Mean-field limit of the Bose-Hubbard model in high dimension

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Abstract

The Bose-Hubbard Hamiltonian effectively describes bosons on a lattice with on-site interactions and nearest-neighbour hopping, serving as a foundational framework for understanding strong particle interactions and the superfluid to Mott-insulator transition. In the physics literature, the mean field theory for this model is known to provide qualitatively accurate results in three or more dimensions. In this talk, I will present results that establishes the validity of the mean-field approximation for bosonic quantum systems in high dimensions. Unlike the standard many-body mean-field limit, the high-dimensional mean-field theory exhibits a phase transition and remains compatible with strongly interacting particles.

Motivations

Study: large system of quantum bosons

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

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

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 limit as $d \to \infty$ of the dynamics and the ground state energy
- Describe a phase transition
- Strong and local particle interactions

Bose-Hubbard model

Lattice: $\Lambda \coloneqq (\mathbb{Z}/L\mathbb{Z})^d$ with $d, L \in \mathbb{N}$ such that $d, L \geqslant 2$ of volume $|\Lambda| = L^d$

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:

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

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

Fock space:

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

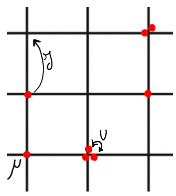
Indeed:

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

If A is an operator on $\ell^2(\mathbb{C})$ and $x \in \Lambda$ 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 $J, \mu, U \in \mathbb{R}$:

$$H_\Lambda \coloneqq -\frac{J}{2d} \overbrace{\sum_{\substack{x,y \in \Lambda \\ x \sim y}} a_x^\dagger a_y}^{\mathcal{O}(2d|\Lambda|)} + (J - \mu) \sum_{x \in \Lambda} \mathcal{N}_x + \frac{U}{2} \sum_{x \in \Lambda} \mathcal{N}_x(\mathcal{N}_x - 1)$$



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

Mean field theory

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

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

mean field energy:

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

Phase transition: Decompose

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

- 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

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

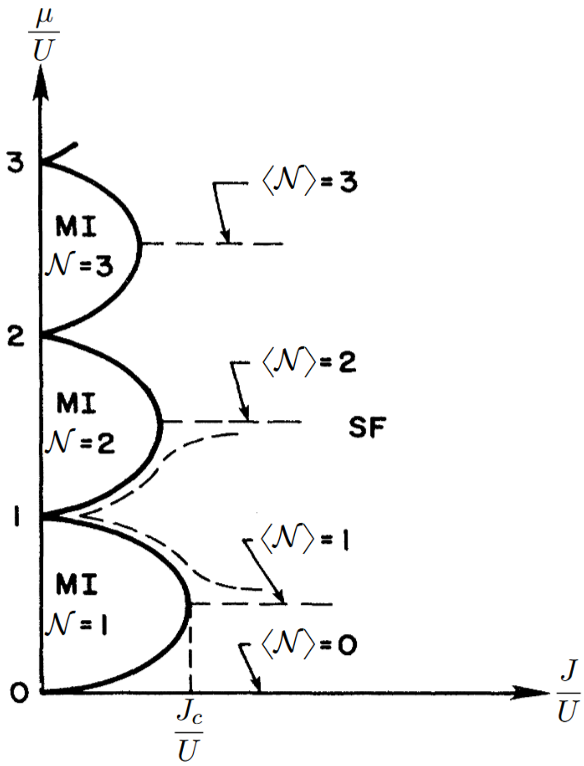


Figure 1: Mott insulator \ Superfluid phase diagram obtained by minimizing E_{mf} [1]

Main result

Theorem .1: *Convergence of the ground state energy (S.Farhat D.P S.Petrat 2025)*

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

$$-\frac{\ln(d)^3}{d} \lesssim \inf_{\substack{\psi_\Lambda \in \mathcal{F} \\ \|\psi_\Lambda\|=1}} \frac{\langle \psi_\Lambda, H_\Lambda \psi_\Lambda\rangle}{|\Lambda|} - \inf_{\substack{\varphi\in\ell^2(\mathbb{C}) \\ \|\varphi\|=1}} E_{mf}(\varphi) \leqslant 0$$

- WIP: convergence of densities
- Dynamics: preprint on ArXiv [4]

Trivial upper bound

Let $\varphi \in \ell^2(\mathbb{C})$,

$$\left\langle \varphi^{\otimes|\Lambda|}, a_x^\dagger a_y \varphi^{\otimes|\Lambda|} \right\rangle = \left\langle \varphi, a^\dagger \varphi \right\rangle \left\langle \varphi, a\varphi \right\rangle = |\alpha_\varphi|^2$$

so

$$\frac{\left\langle \varphi^{\otimes|\Lambda|}, H_\Lambda \varphi^{\otimes|\Lambda|} \right\rangle}{|\Lambda|} = E_{mf}(\varphi)$$

then minimize over φ.

