Superfluidity and BEC in optical lattices and porous media: a path integral Monte Carlo study

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Abstract

We evaluate the Bose-Einstein condensate density and the superfluid fraction of bosons in a periodic external potential using Path-Integral Monte Carlo (PIMC) methods. The periodic lattice consists of a cubic cell containing a potential well that is replicated along 1D using periodic boundary conditions. The aim is to describe bosons in a 1D optical lattice or helium confined in a periodic porous medium. The One-Body Density Matrix (OBDM) is evaluated and diagonalized numerically to obtain the single boson natural orbitals and the occupation of these orbitals. The condensate fraction is obtained as the fraction of Bosons in the orbital that has the highest occupation. The superfluid density is obtained from the winding number. From the condensate orbital and superfluid fraction we investigate (1) the impact of the periodic external potential on the spatial distribution of the condensate, and (2) the correlation of localizing the condensate into separated parts and the loss of superflow along the lattice. For high density systems, as the well depth increases, the condensate becomes depleted in the wells and confined to the plateaus between successive wells, as in pores between necks in a porous medium. For low density systems, as the well depth increases the BEC is localized at the center of the wells (tight binding) and depleted between the wells. In both cases, the localization of the condensate suppresses superflow leading to a superfluid-insulator cross-over. The impact of the external potential on the temperature dependence of the superfluidity is also investigated. The external potential suppresses the superfluid fraction at all temperatures, with a superfluid fraction significantly less than 1 at low temperature. The addition of an external potential does not, however, significantly reduce the transition temperature.

I. Introduction

The two most remarkable properties of Bose liquids at low temperature are superfluidity and Bose-Einstein condensation (BEC). In this paper, we investigate the interdependence of BEC and superfluidity in an ordered, periodic potential. Fritz London first proposed the connection between these two properties in liquid Helium. In contrast, the first successful quantitative theory of superfluidity – that due to Landau – does not explicitly mention BEC. Rather the Landau theory follows from three postulates: (1) a quantum liquid showing superfluidity consists of two components: a superfluid component composed of particles in the ground state, and a normal component composed of elementary excitations, (2) the elementary excitations have a phonon-roton form with no free single particle excitations with energy proportional to \( k^2 \) and (3) the
superfluid component flows irrotationally and carries zero entropy. Starting with this minimal set of postulates, Landau was able to make a remarkable set of predictions, such as dissipationless flow and second sound, all of which were later verified experimentally.

It can, however, be shown that Landau’s postulates follow naturally as a consequence of BEC as long as the superfluid velocity is defined as the gradient of the phase of the condensate wave function. Formally, if the condensate wave function is expressed as

$$\psi_0(\mathbf{r}, t) = \psi(\mathbf{r}, t) e^{i\phi(\mathbf{r}, t)},$$

the superfluid velocity is given by

$$v_s(\mathbf{r}, t) = -\frac{\hbar}{m} \nabla \phi(\mathbf{r}, t).$$

It immediately follows that $$\nabla \times v_s(\mathbf{r}, t) = 0$$, i.e., the flow is irrotational. Also, since no “ignorance” is associated with the single particle state $$\psi_0$$, all the entropy must be carried by the normal component, thereby recovering Landau’s postulates. Elementary excitations of the P-R form with no free particle like excitations also follow from BEC. An important corollary to the above is that for a system to have system-wide superflow, $$\phi(\mathbf{r}, t)$$ must be continuously connected across the whole sample. A transition from extended to localized BEC will therefore result in the loss of macroscopic superflow. The purpose of this paper is to demonstrate the loss of superflow arising from localization of BEC to disconnected islands in space by an external potential in finite sized Bose systems.

![Fig.1: Superfluid fraction, $$\rho_s$$, and condensate fraction, $$\rho_c$$, of an ideal Bose gas of finite size as a function of temperature $$T/T_c$$. The size is set by the number of particles: $$N = 256$$ and $$N = 100,000$$ and the thermodynamic limit (TL). $$T_c$$ is the BEC critical temperature in the TL which involves the density, typically 0.1 m$^{-3}$. In the thermodynamic limit $$n_c = N_c/N = 1 - (T/T_c)^{1/3}$$ and $$n_c$$ and $$\rho_c$$ are identical. At finite $$N$$, $$n_c$$ and $$\rho_c$$ are calculated using analytic expressions given in the appendix and are larger than in the TL and extend to higher temperatures.](image)

The connection between BEC and superfluidity is most clear in an ideal Bose gas, where the two fractions are identical in the thermodynamic limit. As an illustration, in Fig. 1 we show analytically computed values of superfluid fraction and condensate fraction as a function of temperature for an ideal gas of $$N$$ Bosons. At finite $$N$$, the superfluid density exceeds the condensate fraction. For a large number $$N$$ of particles with a commensurately large system size
(i.e., in the thermodynamic limit (TL)), the two fractions are identical at all temperatures (details of the calculation can be found in the appendix). While this equality is illuminating, it is only formal. The critical velocity of an ideal Bose gas is zero because it has a free particle energy spectrum proportional to $k^2$.

