Quantum Phase Transitions and the Bose-Hubbard Model

Eric Fehr
advised by Dr. Fabricio Albuquerque

Swiss Federal Institute of Technology, Zurich

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Outline

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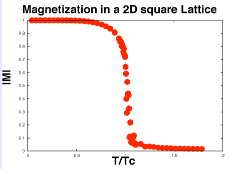
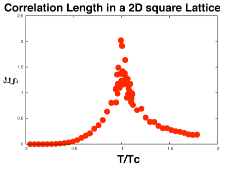
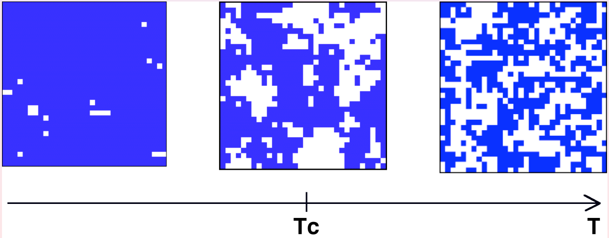
Classical Phase Transitions



Classical Ising model: $H_I = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z$



$M \sim |T - T_c|^{\gamma}$ (Magnetization)
$\xi \sim |T - T_c|^{-\nu}$ (correlation length)



What is a Quantum Phase Transition?

- thermal fluctuations die out at $T = 0$
- quantum fluctuations due to Heisenbergs uncertainty relation
- changes in the ground state at $T = 0$
- level crossing
- competing terms in the Hamiltonian

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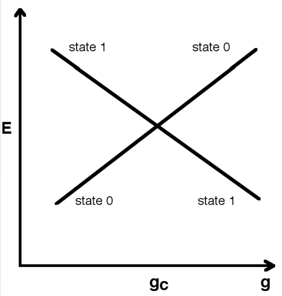

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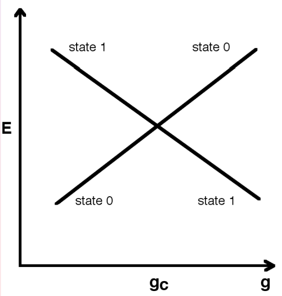
$$H = H_0 + g\,H_1$$

$$\Delta \sim |g - g_c|^{z\nu} \quad \text{(energy gap)}$$



The Bose-Hubbard Hamiltonian and its Symmetry

The Bose-Hubbard Hamiltonian was first studied by Fisher et.al. in '89

$$H_B = -w \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) - \mu \sum_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) \ .$$

Bosonic creation and annihilation operators $b^\dagger$ and b

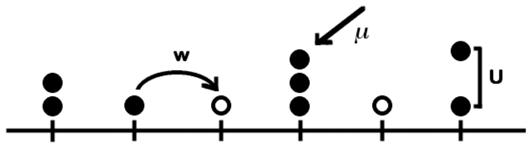
$$\begin{aligned} b^\dagger \, |n\rangle &= \sqrt{n+1} \, |n+1\rangle \\ b \, |n\rangle &= \sqrt{n} \, |n-1\rangle \end{aligned}$$

Fulfilling $[b_i, b_j^\dagger] = \delta_{ij}$ and $[b_i, b_j] = 0$

The occupation number operator: $\hat{n}_i = b_i^\dagger b_i$

The Bose-Hubbard Hamiltonian and its Symmetry

$$H_B = \underbrace{-w\sum_{\langle i,j\rangle}(b_i^\dagger b_j + b_j^\dagger b_i)}_{\text{hopping term}} - \mu\sum_i \hat{n}_i + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1)\ .$$



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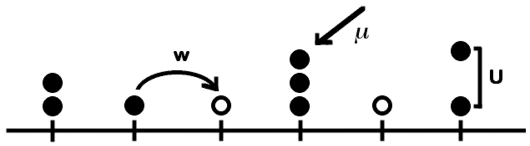

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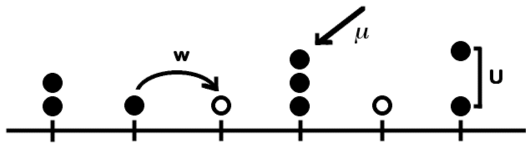
$$H_B = \underbrace{-w \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i)}_{\text{hopping term}} \underbrace{-\mu \sum_i \hat{n}_i}_{\text{offset}} + \underbrace{\frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1)}_{\text{onsite repulsion}} \ .$$



