8. Superfluid to Mott-insulator transition
Overview

Optical lattice potentials
Solution of the Schrödinger equation for periodic potentials
Band structure
Bloch oscillation of bosonic and fermionic atoms in optical lattices
Wannier functions
Bose-Hubbard Hamiltonian
Superfluid to Mott-insulator transition
Optical dipole traps

Potential: \[ U_{\text{Dip}}(r) = \frac{1}{2} \left\langle \vec{d} \cdot \vec{E} \right\rangle = \frac{1}{2\varepsilon_0 c} \text{Re}(\alpha) I(r) \propto \frac{\Gamma}{\Delta} I(r) \]

Loss rate: \[ \gamma_{sc}(r) = \frac{P_{\text{abs}}}{\hbar \omega} = \frac{1}{\hbar \varepsilon_0 c} \text{Im}(\alpha) I(r) \propto \left( \frac{\Gamma}{\Delta} \right)^2 I(r) \]

\( \vec{d} \): induced dipole moment, \( \alpha \): polarizability
\( \Gamma \): Dipole matrix element between ground and excited states, \( \Delta = \omega - \omega_0 \): detuning

\( \Delta < 0 \): red detuned
attractive potential

\( \Delta > 0 \): blue detuned
repulsive potential

\[ I(r) = I_0 e^{-\frac{2r^2}{w^2}} \] Gaussian beam
Optical standing wave fields produce periodic potentials with lattice constants half of the laser’s wavelength ($\lambda \sim 800 \text{ nm} – 10 \mu\text{m}$).

$$I(x) = I_0 \sin^2\left(\frac{2\pi}{\lambda_{\text{laser}}} x + \varphi\right)$$

$$a = \frac{\lambda_{\text{laser}}}{2}$$
Band model

Solutions of the Schrödinger equation in periodic potentials

\[ SE: \quad E\psi = \left(-\frac{\hbar^2}{2m} \Delta + U(z)\right)\psi \quad \text{with} \quad U(x) = \sum U_n e^{in k_0 x}, \quad k_0 = \frac{2\pi}{a} \]

Ansatz: \[ \psi(x) = \sum_k C(k) e^{ikx} \]

Comparing coefficients yields conditional equations for parameters \( C(k) \)

\[ (*) \quad (\lambda_k - E) C(k) + \sum U_n C(k - n k_0) = 0 \quad \text{with} \quad \lambda_k = \frac{\hbar^2 k^2}{2m} \]

For a specific \( k \in [-k_0/2, k_0/2] \) the wavefunction \( \psi_k \) contains also wavevectors \( k+nk_0 \).

\[ \psi_k(x) = \sum_n C(k - nk_0) e^{i(k-nk_0)x} = u_k(x) e^{ikx} \quad \text{Bloch Theorem} \]

In order to find energies and eigenstates for a given \( k \), the equation system \((*)\) has to be solved for all \( k \in [k+nk_0] \).

Note: \(|k>\) is not an eigenstate of the Hamiltonian.
Band model – energies and eigenstates

Example: \( k \in [-k_0/2, k_0/2] \)

\[
U(x) = A \cos k_0 x = \frac{A}{2} \left( e^{i k_0 x} + e^{-i k_0 x} \right)
\]

Solve following \((2n+1) \times (2n+1)\) equation system

\[
\begin{pmatrix}
\frac{\hbar^2 (k-nk_0)^2}{2m} - E & \frac{A}{2} & 0 & 0 & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & \frac{A}{2} & \frac{\hbar^2 k^2}{2m} - E & \frac{A}{2} & 0 \\
0 & 0 & \frac{A}{2} & \frac{\hbar^2 (k+nk_0)^2}{2m} - E & \frac{A}{2}
\end{pmatrix}
\begin{pmatrix}
C(k-nk_0) \\
\vdots \\
C'(k) \\
\vdots \\
C(k+nk_0)
\end{pmatrix} = 0
\]

\[
< k-nk_0 | \psi_k > \\
< k+nk_0 | \psi_k >
\]

