Mean-field analysis of the Bose-Hubbard model

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PHY665: Quantum Phases of Matter and Phase Transitions

Term paper presentation

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Bosons in an optical lattice

Spinless bosons in an optical lattice potential V_{ext}:

$$\hat{H} = \int \mathrm{d}r\, \hat{\psi}^\dagger(r)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(r)\right)\hat{\psi}(r) + \frac{1}{2}\int \mathrm{d}r \int \mathrm{d}r'\, \hat{\psi}^\dagger(r)\hat{\psi}^\dagger(r')\, U_{\text{int}}(r-r')\, \hat{\psi}(r)\hat{\psi}(r')$$

Commutation relations:

$$[\hat{\psi}(r), \hat{\psi}^\dagger(r')] = \delta(r-r') \qquad [\hat{\psi}(r), \hat{\psi}(r')] = 0 = [\hat{\psi}^\dagger(r), \hat{\psi}^\dagger(r')]$$

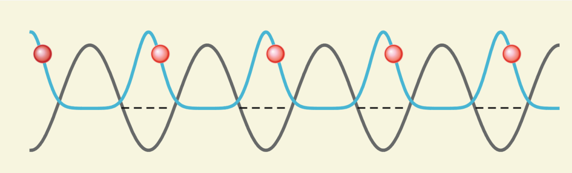

Figure: Bosons in an optical lattice [1].

Bosons in an optical lattice (contd.)

Expanding field operators in terms of Wannier function basis:

$$\hat{\psi}(r) = \sum_j \phi_j(r)\,\hat{a}_j$$

Bosonic operators:

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \qquad [\hat{a}_i, \hat{a}_j] = 0 = [\hat{a}_i^\dagger, \hat{a}_j^\dagger]$$

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Substitute into the Hamiltonian:

$$\hat{H} = \sum_{ij} \hat{a}_i^\dagger \hat{a}_j \int \mathrm{d}r\, \phi_i^*(r) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) \right) \phi_j(r) + \frac{1}{2} \sum_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \int \mathrm{d}r \int \mathrm{d}r'\, \phi_i^*(r) \phi_j^*(r')\, U_{\text{int}}\, \phi_k(r) \phi_l(r')$$

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Substitute into the Hamiltonian:

$$\hat{H} = -\sum_{ij} \hat{a}_i^\dagger \hat{a}_j\, t_{ij} + \frac{1}{2}\sum_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l\, U_{ijkl}$$

Approximations

- Tight-binding approximation: $t_{i+2,i} \gg t_{i+1,1}$.
- Contact interaction approximation: $U_{\text{int}}(r - r') \sim \delta(r - r')$.
- Isotropic lattice approximation: $t_{ij} = t, \quad U_{iiii} = U$.

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Bose-Hubbard Hamiltonian[1]:

$$\boxed{\hat{H} = -t \sum_{\langle i,j \rangle} \left(\hat{a}_i^\dagger \hat{a}_j + \text{h.c.} \right) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i} \tag{1}$$

[1] Grand Canonical Ensemble

Mott insulator phase

Consider the limit $t \ll U$:

$$\hat{H} = \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu \sum_i \hat{n}_i$$

$$\implies E = \sum_i \frac{U}{2} n_i(n_i - 1) - \mu n_i$$

Ground state:

$$n_i = n = \left\lfloor \frac{\mu}{U} \right\rfloor + 1, \quad \forall\, i$$

$$|\psi_{\text{gs}}\rangle = \bigotimes_{i=1}^{L} |n\rangle = \underbrace{|n, n, n, \ldots, n\rangle}_{L \text{ sites}}$$

$T = 0$ Phases of the BHM (contd.)

