Superfluidity and Interference Pattern of Ultracold Bosons in Optical Lattices

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We present a study of the superfluid properties of atomic Bose gases in optical lattice potentials using the Bose-Hubbard model. To do this, we use a microscopic definition of the superfluid fraction based on the response of the system to a phase variation imposed by means of twisted boundary conditions. We compare the superfluid fraction to other physical quantities, i.e., the interference pattern after ballistic expansion, the quasi-momentum distribution, and number fluctuations. We have performed exact numerical calculations of all these quantities for small one-dimensional systems. We show that the superfluid fraction alone exhibits a clear signature of the Mott-insulator transition. Observables like the fringe visibility, which probe only ground state properties, do not provide direct information on superfluidity and the Mott-insulator transition.

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Ultracold atomic gases in optical lattices provide a unique framework for the experimental study of fundamental quantum phenomena in interacting many-body systems. This is especially true for the exploration of quantum phase transitions such as the superfluid to Mott-insulator transition observed in a recent pioneering experiment [1]. The remarkable degree of experimental control over all the relevant parameters—density, interaction strength, lattice geometry and dimensionality—allows much more detailed studies of the complicated mechanisms behind quantum phase transition than conventional solid state systems.

It is clearly the case that the most important quantity for characterizing the superfluid-to-insulator transition is the superfluid density or superfluid fraction f_{s}. The aim of this paper is to set up the general theoretical framework for the calculation of the superfluid fraction within the Bose-Hubbard model and to compare it, on the formal level, with quantities being measured at the moment. These include the interference pattern after ballistic expansion, the quasi-momentum distribution as well as the number fluctuations which are important in applications. We perform exact numerical calculations for the Mott-insulator transition in an one-dimensional system to demonstrate the relationship, and more importantly the differences, between the superfluid fraction and various ground state observables, most notably the visibility of the interference pattern.

Superfluidity. The concept of superfluidity is closely related to the existence of a condensate in the interacting many-boson system [2]. Formally, the one-body density matrix $\rho^{(1)}(\vec{x},\vec{x}')$ has to have exactly one macroscopic eigenvalue which defines the number of particles N_0 in the condensate; the corresponding eigenvector describes the condensate wave function $\phi_0(\vec{x}) = \mathrm{e}^{\mathrm{i}\theta(\vec{x})}|\phi_0(\vec{x})|$. A spatially varying condensate phase $\theta(\vec{x})$ is associated with a velocity field for the condensate, $\vec{v}_0(\vec{x}) = \frac{\hbar}{m}\vec{\nabla}\theta(\vec{x})$. This irrotational velocity field is identified with velocity of the superfluid flow $\vec{v}_{\mathrm{s}}(\vec{x}) \equiv \vec{v}_0(\vec{x})$ [2] and enables us to derive an expression for the superfluid fraction $f_{\mathrm{s}} = N_{\mathrm{s}}/N$. Consider a system with a finite linear dimension L in $\vec{e}_1$-direction and a ground state energy E_0 calculated with periodic boundary conditions. Now we impose a linear phase variation $\theta(\vec{x}) = \Theta\, x_1/L$ with a total twist angle Θ over the length of the system in the $\vec{e}_1$-direction. Technically, this can be achieved by introducing twisted boundary conditions of the form $\Psi(\vec{x}_1,...,\vec{x}_i + L\vec{e}_1,...) = \mathrm{e}^{\mathrm{i}\,\Theta}\;\Psi(\vec{x}_1,...,\vec{x}_i,...)$ with respect to all coordinates of the many-body wave function. The resulting ground state energy E_Θ will depend on the phase twist. For very small twist angles $\Theta \ll \pi$ the energy difference $E_\Theta - E_0$ can be attributed to the kinetic energy T_{s} of the superflow generated by the phase gradient. Thus

$$E_\Theta - E_0 \stackrel{!}{=} T_{\mathrm{s}} = \tfrac{1}{2} m N f_{\mathrm{s}} \vec{v}_{\mathrm{s}}^{\,2}\ , \tag{1}$$

where mNf_{s} is the total mass of the superfluid component. This ansatz corresponds to the macroscopic definition of superfluidity based on the response of the fluid to moving boundaries [3]. Replacing the superfluid velocity $\vec{v}_{\mathrm{s}}$ with the phase gradient leads to a fundamental relation for the superfluid fraction [4, 5]

$$f_{\mathrm{s}} = \frac{2m}{\hbar^2}\frac{L^2}{N}\;\frac{E_\Theta - E_0}{\Theta^2}\ . \tag{2}$$

