Ground state of the Bose-Hubbard model with large coordination number

Périce Denis
dperice@constructor.university

Joint work with: Shahnaz Farhat and Sören Petrat

Walkshop on Mathematical Physics 2026, Universität Kassel, 26/07/2026

Abstract

We consider the ground state energy of the Bose-Hubbard model on a graph with large and homogeneous coordination number. In the limit of infinite coordination number, we prove convergence of the ground state energy to the minimizer of a mean-field energy functional. This functional is obtained by averaging the hopping term over the large number of connected sites, while the interaction energy is not averaged. Hence, the resulting mean-field description is in the strong coupling regime, and is expected to provide a qualitatively correct picture of the phase diagram of the Bose-Hubbard model for large enough coordination number. For our proof, we develop a new version of a de Finetti type theorem, which we call a polaron-type quantum de Finetti theorem, and which we expect to be a more broadly useful extension of existing quantum de Finetti results. Our theorem covers the case where the Hilbert space is a tensor product of some Hilbert space with a Bosonic Fock space. This theorem is applied to the convergence of the ground state energy of the Bose-Hubbard model after reducing it to a polaron-type model.

Context

Study: large system of quantum bosons.

Usually [3]: many-body $N \to \infty$ mean-field:

$$H_N \coloneqq \sum_{i=1}^{N} (-\Delta_i) + \frac{1}{N} \sum_{1 \leqslant i < j \leqslant N} w(X_i - X_j) \quad \text{acting on } L^2(\mathbb{R}^d, \mathbb{C})^{\otimes_+ N}.$$

Statistical description of the interaction for a mean particle $\varphi \in L^2(\mathbb{R}^d)$:

$$h^{\varphi}_{\text{Hartree}} = -\Delta + |\varphi|^2 \star w.$$

Bose-Hubbard model

Interacting bosons on a lattice.

Sequence of graphs: $(V_z, E_z)_{z \in \mathbb{N}}$ with homogeneous coordination number z. Some examples:

- d-dimensional square lattice with periodic boundary conditions and length $L \in \mathbb{N}^*$:

$$V_d \coloneqq (\mathbb{Z}/L\mathbb{Z})^d ,$$

  when $d \to \infty$, with nearest neighbours as edges, so that $z = 2d$.

- cubic lattice V_3 with connections inside a radius $r \leqslant L$, so that

$$z \underset{r \to \infty}{\sim} \frac{4}{3} \pi r^3.$$

One-lattice-site Hilbert space: $\ell^2(\mathbb{C})$ of canonical basis $|n\rangle := (0, \dots, 0, \underbrace{1}_{n^{th}\text{index}}, 0, \dots), n \in \mathbb{N}$

2^{nd} **quantization:** creation and annihilation operators:

$$\begin{aligned} &a\,|0\rangle := 0 \quad \forall n \in \mathbb{N}^*,\ a\,|n\rangle := \sqrt{n}\,|n-1\rangle\,, \\ &\forall n \in \mathbb{N},\ a^\dagger\,|n\rangle := \sqrt{n+1}\,|n+1\rangle\,, \\ &[a, a^\dagger] = 1. \end{aligned} \tag{CCR}$$

Particle number: $\mathcal{N} := a^\dagger a$

Fock space:

$$\mathcal{F}_z := \ell^2(\mathbb{C})^{\otimes|V_z|} \cong \mathcal{F}_+\left(L^2(V_z, \mathbb{C})\right) := \bigoplus_{n\in\mathbb{N}} L^2(V_z, \mathbb{C})^{\otimes_+ n}.$$

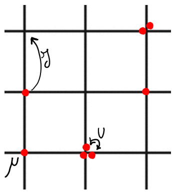
Indeed:

$$\mathcal{F}_+\left(L^2(V_z, \mathbb{C})\right) = \mathcal{F}_+\left(\bigoplus_{x\in V_z} \mathbb{C}\right) \cong \bigotimes_{x\in V_z} \mathcal{F}_+(\mathbb{C}) = \ell^2(\mathbb{C})^{\otimes|V_z|}.$$

If A is an operator on $\ell^2(\mathbb{C})$ and $x \in V_z$ denote A_x the operator on $\mathcal{F}$ acting on site x as A and as identity on other sites.

Bose-Hubbard hamiltonian of parameters $J, \mu, U \in \mathbb{R}$:

$$H_z := -\frac{J}{z} \overbrace{\sum_{\{x,y\}\in E_z} \left(a_x^\dagger a_y + a_y^\dagger a_x\right)}^{\mathcal{O}(z|V_z|)} + (J-\mu)\sum_{x\in V_z} \mathcal{N}_x + \frac{U}{2}\sum_{x\in V_z} \mathcal{N}_x(\mathcal{N}_x - 1). \tag{B-H}$$



- Great success in physics:
  Mott insulator/Superfluid phase transition, experimental observation [2] & theoretical description of mean-field theory [1].
- On the cubic lattice, mean-field justified when $d \to \infty$ and effective in $d = 3$ [5, FIG. 20].
- Strong and local particle interactions unlike many-body mean-field limits.