Diagonalization yields: \((2n+1)\) - Eigenvalues \( E_m(k) \)

\((2n+1)\) - Eigenstates \( \psi^m_k(x) \)

with band index \( m \)

\[
\psi^m_k(x) = \sum_{n} C_m(k-nk_0)e^{i(k-nk_0)x} = u^m_k(x)e^{ikx}
\]
Band model – example

\[ U = 0 \]

\[
\begin{pmatrix}
\frac{\hbar^2(k-nk_0)^2}{2m} & 0 & 0 & 0 & 0 \\
0 & \cdots & \frac{\hbar^2k^2}{2m} & 0 & 0 \\
0 & 0 & \frac{\hbar^2k^2}{2m} & 0 & 0 \\
0 & 0 & 0 & \cdots & \frac{\hbar^2(k+nk_0)^2}{2m}
\end{pmatrix}
\]

\[ U = A \cos k_0x \]

\[
\begin{pmatrix}
\frac{\hbar^2(k-nk_0)^2}{2m} & \frac{A}{2} & 0 & 0 & 0 \\
\frac{A}{2} & \cdots & \frac{\hbar^2k^2}{2m} & \frac{A}{2} & 0 \\
0 & \frac{A}{2} & \frac{\hbar^2k^2}{2m} & \frac{A}{2} & 0 \\
0 & 0 & 0 & \cdots & \frac{\hbar^2(k+nk_0)^2}{2m}
\end{pmatrix}
\]

\[ E_n, \psi_{km}^n(x) = \sum_m C_m(k-nk_0)e^{i(k-nk_0)x} \]
Phase difference between neighboring lattice sites

\[ \phi_j - \phi_i = \frac{(E_j - E_i) \cdot t}{\hbar} \]

Nonlinear dynamics leads to dephasing if gradient is left on for longer times! (2D lattice)

M. Greiner et al. PRL 87, 160405 (2001)
Bloch oscillation of fermionic atoms

Large contrast for more than 100 oscillation periods

Comparison: fermions vs. bosons

(a) Momentum distribution of fermions in the lattice: 1 ms (continuous line) and 252 ms (dashed line).

(b) Momentum distribution of bosons at 0.6 ms (continuous line) and 3.8 ms (dashed line). The much faster broadening for bosons is due to the presence of interactions.

\[ T_B = 1.2 \text{ s} \]

Fermi surfaces
Bose gas in a 3D lattice potential

Resulting potential consists of a simple cubic lattice where the BEC coherently populates about 100,000 lattice sites.

M. Greiner et al. PRL 87, 160405 (2001)
Interference of a superfluid Bose gas from a 3D lattice

M. Greiner et al. PRL 87, 160405 (2001)
Wave function of single particles in a periodic potential

Bloch states: \[ \Psi_k(r) = u_k(r)e^{ikr} \]

Plane waves modulated by a lattice periodic function

Fourier transform

Wannier states: \[ w(r - R_j) = \frac{1}{\sqrt{L}} \sum_{k}^{BZ} e^{ikR_j}\Psi_k(r) \]

Localized wave functions. This picture allows tunneling as well as localized states.

Inverse Fourier transform

\[ \Psi_k(r) = \frac{1}{\sqrt{L}} \sum_{j}^{\text{lattice sites}} e^{-ikR_j}w(r - R_j) \]

The Hamiltonian can be written in Wannier basis (TONS). Second quantization results in the Bose-Hubbard Hamiltonian.