In an interacting Bose fluid, the condensate fraction decreases with increasing interaction strength. However, the connection between superfluidity and BEC via the condensate wave function survives. For example, superfluidity, BEC and well defined P-R excitations still all appear at the same condensation temperature \( T_\lambda \). In strongly interacting liquid helium the condensate fraction is only 7.25% \( \text{9-12} \) but the superfluid fraction is 100% at absolute zero. Thus superfluidity appears to be inseparably linked to the existence of BEC in 3D, uniform fluids, a connection made in Tisza’s two-fluid model of Helium II. On the other hand, Kosterlitz and Thouless \( \text{18} \) have shown that it is possible to have superfluidity in 2-dimensions without BEC although the onset of superfluidity is associated with the onset of algebraically decaying long range order \( \text{19,20} \). Also the dependence of superfluidity on BEC in non-uniform systems in which the condensate may not be continuous is of great current interest \( \text{21} \), the topic investigated here.

In this paper we focus on two broad classes of systems: trapped Bose gases in optical lattices and Bose liquids in porous media. The properties of bosons in external potentials and in disorder have been extensively investigated with primary focus on the nature of superfluid-insulator transition. Fisher and coworkers \( \text{22} \) in their seminal study of bosons on a lattice showed that for commensurate filling of the lattice, a transition from a superfluid state to a Mott insulator (MI) state takes place at a critical ratio of the hopping strength to inter-particle repulsion. Jaksch \( \text{et al.} \) \( \text{23} \) adapted these ideas to bosons confined to an optical lattice, and showed that a transition from a superfluid to MI phase is expected in OLs. The transition was first observed by Greiner \( \text{et al.} \) \( \text{24} \) using Rb\(^{87}\) atoms in a 3D optical lattice. Many examples have been reported \( \text{25,26} \) and OLs with many atoms on a lattice site (in the potential wells at the lattice sites) have been created \( \text{27,28} \), the case we consider here. Most recently, OLs with disorder added have been investigated in search of a superfluid-Bose glass insulating phase \( \text{29-32} \).

In OLs, the existence of superfluidity is inferred from the appearance of a singular peak in the atomic momentum distribution at zero momentum (\( k = 0 \)). This peak signals long range coherence in the BEC. There remains discussion about the precise signature of extended BEC \( \text{33,34} \) since there can be peaks at finite \( k \) without BEC in the MI state. Also, when there are many atoms per site, our results suggest that it is possible to have BEC but negligible superflow along the lattice if the BEC is highly localized in the potential wells. Some coherence in the BEC has been observed in the MI phase \( \text{27} \). Our study is directed at displaying explicitly how localization of the BEC at lattice sites leads to loss of superflow along the lattice.

Equally interesting are high density bose liquids confined in a disordered potential – of which liquid helium in porous media \( \text{35} \) is a prime example. In this case, both disorder and high density introduce different physics into the interdependence of BEC \( \text{36} \) and superfluidity \( \text{35} \). In this context, an interesting observation is evidence of well defined phonon-roton excitations in liquid \(^4\)He above the superfluid transition temperature \( T_c \). Since P-R excitations imply BEC, this means that there is BEC above \( T_c \) of the system, where there is no macroscopic superfluidity. This ostensibly goes against the widely accepted view that in an interacting system the existence of BEC implies the existence of superfluidity. The explanation proposed \( \text{37-41} \) is that above \( T_c \) the BEC is localized to favorable regions (e.g., larger pores) in the porous media separated by regions where depletion has brought the condensate fraction to zero. In the porous media liquid
helium contains islands of BEC separated by normal fluid at temperatures above but close to $T_c$. This results in the loss of phase coherence across the sample and loss of superfluidity at $T_c$ as measured by a torsional oscillator experiment. The islands of BEC still support P-R modes and local superfluidity. In a recent paper, Shams et al. have shown through variational Monte Carlo simulation at 0 K that depletion-mediated localization is indeed a plausible effect in systems where there are regions of high density.

The history of Monte Carlo methods in the study of bose systems is rich and varied, though very few of these studies actually investigate superfluidity and BEC at the same time. The first Monte Carlo study that simultaneously calculated both condensate fraction and superfluid density in disorder was that of Astrakharchik et al. With weak disorder, their results agree with the Bogoliubov model. For strong disorder, their system entered an unusual regime where the superfluid fraction is smaller than the condensate fraction. Recently, Boninsegni, Prokof’ev and Svistunov have studied different solid phases of $^4$He using the Worm Algorithm of PIMC (the method used in the present paper). Starting from a high-$T$ gas phase and "quenching" down to $T = 0.2$ K they created solid helium in a glass phase, denoted a superglass, i.e., a metastable amorphous solid featuring off-diagonal long-range order and superfluidity.

In the light of the above, it seemed appropriate to undertake a program whereby we simultaneously study BEC and superfluidity for a system of bosons, with the goal of investigating their interdependence. We start with the ideal Bose gas, the motivations for doing so being several: (1) the effects of interaction are absent, so that the connection of BEC and superfluidity can be studied at a more fundamental level, (2) analytical expressions for both the condensate and the superfluid fractions can be obtained for a finite sized system, which in turn can be used to check the computer code, (3) finite size effects can be studied by comparing with the known (analytically calculated) behavior of this two quantities in the thermodynamic limit. It is seen (Fig. 1), for example, that the condensate fraction is actually greater than the superfluid fraction for a finite-sized system (as noted above, they are formally identical at the thermodynamic limit). Also, since both of these quantities are non-zero at the critical temperature, we may conclude that the transition temperature for a finite-sized system is greater than it is in the thermodynamic limit (though the smoothing of the transition makes the determination of the transition temperature a bit problematic for a finite-sized system).

