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

[1]

Denis Périce
Joint work with: Shahnaz Farhat & Sören Petrat
Constructor university Bremen

International Workshop on Operator Theory and its Applications
University of Twente
Open session

15/07/2025

1 Motivations

Study: large system of quantum bosons

Usually: 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: $h^{\varphi}_{\text{Hartree}} = -\Delta + |\varphi|^2 \star w$ with $\varphi \in L^2(\mathbb{R}^d)$

Quantum phase transition from a superfluid to a Mott insulator in an ultracold gas of atoms

M. Greiner[a,b,*], O. Mandel[a,b], T. Rom[a,b], A. Altmeyer[a,b], A. Widera[a,b], T.W. Hänsch[a,b], I. Bloch[a,b]

[a] Sektion Physik, Ludwig-Maximilians Universität, Schellingstr. 4/III, D-80799 Munich, Germany
[b] Max-Planck-Institut für Quantenoptik, D-85748 Garching, Germany

Abstract

A quantum phase transition from a superfluid to a Mott insulating ground state was observed in a Bose–Einstein condensate stored in a three-dimensional optical lattice potential. With this experiment a new field of physics with ultracold atomic quantum gases is entered. Now interactions between atoms dominate the behavior of the many-body system, such that it cannot be described by the usual theories for weakly interacting Bose gases anymore.
© 2003 Published by Elsevier Science B.V.

Experimental observation of the phase transition [2]

PHYSICAL REVIEW B VOLUME 40, NUMBER 1 1 JULY 1989

Boson localization and the superfluid-insulator transition

Matthew P. A. Fisher
IBM Research Division, Thomas J. Watson Research Center, Yorktown Heights, New York 10598

Peter B. Weichman
Condensed Matter Physics 114-36, California Institute of Technology, Pasadena, California 91125

G. Grinstein
IBM Research Division, Thomas J. Watson Research Center, Yorktown Heights, New York 10598

Daniel S. Fisher
Joseph Henry Laboratory of Physics, Jadwin Hall, Princeton University, Princeton, New Jersey 08544

Theoretical description of the mean field theory [3]

Bose-Hubbard model: interacting bosons on a lattice

- Great success in physics: Mott-insulator \ Superfluid phase transition
- Mean field justified when $d \to \infty$ and effective in $d = 3$
- Simple mathematical description

Results:

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

2 Bose-Hubbard model

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

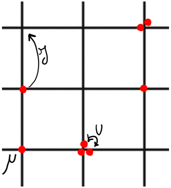
One-lattice-site Hilbert space: $\ell^2(\mathbb{C})$ of canonical basis $|n\rangle := (0, \ldots, 0, \underbrace{1}_{n^{th}\text{index}}, 0, \ldots), n \in \mathbb{N}$

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

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

$$\forall n \in \mathbb{N},\; a^\dagger\,|n\rangle := \sqrt{n+1}\,|n+1\rangle \tag{2}$$

$$[a, a^\dagger] = \mathbb{1}_{\ell^2} \tag{CCR}$$



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

Fock space:

$$\ell^2(\mathbb{C})^{\otimes|\Lambda|} \cong \mathcal{F}_+\left(L^2(\Lambda, \mathbb{C})\right) := \bigoplus_{n\in\mathbb{N}} L^2(\Lambda, \mathbb{C})^{\otimes_+ n} \tag{3}$$

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

$$H_d := -\frac{J}{2d} \overbrace{\sum_{\substack{x,y\in\lambda \\ x\sim y}} a_x^\dagger a_y}^{\mathcal{O}(2d|\Lambda|)} + (J-\mu)\sum_{x\in\Lambda}\mathcal{N}_x + \frac{U}{2}\sum_{x\in\Lambda}\mathcal{N}_x(\mathcal{N}_x - 1) \tag{4}$$

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

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

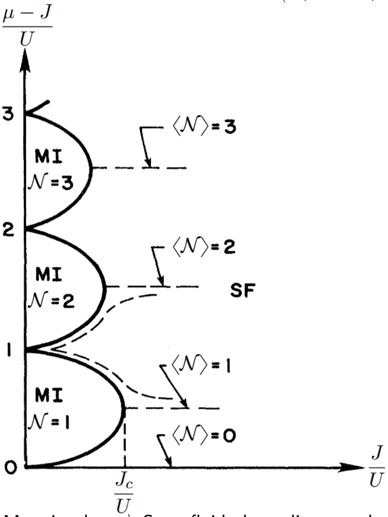
First reduced one-lattice-site density matrix:

$$\gamma_d^{(1)} := \frac{1}{|\Lambda|}\sum_{x\in\Lambda} \mathrm{Tr}_{\Lambda\setminus\{x\}}\left(\gamma_d\right) \tag{5}$$

3 Mean field theory

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

$$h^\varphi := -J\left(\overline{\alpha_\varphi} a + \alpha_\varphi a^\dagger - |\alpha_\varphi|^2\right) + (J-\mu)\mathcal{N} + \frac{U}{2}\mathcal{N}(\mathcal{N}-1) \tag{6}$$