Superfluid phase

Consider the limit $t \gg U$:

$$\hat{H} = -t \sum_{\langle i,j \rangle} \left(\hat{a}_i^\dagger \hat{a}_j + \text{h.c.} \right) - \mu \sum_i \hat{n}_i$$
$$= \sum_k \left(-2t \cos k - \mu \right) \hat{\tilde{a}}_k^\dagger \, \hat{\tilde{a}}_k$$

Ground state:

$$k_{\text{min}} = 0$$

$$|\psi_{\text{gs}}\rangle = \left(\hat{\tilde{a}}_{k=0}^\dagger \right)^N |0\rangle = \left(\frac{1}{\sqrt{L}} \sum_{i=1}^{L} \hat{a}_i^\dagger \right)^N |0\rangle$$

$T = 0$ Phases of the BHM (contd.)

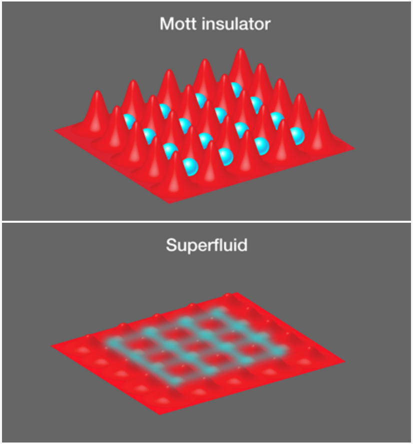

Figure: Ground state phases of the Bose-Hubbard model [2].

Mean-field theory

Mean-field decoupling:

$$\hat{a}_j = \phi_j + \delta\hat{a}_j, \qquad \hat{a}_i^\dagger = \phi_i^* + \delta\hat{a}_i^\dagger.$$

$$\implies \hat{a}_i^\dagger \hat{a}_j \approx \phi_j \hat{a}_i^\dagger + \phi_i^* \hat{a}_j - \phi_i^* \phi_j$$

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Decoupling of the hopping term:

$$H_{\text{hop}} = -t \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \text{h.c.}$$

$$= -t \sum_i \Big(\sum_{j \in \text{nbr}_i} \phi_j \Big) \hat{a}_i^\dagger - t \sum_i \Big(\sum_{j \in \text{nbr}_i} \phi_j^* \Big) \hat{a}_i^\dagger - t \sum_i \Big(\sum_{j \in \text{nbr}_i} \phi_j \Big) \phi_i^*$$

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Reduced to a sum of single-site Hamiltonians!

Mean-field theory (contd.)

Wavefunction ansatz

$$|\psi\rangle = \bigotimes_{i=1}^{L} \left(\sum_{n=0}^{\infty} f_i(n) \, |n\rangle \right)$$

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Further, translation symmetry $\implies \phi_i = \phi, \ \forall \, i$.

$$\boxed{\hat{h}_i(\phi) = -zt\phi\left(\hat{a}_i + \hat{a}_i^\dagger\right) + \frac{U}{2} n_i(n_i - 1) - \mu n_i + zt|\phi|^2} \tag{2}$$

where $z = 2d$ is the coordination number, and $\hat{H}_{\text{MFT}} = \sum_i \hat{h}_i(\phi)$.

Mean-field theory (contd.)

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Solve for single-site Hamiltonian!

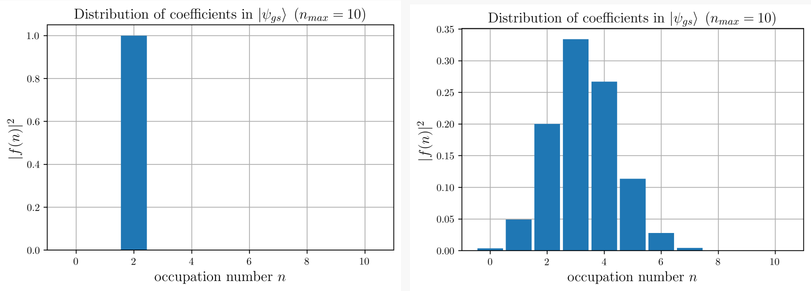
- Order parameter $= \langle \hat{a} \rangle = \phi$.
- Set a cutoff for the maximum boson occupancy n_{max}.
- No dependence on number of lattice sites.
- Solve for the mean-field parameter ϕ recursively.