We then proceed to study dilute and dense interacting systems with periodic external potentials using the Worm Algorithm of Path Integral Monte Carlo (PIMC) to simulate both. We investigate diverse low temperature phenomena, though the focus of the current paper is on the nature of BEC localization and the fate of superfluidity as BEC gets more and more localized. Specifically, we explore the condensate distribution and superfluidity in an external potential demonstrating localization of the condensate by the potential at finite temperature.

II. Bosons in Optical Lattice

The model

Our model consists of a 1D lattice of potential wells. The unit cell of the lattice is shown in the top of Fig. 2. The 1D lattice is periodic along the $z$ axis in Fig. 2. The potential is independent of $x$ and $y$. For square wells, the potential within each unit cell is
\[ V(x, y, z) = \begin{cases} -|V_0| & \text{for } -b < z < b \\ 0 & \text{elsewhere} \end{cases} \]  

where \( b \) is the width of a well, \( |V_0| \) is the depth. The simulation is done within the unit cell only. We use periodic boundary conditions (BCs) along all directions. The periodic BC along the \( z \) direction creates the lattice. The lattice consists of thin "slabs" of attraction at regular intervals along the \( z \) direction as shown in the bottom of Fig. 2.

The specific virtue of this system is that the potential varies in 1D only (along \( z \)). The one-body density matrix (OBDM), defined below, therefore varies along the \( z \) direction only, which enables us to diagonalize it to obtain the condensate orbitals. At the same time, since we are doing PIMC, we can also calculate superfluid fraction along the \( z \) direction using the winding number formula.

In the present work, we consider the simplest system possible, namely one with just one well at the center of the box (see Fig. 2). The rationale for choosing this system was gaining computational efficiency without sacrificing the essential physics. Note that the periodic nature of the potential is recovered through the use of periodic boundary conditions. In other words, what we are simulating is bosons under a periodic external potential with a periodicity of length \( L \).

**OBDM and Single Particles Orbitals**

**General formulation**

Following previous Monte-Carlo work by DuBois and Glyde \(^{47}\), the definition we adopt for the condensate orbital in an interacting system is that given by Onsager and Penrose \(^{48}\), Lowdin \(^{49}\), and others \(^{50}\). According to this approach, the one-body density matrix (OBDM) is the
fundamental quantity that can be defined and evaluated for interacting systems. The single particle orbitals and the condensate orbital in particular are defined in terms of the OBDM. The one-body density matrix is

$$\rho(r', r) = \langle \hat{\Psi}^\dagger(r') \hat{\Psi}(r) \rangle$$

(2)

where \( \hat{\Psi}^\dagger(r) \) and \( \hat{\Psi}(r) \) are the field operators for creating and annihilating a particle at \( r' \) and \( r \), respectively. The single-particle orbitals \( \psi_i \) are then be defined as

$$\rho(r', r) = \sum_i \psi_i^\dagger(r') \psi_i(r) N_i$$

(3)

where \( N_i \) is the number of Bosons in single-particle orbital \( \psi_i \). The index \( i \) here is a shorthand for all the quantum numbers required to uniquely identify a single-particle orbital of the system. The condensate orbital is the single-particle orbital having the largest \( N_i \). BEC arises if \( N_i \) is a macroscopic fraction of \( N \). This provides a definition of BEC for finite sized systems where there is no off diagonal long range order. The natural orbitals and their respective occupation numbers can be found by diagonalizing the OBDM:

$$\int \int \psi_i^\dagger(r') \rho(r', r) \psi_i(r) drdr' = N_i.$$  

(4)

Application to the model

As described above, the external potential inside the rectangular box in our model is independent of \( x \) and \( y \), and depends only on \( z \). For any system uniform in \( x \) and \( y \) direction, the single-particle orbitals should have the form

$$\psi_i \equiv \psi_{mnp} = \frac{1}{\sqrt{L_x L_y}} e^{i k_m x} e^{i l_n y} Z_{mnp}(z)$$

(5)

where \( m, n, p \) are the state indices and \( k_m, l_n \) the wave numbers along \( x \) and \( y \), determined from the boundary conditions along those directions. In this case, Eq. 4 reduces to

$$\int \int Z_{mnp}(z')\rho_{mn}(z', z)Z_{mnp}(z)dzdz' = N_{mnp}$$

(6)

where

$$\rho_{mn}(z', z) = \int \int \rho(r', r)\cos k_m(x' - x)\cos l_n(y' - y)d(x' - x)d(y' - y)$$

(7)

Since our goal is to find \( \psi_0(r) \equiv \psi_{000}(r) \), we only need to concern ourselves with \( m = n = 0 \), in which case equation Eq. 7 becomes

$$\rho_{00}(z', z) = \int \int \rho(r', r)d(x' - x)d(y' - y)$$

(8)
We evaluate \( \rho_{00}(z',z) \) through Monte Carlo simulation and then numerically diagonalize it to find out \( \psi'_0(r) \), that is, the single-particle orbital corresponding to the highest occupation number.