Mott insulator \ Superfluid phase diagram obtained by minimizing $\varphi \mapsto \langle\varphi|h^\varphi\varphi\rangle$[3]

with the order parameter

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

Phase transition: decompose

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

- 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

$$p_\varphi := |\varphi\rangle\langle\varphi|, \quad q_\varphi := \mathbb{1}_{\ell^2} - p_\varphi \tag{7}$$

4 Main result

Recap

$$\gamma_d^{(1)} := \frac{1}{|\Lambda|}\sum_{x\in\Lambda}\mathrm{Tr}_{\Lambda\setminus\{x\}}(\gamma_d) \quad i\partial_t\gamma_d = \left[-\frac{J}{2d}\sum_{\substack{x,y\in\lambda\\ x\sim y}} a_x^\dagger a_y + (J-\mu)\sum_{x\in\Lambda}\mathcal{N}_x + \frac{U}{2}\sum_{x\in\Lambda}\mathcal{N}_x(\mathcal{N}_x-1), \gamma_d\right] \tag{B-H}$$

$$\alpha_\varphi := \langle\varphi|a\varphi\rangle \quad i\partial_t\varphi = \left(-J(\alpha_\varphi a + \overline{\alpha_\varphi}a^\dagger - |\alpha_\varphi|^2) + (J-\mu)\mathcal{N} + \frac{U}{2}\mathcal{N}(\mathcal{N}-1)\right)\varphi \tag{mf}$$

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

Assume

- γ_d solves (B-H) with $\gamma_d(0)\in S^1\left(\ell^2(\mathbb{C})^{\otimes|\Lambda|}\right)$ 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 $\forall n\in\mathbb{N}$,

$$\mathrm{Tr}\,(p_\varphi(0)\mathbb{1}_{\mathcal{N}=n}) \leqslant c_1 e^{-\frac{n}{c_2}}, \quad \mathrm{Tr}\left(\gamma_d^{(1)}(0)\mathbb{1}_{\mathcal{N}=n}\right) \leqslant c_1 e^{-\frac{n}{c_2}}. \tag{8}$$

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

$$\left\|\gamma_d^{(1)}(t) - p_\varphi(t)\right\|_{S^1} \leqslant C\left(\left\|\gamma_d^{(1)}(0) - p_\varphi(0)\right\|_{S^1} + \frac{1}{d\sqrt{\ln(d)}}\right)e^{Cte^{Ct}\sqrt{\ln(d)}} \tag{9}$$

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

$$\left\|\gamma_d^{(1)}(t) - p_\varphi(t)\right\|_{S^1} \lesssim e^{Cte^{Ct}\sqrt{\ln(d)}-\ln(d)} \underset{d\to\infty}{\longrightarrow} 0$$

5 Convergence of the order parameter:

Use $a \leqslant \mathcal{N} + 1$ and insert a $\mathcal{N}$-cut-off:

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

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

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

6 Sketch of the proof

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

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

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

- Gronwall estimate tentative

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

  with

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

- 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:

$$\underbrace{\frac{M}{d}}_{\mathcal{N}<M \text{ error}} = \underbrace{e^{-M}}_{\mathcal{N}\geqslant M \text{ error}} \iff Me^M = d \iff M = \ln\left(\frac{d}{\ln\left(\frac{d}{\ln(\dots)}\right)}\right)$$

7 WIP: Ground-state energy

Recap

$$H_d = -\frac{J}{2d} \sum_{\substack{x,y\in\lambda \\ x\sim y}} a_x^\dagger a_y + (J-\mu)\sum_{x\in\Lambda}\mathcal{N}_x + \frac{U}{2}\sum_{x\in\Lambda}\mathcal{N}_x(\mathcal{N}_x - 1) \quad (10)$$

$$\alpha_\varphi := \langle\varphi|a\varphi\rangle \qquad h^\varphi = -J(\alpha_\varphi a + \overline{\alpha_\varphi} a^\dagger - |\alpha_\varphi|^2) + (J-\mu)\mathcal{N} + \frac{U}{2}\mathcal{N}(\mathcal{N}-1) \quad (11)$$

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

$$\inf_{\substack{\psi_d\in\ell^2(\mathbb{C})^{\otimes|\Lambda|} \\ \|\psi_d\|=1}} \frac{\langle\psi_d|H_d\psi_d\rangle}{|\Lambda|} \underset{d\to\infty}{\longrightarrow} \inf_{\substack{\varphi\in\ell^2(\mathbb{C}) \\ \|\varphi\|=1}} \langle\varphi|h^\varphi\varphi\rangle$$

Upper bound: for $\varphi\in\ell^2(\mathbb{C})$,

$$\frac{\left\langle\varphi^{\otimes|\Lambda|}\middle|H_d\varphi^{\otimes|\Lambda|}\right\rangle}{|\Lambda|} = \langle\varphi|h^\varphi\varphi\rangle$$

Lower bound: for $\gamma_d\in S^1\left(\ell^2(\mathbb{C})^{\otimes|\Lambda|}\right)$, consider

$$\mathrm{Tr}_{\Lambda\setminus\{e_0,e_1,\dots e_d\}}(\gamma_d)$$

with $e_0\in\Lambda$ and $e_1,\dots,e_d$ a unit cell basis of nearest neighbours of e_0.
Key steps: ground state symmetries & partially symmetric quantum De-Finetti theorem

Thank you for your attention

References

[1] 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.

[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.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.