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:

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

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

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

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

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

Fock space:

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

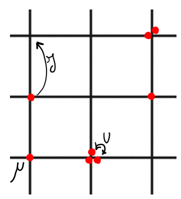
Indeed:

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

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.

Dynamics for $\gamma_d \in L^\infty\left(\mathbb{R}_+, S^1\left(\ell^2(\mathbb{C})^{\otimes|\Lambda|}\right)\right)$:

$$i\partial_t \gamma_d(t) = [H_d, \gamma_d(t)] \tag{B-H}$$

First reduced one-lattice-site density matrix:

$$\gamma_d^{(1)} \coloneqq \frac{1}{|\Lambda|} \sum_{x\in\Lambda} \mathrm{Tr}_{\Lambda\setminus\{x\}}\left(\gamma_d\right)$$

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:

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

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

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

  optimal when

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

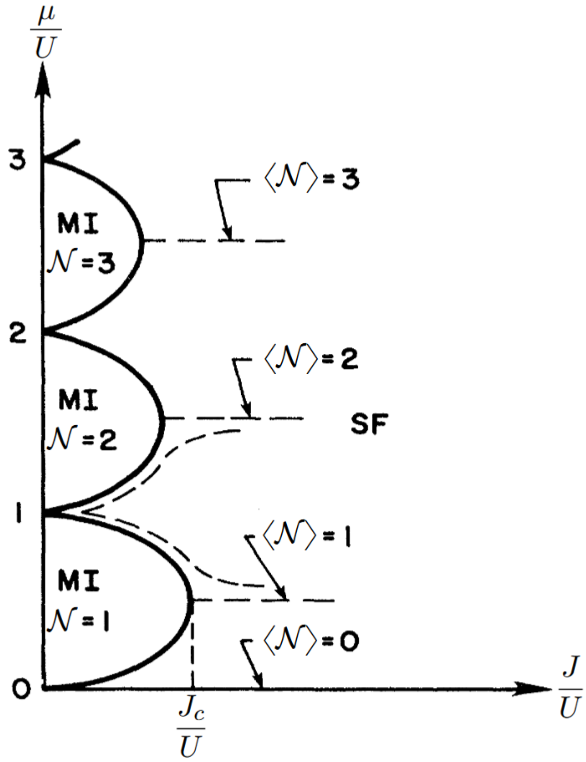


Figure 1: Mott insulator \ Superfluid phase diagram obtained by minimizing E_{mf} [1]

Dynamics:

$$i\partial_t\varphi(t) = h^{\varphi(t)}\varphi(t), \quad p_\varphi \coloneqq |\varphi\rangle\langle\varphi| \tag{mf}$$

Main result

Theorem .1: *S.Farhat D.P S.Petrat 2025 [4]*

Assume

- γ_d solves (B-H) with $\gamma_d(0) \in \mathcal{L}^1(\mathcal{F})$ such that $\mathrm{Tr}(\gamma_d(0)) = 1$
- φ solves (mf) with $\varphi(0) \in \ell^2(\mathbb{C})$ such that $\|\varphi\|_{\ell^2} = 1$
- $\exists c_1, c_2 > 0$ such that $\forall n \in \mathbb{N}$,

$$\mathrm{Tr}\left(p_\varphi(0)\mathbb{1}_{\mathcal{N}=n}\right) \leqslant c_1 e^{-\frac{n}{c_2}} \quad \mathrm{Tr}\left(\gamma_d^{(1)}(0)\mathbb{1}_{\mathcal{N}=n}\right) \leqslant c_1 e^{-\frac{n}{c_2}}.$$

Then $\exists\ C := C\left(J, c_1, c_2, \mathrm{Tr}\left(p_\varphi(0)\mathcal{N}\right)\right) > 0$ such that $\forall t \in \mathbb{R}_+$,

$$\left\|\gamma_d^{(1)}(t) - p_\varphi(t)\right\|_{\mathcal{L}^1} \leqslant e^{te^{C(t+1)}\sqrt{\ln(d)}}\left(\left\|\gamma_d^{(1)}(0) - p_\varphi(0)\right\|_{\mathcal{L}^1} + \frac{1}{d\sqrt{\ln(d)}}\right)$$