**Superfluid Fraction**

In path integral Monte Carlo, each particle is represented by a “polymer”, where a specific “molecule” along the polymer chain represents one specific space-time position of the particle (time in the imaginary sense), the complete polymer being the path of the particle as it “evolves” from its initial space-time position to the final one. The simulation consists in moving/changing the paths in a stochastic way, and accepting/rejecting the moves using the Metropolis condition. A “measurement” is taken of various properties after each move and the average of such properties give us the equilibrium quantum mechanical expectation value of the properties concerned. The boundary conditions are such that the last “bead” of the polymer connects with the first one, giving us a “ring” polymer. To allow for Bose symmetry, however, the polymers are allowed to connect with each other too, so that one can have very long polymers that “wind” around the box, possibly multiple times. Each such polymer has a certain “winding number” (roughly, the net number of times it winds around the boundaries in a certain direction), and the superfluid fraction is computed using the winding number formula, given by

\[
\frac{\rho_s}{\rho} = \frac{\langle W^2 \rangle}{2\lambda \beta N}
\]  

(9)

where \( W \) is the winding number, \( \lambda = \hbar^2 / 2m \), \( \beta = 1 / k_B T \), \( T \) is the temperature, \( m \) is the mass of the bosons, and \( N \) is the total number of particles. Details of the procedure for calculating the winding number in the Path Integral methodology can be found in Ref. 12, and the details of the Worm Algorithm of PIMC can be found in Ref. 10.

**III. Results**

In Fig. 3 we show the superfluid fraction and the associated condensate density for Bosons in the simulation cell depicted in Fig. 2 with a square well at the center of the cell. The simulation was carried out with 64 particles having helium mass and a hard-core diameter of \( a = 0.22a_{He} \) at temperature \( T = 1.053T_c \). Since the mass of particles equals that of helium, but the hard-core diameter is much less than the helium scattering length 2.2Å, what we are simulating here could be described as very weakly interacting liquid helium. The well width was chosen to be \( b = 2.2a_{He} \), and the well depth, \( V_0 \), was varied from 0.13 to 5.26\( T_c \). Since we are using periodic boundary conditions along \( z \), we are essentially simulating a 1D array of wells with a periodicity of \( L_z \). In all subsequent calculations the particles also have helium mass.
Fig. 3: The central plot shows the superfluid fraction for flow of bosons along the 1-D periodic system with depicted in Fig. 2. The unit cell of side $L$ in the 1-D periodic system contains a potential well of depth $V_0$ at the center of the cell and $\rho_s$ is plotted vs. $V_0$. There are $N = 64$ hard-core bosons in each cell of volume $V = L^3$. $T_c$, is the BEC transition temperature for a uniform ideal Bose gas at the same density and mass in the thermodynamic limit (TL). The satellite plots show the corresponding condensate density within a cell (in arbitrary units) along the direction of the 1D lattice. In the present example, the bosons have helium mass at a density parameter $n a^3 = 10^{-3}$ at temperature $T = 2.0 K = 1.053 T_c$ ($T_c = 1.9 K = 10.8 E_R$ in TL), where $E_R$ is the recoil energy defined in the text). In terms of the helium scattering length $a_{\text{He}} = 2.2 \text{Å}$, the relevant length scales are, hardcore diameter $a = 0.22 a_{\text{He}}$, well width $b = 2.2 a_{\text{He}}$, and site-to-site separation $L = 8.4 a_{\text{He}}$. The average number density in the cell $n = 1.01 \times 10^{22} \text{ atoms/cm}^3$. The ratio of hard-core diameter to site-to-site separation is $a/L = 0.03$, which is typical for porous media, if we take $L$ to be the pore diameter. The parameters represents liquid helium in porous media, albeit very weakly interacting, or helium in an optical lattice. As can be seen, the superfluid fraction approaches zero as the condensate gets more and more localized at the center of each unit cell. As evidenced by the superfluid fraction $\sim 0.25$ at $V_0 = 0$, the system is just below its superfluid transition temperature, which is higher than the TL value due to finite size effects.

The main plot in Fig. 3 shows the superfluid fraction for flow along the $z$ direction for various well depths, and the smaller plots surrounding it shows the condensate density distribution at specific values of the condensate fraction. As can be seen, when $V_0$ is small, the condensate is distributed more or less evenly throughout the box and the corresponding superfluid fraction along $z$ direction is highest. As the well depth, $V_0$, is increased, the condensate becomes increasingly localized around the well, and the superfluid fraction for superflow along $z$ direction decreases. Eventually the superfluid fraction vanishes for $V_0 \gg 3T_c$ and the condensate density goes to near zero at the edges of the box. A strong correlation of BEC localization and the vanishing of superflow along $z$ direction thus clearly emerges at finite temperature.
The distribution of condensate density for this system is straightforward to explain. As the well-depth is increased, particles are increasingly attracted towards the center of the box, so the overall density goes up at the center. The (average) density parameter for this system is \( na^3 = 0.001 \) which is 2000 times lower than that for liquid helium. Note that though the number density for our system is quite high, it is still very weakly interacting because of the small hard-core diameter. The \( na^3 = 0.001 \) value is more characteristic of gases in optical lattices which are very weakly interacting because they are dilute and where there are similar localization effects in individual wells (see, for example, Schulte et al.\textsuperscript{52}). Thus, although the number density is significantly higher at the center than it is near the edges, the system still remains sufficiently weakly interacting everywhere. This means there is no significant depletion of the condensate caused by particle correlations and the condensate density simply tracks the overall density, peaking at the center.