Hence the superfluid fraction can be interpreted as a measure for the stiffness of the system under an imposed phase variation. This demonstrates that superfluidity is not a static ground state property but rather the response of the system to an external perturbation. We should note that this definition of superfluidity does not tell anything about the stability of the superfluid flow at finite velocities [6]. However, it is equivalent to the helicity modulus [5] and the concept of winding numbers used in Monte Carlo approaches [3].

We now transfer these findings to a lattice system described in the framework of the Bose-Hubbard model [4, 7, 8]. For simplicity we restrict ourselves to a regular one-dimensional lattice composed of I sites described by the Bose-Hubbard Hamiltonian

$$\mathbf{H}_0 = -J\sum_{i=1}^{I}(\mathbf{a}_i^\dagger \mathbf{a}_{i+1} + \text{h.a.}) + \frac{V}{2}\sum_{i=1}^{I}\mathbf{n}_i(\mathbf{n}_i - 1)\ , \tag{3}$$

where $\mathbf{a}_i^\dagger$ creates a boson in the lowest Wannier state localized at site i and $\mathbf{n}_i = \mathbf{a}_i^\dagger\mathbf{a}_i$. The first term describes the hopping or tunneling between adjacent sites with a tunneling strength J, the second term characterizes the on-site two-body interaction with a strength V [7, 9]. The hopping between the first and the last site of the lattice is included ($I+1\hat{=}1$), which corresponds to periodic boundary conditions. The generalization to three-dimensional lattices is straight forward.

In order to compute the energy of the system with an imposed phase twist Θ we map the twisted boundary conditions by means of a local unitary transformation onto the Hamiltonian [10, 11]. This leads to a twisted Hamiltonian of the form

$$\mathbf{H}_\Theta = -J \sum_{i=1}^{I} (\mathrm{e}^{-\mathrm{i}\,\Theta/I}\ \mathbf{a}_{i+1}^\dagger \mathbf{a}_i + \text{h.a.}) + \frac{V}{2} \sum_{i=1}^{I} \mathbf{n}_i(\mathbf{n}_i - 1) \tag{4}$$

with a modified hopping term that contains the so-called Peierls phase factors $\mathrm{e}^{\pm\mathrm{i}\,\Theta/I}$ [11]. The energy E_Θ in the presence of the phase twist is given by the lowest eigenvalue of the twisted Hamiltonian using periodic boundary conditions. From the difference of the ground state energies $E_\Theta - E_0$ we obtain the superfluid fraction [12]

$$f_\text{s} = \frac{I^2}{N}\, \frac{E_\Theta - E_0}{J\,\Theta^2}\ , \tag{5}$$

now expressed in terms of the parameters of the Bose-Hubbard model.

One can get a more detailed insight into the dependency of the superfluid fraction on the structure of the eigenstates of the system by considering a perturbative calculation of the energy difference $E_\Theta - E_0$. We expand the the twisted Hamiltonian up to second order in the twist angle Θ thus,

$$\mathbf{H}_\Theta \approx \mathbf{H}_0 + \frac{\Theta}{I}\,\mathbf{J} - \frac{\Theta^2}{2I^2}\,\mathbf{T} = \mathbf{H}_0 + \mathbf{H}_\text{pert}\ . \tag{6}$$