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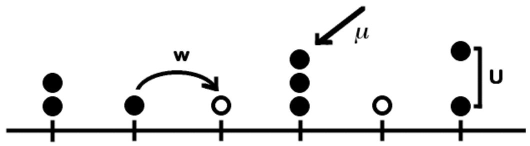

H_B is invariant under a global U(1)≡O(2) phase transformation under which $\hat{b}_i \rightarrow \hat{b}_i e^{i\Phi}$.

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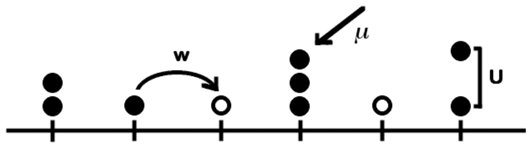


H_B is invariant under a global U(1)≡O(2) phase transformation under which $\hat{b}_i \rightarrow \hat{b}_i e^{i\Phi}$.

We do have conservation of the total number of bosons as $\hat{N}_b = \sum_i \hat{n}_{bi}$ commutes with H_B.

Competing Terms

$$\frac{w}{U} \rightarrow 0 : \quad H_o = \sum_i \frac{U}{2} \hat{n}_i(\hat{n}_i - 1) \quad \text{its ground state would be } |n_0\rangle$$

$$b_q = \frac{1}{\sqrt{M}} \sum_i b_i\, e^{\imath q r_i} \qquad b_i = \frac{1}{\sqrt{M}} \sum_q b_q\, e^{\imath q r_i}$$

$$\langle b_q^\dagger b_q \rangle = \frac{1}{M} \left\langle \sum_{ij} b_i^\dagger b_j\, e^{\imath\, q(r_j - r_i)} \right\rangle = \frac{1}{M} \sum_{ij} \left\langle b_i^\dagger b_j \right\rangle\, e^{\imath\, q(r_j - r_i)}$$

$$= \frac{1}{M} \sum_{ij} \delta_{ij} n\, e^{\imath\, q(r_j - r_i)} = n$$

$\Rightarrow$ Featureless!

Competing Terms

$$
\begin{aligned}
\frac{w}{U} \quad &\rightarrow \quad \infty : \quad H_h = -w \sum_{\langle i,j \rangle} b_i^\dagger b_j + b_j^\dagger b_i \\
b_q \quad &= \quad \frac{1}{\sqrt{M}} \sum_i b_i \, e^{\imath q r_i} \qquad b_i = \frac{1}{\sqrt{M}} \sum_q b_q \, e^{\imath q r_i} \\
H_h \quad &= \quad -\frac{w}{M} \sum_{\langle i,j \rangle, q, k} \left(b_q^\dagger b_k \, e^{\imath \, (r_j k - r_i q)} + \text{h.c.} \right) \\
&= \quad -\frac{w}{M} \sum_{i,q,k,a} \left(b_q^\dagger b_k \, e^{\imath \, (r_i (k-q) + ak)} + \text{h.c.} \right) \\
&= \quad -w \sum_{q,k,a} \hat{n}_q \delta_{qk} \left(e^{\imath ak} + e^{-\imath ak} \right) = -w \sum_q \hat{n}_q \cos(q)
\end{aligned}
$$

Ground state is at $q = 0 \Rightarrow \langle b_q^\dagger b_q \rangle = \delta_{q,0} \Rightarrow$ only one momentum contributes!

