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

Périce Denis
dperice@constructor.university

Joint work with: Shahnaz Farhat and Sören Petrat

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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 $N \rightarrow \infty$ mean field:

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

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

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

Bose-Hubbard model: interacting bosons on a lattice

- Great success in physics:
Mott-insulator \ Superfluid phase transition, experimental observation [2] & theoretical description of the mean field theory [1]
- Mean field justified when $d \rightarrow \infty$ and effective in $d = 3$

- Simple mathematical description

Goals:

- Mean field description as $z \rightarrow \infty$ (coordination number) of the ground state (for example $d \rightarrow \infty$)
- Describe a phase transition
- Strong and local particle interactions

Bose-Hubbard model

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

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

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

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

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

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

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

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

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

(CCR)

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

Fock space:

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

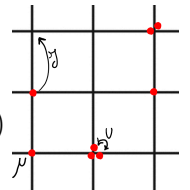
Indeed:

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

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 $J, \mu, U \in \mathbb{R}$:

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



Mean field with respect to sites interactions and not particle interactions due to large coordination number.

Mean field theory

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

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

mean field energy:

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

Main result

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

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

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

Phase transition: Let $\varphi_0 := \varphi_0(J, \mu, U)$ be a normalized minimizer of (.2) and $\alpha_0 := \langle \varphi_0, a\varphi_0 \rangle$.

- Mott Insulator (MI): $\alpha_0 = 0$

If $J = 0$,

$$E_{mf}(\varphi) = \frac{U}{2} \left\langle \varphi, \underbrace{\mathcal{N} \left(\mathcal{N} - \left(1 + 2\frac{\mu}{U} \right) \right)}_{\text{minimal at } \mathcal{N} = \frac{\mu}{U} + \frac{1}{2}} \varphi \right\rangle.$$

So $\varphi_0 = \left| \left\lfloor \frac{\mu}{U} + \frac{1}{2} \right\rfloor \right\rangle$ with degeneracy at $\frac{\mu}{U} \in \mathbb{N}$.

- Superfluid (SF): $\alpha_0 > 0$

If $J \rightarrow \infty$, by Cauchy-Schwarz

$$|\alpha_\varphi|^2 \leq \|\varphi\|_{\ell^2}^2 \|a\varphi\|_{\ell^2}^2 = \langle \varphi, \mathcal{N}\varphi \rangle$$

optimal when

$$|\alpha_\varphi| = \sqrt{\langle \varphi, \mathcal{N}\varphi \rangle},$$

then $\varphi_0 = e^{-\frac{|\alpha_0|^2}{2} + \alpha_0 a^\dagger} |0\rangle$.

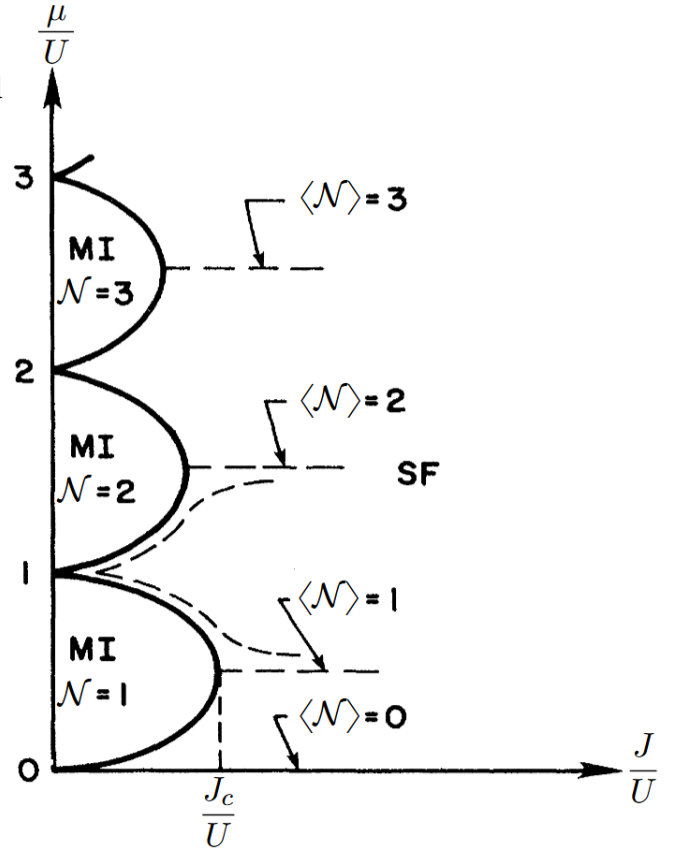


Figure 1: Mott insulator \ Superfluid phase diagram [1]

Some comments

- Convergence of states: let $\gamma_z \in \mathcal{L}^1(\mathcal{F}_z)$ be the projection on the ground state of (.1) (unique if V_z is connected and $J > 0$), then there exist

- a probability measure \mathbb{P} on the sphere of $\ell^2(\mathbb{C})$ concentrated on minimizers of (.2),
- a trace-class valued function $\zeta \in L^1(\mathbb{P}, \mathcal{L}_+^1(\ell^2(\mathbb{C})))$ such that \mathbb{P} -a.e., $\text{Tr}(\zeta) = 1$,

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

$$\text{Tr}_{V_z \setminus \{x_{0:k}\}}(\gamma_z) \xrightarrow{z \rightarrow \infty} \int_{S_{\ell^2(\mathbb{C})}} \zeta(u) \otimes p_u^{\otimes k} d\mathbb{P}(u). \quad (.3)$$

where $\text{Tr}_{V_z \setminus \{x_{0:k}\}}$ is tracing every variables except $x_{0:k}$, with convergence holding when tested against \mathcal{N}^2 .

- We previously proved the mean field limit for the dynamics [5].
- Main difficulty: no lattice site symmetry.
- Main idea of the proof:
 - upper bound is trivial: test state can be chosen factorized,
 - for the lower bound:
 - * Reduce the system by translation invariance to $x \in V_z$ and its nearest neighbours shell,
 - * De Finetti theorem making use of the symmetries inside the neighbouring shell (for V_d these are rotations and reflections of the lattice).
- WIP: convergence rate and uniqueness of minimizer for (.2).

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