Fixed point iteration

$$\phi^{(0)} \longrightarrow \text{ Diagonalize } h(\phi) \text{ and find } \psi_{\mathrm{gs}} \longrightarrow \text{calculate } \phi^{(1)} = \langle \hat{a} \rangle_{\mathrm{gs}}$$

Repeat!

Wavefunction of the phases



(a) Mott insulator at $(t/U, \mu/U) = (0.025, 1.5)$.

(b) Superfluid at $(t/U, \mu/U) = (0.75, 1.5)$.

Figure: Distribution of modes in different phases.

Average occupation number

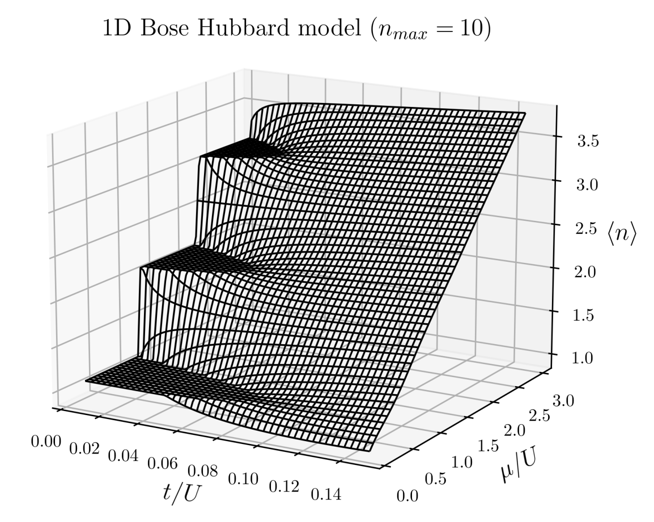


Figure: Jumps in average occupation number between different Mott insulator lobes.

Occupation number variance

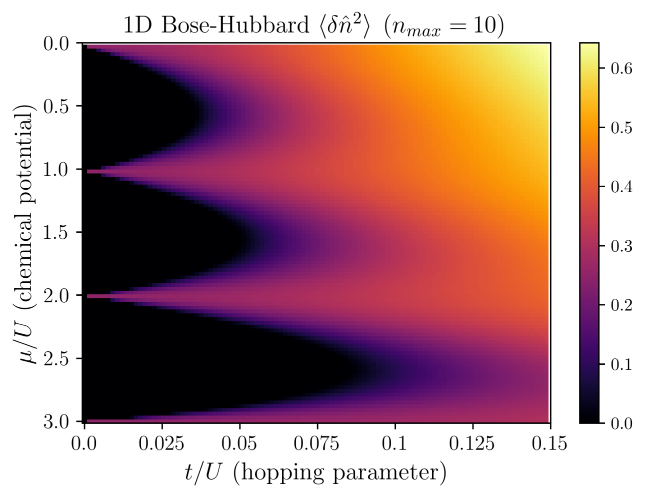


Figure: Variance in the occupation number $\langle \delta \hat{n}^2 \rangle$ roughly distinguishes phases.

