bose gas
without condensate



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

Theorem [ADAMS/COLLEVECCHIO/K. 2011]

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

$$f(\beta,\rho) \le q + \inf\Big\{ I(P) + P(\Phi_{U,\mathbb{R}^d}) \colon P \in \mathcal{M}_1^{(\mathrm{s})}(\Omega), P(N_U^{(\ell)}) = \rho \Big\},$$

where we write $P(f) = \int f \, \mathrm{d}P = \langle P, f \rangle$, and

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

is the specific relative entropy w.r.t. the reference process.

- One result of [ACK 2011] is also '$\ge$' with a slightly different formula, for small ρ.
- Proof via level-three large deviations, based on an LDP by [GEORGII/ZESSIN (1993)] for the empirical stationary field.
- Technical problems: unboundedness of $\Phi_{U,\mathbb{R}^d}$, lack of continuity of $P \mapsto P(N_U^{(\ell)})$.

- '$=$' holds true for any ρ.
- Existence of minimizer $P \quad \Longleftrightarrow \quad$ absence of condensate.
- 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 $\rho > \rho_{\mathrm{c}}$.
- That is,

$$\rho_{\mathrm{c}} = \sup \big\{ \rho \in (0,\infty) \colon f(\beta,\rho) \text{ has a minimizer } P \big\}.$$

- There is a variational formula on an extended space that describes also the condensate.

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

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

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.

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

Largest achievable value of ρ is

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

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, MEOLA, 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, TAGGI,… (2014 –): various models of random loop ensembles, reflection positivity (a correlation inequality)
- FRÖHLICH, KNOWLES, SCHLEIN, SOHINGER,… (2017 –): various rescalings of box sizes, interaction lengths etc.
- 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

Simplified model:

- $\mathbb{Z}^d$ instead of $\mathbb{R}^d$,
- deterministic centred boxes instead of Brownian cycles.
- arbitrary $q = (q_k)_{k\in\mathbb{N}}$ satisfying $\sum_k q_k < \infty$.

Mark $G_k =$ discrete regular centred box with k particles.

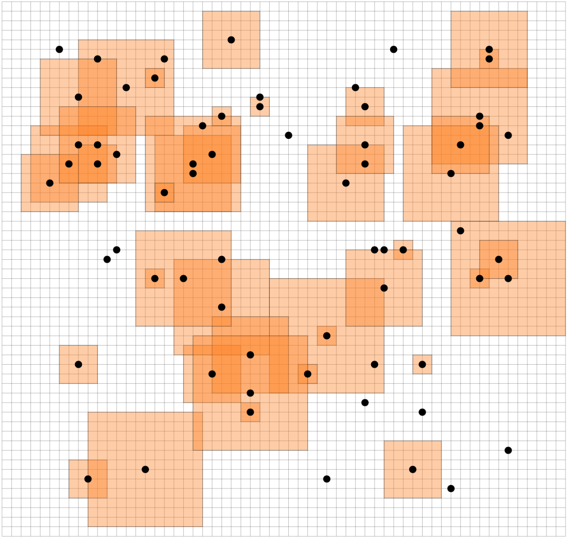
Marked PPP: $$\omega_{\rm P} = \sum_{k\in\mathbb{N}} \sum_{x\in\mathbb{Z}^d} \xi_{\rm P}^{(k)}(x)\delta_{(x,G_k)}$$

intensity measure: $$\sum_{k\in\mathbb{N}} q_k \mathrm{Leb}(\mathrm{d}x) \otimes \delta_{G_k}.$$

Interaction $\Phi_{\Lambda,\Lambda'}(\omega)$ as before (sum of $v(i-j)$ over all pairs (i,j) of particles of points in Λ resp. in Λ').