![Fig. 4: Superfluid fraction vs. well depth \( V_0/T_c \) for the system shown in Fig. 3 (\( na^3 = 10^{-3} \)) at different temperatures, \( T = 0.53T_c \), 0.79\( T_c \) and 1.05\( T_c \), where \( T_c \) is the BEC critical temperature for a uniform Bose gas in the TL with the same particle density and mass (See Fig. 3 for further system parameters). As can be seen, the superfluid density goes to zero at approximately the same value of potential \( V_0/T_c \) independent of temperature.](image)

In this scenario, not only the condensate, but particles themselves are getting localized, and successive wells are getting almost physically disconnected from each other by empty regions near the edges of the simulation box. There is no flow, let alone superflow, across the boundary of the box because there are no particles, condensed or otherwise, to carry the flow in that region. It could be said that, in this case, the loss of superfluidity is caused by a localization effect that is classical – even trivial – in nature.

To show how the suppression of superfluidity by an external potential depends on temperature, we have plotted the superfluid fraction vs. \( V_0/T_c \) for three different temperatures in Fig. 5. As expected the superfluid fraction, \( \rho_s(T)/\rho \), increases with decreasing temperature.
when $V_0$ is small and approaches unity at low $T$ when $V_0 = 0$. At each temperature the superfluid fraction decreases with increasing $V_0$ and the unexpected result is that $\rho_s(T)$ goes to zero at the same value of $V_0$ independent of temperature. This suggests that zero temperature calculations of the optical lattice potential needed to bring $\rho_s(T)$ to zero will be valid at finite temperatures.

Fig. 5: Superfluid fraction vs. well depth $V_0/T_c$ as shown in Fig. 3 but for strongly interacting bosons with large hard-core diameter $a = 0.91a_{\text{He}}$ and density parameter $na^3 = 0.16$, where $a_{\text{He}} = 2.2$ Å is the helium scattering length. Specifically, we simulate 128 particles having helium mass with average number density in the cell $n = 2.02 \times 10^{22}$ atoms/cm$^3$. The well width is $b = 0.91a_{\text{He}}$, and all other parameters are the same as in Fig. 3. Note that in a strongly interacting system, the condensate density is lowest at the center of the well, where the total number density is highest. The condensate is depleted by strong interaction. $T_c = 2.98$K.

Fig. 5 shows $\rho_s(T)/\rho$ and the condensate density for a strongly interacting system. In this case, we simulated 128 particles of helium mass having a hard-core diameter of $a = 0.91a_{\text{He}}$. The square well at the center of the box had a width of $b = 0.91a_{\text{He}}$, and the depth was varied from zero to approximately $40T_c$. The well in this case was therefore narrower and much stronger than in the system shown in Fig. 3. The goal was to push the density as high as possible at the center of the box, so that correlation effects and depletion manifest themselves. For this system the density parameter $na^3 = 0.16$ is close to that in liquid helium. Again, we find the superfluid fraction to be maximum when the when $V_0$ is small and the condensate is uniformly distributed throughout the length of the box. As the well depth is increased, the condensate distribution becomes non-uniform, but in a way which is drastically different from the low-density case: the condensate is depleted in the wells where the density is high and localized primarily in the region between two consecutive wells (remember that even though there is only one well inside our
simulation cell, because of the periodic boundary conditions the particles essentially see a periodic array of wells along \( z \) direction). The superfluid fraction is seen to go down as the condensate gets depleted from the center, but not as sharply as the low-density case. A possible explanation could be that the region of depletion is narrower than that of Fig. 3, so there is more tunneling of the condensate into the depleted region.

The reason the condensate density goes to near zero inside of the well is that the extremely high number density together with a large hard-core diameter gives rise to a system that is highly correlated in that narrow strip. This results in a significant depletion of the condensate (intuitively, the more important many-body interactions become, the less the system is describable by a macroscopically occupied single-particle orbital – the definition of BEC). Outside the well, two competing effects determine the condensate density. Since the condensate density cannot exceed the total density, it has to go down as the total density goes down. However, since low density also means little depletion, we have a higher condensate fraction. In our case, the latter effect overrides the former, resulting in a greater condensate density outside the well than inside.

In Fig. 5, if we examine the condensate density profile at higher values of the potential depth, we notice there are spikes just at the edges of the potential well. At this point these spikes are not well understood. These spikes disappear for low density and for smoother (such as a Gaussian) potentials. It could be an artifact of the sudden discontinuity of the square potential well. We are using the fourth-order propagator that has terms depending on the derivative of the potential, and it is conceivable that pathological features could result when the formula is applied to a potential that has discontinuities.