Goal: mean-field description of the ground state for large coordination numbers. Mean-field is with respect to lattice-sites interactions and not particle interactions.

Mean field theory

Mean field hamiltonian for $\varphi \in \ell^2(\mathbb{C})$:

$$h_\varphi := -J\left(\overline{\alpha_\varphi} a + \alpha_\varphi a^\dagger - |\alpha_\varphi|^2\right) + (J-\mu)\mathcal{N} + \frac{U}{2}\mathcal{N}(\mathcal{N}-1) \quad \text{with} \quad \alpha_\varphi := \langle \varphi, a\varphi\rangle.$$

mean field energy:

$$E_{mf}(\varphi) := -J\,|\alpha_\varphi|^2 + (J-\mu)\,\langle \varphi, \mathcal{N}\varphi\rangle + \frac{U}{2}\,\langle \varphi, \mathcal{N}(\mathcal{N}-1)\varphi\rangle\,. \tag{Emf}$$

Main result

Theorem 1: *S.Farhat & D.P & S.Petrat 2026 [4]*

If $U > 0$ and $J \geqslant 0$, then

$$\inf_{\substack{\psi \in \mathcal{F}_z \\ \|\psi\|_{\mathcal{F}_z}=1}} \frac{\langle \psi, H_z \psi \rangle}{|V_z|} \underset{z\to\infty}{\longrightarrow} \inf_{\substack{\varphi \in \ell^2(\mathbb{C}) \\ \|\varphi\|_{\ell^2}=1}} E_{mf}(\varphi).$$