Here we defined a current operator $\mathbf{J} = \mathrm{i}J\sum_i(\mathbf{a}_{i+1}^\dagger\mathbf{a}_i - \text{h.a.})$ and the usual kinetic energy or hopping operator $\mathbf{T} = -J\sum_i(\mathbf{a}_{i+1}^\dagger\mathbf{a}_i + \text{h.a.})$. We can calculate the energy shift $E_\Theta - E_0$ caused by the perturbation $\mathbf{H}_\text{pert}$ in second order perturbation theory. Retaining the terms up to the quadratic order in the twist angle Θ we obtain for the superfluid fraction using Eq. (5)

$$\begin{aligned} f_\text{s} &= f_\text{s}^{(1)} - f_\text{s}^{(2)} \\ &= \frac{1}{NJ}\bigg(-\frac{1}{2}\langle\Psi_0|\,\mathbf{T}\,|\Psi_0\rangle - \sum_{\nu\neq 0} \frac{|\langle\Psi_\nu|\,\mathbf{J}\,|\Psi_0\rangle|^2}{E_\nu - E_0} \bigg), \end{aligned} \tag{7}$$

where the $|\Psi_\nu\rangle$ ($\nu = 0, 1...$) are the eigenstates of the non-twisted Bose-Hubbard Hamiltonian $\mathbf{H}_0$. The ground state expectation value of the hopping operator describes the first order contribution ${f_\text{s}}^{(1)}$. The sum over the excited states involving the current operator constitutes the second order term ${f_\text{s}}^{(2)}$. It is this second order term which introduces a significant dependence of the superfluid fraction on the excitation spectrum and thus goes beyond the static ground state properties of the system.

Equation (7) corresponds to the Drude weight used to characterize the DC conductivity of charged fermionic systems [13]. This demonstrates that the phase factors appearing in the twisted Hamiltonian (4) can actually be realized experimentally, i.e., by an external electric field for charged particles or by some linear external potential or even by accelerating the lattice.

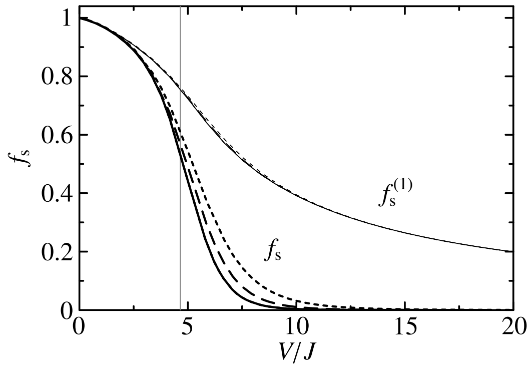

FIG. 1: Superfluid fraction f_s as function of the interaction strength V/J for filling $N/I = 1$ and different lattice sizes: $I = 12$ (full line), 10 (dashed), 8 (dotted). The thin lines show the first order term $f_\text{s}^{(1)}$. The vertical line marks the critical interaction strength $(V/J)_\text{crit} \approx 4.65$ for the infinite system.

To illustrate the generic behavior of the superfluid fraction as function of the interaction parameter V/J, and hence the appearance of the Mott insulator phase, we solve the eigenvalue problems of the non-twisted Hamiltonian (3) and the twisted Hamiltonian (4) numerically. We construct the corresponding Hamilton matrices using a complete basis of Fock states $|n_1, ..., n_I\rangle$ with all compositions of the occupation numbers n_i. The ground state energies E_0 and $E_{\Theta=0.1}$ are obtained with an efficient iterative Lanczos algorithm [8]. The perturbative expression (7) is then used to separate the contributions of ground and excited states.