Lower bound

Difficulty: no symmetry under sites exchange

Translation invariance: let $(e_{1:d})$ be the canonical basis of Λ, rewrite

$$H_\Lambda = \sum_{x\in\Lambda} \frac{1}{2d} \sum_{i=1}^{d} \left(a_{x+e_i}^\dagger a_x + a_x^\dagger a_{x+e_i} + (J-\mu)(\mathcal{N}_x + \mathcal{N}_{x+e_i}) + \frac{U}{2} \left(\mathcal{N}_x(\mathcal{N}_x - 1) + \mathcal{N}_{x+e_i}(\mathcal{N}_{x+e_i} - 1) \right) \right)$$

Let $\psi_\Lambda \in \mathcal{F}$, introduce the reduced densities: $\forall k \in [\![0,d]\!]$,

$$\gamma_\Lambda^{(1,k)} \coloneqq \frac{1}{|\Lambda|} \sum_{x\in\Lambda} \mathrm{Tr}_{\Lambda\setminus\{x,x+e_1,\dots,x+e_k\}} \left(|\psi_\Lambda\rangle \langle \psi_\Lambda| \right)$$

Let

$$H_{1,d} \coloneqq \sum_{i=1}^{d} \left(a_i^\dagger a_0 + a_0^\dagger a_i + (J-\mu)(\mathcal{N}_0 + \mathcal{N}_i) + \frac{U}{2} \left(\mathcal{N}_0(\mathcal{N}_0 - 1) + \mathcal{N}_i(\mathcal{N}_i - 1) \right) \right)$$

acting on $\ell^2(\mathbb{C})^{\otimes(d+1)}$, symmetrically on the last d variables (lattice axis permutation). Then,

$$\frac{\langle \psi_\Lambda, H_\Lambda \psi_\Lambda \rangle}{|\Lambda|} = \frac{\mathrm{Tr}\left(\gamma_\Lambda^{(1,d)} H_{1,d} \right)}{2d} = \frac{\mathrm{Tr}(\gamma_{1,d}^{(1,1)} \overbrace{H_{1,1}}^{\text{symmetric}})}{2}$$

Partially symmetric quantum De Finetti theorem:

Let $\gamma_{1,d}$ be a non-negative operator on $\ell^2(\mathbb{C}) \otimes \ell^2(\mathbb{C})^{\otimes_+ d}$ such that $\mathrm{Tr}\left(\gamma_{1,N}\right) = 1$, then there exists a probability $\mathbb{P}_m$ (constructed from the Haar measure) on $S^m \subseteq \mathbb{C}^{m+1}$ such that

$$\gamma_m \coloneqq \int_{S^m} \gamma_1(u) \otimes |u\rangle \langle u|^{\otimes d} \, d\mathbb{P}_m(u) \quad \text{with} \quad \gamma_1(u) \coloneqq \frac{\left(\mathbb{1}_{\ell^2} \otimes |u\rangle \langle u|^{\otimes d} \ \ \gamma_{1,d} \right)^{(1,0)}}{\mathrm{Tr}\left(\mathbb{1}_{\ell^2} \otimes |u\rangle \langle u|^{\otimes d} \ \ \gamma_{1,d} \right)}$$

satisfies

$$\operatorname{Tr}\left|\left(\gamma_{1,d}^{(1,1)} - \gamma_m^{(1,1)}\right) H_{1,1}\right| \lesssim \frac{m^3}{d} + d\,\underbrace{\operatorname{Tr}\left(\mathbb{1}_{\ell^2} \otimes \mathbb{1}_{\mathcal{N}>m}\mathcal{N}^2\ \gamma_{1,d}^{(1,1)}\right)^{\frac{1}{2}}}_{\text{exp decay in } m \text{ for G.S. of } H_{1,d}}$$

Cut-off optimization: $\frac{m^3}{d} = de^{-cm} \iff m = \frac{3}{c}\ln\left(\frac{cd^{\frac{2}{3}}}{3\ln\left(\frac{cd^{\frac{2}{3}}}{3\ln(\dots)}\right)}\right) \implies \frac{m^3}{d} \lesssim \frac{\ln(d)^3}{d}$

Conclusion:

$$\operatorname{Tr}\left(a^\dagger \otimes a\gamma_1(u) \otimes |u\rangle\langle u|\right) = \overline{\alpha_{\gamma_1(u)}}\alpha_u \leqslant \frac{\left|\alpha_{\gamma_1(u)}\right|^2 + |\alpha_u|^2}{2}$$

so

$$\operatorname{Tr}\left(\gamma_m^{(1,1)} H_{1,1}\right) \geqslant \int_{S^m} \frac{E_{mf}(\gamma_1(u)) + E_{mf}(u)}{2} d\mathbb{P}_m(u) \geqslant \inf_{\substack{\varphi\in\ell^2(\mathbb{C})\\ \|\varphi\|=1}} E_{mf}(\varphi)$$

Bibliography

[1] M.P.A. Fisher P.B.Weichman G.Grinstein D.S.Fisher. “Boson localization and the superfluid-insulator transition”. In: *Phys. Rev. B* (1989). DOI: https://doi.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”. In: *Physica B: Condensed Matter* (2003). DOI: https://doi.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”. In: *Advances in Mathematics* 254 (2014). DOI: https://doi.org/10.1016/j.aim.2013.12.010.

[4] S.Farhat D.Périce S.Petrat. “Mean-Field Dynamics of the Bose-Hubbard Model in High Dimension”. In: (2025). DOI: https://doi.org/10.48550/arXiv.2501.05304.