

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

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Motivation

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 mean-field theory [1].

- Mean-field justified when $d \rightarrow \infty$ and effective in $d = 3$ [5, FIG. 20].

Goals:

- Mean-field description of the ground state for large coordination numbers.
- Strong and local particle interactions.
- Describe a phase transition.

Bose–Hubbard model

Graphs: $(V_z, E_z)_{z \in \mathbb{N}}$ with constant coordination number z . Examples:

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

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

when $d \rightarrow \infty$, so that $z = 2d$.

- Cubic lattice V_3 with edges up to 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:

$$a|0\rangle := 0 \quad \forall n \in \mathbb{N}^*, \quad a|n\rangle := \sqrt{n}|n-1\rangle,$$

$$\forall n \in \mathbb{N}, \quad a^\dagger|n\rangle := \sqrt{n+1}|n+1\rangle,$$

$$[a, a^\dagger] = 1.$$

(CCR)

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

Fock space:

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

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

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

(B-H)

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:

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

References

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Mean-field theory

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

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

with $\alpha_\varphi := \langle \varphi, a\varphi \rangle$. Mean-field energy:

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

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 $J = 0$,

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

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

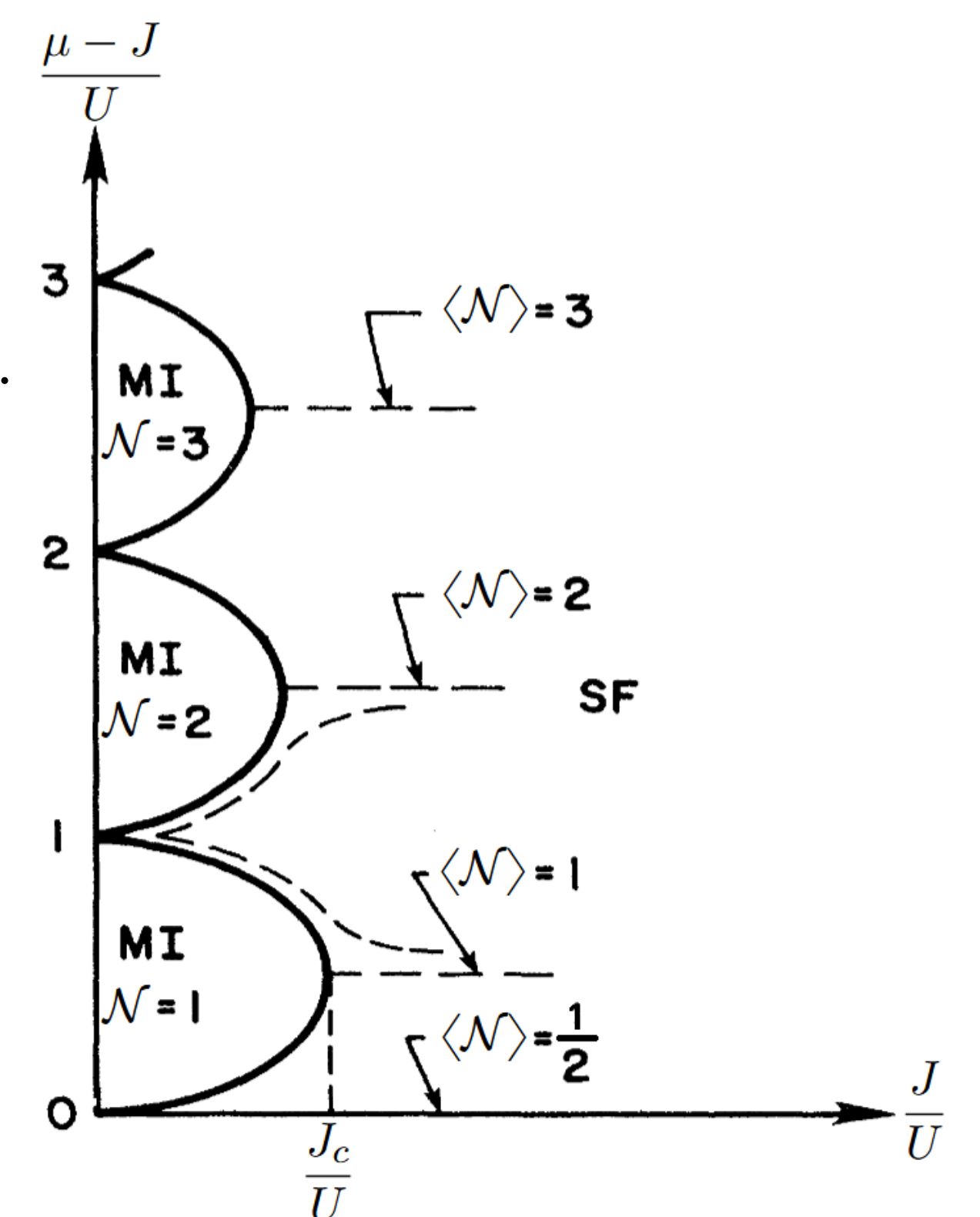
- Superfluid (SF): $\alpha_0 > 0$.

If $J \rightarrow \infty$, the Cauchy-Schwarz inequality

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

is sharp iff $|\alpha_\varphi| = \sqrt{\langle \varphi, \mathcal{N}\varphi \rangle}$, then

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



Results [4]

Theorem: Convergence of ground state energy

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

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

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 $\text{Tr}_{V_z \setminus X}(\gamma_z) \in \mathcal{L}^1(\ell^2(\mathbb{C})^{\otimes |X|})$.

Theorem: Convergence of ground state [4]

If $U > 0$ and $J \geq 0$, 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., $\text{Tr}(\zeta) = 1$,
- such that $\forall x_0 \in V_z$ and $x_{1:k} \subseteq V_z$ different nearest neighbours of x_0 ,

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

Comments:

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