Figure 1 shows the superfluid fraction f_s for one-dimensional lattices with up to $I = 12$ sites and fixed filling factor $N/I = 1$. The superfluid fraction is 1 for the non-interacting system and decreases slowly for small V/J. In the region of the Mott transition f_s drops rapidly and goes to zero in the Mott-insulator phase. The sequence of curves for increasing system size shows a moderate size dependence around the onset of the insulator phase. One can extrapolate the curves to $I \to \infty$ and finds a vanishing superfluid fraction above a critical interaction strength which is in good agreement with the value $(V/J)_\text{crit} \approx 4.65$ obtained by strong coupling expansion [14] and Monte Carlo methods [15]. The thin lines in Fig. 1 depict the isolated first order contribution ${f_\text{s}}^{(1)} = -\frac{1}{2NJ}\langle\Psi_0|\,\mathbf{T}\,|\Psi_0\rangle$ to the superfluid fraction (7), which is just the reduced expectation value of the hopping operator. This quantity decreases much slower than the total superfluid fraction. Thus even deep in the Mott regime the hopping operator has a considerable expectation value (up to 30% of its value in the non-interacting system) although the system is already an insulator, i.e., the superfluid fraction is zero. The rapid decrease of the total superfluid fraction is largely due to the second order contribution ${f_\text{s}}^{(2)}$, which vanishes for small V/J and shows a threshold-like behavior around the Mott transition. The vanishing of the superfluid fraction in the insulating phase is generated by a strong cancellation between the first and second order term. This emphasizes that the superfluid fraction depends crucially on the properties of the excited states.

Interference Pattern. The standard experimental approach to investigate the state of the Bose gas in an optical lattice relies on the matter-wave interference pattern after the gas was released from the lattice. How much can the presence or absence of interference fringes tell about superfluidity?

In the simplest model of the expansion for the system after release from the lattice the effects of interactions are neglected. We can write the intensity observed after some time-of-flight τ at a point $\vec{y}$ as

$$\mathcal{I}(\vec{y}) = \langle\Psi_0|\, \mathbf{A}^\dagger(\vec{y})\mathbf{A}(\vec{y})\, |\Psi_0\rangle \ . \tag{8}$$

We assume that the Wannier functions $w(x-\xi_i)$ can be described by Gaussians. The amplitude operator is given by $\mathbf{A}(\vec{y}) = \frac{1}{\sqrt{I}} \sum_{i=1}^{I} \chi_i(\vec{y})\ \mathbf{a}_i$, where $\chi_i(\vec{y})$ denotes the Gaussian wave packet associated with site i after a free evolution for a time τ. Since we are interested only in the generic features of the interference pattern we discard all terms related to the spatial structure of the envelope of $\chi_i(\vec{y})$ and only retain the phase terms. This leads to

$$\mathbf{A}(\vec{y}) = \frac{1}{\sqrt{I}} \sum_{i=1}^{I} \mathrm{e}^{\mathrm{i}\,\phi_i(\vec{y})}\ \mathbf{a}_i \ , \tag{9}$$

where $\phi_i(\vec{y})$ is the total phase acquired on the path from site i to the observation point $\vec{y}$. In the far-field approximation we can assume a constant phase difference $\delta\phi(\vec{y}) = \phi_{i+1}(\vec{y}) - \phi_i(\vec{y})$ for adjacent sites (gravity neglected). Calculating the intensity (8) as function of the phase difference $\delta\phi$, using the far-field form of the amplitude operator (9), leads to the following expression:

$$\begin{aligned}\mathcal{I}(\delta\phi) &= \frac{1}{I} \sum_{i,j=1}^{I} \mathrm{e}^{\mathrm{i}\,(j-i)\delta\phi}\ \langle\Psi_0|\, \mathbf{a}_i^\dagger \mathbf{a}_j\, |\Psi_0\rangle \\ &= \frac{1}{I}\left[N + \sum_{d=1}^{I-1} B_d\ \cos(d\,\delta\phi)\right] .\end{aligned} \tag{10}$$

In the last step we rearranged the double summation into a sum over the hopping distance $d = j - i$. The coefficients B_d are given by the expectation values of the dth neighbour hopping operators, $B_d = \sum_{i=1}^{I-d} \langle\Psi_0|\, \mathbf{a}_{i+d}^\dagger \mathbf{a}_i + \mathbf{a}_i^\dagger \mathbf{a}_{i+d}\, |\Psi_0\rangle$. The leading coefficient B_1 is related to the first order term of to the superfluid fraction (7) through $B_1 = 2(I-d)\, f_\mathrm{s}{}^{(1)}$. Clearly, there is no contribution corresponding to the important second order term $f_\mathrm{s}{}^{(2)}$ of the superfluid fraction, because the intensity (8) involves only the ground state. Thus the interference pattern cannot provide full information on the superfluid properties, as it only measures the first order term of the superfluid fraction.