Partition function: $$Z_{N,\Lambda} = \mathbb{E}\Big[\mathrm{e}^{-\Phi_{\Lambda,\Lambda}(\omega_{\rm P})} \mathbb{1}\{N_\Lambda^{(\ell)}(\omega_{\rm P}) = N\}\Big].$$

An Illustration



Theorem [COLLIN/JAHNEL/K. 2022]

For any $\rho \in (0,\infty)$, for a centred box satisfying $|\Lambda_N| = N/\rho$, the limiting free energy

$$\lim_{N\to\infty} \frac{1}{|\Lambda_N|} \log Z_{N,\Lambda_N} = -\chi(\rho)$$

exists, where

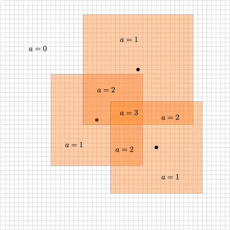
$$\chi(\rho) = \inf\Big\{\varphi(m,\psi) \colon m \in [0,\infty)^{\mathbb{N}}, \psi \in \mathcal{M}_1(\mathbb{N}_0), \sum_{k\in\mathbb{N}} k m_k + \sum_{a\in\mathbb{N}_0} a\psi(a) = \rho\Big\},$$

and

$$\varphi(m,\psi) = \inf\Big\{ \sum_{a\in\mathbb{N}_0} \psi(a)\Big[I(P_a) + P_a(\Phi_{0,\mathbb{Z}^d}) + 2aC_v P_a(N_0^{(\ell)}) + a^2 C_v\Big] \colon$$

$$P_0, P_1, P_2, \dots \in \mathcal{M}_1^{(\mathrm{s})}(\Omega), \sum_{a\in\mathbb{N}_0} \psi(a) P_a(N_0^{(\delta_k)}) = m_k \ \forall k\Big\}.$$

- $\rho_{\mathrm{mi}} = \sum_k k m_k$ is the microscopic particle density, $\rho_{\mathrm{ma}} = \sum_a a\psi(a)$ the condensate density.
- $\psi(a) =$ percentage of area covered by a macro boxes.
- $P_a =$ microscopic box distribution in a-areas.
- condensate does not exist $\iff \psi = \delta_0$ minimizes.



- Decompose $_N$ regularly into meso boxes of radius R.
- Estimate away all interactions between different mesoboxes.
- Marks G_k are called L-condensate if $k > L$.
- Count the number of meso boxes with precisely a overlapping condensate marks; call this $\psi(a)|\Lambda_N|/R^d$.
- Apply a Sanov-type LDP with many different types (indexed by a).
- Make $R \to \infty$ in the resulting variational formula, using the spatial ergodic theorem and the definition of the specific relative entropy I.

Lemma [Collin/Jahnel/K. 2022]

- φ and hence χ are convex and hence continuous.
- $\chi(0) = \sum_k q_k$ and $\chi'(0) = -\infty$.
- $\chi^{(v=0)}(\rho) + C_v\rho^2 \leq \chi(\rho) \leq \chi^{(v=0)}(\rho) + C_v(\rho^2 + \rho)$ for any ρ.
- $m \mapsto \varphi(m, \psi)$ is differentiable for any ψ (and we have two formulas).

Occurrence of condensation cannot be seen from existence of minimizers $(\rho_{\rm mi}, \rho_{\rm ma})$:

Lemma [Collin/Jahnel/K. 2022]

$$\chi(\rho) = \min_{\rho_{\rm mi}, \rho_{\rm ma} \geq 0 \colon \rho_{\rm mi} + \rho_{\rm ma} = \rho} \chi(\rho_{\rm mi}, \rho_{\rm ma}),$$

where $\chi(\rho_{\rm mi}, \rho_{\rm ma})$ is defined with infimum ranging over m and ψ satisfying $\rho_{\rm mi} = \sum_{k\in\mathbb{N}} k m_k$ and $\rho_{\rm ma} = \sum_{a\in\mathbb{N}_0} a\psi(a)$.

- The proof shows that any configuration (also if it contains a condensate) can also be approximated by an entirely microscopic configuration: one re-organises all the condensate part in boxes of size K and lets $K \to \infty$.

For given m and ψ, there is always a corresponding minimizing family $(P_a)_{a\in\mathbb{N}_0}$ of (distributions of) micro box configurations, i.e., the variational formula for $\varphi(m,\psi)$ always has minimizer(s). The number of minimizers is unknown to us.