![Graph](image)

Fig. 6: The matrix element \(|J|\) for hopping between sites defined in Eq. 10 (arbitrary units) vs. well depth \(V_0/T_c\) for density parameter \(n_0a^3 = 10^{-3}\). The tunneling between sites \(|J|\) decreases with increasing potential well depth \(V_0\) in the unit cell. \(T_c\) is the BEC critical temperature for a uniform ideal Bose gas in the TL at the same particle density and mass. \(J\) goes to zero at the roughly the same \(V_0/T_c\) as the superfluid density shown in Figs. 3 and 5.
To quantify the dependence of superfluidity on the localization of BEC and to compare our results with Hubbard model calculations, we have calculated the hopping matrix element corresponding to various well depths for a low density system. The hopping matrix element between two adjacent sites $i$ and $j$, as defined by Jaksch et al.\textsuperscript{23} is given by

$$J = \int w(\mathbf{r} - \mathbf{r}_i) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] w(\mathbf{r} - \mathbf{r}_j) d^3 \mathbf{r}$$

where $w(\mathbf{r} - \mathbf{r}_i)$ is the localized Wannier orbital at site $i$. Since in our case, when the potential is strong, the condensate essentially separates into Wannier-like localized orbitals, the hopping matrix element as defined above can be used as a quantitative measure of the tunneling of the condensate between successive wells. The condensate orbital was first decomposed into a sum of double Gaussians centered at each well, then two such consecutive orbitals were used to compute $J$. The result is shown in Fig. 6. As can be seen, tunneling between wells as signaled by the magnitude of $J$ is increasingly suppressed as well depth is increased. This is what one expects in the tight binding regime.

![Fig. 6: Superfluid fraction vs. $|1/J|$](image)

Fig. 7: Superfluid fraction vs. $|1/J|$ (arbitrary units) where $J$ is the matrix element for hopping between the sites defined in Eq. 10. The superfluid fraction falls rapidly as tunneling between adjacent sites is suppressed by increasing the potential well depth.

In Fig. 7, we plot the superfluid fraction vs. $1/J$, again for the low density system shown in Fig. 1. Krauth et al.\textsuperscript{53} have found a similar dependence of the superfluid fraction on the interaction strength defined by $U/J$, where $U$ is the on-site repulsive interaction among bosons (see Fig. 1 of Ref. 53).

Fig. 8 shows the temperature dependence of the superfluid fraction, $\rho_s(T)/\rho$, for a weakly interacting system ($na^3 = 0.0025$) for several values of the depth, $V_0$, of the potential.
well. The observed $\rho_s(T)/\rho$ of liquid helium in different porous media is typically presented in this manner. As can be seen in Fig. 8, the external potential suppresses the $\rho_s(T)/\rho$ at all temperatures, and in contrast to a uniform system, the system is not 100% superfluid even at 0°K. The shape of the $\rho_s(T)/\rho$ curves also changes as the well depth increases with the curvature going from positive to negative around $T_c$. The most significant fact that emerges, however, is that all the curves approach zero at approximately the same temperature. In other words, the “transition temperature” does not seem to change with increasing well depth.

![Fig. 8: Superfluid fraction for superflow along the lattice vs. $T$ for density parameter $na^3 = 0.0025$ and potential well depths in the unit cell of $V_0 = 0, 1.68, 2.34, \text{ and } 3.36$. The particle and cell parameters are: hard-core diameter $a = 0.22a_{He}$, well width $b = 2.27a_{He}$, number of particles $N = 128$, cell side $L = 8.41a_{He}$, well type = Gaussian. The BEC critical temperature for the corresponding uniform ideal Bose gas is $T_c = 2.98$ K. The solid lines are fits of $\rho_s/\rho = A(T_c - T)^\zeta$. The apparent critical exponent increases from $\zeta = 0.64$ for $V_0 = 0$ to $\zeta = 1.0$ for $V_0 = 10$.](image)

To estimate the critical exponent, $\zeta$, and transition temperature of $\rho_s(T)$, we have fitted a power law relationship to the superfluid fraction of the form $\rho_s/\rho = A(T_c - T)^\zeta$. Strictly, this power law dependence is expected to be valid only for an infinite system very close to the critical region. This makes such a fitting problematic for a finite system, because it is exactly in the critical region that $\rho_s(T)/\rho$ starts to deviate from the power law behavior because of finite size effects (the “tail effect”). Nevertheless, the prevailing practice is to fit the power law considerably beyond the critical temperature. Following this approach, we find that the apparent critical exponent increases for increasing well depth. Reppy has observed similar behavior for liquid helium in porous media where $\zeta$ increases with decreasing porosity which implies...
increasing interaction with pore walls. However, $\zeta$ does not increase uniformly with decreasing pore size. For example $\zeta$ is smaller in Vycor than in aerogel. Huang and Meng\textsuperscript{54} suggest that the apparent $\zeta$ depends on the distribution of pore sizes in the porous media and that $\zeta$ increases with increasing width in the pore size distribution. The observed $T_c$ decreases with decreasing pore size (increasing interaction with the walls), whereas we find that $T_c$ remains unchanged as the well depth increases.

![Graph](image)

Fig. 9: As Fig. 8 but larger density parameter $na^3 = 0.02$. The potential well depths are $V_0 = 0, 3.36,$ and $6.71T_c$ (top to bottom). The boson and cell parameters are: hard-core diameter $a = 0.45a_{1\text{ig}},$ well width $b = 2.27a_{1\text{ig}},$ number of particles $N = 128,$ box side $L = 8.41a_{1\text{ig}},$ well type = Gaussian. The $T_c$ BEC in the corresponding uniform ideal Bose gas is $T_c = 2.98$ K. Fits of $\rho_s(T)/\rho = A(T_c - T)^\zeta$ again show an exponent $\zeta$ that increases with increasing $V_0$ as in Fig. 8.