Phase diagram for the order parameter ϕ

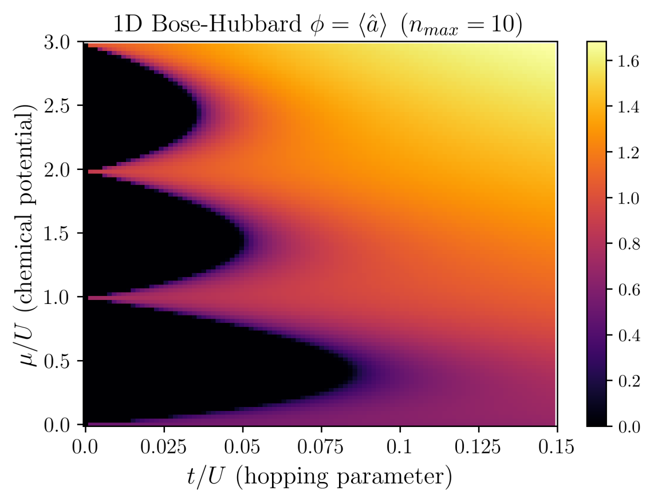


Figure: Order parameter ϕ distinguishing the Mott insulator and the superfluid phases.

Varying $n_{\max}$

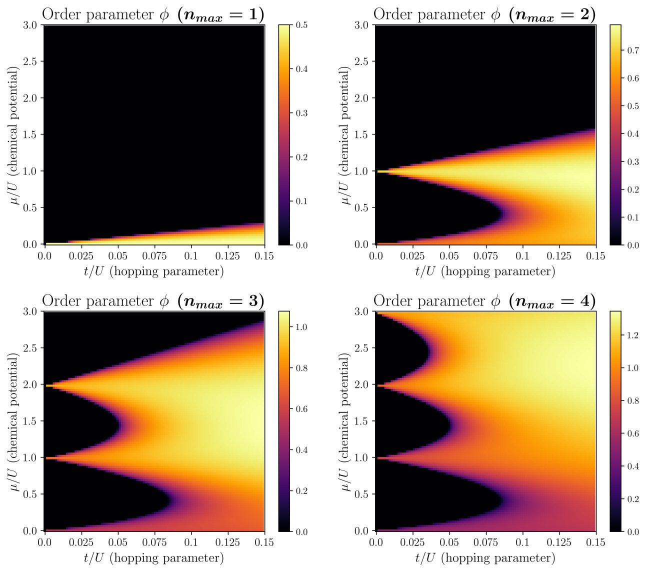


Figure: $n_{\max} \overset{!}{=} n + 1$ where n is the occupation number of the MI lobe.

Perturbative analysis of mean-field theory

Mean-field decoupled BHM Hamiltonian:

$$\hat{H}_{\mathrm{MFT}} = \underbrace{\sum_i \left(\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i + zt|\phi|^2 \right)}_{h^{(0)}} \underbrace{- zt \sum_i \left(\phi \hat{a}_i^\dagger + \phi^* \hat{a}_i \right)}_{V}$$

Eigenstates of $h^{(0)}$ are

$$\left| n_0^{(0)} \right\rangle = \bigotimes_{i=1}^{N} \frac{1}{\sqrt{n_0}} (b_i^\dagger)^{n_0} \left| 0 \right\rangle$$

with eigenenergies

$$E_{n_0}^{(0)} = \frac{U}{2} n_0 (n_0 - 1) - \mu n_0 + tz|\phi|^2$$

The p^{th} order correction for eigenstates

$$\left|n_0^{(p)}\right\rangle = \sum_{m\neq n}\left|m_0^{(0)}\right\rangle \frac{\left\langle m_0^{(0)}\right| V \left|n_0^{(p-1)}\right\rangle}{E_{n_0}^{(0)} - E_{m_0}^{(0)}} - \sum_{j=1}^{p} E_{n_0}^{(j)} \sum_{m\neq n}\left|m_0^{(0)}\right\rangle \frac{\left\langle m_0^{(0)} \middle| n_0^{(p-j)}\right\rangle}{E_{n_0}^{(0)} - E_{m_0}^{(0)}}$$

and p^{th} order energy correction is

$$E_{n_0}^{(p)} = \left\langle n_0^{(0)}\right| V \left|n_0^{(p-1)}\right\rangle$$

