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

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Effective Approximation and Dynamics of Many-Body Quantum Systems Mini Workshop

Université de Rennes

06/03/2025

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:

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

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:

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

 $\forall n \in \mathbb{N}, \ a^{\dagger} |n\rangle \coloneqq \sqrt{n+1} |n+1\rangle$
 $[a, a^{\dagger}] = 1$ (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 $J, \mu, U \in \mathbb{R}$:

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

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

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

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

First one-lattice-site reduced density matrix:

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

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 the order parameter

$$\alpha_{\varphi} := \langle \varphi | a\varphi \rangle$$

Phase transition: Decompose

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

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

Dynamics

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

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

Corresponding projection

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

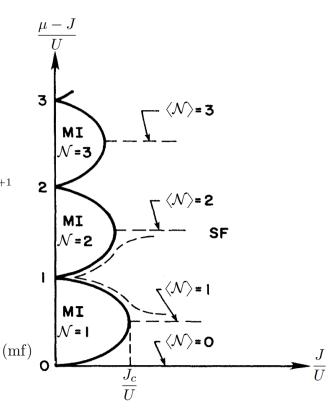


Figure 1: Mott insulator \ Superfluid phase diagram obtained by minimizing $\varphi \mapsto \langle \varphi | h^{\varphi} \varphi \rangle [1]$

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 $\operatorname{Tr}(\gamma_d(0)) = 1$
- φ solves (mf) with $\varphi(0) \in \ell^2(\mathbb{C})$ such that $\|\varphi\|_{\ell^2} = 1$
- $\exists c_1, c_2 > 0 \text{ such that } \forall n \in \mathbb{N},$

$$\operatorname{Tr}\left(p_{\varphi}(0)\mathbb{1}_{\mathcal{N}=n}\right) \leqslant c_{1}e^{-\frac{n}{c_{2}}} \quad \operatorname{Tr}\left(\gamma_{d}^{(1)}(0)\mathbb{1}_{\mathcal{N}=n}\right) \leqslant c_{1}e^{-\frac{n}{c_{2}}}.$$

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

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

• If $\left\| \gamma_d^{(1)}(0) - p_{\varphi}(0) \right\|_{\mathcal{C}^1} = \mathcal{O}\left(\frac{1}{d}\right)$, 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 $a \leq \mathcal{N} + 1$ Insert a cut-off

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

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} :

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

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

• Gronwall estimate tentative

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

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

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

• Close Gronwall and optimize in M.





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- [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.
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