(Necessary condition: only the lowest band is populated \(\leftrightarrow\) excitation energies are larger than the energy gap.)
Bose-Hubbard Hamiltonian

Expanding the field operator in the Wannier basis of localized wave functions on each lattice site, yields:

\[
\hat{\psi}(x) = \sum_i \hat{a}_i w(x - x_i)
\]

Bose-Hubbard Hamiltonian

\[
H = -J \sum_{\langle i,j \rangle} \hat{a}_i^+ \hat{a}_j + \sum_i \epsilon_i \hat{n}_i + \frac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1)
\]

Single particle energy in the trapping potential

\[
J = -\int d^3x \, w(x - x_i) \left( -\frac{\hbar^2}{2m} \nabla^2 + V_{lat}(x) \right) w(x - x_j)
\]

Tunnel matrix element (hopping element)

\[
U = \frac{4\pi \hbar^2 a}{m} \int d^3 x |w(x)|^4
\]

Onsite interaction matrix element

Bosonic operators

- **annihilation** \( \hat{a}_i |..., N_i, ...\rangle = \sqrt{N_i - 1} |..., N_i - 1, ...\rangle \)
- **creation** \( \hat{a}_i^+ |..., N_i, ...\rangle = \sqrt{N_i + 1} |..., N_i + 1, ...\rangle \)
- \( (\hat{a}_i)^* = \hat{a}_i^+ \quad [\hat{a}_i, \hat{a}_j^+] = \delta_{ij} \)
- **number** \( \hat{a}_j^+ \hat{a}_j = n_j \)

Superfluid Limit

The kinetic energy dominates (weakly interacting bosonic system).

\[ H = -J \sum_{i,j} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} U \sum_{i} \hat{n}_i (\hat{n}_i - 1) \]

Atoms are delocalized over the entire lattice, macroscopic wave function describes this state.

\[ |\Psi_{SF}\rangle \propto \left( \sum_{i=1}^{M} \hat{a}_i^\dagger \right)^N |0\rangle \quad \langle a_i \rangle \neq 0 \]

Poissonian atom number distribution per lattice site.
Mott-insulator

Interaction energy dominates (strongly correlated bosonic system).

\[
H = -J \sum_{i,j} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} U \sum_i \hat{n}_i(\hat{n}_i - 1)
\]

Atoms are completely localized to lattice sites.

\[
|\Psi_{Mott}\rangle \propto \prod_{i=1}^{M} \left(a_i^\dagger\right)^n |0\rangle \quad \langle a_i \rangle = 0
\]

Fock states with a vanishing atom number fluctuation are formed, e.g. n=1.
Momentum distribution for different potential depths ($E_{\text{recoil}}$)

Restoring coherence

a) Ramp up the potential for generating the Mott-insulator state and subsequent ramp down.

b) Width of the zero momentum central peak

The coherence is restored within the tunneling time to the neighboring lattice site.

Quantum phase transition from a superfluid to a Mott-insulator

At the critical point $g_c$ the system will undergo a phase transition from a superfluid to an insulator.

This phase transition occurs even at $T=0$ and is driven by quantum fluctuations!

Characteristic of the quantum phase transition

- Excitation spectrum is dramatically modified at the critical point.
- $U/J < g_c$ (Superfluid regime)
  Excitation spectrum is gapless
- $U/J > g_c$ (Mott-Insulator regime)
  Excitation spectrum is gapped

Critical ratio: $U/J = z \times 5.8$

number of next neighbors (for a cubic lattice 6)
Creating excitations in the MI phase

Mott-insulator with $n_i = 1$ atom per lattice site

Energy Scales:
\[
\hbar \omega_v \approx 20 \cdot U
\]
\[
U \approx 10 - 300 \cdot J
\]

Without gradient potential

With gradient potential

Special case: $\Delta E_{ij} = U$
Measuring the excitation gap in the MI phase
(probability vs. gradient)

10 $E_{\text{recoil}} t_{\text{perturb}} = 2$ ms

13 $E_{\text{recoil}} t_{\text{perturb}} = 4$ ms

16 $E_{\text{recoil}} t_{\text{perturb}} = 9$ ms

20 $E_{\text{recoil}} t_{\text{perturb}} = 20$ ms

Literature

Bose-Einstein condensates in 1D- and 2D optical lattices

Exploring the phase coherence in a 2D lattice of Bose-Einstein condensates
M. Greiner et al. PRL 87, 160405 (2001)

Fermionic atoms in a three dimensional optical lattice: observing Fermi surfaces, dynamics and interactions, M. Köhl et al., PRL94, 080403 (2005)

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