Ultracold Bose Gases in Optical Lattices

Superfluidity, Interference Pattern, Disorder

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Mission Statement

- recent experiments on the Mott-insulator transition for bosonic atoms in optical lattices [1] reveal a huge potential for the study of the complex mechanisms behind quantum phase transitions
- we discuss the microscopic definition of the superfluid fraction (order parameter) in the framework of the Bose-Hubbard model and relate it to experimental observables like the interference pattern after expansion
- we perform exact numerical calculations for the superfluid to Mott-insulator transition in one-dimensional systems and compare superfluid fraction, number fluctuations, and fringe visibility
- we study the influence of simple non-uniform lattice potentials as they can be produced in two-color lattices and map out a phase diagram as function of modulation amplitude and interaction strength

Summary of Results

- the superfluid fraction is not a static ground state property but the response of the system to a perturbation (phase twist)
- it depends crucially on the excited states of the system; they are responsible for the vanishing of f_s in the insulating phase
- ground state observables like the matter wave interference pattern cannot provide full information on superfluid properties and the Mott-insulator transition
- a sinusoidal modulation of the well depth together with the two-body interaction generates a rich phase diagram with several distinct insulating phases (localized, Bose glass, Mott insulator) which can be detected through their interference patterns
- one has to devise specialized experimental schemes to probe superfluidity; e.g. accelerate the lattice (impose phase variation) and measure flow velocity after expansion

Bose-Hubbard Model

- one-dimensional lattice with I sites and N bosons
- single-particle states described in terms of Wannier functions $w(x-\xi_i)$ of the lowest band; define operator $\mathbf{a}_i^\dagger$ that creates a boson in the Wannier state at site i
- usual Hamiltonian of the interacting many-boson system translates into the Bose-Hubbard Hamiltonian [2]

$$\mathbf{H} = -J\sum_{i=1}^{I}(\mathbf{a}_{i+1}^\dagger \mathbf{a}_i + \text{h.a.}) + \sum_{i=1}^{I}\epsilon_i\,\mathbf{n}_i + \frac{V}{2}\sum_{i=1}^{I}\mathbf{n}_i(\mathbf{n}_i-1)$$

J : tunneling strength between adjacent sites
ϵ_i : on-site single-particle energies
V : on-site two-body interaction strength

- ground state $|\Psi_0\rangle$ is obtained from the exact solution of eigenvalue problem in a complete basis of Fock states $|n_1,\dots,n_I\rangle$ with all compositions of occupation numbers n_i
- alternative representation in terms of Bloch functions $\psi_q(x)$ for quasi-momentum q; from the relation between Bloch and Wannier functions we can construct the creation operators for a boson in a Bloch state

$$\mathbf{c}_q^\dagger = \sum_{i=1}^{I} e^{-iq\xi_i}\,\mathbf{a}_i^\dagger \qquad \text{with } q = \text{multiples of } \tfrac{2\pi}{Ia}$$

- this allows us to determine occupation numbers for the Bloch states, i.e., the quasi-momentum distribution

$$\tilde{n}_q = \langle\Psi_0|\,\mathbf{c}_q^\dagger\mathbf{c}_q\,|\Psi_0\rangle$$

- the quasi-momentum $q=0$ state describes the condensate, i.e., we can define the condensate fraction $f_c = \tilde{n}_{q=0}/N$

Interference Pattern

- simplest experimental observable is the matter-wave interference pattern after release from the lattice and expansion
- intensity at a detection point $\vec{y}$ after a time-of-flight τ is given by (interactions neglected) [3]

$$\mathcal{I}(\vec{y}) = \langle\Psi_0|\,\mathbf{A}^\dagger(\vec{y})\,\mathbf{A}(\vec{y})\,|\Psi_0\rangle$$

- approximating the expanded wave packets from the individual sites by Gaussians $\chi_i(\vec{y})$ and neglecting the spatial structure of the envelope leads to the amplitude operator

$$\mathbf{A}(\vec{y}) = \sum_{i=1}^{I}\chi_i(\vec{y})\,\mathbf{a}_i \sim \sum_{i=1}^{I} e^{i\phi_i(\vec{y})}\,\mathbf{a}_i$$

where $\phi_i(\vec{y})$ is the phase accumulated on the path from site i to the detection point

- intensity as function of the phase difference $\delta\phi = \phi_{i+1}-\phi_i$ between adjacent sites

$$\mathcal{I}(\delta\phi) = \frac{1}{I}\Big[N + \sum_{d=1}^{I-1} B_d\,\cos(d\,\delta\phi)\Big]$$

with the exp. values of the dth neighbor hopping operators

$$B_d = \sum_{i=1}^{I-d}\langle\Psi_0|\,\mathbf{a}_{i+d}^\dagger\mathbf{a}_i + \mathbf{a}_i^\dagger\mathbf{a}_{i+d}\,|\Psi_0\rangle$$

- there is a one-to-one correspondence between intensity and quasi-momentum distribution

$$\tilde{n}_q = \langle\Psi_0|\,\mathbf{c}_q^\dagger\mathbf{c}_q\,|\Psi_0\rangle = \mathcal{I}(\delta\phi = qa)\,.$$

i.e. the interference pattern provides full information about the quasi-momentum distribution

Superfluidity

- superfluidity is the rigidity of the system under variations of the condensate phase, i.e., it measures the response to a perturbation and not a mere ground state property
- assume a condensate wave function $\Phi(\vec{x}) = e^{i\theta(\vec{x})}|\Phi(\vec{x})|$ with a spatially varying phase $\theta(\vec{x})$; the phase variation gives rise to a velocity field

$$\vec{v}_s(\vec{x}) = \frac{\hbar}{m}\,\vec{\nabla}\theta(\vec{x})$$

which describes the irrotational, non-dissipative flow of the superfluid component