Competing Terms

$$\frac{w}{U} \rightarrow 0 : \quad H_o = \sum_i \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) \quad \text{its ground state would be } |n_0\rangle$$

$$\langle b_q^\dagger b_q \rangle = n \quad \Rightarrow \text{Particles well localized in space!}$$

$$\Rightarrow \text{Mott insulating state}$$

$$\frac{w}{U} \rightarrow \infty : \quad H_h = -w \sum_{\langle i,j \rangle} b_i^\dagger b_j + b_j^\dagger b_i$$

$$\langle b_q^\dagger b_q \rangle = \delta_{q,0} \quad \Rightarrow \text{Particles spread out over the hole system!}$$

$$\Rightarrow \text{Superfluid state}$$

Mean-Field Hamiltonian

We choose a mean-field Hamiltonian with the same on-site terms as H_B and add an additional term with a "field" Ψ_B to represent the influence of the neighboring sites.

$$H_{MF} = \sum_i \left(-\mu \hat{n}_i + \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) \underbrace{-\Psi_B^* \hat{b}_i - \Psi_B \hat{b}_i^\dagger}_{\text{breaks U(1) symm.}} \right) .$$

$\Psi_B = 0 \rightarrow$ symmetric phase $\Rightarrow |\Psi_B|^2$ acts as order parameter

Mean-Field ground state: $|\psi_{MF}\rangle = |n_0\rangle_1 \otimes \cdots \otimes |n_0\rangle_M$

Expectation value of H_B in the Mean-Field

$$H_B = -w\sum_{\langle i,j\rangle}(b_i^\dagger b_j + b_j^\dagger b_i) - \mu\sum_i \hat{n}_i + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1)$$

$$H_{MF} = \sum_i \left(-\mu\hat{n}_i + \frac{U}{2}\hat{n}_i(\hat{n}_i-1)\underbrace{-\Psi_B^*\hat{b}_i - \Psi_B\hat{b}_i^\dagger}_{\text{breaks U(1) symm.}}\right)$$

Expectation value of H_B in the Mean-Field ground state:

$$E_0 = \langle\Psi_{MF}|(H_{MF} + (H_B - H_{MF}))|\Psi_{MF}\rangle$$

$$= E_{MF}(\Psi_B) - Z\,M\,w\langle b^\dagger\rangle\langle b\rangle + \Psi_B^*\langle b\rangle + \Psi_B\langle b^\dagger\rangle$$

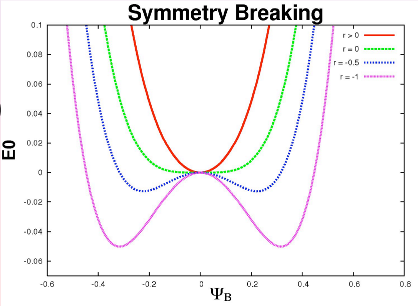
Symmetry Breaking and the Landau Argument

Expectation value of H_B in the Mean-Field ground state:

$$E_0 = E_{MF}(\Psi_B) - Z\,M\,w\langle b^\dagger\rangle\langle b\rangle + \Psi_B^*\langle b\rangle + \Psi_B\langle b^\dagger\rangle$$

Landau argument:

$$E_0 = E_{00} + r\,|\Psi_B|^2 + s\,|\Psi_B|^4 + O(|\Psi_B|^6)$$



Deriving the Phase Diagram

Using second order perturbation theory to calculate E_{MF} and hence E_0

$$\frac{E_0}{M} = \frac{U}{2} n_0(n_0 - 1) - \mu n_0 - \chi_0(1 - Zw\chi_0)|\Psi_B|^2$$

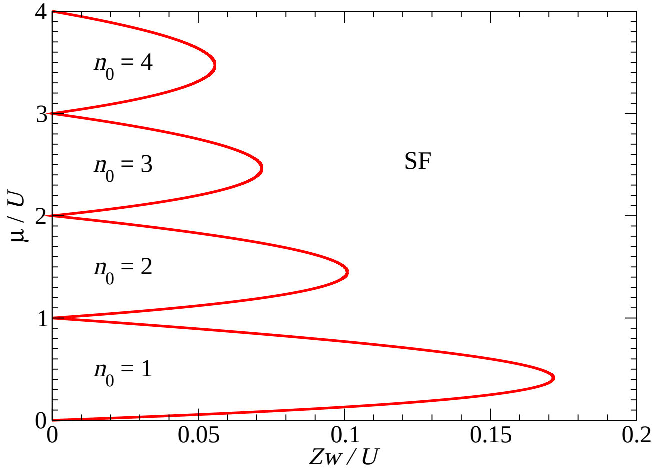
therefore

$$r = \chi_0(1 - Zw\chi_0) \quad \text{where} \quad \chi_0 = \frac{n_0+1}{Un_0-\mu} + \frac{n_0}{\mu-U(n_0-1)} \quad .$$