Figure 2 shows the intensities $\mathcal{I}(\delta\phi)$ resulting from the exact numerical calculation for different interaction strengths. The interference peaks around $\delta\phi = 0, \pm 2\pi, ...$ correspond to the prominent peaks observed experimentally. Recall that terms describing the overall envelope were neglected in (9).

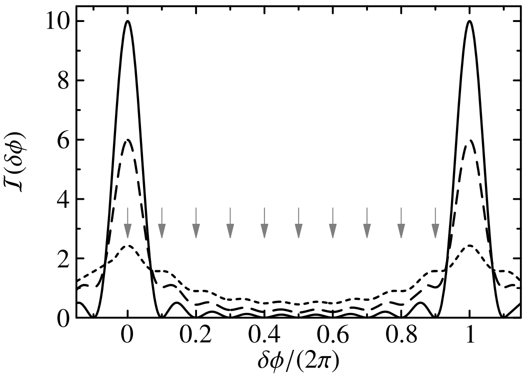

FIG. 2: Intensity $\mathcal{I}(\delta\phi)$ as function of the phase difference $\delta\phi$ for a system with $I = N = 10$ and $V/J = 0$ (full line), 5 (dashed line), 10 (dotted line).

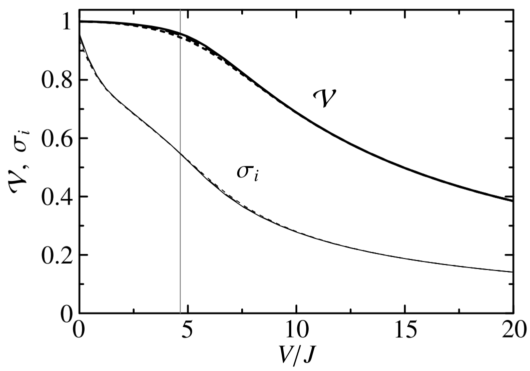

FIG. 3: Fringe visibility $\mathcal{V}$ and number fluctuations σ_i as function of the interaction strength V/J for $N/I = 1$ and $I = 12$ (full), 10 (dashed), and 8 (dotted). Both quantities show practically no size dependence.

With increasing V/J the intensity $\mathcal{I}_\mathrm{max}$ of these principal peaks reduces. At the same time an incoherent background emerges such that the minimum intensity $\mathcal{I}_\mathrm{min}$ between the principal peaks grows. Thus the interference fringes are increasingly washed-out and eventually only a flat intensity distribution remains.

As a quantitative measure for the vanishing of the interference pattern the full line in Fig. 3 shows the fringe visibility $\mathcal{V} = (\mathcal{I}_\mathrm{max} - \mathcal{I}_\mathrm{min})/(\mathcal{I}_\mathrm{max} + \mathcal{I}_\mathrm{min})$ as function of V/J. In addition, the dashed curve shows the on-site number fluctuations $\sigma_i = (\langle \mathbf{n}_i^2\rangle - \langle \mathbf{n}_i\rangle^2)^{1/2}$ of the ground state. Obviously, the visibility of the fringes has no immediate relation to the number fluctuations. For small interaction strengths $V/J \lesssim 5$ the visibility remains almost constant at $\mathcal{V} \approx 1$ whereas the number fluctuations drop to 0.5 in the same interval.