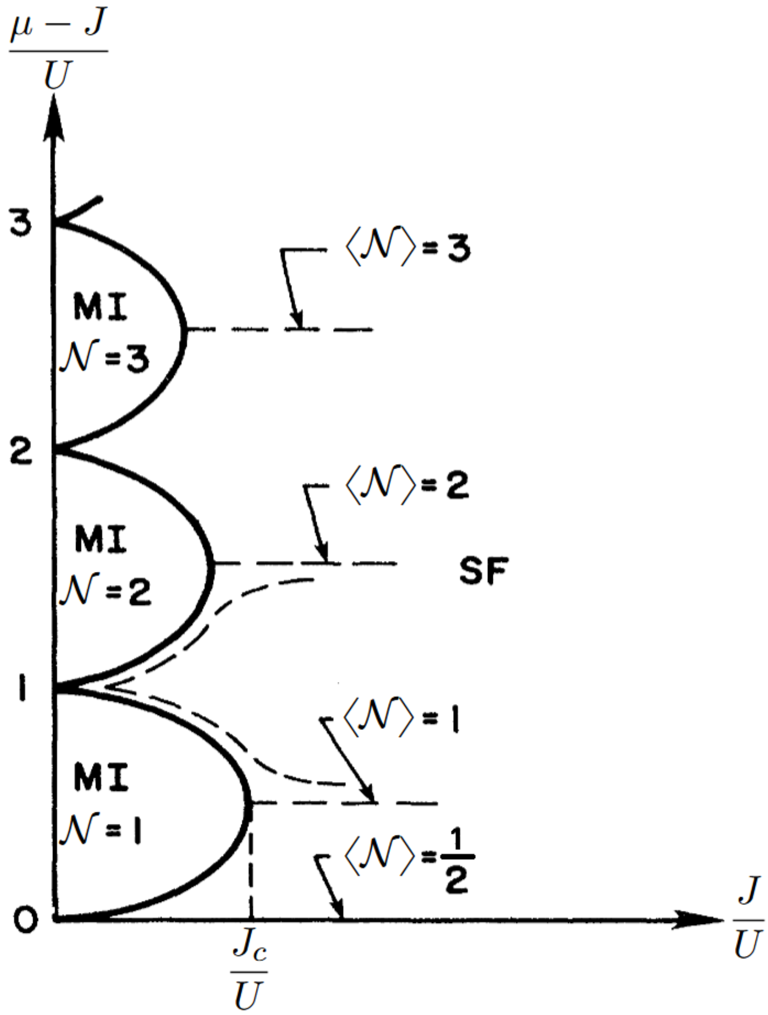
Phase transition [1]: let

$$\varphi_0 := \varphi_0(J, \mu, U)$$

be a normalized minimizer of (*Emf*) and

$$\alpha_0 := \langle \varphi_0, a\varphi_0 \rangle .$$

- Mott Insulator (MI): $\alpha_0 = 0$.
  If $J = 0$,
  $$E_{mf}(\varphi) = \frac{U}{2} \langle \varphi, \overbrace{\mathcal{N}\left(\mathcal{N} - \left(1 + 2\frac{\mu}{U}\right)\right)}^{\text{minimal at } \mathcal{N}=\frac{\mu}{U}+\frac{1}{2}} \varphi \rangle .$$
  So $\varphi_0 = \left|\left\lfloor \frac{\mu}{U} + \frac{1}{2} \right\rceil\right\rangle$, degeneracy at $\frac{\mu}{U} \in \mathbb{N}$.
- Superfluid (SF): $\alpha_0 > 0$.
  If $J \to \infty$, the Cauchy-Schwarz inequality
  $$|\alpha_\varphi|^2 \leqslant \|\varphi\|^2_{\ell^2} \|a\varphi\|^2_{\ell^2} = \langle \varphi, \mathcal{N}\varphi \rangle$$
  is sharp iff $|\alpha_\varphi| = \sqrt{\langle \varphi, \mathcal{N}\varphi \rangle}$, then
  $$\varphi_0 = e^{-\frac{|\alpha_0|^2}{2} + \alpha_0 a^\dagger} |0\rangle .$$



Notation:

- Let $\gamma_z \in \mathcal{L}^1(\mathcal{F}_z)$ be the projection onto the ground state of (B-H) (unique if V_z is connected and $J > 0$).
- The state reduced to $X \subseteq V_z$ is denoted $\mathrm{Tr}_{V_z \setminus X}(\gamma_z) \in \mathcal{L}^1\left(\ell^2(\mathbb{C})^{\otimes |X|}\right)$.

Theorem 2: *Convergence of ground state [4]*

If $U > 0$ and $J \geqslant 0$, then there exist

- $\mathbb{P} \in \mathcal{P}(\ell^2(\mathbb{C}))$ concentrated on normalized minimizers of ((Emf)),
- $\zeta \in L^1(\mathbb{P}, \mathcal{L}^1_+(\ell^2(\mathbb{C}))$ such that $\mathbb{P}$-a.e., $\mathrm{Tr}(\zeta) = 1$,

such that $\forall x_0 \in V_z$ and $x_{1:k} \subseteq V_z$ different nearest neighbours of x_0,

$$\mathrm{Tr}_{V_z \setminus \{x_{0:k}\}}(\gamma_z) \underset{z\to\infty}{\rightharpoonup} \int_{\ell^2(\mathbb{C})} \zeta(u) \otimes p_u^{\otimes k} \, d\mathbb{P}(u).$$

Comments:

- Convergence holds when tested against $\mathcal{N}^2$.
- WIP: convergence rate and uniqueness of minimizer for (Emf).

1 About the proof

Upper bound: lattice-site factorized test states: $\forall \varphi \in \ell^2(\mathbb{C})$, $\langle \varphi^{\otimes |V_z|}, H_z \varphi^{\otimes |V_z|} \rangle = |V_z| \, E_{mf}(\varphi)$.

Lower bound: problem: no lattice-site permutation symmetry.
Key idea: Polaron-type quantum de Finetti theorem after reducing by translation invariance to the nearest-neighbours shell model:

$$\widetilde{H}_z \coloneqq \sum_{i=1}^{z} \left(-J \left(a_0^\dagger a_i + a_i^\dagger a_0 \right) + (J-\mu)(\mathcal{N}_0 + \mathcal{N}_i) + \frac{U}{2} \left(\mathcal{N}_0(\mathcal{N}_0 - 1) + \mathcal{N}_i(\mathcal{N}_i - 1) \right) \right).$$

Bibliography

[1] M.P.A. Fisher P.B.Weichman G.Grinstein D.S.Fisher. “Boson localization and the superfluid-insulator transition”. *Phys. Rev. B* (1989). URL: https://url.org/10.1103/PhysRevB.40.546.

[2] M.Greiner O.Mandel T.Rom A.Altmeyer A.Widera T.W.Hänsch I.Bloch. “Quantum phase transition from a superfluid to a Mott insulator in an ultracold gas of atoms”. *Physica B: Condensed Matter* (2003). URL: https://url.org/10.1016/S0921-4526(02)01872-0.

[3] M.Lewin, P.T.Nam, and N.Rougerie. “Derivation of Hartree’s theory for generic mean-field Bose systems”. *Advances in Mathematics* 254 (2014). URL: https://url.org/10.1016/j.aim.2013.12.010.

[4] S.Farhat D.Périce S.Petrat. “Ground state energy of the Bose–Hubbard model with large coordination number with a polaron-type quantum de Finetti theorem”. *preprint* (2026). URL: https://arxiv.org/abs/2603.29562.

[5] Niklas Teichmann et al. “Process-chain approach to the Bose-Hubbard model: Ground-state properties and phase diagram”. *Phys. Rev. B* (2009). DOI: 10.1103/PhysRevB.79.224515.