Multi-state condensation in Berlin–Kac spherical models

Jani Lukkarinen

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UNIVERSITY OF HELSINKI

CENTRES OF EXCELLENCE IN RESEARCH

Bose–Einstein condensation: ideal gas

Consider an *ideal gas* of N bosons, confined into a box ($d \geq 3$):

supercritical density $\rho > \rho_{\mathrm{c}}$

$\downarrow$ ($N \gg 1$)

condensation of "extra" mass

$\downarrow$ $\rho - \rho_{\mathrm{c}}$ $\qquad$ $\searrow$ ρ_{c}

lowest energy state
(in the box)

$\sim$ quasifree state
with critical density ρ_{c}

- Boundary conditions affect the lowest energy state
- What happens if the ground state is not unique?
- How accurate is the quasifree approximation?
  Is error $O(N^{-p})$ for some $p > 0$?

Berlin–Kac spherical model

Berlin and Kac proposed in 1952 a *spherical model* as a modification of the Ising model of a ferromagnet:

- *Nearest neighbour interactions* on a finite lattice Λ, $N = |\Lambda|$,
  $\Rightarrow$ energy given by $E_\Lambda[s] := J \sum_{x\sim y} s_x s_y$, $J > 0$
- *Continuum spin* variables $s_x \in \mathbb{R}$, $x \in \Lambda$
  (instead of discrete $s_x = \pm 1$)
- Just as for Ising spins, require that

$$\sum_{x\in\Lambda} s_x^2 = N$$

$\Rightarrow$ spin configurations lie on the sphere of radius N in $\mathbb{R}^\Lambda$
$\Rightarrow$ Hence, the name *spherical model*

Explicitly, Berlin and Kac consider $N \to \infty$ limit of the *partition function* $Z = Z_{\mathrm{BK},\Lambda,\beta}$ normalizing the measure

$$\mu_{\mathrm{BK},\beta}[\mathrm{d}s] = \frac{1}{Z} \mathrm{e}^{-\beta E_\Lambda[s]}\, \delta\Big(\sum_{x\in\Lambda} s_x^2 - V\Big) \prod_{x\in\Lambda} \mathrm{d}s_x$$

for inverse temperature $\beta > 0$ and at $d = 3$. They showed that

- There is a phase transition corresponding to spontaneous magnetisation
- In the phase with spontaneous magnetisation, the fluctuations cannot be Gaussian

Later (1965), Yan and Wannier studied single site marginal for $N \to \infty$:

- In the phase without magnetisation (*subcritical*), the distribution is centred Gaussian
- Otherwise (*supercritical*), the distribution is sum of a random constant ("condensate") and a centred Gaussian

Generalized spherical model

To better emulate the bosonic case, slightly modify the BK-model:

- Take a *complex-valued* field, $\phi_x \in \mathbb{C}$, $x \in \Lambda$
- Consider an equal-sided box (*length L*) with *periodic BC*, $\Lambda_L = (\mathbb{Z}/L)^d$
- Allow for arbitrary densities $\rho > 0$
- Take an arbitrary *translation invariant* interaction and include β in its definition:

$$\beta E_\Lambda[\phi] = H_L[\phi] := \sum_{x,y\in\Lambda_L} \phi_x^* \alpha(x-y;L)\phi_y$$

Generalized spherical model

$$\mu_{\rho,\beta}[\mathrm{d}\phi] = \frac{1}{Z_{\rho,\beta}} \mathrm{e}^{-H_L[\phi]}\, \delta\!\left(\sum_{x\in\Lambda} |\phi_x|^2 - \rho V\right) \prod_{x\in\Lambda} \left[\mathrm{d}\big(\mathrm{Re}\,\phi_x\big)\mathrm{d}\big(\mathrm{Im}\,\phi_x\big)\right]$$

Summary of the main results

Consider the generalized spherical model:

1. There is a natural definition of a critical density ρ_c
2. There is a finite collection of condensate modes Λ_0^*, determined by their relative energy gap

supercritical density $\rho > \rho_c$

$\downarrow \quad (L \gg 1)$

condensation of "extra" mass

$\downarrow \quad \rho - \rho_c$ $\qquad\qquad \searrow \quad \rho_c$

modes in Λ_0^*
(nontrivial fluctuations?)