A second observation concerns the relation with the superfluid fraction shown in Fig. 1. The superfluid fraction f_s vanishes much faster than the visibility $\mathcal{V}$ and the number fluctuations σ_i. For values of V/J where the superfluid fraction has practically vanished the visibility is still larger than 0.7. Thus neither fringe visibility nor number fluctuations are suitable indicators for the superfluid properties and the Mott-insulator transition in lattice systems. Because neither $\mathcal{V}$ nor σ_i show noticable finite-size effects (see Fig. 3), this also holds for large one-dimensional systems. A similar conclusion can be drawn from Monte Carlo simulations including the influence of an additional parabolic trapping potential [16].

Quasi-Momentum Distribution. The interference pattern after ballistic expansion is closely related to the quasi-momentum distribution of the Bose gas in the lattice. Formally, the connection is revealed by constructing an expression for the occupation numbers for the Bloch states of the lowest band. We can use the relation between localized Wannier functions $w(x-\xi_i)$ and Bloch functions $\psi_q(x)$ to define a creation operator $\mathbf{c}_q^\dagger$ for a boson in Bloch state with quasi-momentum q [9]

$$\mathbf{c}_q^\dagger = \frac{1}{\sqrt{I}} \sum_{i=1}^{I} \mathrm{e}^{-\mathrm{i}\,q\,\xi_i}\ \mathbf{a}_i^\dagger \ , \tag{11}$$

where ξ_i is the coordinate of the center of the ith lattice site. This relation is identical to the definition of the amplitude operator $\mathbf{A}(\vec{y})$ in (9) if we identify the phase $\phi_i(\vec{y})$ with $q\xi_i$ or the phase difference $\delta\phi$ with qa, where $a=\xi_{i+1}-\xi_i$ is the lattice spacing. The occupation numbers $\tilde{n}_q$ for the Bloch states with quasi-momenta q are, therefore, directly related to the intensity (10) through

$$\tilde{n}_q = \langle\Psi_0|\,\mathbf{c}_q^\dagger\mathbf{c}_q\,|\Psi_0\rangle = \mathcal{I}(\delta\phi = qa) \ . \tag{12}$$

Notice that in a finite system of length L the quasi-momentum q has discrete values which are integer multiples of $2\pi/L$. The values of $\delta\phi = qa$ for these allowed quasi-momenta are marked by gray arrows in Fig. 2.

Because of this intimate relation the interference pattern provides complete information on the quasi-momentum distribution of the trapped system. The intensity of the principal interference peak is proportional to the occupation number of the $q=0$ Bloch state, i.e., it describes the number of particles in the condensate. The washing out of the interference peaks with increasing interaction strength is linked to the successive redistribution of the population from the condensate state with $q=0$ to states of higher quasi-momenta. In the limit of large V/J the intensity distribution is flat, i.e., all quasi-momentum states of the lowest band are occupied uniformly. On the basis of this one-to-one correspondence between interference pattern and quasi-momentum distribution we can reinterpret the visibility $\mathcal{V}$ of the interference fringes as measure for the uniformity of the quasi-momentum distribution. Vanishing visibility corresponds to a completely uniform quasi-momentum distribution, whereas visibility $\mathcal{V}=1$ means that at least one quasi-momentum state is unoccupied.

Conclusions. We have shown that the matter-wave interference pattern observed experimentally contains all the information on the quasi-momentum distribution of the lattice system but no direct information on the superfluid fraction. The behavior of the superfluid fraction shown in Fig. 1 depends strongly on the properties of the excitation spectrum, which enters through the second order contribution $f_s{}^{(2)}$. The importance of this second order term shows that one cannot probe superfluidity through quantities which are only sensitive to the ground state of the system (like number fluctuation, condensate fraction, coherence properties, etc.). One has to devise an experimental scheme that measures superfluidity directly. The formal definition of superfluidity gives a hint how to accomplish this. As mentioned earlier there are several methods to create the phase factor appearing in $\mathbf{H}_\Theta$ experimentally, e.g. by accelerating the lattice. By observing the resulting flow behavior after release from the lattice one should be able to distinguish superfluid and non-superfluid components and determine the superfluid fraction.

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