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

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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 $N \to \infty$ 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

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

- Simple mathematical description

Goals:

- Mean field description as $z \to \infty$ (coordination number) of the ground state (for exemple $d \to \infty$)
- 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 exemples:

- 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 $|n\rangle \coloneqq (0, \dots, 0, \underbrace{1}_{n^{th}\text{index}}, 0, \dots), n \in \mathbb{N}$

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

$$a|0\rangle \coloneqq 0 \quad \forall n \in \mathbb{N}^*,\ a|n\rangle \coloneqq \sqrt{n}\,|n-1\rangle\,,$$
$$\forall n \in \mathbb{N},\ a^\dagger|n\rangle \coloneqq \sqrt{n+1}\,|n+1\rangle$$
$$[a, a^\dagger] = 1 \tag{CCR}$$

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

Fock space:

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

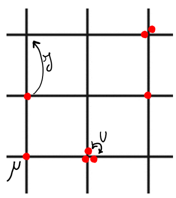
Indeed:

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

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

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



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

Mean field theory

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

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

mean field energy:

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

Main result

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

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

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

Phase transition:

Decompose

$$\varphi \eqqcolon \sum_{n\in\mathbb{N}} \lambda_n\,|n\rangle \implies \alpha_\varphi = \sum_{n\in N} \sqrt{n+1}\;\overline{\lambda_n}\lambda_{n+1}$$

- Mott Insulator (MI): $\alpha_\varphi = 0$

  If $J = 0$,

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

- Superfluid (SF): $\alpha_\varphi > 0$

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

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

  optimal when

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

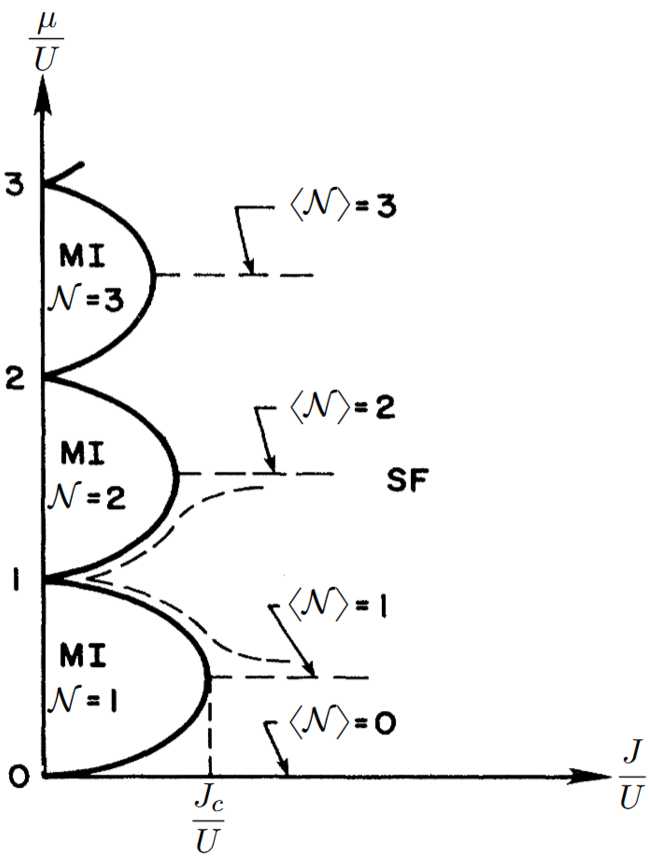


Figure 1: Mott insulator \ Superfluid phase diagram obtained by minimizing E_{mf} [1]

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., $\mathrm{Tr}\,(\zeta) = 1$,

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

$$\mathrm{Tr}_{V_z \setminus \{x_{0:k}\}}(\gamma_z) \underset{z\to\infty}{\longrightarrow} \int_{S_{\ell^2(\mathbb{C})}} \zeta(u) \otimes p_u^{\otimes k} \, d\mathbb{P}(u). \tag{.3}$$

where $\mathrm{Tr}_{V_z \setminus \{x_{0:k}\}}$ 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.

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