In Fig. 9 we show $\rho_s(T)/\rho$ for several values of $V_0$, as in Fig. 8, for a moderately strongly interacting system ($na^3 = 0.02$). Qualitatively, we get the same behavior as in Fig. 8, although a much stronger potential $V_0$ is needed to suppress the superfluid fraction. There is a simple explanation for this in the path integral picture. For an interacting system, the particles are more resilient to clustering because of their mutual repulsion, so the external potential cannot readily distort the uniform density distribution. Each particle thus always has a high number of neighbors to form macroscopic exchange cycles that gives rise to superfluidity.

**Discussion and Conclusion**

The chief goal of this paper is to investigate how a periodic external potential modifies the condensate distribution and how that in turn affects the superflow along the direction of potential variation. We used periodic boundary conditions along the $z$ direction because we are using the winding number formula to calculate the superfluid fraction which relies on the system being periodic. Because of this periodic boundary condition we can focus on a single cell
containing a potential well and the particles see an array of potential wells along the \( z \) direction. In this way our system maps directly onto those found in optical lattice experiments. For strong enough potential wells, we see localization of the condensate to islands and loss of superflow along the lattice. The localization of the condensate to islands that we see could be similar to that observed in disordered systems like helium in porous media \(^{37-42}\), because the localization in porous media is thought to be depletion mediated \(^{41,42}\), rather than caused by disorder \textit{per se}. Depletion can localize the condensate whenever there are sharp changes in the density profile and that can happen either in periodic or aperiodic (disordered) systems.

In high temperature superconductors, recent measurements \(^{55}\) show that at temperatures above \( T_c \), between \( T_c \) and \( T^* \), and for certain doping levels, there can be isolated islands of superconductivity within the normal material. The superconducting to insulator transition at \( T_c \) is associated with a cross-over from an extended, connected superconducting state to one in which there are only separated islands of superconductivity. In the islands there is pairing and an energy gap. In this case the localization of the superconducting state to islands is believed to arise from disorder. Also the localization is more complicated than simple localization of the condensate to islands as in helium in porous media at \( T_c \). It is also interesting that Ghosal \textit{et al}. \(^{56,57}\) have shown that localization of the superconducting state to islands can be induced by a homogeneous disordered potential which is a different phenomena from that considered here.

Specifically, we have shown that for a low density system, the condensate can be highly localized inside the potential wells. Schulte \(^{52}\) \textit{et al}. have shown both experimentally and by numerically solving Gross-Pitaevskii equation that the BEC wave function in the presence of a disordered optical potential at low densities mimics a superposition of localized, and practically non-overlapping states. This is exactly the type of localization that we see in Fig. 3 for the deeper well values, where it is seen that the individual islands of BEC are localized in successive wells with practically zero overlap with each other. Fort \textit{et al}. \(^{32}\) have found that even in the weak-binding regime, the effect of trapping in the deepest wells cannot be avoided, so the effect of disorder is mostly classical in nature, as we have found in our present simulation. To date, genuinely quantum effects, such as Anderson localization, in disordered Bose systems have not yet been realized experimentally. To explain this, Modugno \(^{58}\) did a detailed analysis of the Fort experiment using Gross-Pitaevskii theory, and reached the conclusion that one would need a shorter correlation length of the random potential than is attainable experimentally to obtain Anderson localization. We will attempt to verify this assertion in a future project.

An important feature of the present method is the representation of the optical lattice by the periodic images of the single well at the center of the simulation cell. Essentially, we are assuming the single particle orbitals to have the same periodicity as that of the lattice. This is strictly true for the condensate orbital in a mean-field approximation, because then the single-particle wave-functions are given by the Bloch expression \(^{59}\)

\[
\psi_k(z) = u_k(z) \exp(ikz)
\]

where \( u_k(z) \) is a periodic function having the periodicity of the lattice, \( k = \frac{2\pi s}{NL_z} \), \( N \) is the number of cells constituting the 1D lattice, \( L_z \) is the lattice periodicity, and \( s = 0, 1, 2, \ldots, N - 1 \). Putting \( s = 0 \) for the condensate orbital, we get

\[
\psi_0(z) = u_0(z)
\]
showing \( \psi_0(z) \), like \( u_0(z) \), has the periodicity of the lattice.

To convince ourselves that this indeed is the case, we doubled the size of the simulation cell to consist of two cells rather than one. That is, we extended the period length of the simulation from \( L \) to \( 2L \) to test whether the condensate was sensitive to the period length. In Fig. 10 we compare the condensate orbitals for the two periods. The orbitals for the two periods are clearly the same showing that the orbital is insensitive to period increase from \( L \) to \( 2L \). By extension, simulation of a single cell plus periodic boundary conditions appears to be equivalent to simulating a full lattice.