- If $\left\|\gamma_d^{(1)}(0) - p_\varphi(0)\right\|_{\mathcal{L}^1} = \mathcal{O}\left(\frac{1}{d}\right)$, then $\forall t \in \mathbb{R}_+$,

$$\left\|\gamma_d^{(1)}(t) - p_\varphi(t)\right\|_{\mathcal{L}^1} \leqslant 2e^{te^{C(t+1)}\sqrt{\ln(d)} - \ln(d)} \underset{d\to\infty}{\longrightarrow} 0$$

- Proof relies on propagation of moments of $\mathcal{N}$
- Article has another result without the double exponential in t working with less assumptions on initial moments but requiring $U > 0$
- Well-posedness of the mean field equation treated
- Further works: improve error with corrections to the dynamics to get something small when $d = 3$
- WIP ground state energy: if $J, \mu \geqslant 0, U > 0$, then

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

Convergence of the order parameter: since $a \leqslant \mathcal{N} + 1$ Insert a cut-off

$$\begin{aligned}
&\left|\mathrm{Tr}\left(\gamma_d^{(1)} a\right) - \mathrm{Tr}\left(p_\varphi a\right)\right| \\
&\leqslant \left\|\left(\gamma_d^{(1)} - p_\varphi\right) a\right\|_{\mathcal{L}^1} \\
&\leqslant \left\|\left(\gamma_d^{(1)} - p_\varphi\right) a\left(\mathcal{N}+1\right)^{-1}\left(\mathcal{N}+1\right)\mathbb{1}_{\mathcal{N}<M}\right\|_{\mathcal{L}^1} + \left\|\left(\gamma_d^{(1)} - p_\varphi\right) a\left(\mathcal{N}+1\right)^{-1}\left(\mathcal{N}+1\right)\mathbb{1}_{\mathcal{N}\geqslant M}\right\|_{\mathcal{L}^1} \\
&\leqslant M\left\|\gamma_d^{(1)} - p_\varphi\right\|_{\mathcal{L}^1} + \underbrace{\mathrm{Tr}\left(\gamma_d^{(1)}(\mathcal{N}+1)\mathbb{1}_{\mathcal{N}\geqslant M}\right) + \mathrm{Tr}\left(p_\varphi(\mathcal{N}+1)\mathbb{1}_{\mathcal{N}\geqslant M}\right)}_{\to 0 \text{ when } M\to\infty \text{ since the particle numbers are conserved}}
\end{aligned}$$

Any choice of $M \gg 1$ such that $M \left\|\gamma_d^{(1)} - p_\varphi\right\|_{\mathcal{L}^1} \ll 1$ as $d \to \infty$ is sufficient to prove that

$$\left\|\left(\gamma_d^{(1)} - p_\varphi\right) a\right\|_{\mathcal{L}^1} \underset{d\to\infty}{\to} 0$$

Sketch of the proof

- Propagation of moments of $\mathcal{N}$:

$$\operatorname{Tr}\left(p_\varphi(t)\mathcal{N}^k\right) \leqslant \left(\operatorname{Tr}\left(p_\varphi(0)\mathcal{N}^k\right) + k^k\right) e^{C(t+1)},$$

  and same for $\operatorname{Tr}\left(\gamma_d^{(1)}(t)\mathcal{N}^k\right)$

- Gronwall estimate tentative

$$\left|\partial_t \operatorname{Tr}\left(\gamma_d^{(1)} q_\varphi\right)\right| \leqslant C\left(\operatorname{Tr}\left(\gamma_d^{(1)} q_\varphi\right) + \operatorname{Tr}\left(\gamma_d^{(1)} q_\varphi\right)^{\frac{1}{2}} \underbrace{\operatorname{Tr}\left(\gamma_d^{(1)} q_\varphi\left(\mathcal{N}+1\right) q_\varphi\right)^{\frac{1}{2}}}_{\text{Insert cut-off } \mathbb{1}_{\mathcal{N}<M}+\mathbb{1}_{\mathcal{N}\geqslant M}} + d^{-1}\right).$$

  since

$$\left\|\gamma_d^{(1)} - p_\varphi\right\|_{\mathcal{L}^1} \lesssim \sqrt{\operatorname{Tr}\left(\gamma_d^{(1)} q_\varphi\right)}$$

- Controlling large $\mathcal{N}$ terms

$$\operatorname{Tr}\left(\gamma_d^{(1)} q_\varphi\left(\mathcal{N}+1\right)\mathbb{1}_{\mathcal{N}\geqslant M} q_\varphi\right) \leqslant e^{C(t+1) - Me^{-C(t+1)}} \underset{M\to\infty}{\to} 0$$

- Close Gronwall and optimize in M.

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