Lemma [Collin/Jahnel/K. 2022]

For any $\rho \in (0,\infty)$, there is a minimizer (m,ψ) in the formula

$$\chi(\rho) = \inf\Big\{\varphi(m,\psi)\colon m \in [0,\infty)^{\mathbb{N}}, \psi \in \mathcal{M}_1(\mathbb{N}_0), \sum_{k\in\mathbb{N}} k m_k + \sum_{a\in\mathbb{N}_0} a\psi(a) = \rho\Big\}.$$

- Proof is a by-product of the proof of the upper bound for the free energy.
- There is at least one minimizer (m,ψ) such that ψ has at most two atoms.
- Minimizing w.r.t. m is amenable to differentiation techniques, while minimizing w.r.t. ψ is a linear-programming question.

- Big open question: Is the critical density $\rho_{\rm c}$ finite?

$$\rho_{\rm c} = \sup\{\rho\colon \chi(\rho) \text{ has a minimizer } (m,\delta_0)\} \in (0,\infty].$$

- Conjecture: $\rho_{\rm c} < \infty \quad \Longrightarrow \quad \sum_{k\in\mathbb{N}} kq_k < \infty$, perhaps also $\Longleftarrow$.
- Criterion for condensation: non-existence of a miminizer (m,δ_0) for ρ sufficiently large.
- The Euler–Lagrange equations for m:

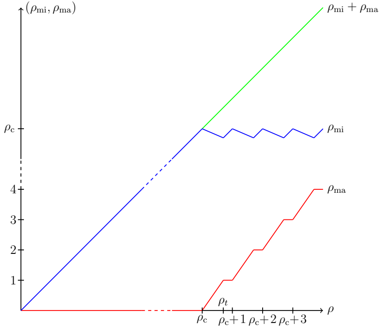
$$m_k = q_k \mathrm{e}^{-\alpha k} \mathrm{e}^{-t_k} \max_P P\big[\mathrm{e}^{-2\Phi^{(k)}}\big], \qquad k\in\mathbb{N},$$

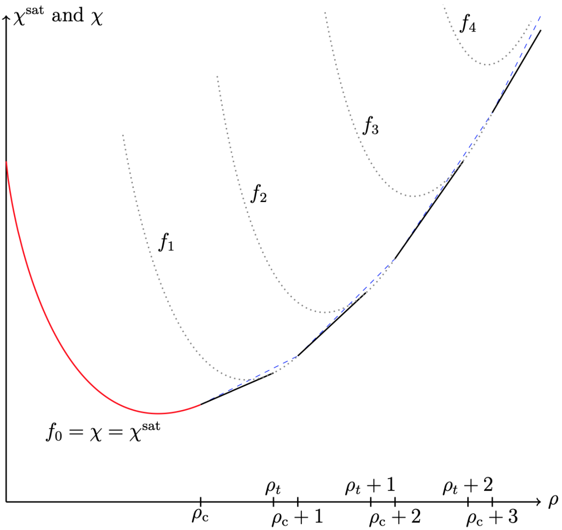
  where $t_k \approx C_v k - Ck^{1-1/d}$ is the internal energy of G_k, and $-2\Phi^{(k)}$ is the mutual energy of $\delta_{(0,G_k)}$ with the configuration, and α is the Lagrange multiplier, and P is a minimizer for $\chi(\rho,0)$ with $P(N_0^{(\ell)}) = \rho$.
- Does an m like that exist with $\sum_{k\in\mathbb{N}} km_k = \rho$? This is difficult to analyse, since m and P depend on ρ.

- The conjecture for the interacting Bose gas is that the micro total mass (as a function of ρ) is first equal to ρ and from ρ_c on constant. Accordingly, the macro total mass (the condensate total mass) is first zero and then equal to $\rho - \rho_c$.
- For our model, this would mean that the minimizer (m, ψ) should satisfy

$$\rho_{mi} = \sum_{k\in\mathbb{N}} k m_k = \rho \wedge \rho_c \qquad \text{and} \qquad \rho_{ma} = \sum_{a\in\mathbb{N}} \psi(a) a = [\rho - \rho_c]^+.$$

- However, this is not true in our model! Instead, assuming that $\rho_c < \infty$,





χ^{sat} and χ
f_1
f_2
f_3
f_4
$f_0 = \chi = \chi^{\mathrm{sat}}$
ρ_t
$\rho_t + 1$
$\rho_t + 2$
ρ
ρ_c
$\rho_c + 1$
$\rho_c + 2$
$\rho_c + 3$