For $r = 0$ we get the phase boundary

$$Zw = \frac{(n_0-\frac{\mu}{U})(\frac{\mu}{U}-n_0+1)}{n_0(n_0-\frac{\mu}{U})+(n_0+1)(\frac{\mu}{U}-n_0+1)} \quad .$$

Phase Diagram for the BHM



Monte Carlo Simulations of the BHM

Figures taken from G.G. Batrouni Phys. Rev. Lett. Vol 65 Number 14

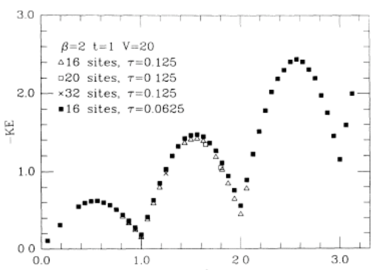
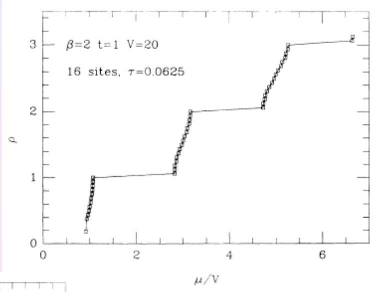
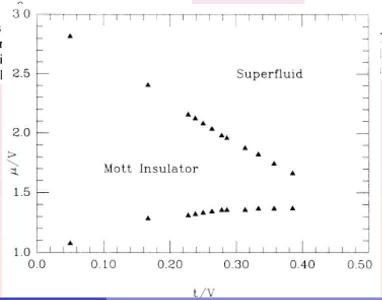


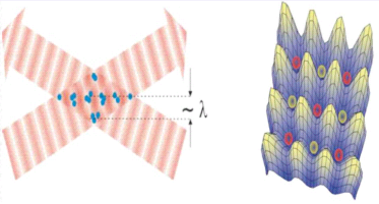
FIG. 1. The kinetic energy is
tion ρ for $t=1$, $V=20$. Differ
choices of lattice size and imagi
τ. Error bars are smaller than tl

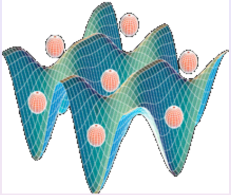


he occupation (density) ρ as a function of chemi-
, $\mu=E_{N+1}-E_N$, going across the first three lobes
lator regions. The solid line is to guide the eye.



Ultracold bosonic gas in an optical lattice potential





The Hamiltonian for an ultracold bosonic gas in an optical lattice potential:

$$H = \int d^3x\, \psi^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) + V_T(\mathbf{x}) \right) \psi(\mathbf{x})$$
$$+ \frac{1}{2} \frac{4\pi a_s \hbar^2}{m} \int d^3x\, \psi^\dagger(\mathbf{x}) \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) \psi(\mathbf{x})$$

Ultracold bosonic gas in an optical lattice potential

The Hamiltonian for an ultracold bosonic gas in an optical lattice potential:

$$
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H &= \int d^3x\, \psi^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m} \bigtriangledown^2 + V(\mathbf{x}) + V_T(\mathbf{x}) \right) \psi(\mathbf{x}) \\
&\quad + \frac{1}{2} \frac{4\pi a_s \hbar^2}{m} \int d^3x\, \psi^\dagger(\mathbf{x}) \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) \psi(\mathbf{x})
\end{aligned}
$$

Bloch wavefunctions expanded as wannierfunctions :

$$
\psi(\mathbf{x}) = \sum_i b_i\, w(\mathbf{x} - \mathbf{x}_i)
$$

Keeping only lowest vibrational states this leads us to :

$$
H_B = -w \sum_{\langle i,j \rangle} b_i^\dagger b_j - \mu \sum_i \hat{n}_i + \frac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1) \ .
$$

Coherence Measurement

Figures taken from Greiner et.al. Nature Vol 415 3 January 2002