- to probe the superfluid content of a system we impose a linear phase variation by means of twisted boundary conditions or phase factors in the hopping term

$$\mathbf{a}_{i+1}^\dagger\mathbf{a}_i \to e^{-i\Theta/I}\,\mathbf{a}_{i+1}^\dagger\mathbf{a}_i$$

- the energy change $E_\Theta - E_0$ caused by the imposed phase variation is for small twist angles Θ identical to the kinetic energy of the superflow $T_s = \frac{1}{2}mNf_s v_s^2$
- by computing the ground state energies of the twisted and the non-twisted Hamiltonian we can determine the superfluid fraction [3]

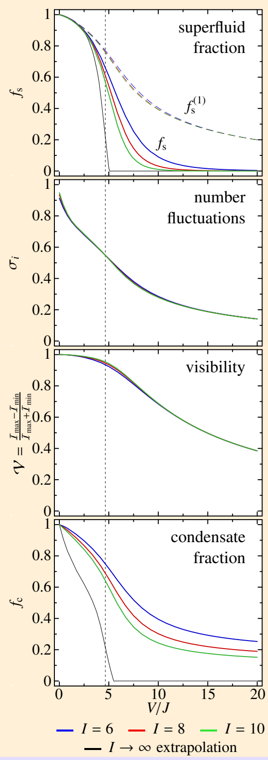
$$f_s = \frac{I^2}{N}\,\frac{E_\Theta - E_0}{J\,\Theta^2}$$

- alternatively we can calculate the energy difference in second order perturbation theory (analogous Drude weight)

$$f_s = f_s^{(1)} - f_s^{(2)} = \frac{1}{NJ}\Big(-\frac{1}{2}\langle\Psi_0|\,\mathbf{T}\,|\Psi_0\rangle - \sum_{\nu\neq0}\frac{|\langle\Psi_\nu|\,\mathbf{J}\,|\Psi_0\rangle|^2}{E_\nu - E_0}\Big)$$

$$\mathbf{T} = -J\sum_{i=1}^{I}(\mathbf{a}_{i+1}^\dagger\mathbf{a}_i + \text{h.a.})\;,\qquad \mathbf{J} = iJ\sum_{i=1}^{I}(\mathbf{a}_{i+1}^\dagger\mathbf{a}_i - \text{h.a.})$$

Superfluid to Mott-Insulator Transition $(N/I = 1)$



- the repulsive two-body interaction drives a quantum phase transition from a superfluid phase at small V/J to the Mott-insulator at large V/J
- exact Monte Carlo calculations and strong coupling expansions predict the transition at $(V/J)_{\text{crit}} = 4.65$ for a 1D system with filling $N/I = 1$ [5]
- the order parameter for this transition is the superfluid fraction f_s which, in an infinite lattice, vanishes above $(V/J)_{\text{crit}}$
- our exact calculations show that the vanishing of f_s in the insulator phase is due to a cancellation of
  - *a)* the first order contribution $f_s^{(1)}$ which depends only on the ground state and still has a substantial size in the insulating phase
  - *b)* the second order term $f_s^{(2)}$, which involves the full excitation spectrum, exhibits a threshold-like increase around $(V/J)_{\text{crit}}$

➤ properties of the excitation spectrum are crucial for superfluidity and the Mott-insulator transition; hence ground state observables cannot provide full information on the phase transition

- number fluctuations and fringe visibility decrease much slower than the superfluid fraction and do not show a clear signature for the phase transition
- e.g. in the insulating phase where f_s vanishes the visibility can still be up to 75%
- however, the visibility measures the non-uniformity of the quasi-momentum distribution; vanishing visibility indicates uniform occupation of the band

Two-Color Lattices: Localization & Bose Glass

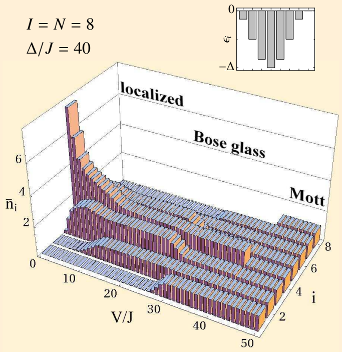
- the superposition of two standing wave lattices with different wavelengths generates a superlattice with sinusoidal modulation of the well depth, i.e., the on-site energies ϵ_i
- the interplay between interaction and "disorder" generates a rich phase diagram with various insulating phases [4]:

localized phase: all particles at the deepest well of each unit cell; in the presence of weak interactions a few sites are populated; large number fluctuations

Bose glass: integer occupation with sudden rearrangements between different distributions; small number fluctuations except near rearrangements; disordered Mott insulator

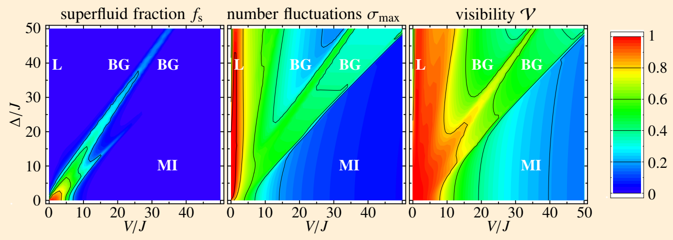
Mott insulator: despite non-uniform on-site energies a Mott insulator with an uniform population appears for $V > \Delta$

- superfluidity is destroyed by both interaction and disorder; however, their competition can also restore superfluidity



➤ **again**: the fringe contrast is not suitable as a measure for the superfluid properties

➤ **but**: the interference pattern and the variations in the visibility can be used to distinguish the various insulating phases experimentally



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