Energy expansion

Since $V = -zt\sum_{\langle i,j\rangle}\left(\phi a_i^\dagger + \phi^* a_j\right)$ is linear, $\implies$ all odd order corrections of energy are 0, i.e.,

$$\boldsymbol{p^{\text{th}}\ \textbf{order perturbation theory} \sim V^p}$$

Therefore, the energy anstaz looks as follows

$$E_{n_0} = E_{n_0}^{(0)} + E_{n_0}^{(2)}|\phi|^2 + E_{n_0}^{(4)}|\phi|^4 + \mathcal{O}(|\phi|^6) \tag{3}$$

First and second order corrections

We get

$$\left|n_0^{(1)}\right\rangle = -tz\left(\frac{\phi\sqrt{n_0+1}|n_0+1\rangle}{\mu - Un_0} + \frac{\phi^*\sqrt{n_0}|n_0-1\rangle}{U(n_0-1)-\mu}\right)$$

and

$$\left|n_0^{(2)}\right\rangle = (tz)^2\Big(\frac{\phi^2\sqrt{n_0+1}\sqrt{n_0+2}\,|n_0+2\rangle}{(\mu - Un_0)(2\mu - U(2n_0+1))} + \frac{\phi^{*2}\sqrt{n_0}\sqrt{n_0-1}\,|n_0-2\rangle}{(U(n_0-1)-\mu)(U(2n_0-3)-2\mu)}\Big)$$

Third order correction

$$\left|n_0^{(3)}\right\rangle = (-tz)^3 \Big(\frac{\phi|\phi|^2\sqrt{n_0+1}(n_0+2)|n_0+1\rangle}{(\mu - Un_0)^2(2\mu - U(2n_0+1))} + \frac{\phi^*|\phi|^2\sqrt{n_0}(n_0-1)|n_0-1\rangle}{(U(n_0-1)-\mu)^2(U(2n_0-3)-2\mu)} \Big) - (tz)^3|\phi|^2\left[\frac{n_0+1}{\mu - Un_0} + \frac{n_0}{U(n_0-1)-\mu}\right] \times \left[\frac{\phi\sqrt{n_0+1}|n_0+1\rangle}{(\mu - Un_0)^2} + \frac{\phi^*\sqrt{n_0}|n_0-1\rangle}{(U(n_0-1)-\mu)^2}\right] + C_{n_0+3}\left|n_0+3\right\rangle + C_{n_0-3}\left|n_0-3\right\rangle$$

Energy corrections

$$E_{n_0}^{(0)} = \frac{U}{2} n_0(n_0 - 1) - \mu n_0,$$

$$E_{n_0}^{(2)} = (tz)^2 \left(\frac{n_0 + 1}{\mu - U n_0} + \frac{n_0}{U(n_0 - 1) - \mu} \right) + tz$$

and

$$E_{n_0}^{(4)} = (tz)^4 \Big(\frac{(n_0+1)(n_0+2)}{(\mu - U n_0)^2 (2\mu - U(2n_0+1))} + \frac{n_0(n_0-1)}{(U(n_0-1)-\mu)^2 (U(2n_0-3) - 2\mu)} \Big)$$

Minimizing energy in equation (3)

$$\frac{\partial E}{\partial \phi^*} = E_{n_0}^{(2)}\phi + 2E_{n_0}^{(4)}|\phi|^2\phi = 0$$

$$\implies \phi = 0 \quad or \quad |\phi|^2 = -\frac{E_{n_0}^{(2)}}{2E_{n_0}^{(4)}}$$

and

$$\frac{\partial^2 E}{\partial \phi \partial \phi^*} = E_{n_0}^{(2)} + 4E_{n_0}^{(4)}|\phi|^2 > 0$$

This implies

$$|\phi| = \begin{cases} 0 & \text{for } E_{n_0}^{(2)} > 0 \\ \sqrt{\frac{-E_{n_0}^{(2)}}{2E_{n_0}^{(4)}}} & \text{for } E_{n_0}^{(2)} < 0 \end{cases}$$