"normal fluid" modes
$\sim$ critical field
(grand canonical, Gaussian)

- All finite moments of ϕ_x agree up to errors which are $O(L^{-p})$

The problem can be "diagolized" by discrete Fourier transform:

- Define the *dual lattice* by $\Lambda^*(L) = \Lambda_L / L \subset \left]-\frac{1}{2}, \frac{1}{2}\right]^d$ and set

$$\widehat{f}(k) = \sum_{x \in \Lambda} f(x) \mathrm{e}^{-\mathrm{i}2\pi k \cdot x}\,, \qquad k \in \Lambda^*$$

- Denote *volume* $V = |\Lambda| = L^d$
- With the *shorthand notation* $\displaystyle\int_{\Lambda^*} \mathrm{d}k \cdots = \frac{1}{V} \sum_{k \in \Lambda^*} \cdots$

  we may rewrite

$$H_L[\phi] = \int_{\Lambda^*} \mathrm{d}k\, \omega(k) |\Phi_k|^2\,, \quad N[\phi] := \int_{\Lambda^*} \mathrm{d}k\, |\Phi_k|^2 = \sum_{x \in \Lambda_L} |\phi_x|^2$$

  where $\Phi = \widehat{\phi}$, and $\omega = \widehat{\alpha}$ is real-valued

- *Analogy with the bosonic system:* N corresponds to the *number operator*; $k \in \Lambda^*$ labels the eigenvectors and $\omega(k)$ the eigenvalues of the self-adjoint operator "βH"

- Let μ_0 denote the spherical model measure after the Fourier transform $\phi \to \Phi$,

$$\mu_0[\mathrm{d}\Phi] = \frac{1}{Z_\rho} \mathrm{e}^{-H[\Phi]} \delta(N[\Phi] - \rho V) \prod_{k \in \Lambda^*} [\mathrm{d}\Phi_k^* \mathrm{d}\Phi_k]$$

- Goal is to find a simplified translation invariant measure μ_1 such that its 2-Wasserstein distance from μ_0 is $O(L^{-p+d/2})$ for some $p > 0$

- *Reminder:* p-Wasserstein distance between probability measures μ_0 and μ_1 on Y is defined by

$$W_p(\mu_0, \mu_1)^p := \inf_\gamma \int_{Y \times Y} \gamma(\mathrm{d}y_1, \mathrm{d}y_2) \, \|y_1 - y_2\|^p$$

  where the infimum is taken over *couplings* γ between μ_0 and μ_1

- Then by using translation invariance, for any finite moment of ϕ_x the difference between the expectations under μ_0 and μ_1 is bounded by const. $\times\, L^{-p}$

Identification of the condensate modes

- *Minimum energy* $\omega_0 := \min_{k\in\Lambda^*} \omega(k)$
- *Shifted energies* $e_k := \omega(k) - \omega_0,\ k \in \Lambda^*$
- We call a pair $(\Lambda^*_0, \Lambda^*_+)$ of nonempty disjoint subsets of Λ^* whose union covers the whole Λ^*, a *split of* Λ^*
- The split is *separated by the energy interval* $[a, b]$, if $e_k \le a$, $k \in \Lambda^*_0$, and $e_k \ge b$, $k \in \Lambda^*_+$
- *Relative energy gap of the split* is defined as δ^{-1} where

$$\delta := \frac{\max_{k\in\Lambda^*_0} e_k}{\min_{k\in\Lambda^*_+} e_k} \le \frac{a}{b} < 1$$

- If $b > 0$, may define the *critical density* as $\rho_c(L) := \int_{\Lambda^*_+} \mathrm{d}k\, \frac{1}{e_k}$

Condensate on a finite lattice

1. $(\Lambda_0^*, \Lambda_+^*)$ is a split with $0 \le a < b$, and has a relative energy gap $\delta^{-1} \ge 2$; denote $V_0 = |\Lambda_0^*|$, $V_+ = |\Lambda_+^*| = V - V_0$
2. $\rho > \rho_{\rm c}$; denote $\Delta = \rho - \rho_{\rm c}$
3. $\varepsilon := \max\left(2\delta, \frac{1}{V^2 \rho_{\rm c}^2} \sum_{k \in \Lambda_+^*} \frac{1}{e_k^2}\right) \le \frac{\Delta^2}{2^5 V_0^2 \rho^2}$

$$\mu_1[\mathrm{d}\Phi] := \frac{1}{Z_1} \prod_{k \in \Lambda_+^*} [\mathrm{d}\Phi_k^* \mathrm{d}\Phi_k]\, \mathrm{e}^{-E_+[\Phi]}$$

$$\times \prod_{k \in \Lambda_0^*} [\mathrm{d}\Phi_k^* \mathrm{d}\Phi_k]\, \mathrm{e}^{-E_0[\Phi]\left(1 - \frac{\rho_{\rm c}}{\Delta}\right)} \prod_{k \in \Lambda_+^*} \left(1 - \frac{E_0[\Phi] L^{-d}}{e_k \Delta}\right)^{-1} \delta(\rho_0[\Phi] - \Delta)$$

$$E_+ = \int_{\Lambda_+^*} \mathrm{d}k\, e_k |\Phi_k|^2,\ E_0 = \int_{\Lambda_0^*} \mathrm{d}k\, e_k |\Phi_k|^2,\ \rho_0 = V^{-1} \int_{\Lambda_0^*} \mathrm{d}k\, |\Phi_k|^2$$