An oft-used energy scale in optical lattice experiments is the photon recoil energy \( E_R \), which is defined by \( E_R \equiv h^2/2m\lambda^2 \) where \( m \) is the mass of bosons and \( \lambda \) is twice the separation between wells. In terms of this quantity, \( T_c = 10.8E_R \) for the system shown in Fig. 3, which means the superflow almost completely vanishes at around a well depth of \( 30E_R \). Fertig et al.\(^{60}\) have found that the dipole oscillations of a 1D Bose gas under a combined harmonic and optical lattice potential gets totally inhibited around a lattice well depth of \( 3E_R \). The much lower value they observe could be attributed to the diluteness of the gas they use. With a peak density of \( n = 4.7 \times 10^4 \) cm\(^{-3} \) and a Rubidium scattering length of \( a = 53 \) Å\(^4\), the density parameter in the Fertig experiment turns out to be \( na^3 \approx 10^{-15} \). This is extremely low compared to the value of \( na^3 \approx 10^{-3} \) for the system shown in Fig. 3. As is obvious from Fig. 5, the stronger the interaction...
(signified by the density parameter), the more resilient the superflow is to the inhibitory effect of the lattice potential. Schulte et al.\textsuperscript{52} have also found by solving the Gross-Pitaevskii equation that the superfluid fraction of a Bose fluid in a 1D pseudo-random potential goes up with increasing strength of the interaction.

Experimentally, it is found that the introduction of a disordered potential decreases both the critical temperature and the superfluid fraction of helium\textsuperscript{35,61}. In Figures. 8 and 9 we see what happens to these two quantities when a periodic external potential is introduced. While we do see a definite reduction of the superfluid fraction, the transition temperature is apparently largely unchanged. Gordillo and Ceperley\textsuperscript{62} have found similar results in PIMC simulation of a system of hard-core bosons in quenched disorder, i.e. when disorder is introduced $T_c$ is unchanged. The conclusion could therefore be drawn that, as far as PIMC simulations of Bose fluids are concerned, the superfluid transition temperature is largely insensitive to the presence external potentials, disordered or not.

Referring to Fig. 8 and 9, it should be mentioned that Huang and Meng\textsuperscript{54} have called into question the standard procedure (also followed in this paper) of fitting a power law relationship between the superfluid fraction and temperature of the form $\rho_s/\rho = A(T_c - T)^\zeta$ when $T$ is outside the critical region. In these authors’ opinion, the different critical exponents for Vycor, Aerogel and Xerogel observed experimentally are actually the result of fitting data points that are not in the critical region, and a universal critical exponent of 1.7 cannot actually be ruled out in the truly critical region.

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References

61. See Gordillo and Ceperley (Ref. 62 below) and references therein.
Appendix

Condensate fraction for an ideal Bose gas with a finite number of particles

The Bose-Einstein distribution function is given by

\[ N_i = \left[ e^{\beta(E_i - \mu)} + 1 \right]^{-1} \]  \hspace{1cm} (A1)

where \( N_i \) is the occupation number for the \( i \)th state, \( E_i \) is the energy of that state, \( \mu \) is the chemical potential, \( \beta \equiv 1/k_B T \), and \( T \) is the temperature. The chemical potential \( \mu \) is found from the condition

\[ \sum_{i=0}^{\infty} N_i = N \]  \hspace{1cm} (A2)

In practice, for low temperatures, the summation above converges quite rapidly, and the upper limit can be replaced by a cut-off value \( i_{\text{max}} \). One then finds \( \mu \) by plotting \( \sum_{i=0}^{i_{\text{max}}} N_i - N \) vs. \( \mu \), and locating the point where the curve intersects the abscissa.

Once \( \mu \) is determined, the condensate fraction follows from

\[ n_0 \equiv \frac{N_0}{N} = \frac{1}{N \left[ e^{\beta(E_0 - \mu)} + 1 \right]} \]  \hspace{1cm} (A3)

where \( E_0 = 0 \) for an ideal Bose gas in a uniform system.

Superfluid fraction for an ideal Bose gas with a finite number of particles

For a uniform system with a cubic geometry, the superfluid fraction can be shown to be given by [Ref. 8]

\[ \frac{\rho_s}{\rho} = 1 - \sum_i \left[ \frac{2\beta}{3N} E_i \langle N_i \rangle + \frac{6\beta}{mN^2} i |l_z|^2 \langle N_i \rangle \right] \]  \hspace{1cm} (A3)

where \( \beta \equiv 1/k_B T \), \( l_z \) is the \( z \)-component of the angular momentum operator, \( E_i \) is the energy corresponding to the energy eigenstate \( |i\rangle \), \( N \) the total number of particles, and \( \langle N_i \rangle \) is the expectation value of the corresponding occupation number given by (A1).

In the coordinate representation, we have

\[ l_z \equiv (\mathbf{r} \times \mathbf{p})_z = -i\hbar \left( \frac{x}{\partial y} - \frac{y}{\partial x} \right) \]  \hspace{1cm} (A4)

and for a cubic system with sides equal to \( L \), the eigenstates are

\[ |i\rangle \equiv |pqr\rangle = A e^{\frac{2\pi px}{L}} e^{\frac{2\pi qy}{L}} e^{\frac{2\pi rz}{L}} \]  \hspace{1cm} (A5)

Using (A4) and (A5), we can numerically evaluate (A3), replacing the upper limit of the summation with a cut-off value that gives us convergence to the desired degree of precision.