Second order phase transitions occur at $E^{(2)}_{n_0} = 0$

$$(tz)^2 \left(\frac{n_0 + 1}{\mu - U n_0} + \frac{n_0}{U(n_0 - 1) - \mu} \right) + tz = 0$$

Taking $\bar{\mu} \equiv \mu / U$ and $w \equiv zt/U$

$$w = \frac{(n_0 - \bar{\mu})(\bar{\mu} - (n_0 - 1))}{\bar{\mu} + 1} \tag{4}$$

Numerical vs. Perturbation theory

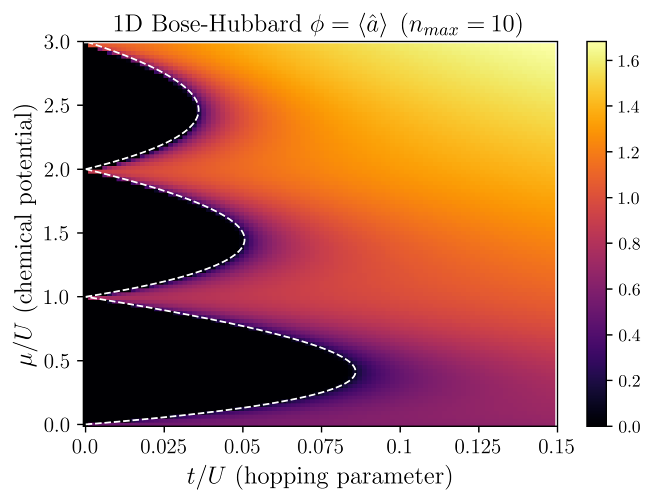


Figure: Phase diagram with $\langle a \rangle = \phi$ as the order parameter, compared to PT results.

Numerical vs. Perturbation theory (contd.)

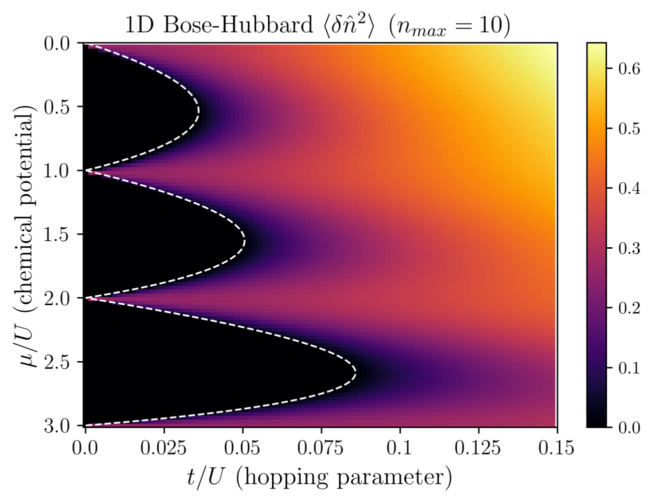


Figure: Variance $\langle \delta\hat{n}^2 \rangle$ compared to PT results.

Average particle number can be calculated using the relation

$$\langle n \rangle = -\frac{\partial E}{\partial \mu}$$

$$= -\frac{\partial}{\partial \mu} E_{n_0}^{(0)} - \frac{\partial}{\partial \mu}(E_{n_0}^{(2)} |\phi|^2) - \frac{\partial}{\partial \mu}(E_{n_0}^{(4)} |\phi|^4)$$

$$= n_0 - \frac{\partial}{\partial \mu}(E_{n_0}^{(2)} |\phi|^2 - E_{n_0}^{(4)} |\phi|^4)$$

Perturbative analysis of mean-field theory (contd.)

In Mott-insulating state,

$$\langle n \rangle = n_0$$

For superfluid state,

$$\langle n \rangle = n_0 + \frac{\partial}{\partial \mu}\left(\frac{(E_{n_0}^{(2)})^2}{4E_{n_0}^{(4)}}\right)$$

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