Mean-Field Dynamics of the Bose-Hubbard Model in High Dimension

Périce Denis
dperice@constructor.university

Joint work with: Shahnaz Farhat and Sören Petrat

44th Northwest German Functional Analysis Colloquium

University of Oldenburg

10/05/2025

Abstract

The Bose-Hubbard model 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. We present a result establishing the validity of a mean-field approximation for the dynamics of quantum systems in high dimension, using the Bose-Hubbard model on a square lattice as a case study. Our result is a trace norm estimate between the one-lattice-site reduced density of the Schrödinger dynamics and the mean-field dynamics in the limit of large dimension.

Motivations

Goal: rigorously derives large dimensional mean field limits since claim from physics literature: mean field theory exact in $d = +\infty$.

Usual many-body $N \to \infty$ mean field:

$$H_N \coloneqq \sum_{i=1}^{N} (-\Delta_i) + \frac{1}{N} \sum_{1 \leqslant i < j \leqslant N} w(X_i - X_j)$$

Bose-Hubbard model: interacting bosons on a lattice

- Simple mathematical description: finite lattice model
- Great success in physics: description of Mott-insulator \ Superfluid phase transition experimental observation [2] and theoretical description of mean field theory [1]
- Numerics shows mean field already effective in $d = 3$

Result: [3]

- Convergence of the many-body dynamics to the mean field dynamics when $d \to \infty$
- Describe a phase transition
- Strong 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:

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

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

Fock space:

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

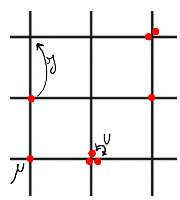
Indeed:

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

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

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



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

Dynamics for $\gamma_d \in L^\infty\left(\mathbb{R}_+, \mathcal{L}^1\left(\mathcal{F}\right)\right)$:

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

First one-lattice-site reduced 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 $\varphi \in \ell^2(\mathbb{C})$:

$$h^{\varphi} \coloneqq -J\left(\overline{\alpha_{\varphi}}a + \alpha_{\varphi}a^{\dagger} - |\alpha_{\varphi}|^2\right) + (J-\mu)\mathcal{N} + \frac{U}{2}\mathcal{N}(\mathcal{N}-1)$$

with the order parameter

$$\alpha_{\varphi} \coloneqq \langle \varphi | a\varphi \rangle$$

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

Dynamics

For $\varphi \in L^{\infty}\left(\mathbb{R}_+, \ell^2(\mathbb{C})\right)$,

$$i\partial_t\varphi(t) = h^{\varphi(t)}\varphi(t) \tag{mf}$$

Corresponding projection

$$p_{\varphi} \coloneqq |\varphi\rangle\langle\varphi| \quad q_{\varphi} \coloneqq 1 - p_{\varphi}$$

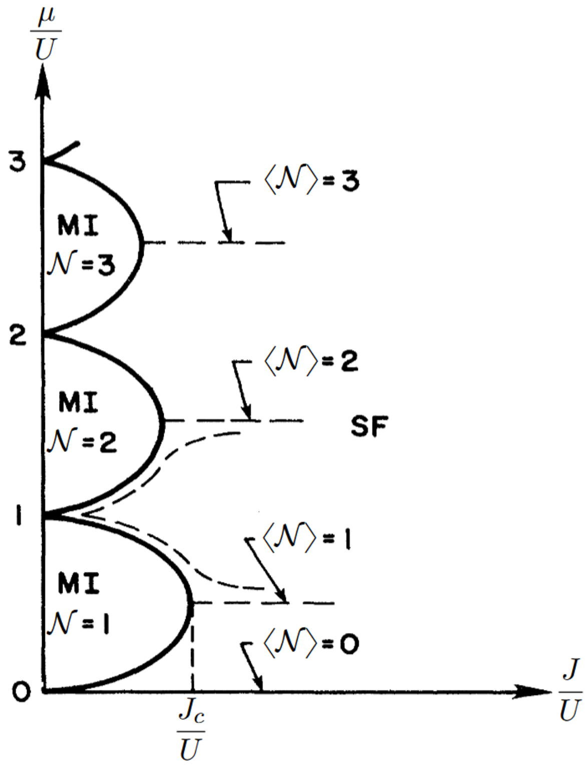


Figure 1: Mott insulator \ Superfluid phase diagram obtained by minimizing $\varphi \mapsto \langle\varphi|h^{\varphi}\varphi\rangle$[1]

Main result

Theorem .1: *S.Farhat D.P S.Petrat 2025*

Assume

- γ_d solves (B-H) with $\gamma_d(0) \in \mathcal{L}^1(\mathcal{F})$ such that $\mathrm{Tr}\left(\gamma_d(0)\right) = 1$
- 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 $d = 3$

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

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

Sketch of the proof

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

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

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

- Gronwall estimate tentative

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

since

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

- Controlling large $\mathcal{N}$ terms

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

- Close Gronwall and optimize in M.

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