Then the 2-Wasserstein distance $W_2(\mu_0, \mu_1) \le C_2 L^{\frac{d}{2}} \varepsilon^{\frac{1}{4}}$, at least for $C_2 = 2^4 (\rho/\Delta)^{V_0/2} \sqrt{(\rho + \Delta) V_0}$

Simplified condensate fluctuations

Let Φ^+ denote the *Gaussian lattice field* distributed by

$$\mu_+[\mathrm{d}\Phi] := \frac{1}{Z_+} \prod_{k\in\Lambda_+^*} [\mathrm{d}\Phi_k^* \mathrm{d}\Phi_k]\, \mathrm{e}^{-L^{-d} \sum_{k\in\Lambda_+^*} (\omega(k)-\omega_0)|\Phi_k|^2}$$

- If $V_0 = 1$, then $\Phi = \Phi^+ + L^d\sqrt{\Delta}\mathrm{e}^{\mathrm{i}\theta}$ in distribution, θ is independent and uniformly distributed on $[0, 2\pi]$
- If $\omega(k)$ is a constant for $k \in \Lambda_0^*$, then in distribution $\Phi = \Phi^+ + L^d\sqrt{\Delta}X$, where X is independent and uniformly distributed on the unit sphere S^{2V_0-1}
- If $e_k \le \frac{1}{2\rho} L^{-d}\sqrt{\varepsilon}$ for $k \in \Lambda_0^*$, then the previous item can also be realised, possibly needing a larger C_2

Condensate with a fixed dispersion relation

Consider energies $\omega(k)$, $k \in \Lambda^*$, which are obtained from a fixed continuum *dispersion relation* $\omega : \mathbb{T}^d \to \mathbb{R}$. Suppose that

1. $d \geq 3$
2. The periodic extension of ω into a function $\mathbb{R}^d \to \mathbb{R}$ is twice continuously differentiable
3. Then ω has a unique minimum value $\omega_{\min}$. We assume that the set of global minima, $T_0 := \{k \in \mathbb{T}^d \,|\, \omega(k) = \omega_{\min}\}$, is finite and whenever $k_0 \in T_0$ the Hessian $D^2\omega(k_0)$ is invertible

Theorem

Then for all large enough L, we can find a split $(\Lambda_0^*, \Lambda_+^*)$ of Λ^* for which $|\Lambda_0^*|$ remains bounded by $M_0 < \infty$ and the required Wasserstein bound can be satisfied with

$$p = \frac{d/2 - 1}{2M_0 + 1}$$

Nearest neighbour interactions

$$\omega(k) = a + b\sum_{i=1}^{d} \sin^2(\pi k_i)\,, \quad a \in \mathbb{R},\ b > 0$$

- $k = 0$ is the unique minimum point on $\mathbb{T}^d$ and $\omega_{\min} = \omega(0) = a$
- $\Lambda_0^* = \{0\}$ and $\Lambda_+^* = \Lambda^* \setminus \{0\}$, results in a split of Λ^* which is separated by the energy interval $[0, 4bL^{-2}] \quad \Rightarrow \quad \delta_L = 0$
- $W_2(\mu_0, \mu_1) \leq C_2 L^{\frac{d}{2}-p}$ with $p = \frac{d}{4}$ for $d \geq 5$ ($p = \frac{1}{2}$, for $d = 3$)
- Acoustic phonon -type dispersion relation obtained by replacing $\omega \to \sqrt{\omega}$ can be used already for $d \geq 2$

Dispersion relation with several minima

$$\omega(k) = \sum_{i=1}^{d} \sin^2(2\pi k_i)$$

- Has 2^d global minima at points with components $k_i \in \{0, \frac{1}{2}\}$
- $k = 0$ is a minimum and thus for all L the minimum value is reached, $\omega_{\min} = 0 = \omega_0$
- If *L is odd*, $e_k \geq L^{-2}$ for all $k \in T_0 \setminus \{0\}$
  $\Rightarrow$ one finds a *single-component condensate*,
  even though $|T_0| = 2^d$
- If *L is even*, $T_0 \subset \Lambda_L/L \Rightarrow \Lambda_0^* = T_0$
  $\Rightarrow$ the condensate is 2^d*-fold degenerate*
- Since odd and even lattice sizes behave differently, it does not make sense to talk about $L \to \infty$ limit of μ_0

More complex examples

$$\omega(k;\zeta) = \sum_{i=1}^{d} \sin^2(\pi(k_i - \zeta_i))$$

- The minimum point is unique ($k = \zeta$) on the torus. However, if $\zeta \neq 0$, it does not need to belong to Λ^* and then there might be several minimum points in Λ^*
  $\Rightarrow$ Multi-state condensate but unique continuum minimum

Other examples:

- It is possible to have nontrivial condensate fluctuations
- For anisotropic dispersion relations, the minimum does not need to be the nearest point on the lattice; V_0 might also be surprisingly large

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