Quantum phase transitions in dilute bosonic superfluids on a lattice

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It has been well known that quantum fluctuations induce a macroscopic phase transition from a superfluid to a Mott insulator phase driven by the repulsive potential energy in the ground state of dense bosonic systems on a lattice. We find a quantum phase transition from the homogeneous to an inhomogeneous Bose-condensate strongly affected or sometimes driven by the kinetic energy dispersion in dilute bosonic superfluids, which provides a clear identification of the superfluid state.

The experimental realization of the quantum phase transition (QPT) from a superfluid liquid to a Mott insulator phase in an atomic gas trapped in an optical lattice \(^{[1]}\) triggered remarkable experimental and theoretical activity. This experiment heralded a new regime in exploration of the many body physics dominated by an interplay between atom-atom interactions and the boson kinetic energy as described by the Bose-Hubbard model \(^{[2]}\). The competition between kinetic and interaction energy terms in the underlying Hamiltonian has been considered to be fundamental to quantum phase transitions not only in neutral but also in charged Bose liquids in the context of granular superconductors and Josephson junction arrays \(^{[3]}\) and preformed real-space electron pairs as bipolarons \(^{[4]}\).

The Bose superfluid to Mott insulator transition takes place only at fixed density in a homogeneous dense system when the number of bosons is commensurate with the number of lattice sites. At first glance, one would not expect any phase transformation in a dilute Bose superfluid well described by the Bogoliubov theory \(^{[5]}\). Surprisingly (as we shall show), this wisdom is not always applicable to bosons in a periodic potential, whose ground state is described by a Gross-Pitaevskii-type (GP) equation \(^{[6]}\) including lattice, \(V(r)\), and interaction, \(U(r)\), potentials,

\[
\left(-\frac{\hbar^2 \nabla^2}{2m} + V(r) - \mu + \int dr' U(r-r')|\psi(r')|^2\right)\psi(r) = 0. \tag{1}
\]

Here the condensate wave-functions \(\psi(r)\), which is also the order parameter, is normalized by the number of bosons as \(\int dr |\psi(r)|^2 = N_b\), \(m\) is the boson mass, and \(\mu\) is the chemical potential, which controls the total number of particles in the system. One can solve equation (1) variationally on a representative lattice with a large number of sites, \(N\), using a complete set of orthogonal Wannier (site) functions \(w(r)\). Transforming the order parameter as \(\psi(r) = \sum_m \phi_m w(r-m)\) we reduce (1) to a discrete set of equations for the site amplitudes \(\phi_m\),

\[-\sum_m \left[t(m-m') + \mu \delta_{m,m'}\right] \phi_m + \sum_{m,n} U_{m'n'} \phi_{n'} \phi_m = 0. \tag{2}\]

Here \(t(m) = \int dr w^*(r)(-\hbar^2 \nabla^2/2m + V(r))w(r-m)\) is the hopping integral, and \(U_{m'n'} = \int dr dr' U(r-r') w^*(r-m') w^*(r'-n') w(r'-n) w(r-m)\) is the matrix element of the interaction potential.

We are interested in the dilute liquid regime far away from the Bose liquid-Mott transition. It is accustomed to keeping only the density-density interactions, \(U_{m'n'} \delta_{m,m'} \delta_{n,n'}\). Solving the GP equation (2) is then equivalent to minimization of the energy functional,

\[E(\phi_m) = -\sum_{m,n} \left[t(m-n) + \mu \delta_{m,n} + \frac{1}{2} U_{m'n'} \phi_m^* \phi_n\right] \phi_n^* \phi_m. \tag{3}\]

Importantly, rescaling the order parameter as \(\phi_m = n^{1/2}f_m\) and the interaction as \(U_{m'n'} = u_{m'n}/n\) yields a universal functional, \(\tilde{E}(f_m) = E(\phi_m)/n\) that is independent of \(n = N_b/N\), the number of bosons per lattice valley:

\[\tilde{E}(f_m) = -\sum_{m,n} \left[t(m-n) + \mu \delta_{m,n} + \frac{1}{2} u_{m'n} f_m f_n\right] f_n^* f_m. \tag{4}\]

A solution to the tight-binding form of (1) corresponds to the minimum of this functional when the following constraint is imposed, \(\sum_m |f_m|^2 = N\). Solutions for different particle densities are mapped on to each other by a simple rescaling of the interaction.

The noninteracting part of Eq.(1) can be solved using the Bloch eigenfunctions, and the Wannier states are constructed by summing the Bloch states with appropriate phase factors. Having obtained the Wannier states the hopping integrals and the interaction matrix elements can be evaluated for any periodic lattice potential \(V(r)\). When the lattice potential is deep enough, the nearest-neighbor hopping, \(t_1\) dominates over the next-nearest (nn), \(t_2\) and the next-next (nnn), \(t_3\) nearest neighbor tunneling \(^{[6]}\). Lowering the lattice potential causes \(t_2\) and/or \(t_3\) hopping integrals to be of the same order as \(t_1\). Also lowering the boson density reduces the rescaled repulsion between bosons. That allows us to investigate QPTs in the superfluid state which might be driven by the kinetic energy dispersion, \(E(k) = \sum_m t(m) \exp(ik \cdot m)\) rather than by the repulsion under certain conditions.

We have randomly generated starting values for real site amplitudes, \(f_m\). The kinetic portion of the functional is calculated in the momentum space using the Fourier transformed values of the amplitudes at each lattice site.
Then it is inverse Fourier-transformed back into the Wannier space, where the effects of the interaction energy are applied; note that the minimization procedure tends to fail in the absence of any repulsion. The functional \( \mathcal{H} \) is minimized for a given value of \( \mu \) using the NAG optimization routine E04DGF. The value of \( \mu \) is then fine-tuned so that the constraint \( \sum_m |f_m|^2 = N \) is imposed. There are virtually no significant size effects as verified by our simulations on \( N = 25 \times 25 \) and \( N = 50 \times 50 \) lattices.

Some of our results are illustrated in Figs. (1,2,3). Fig. (1a) represents the single particle dispersion, \( E(k) \), for a deep square lattice potential, where \( t_1 \) is positive and \( t_2 \) and \( t_3 \) are negligible. The level position in a single lattice valley is taken as zero, \( t(0) = 0 \), and all energies are measured in units of \( t_1 = 1 \). The order parameter and the density are uniform in this case, \( f_m^2 = 1 \), and there is no phase transition with increasing but moderate on-
site repulsion, \( u_{00} \lesssim 1 \). Effects driven by the strength of the repulsion will be typically seen when \( u_{00} \approx 4.0 \) or larger; these effects destroy the homogeneity of the condensate. Fig. 1(b) shows an example of such an inhomogeneous condensate. Fig 1(c) shows how the value of the on-site repulsion \( u_{00} \) at which the homogeneity is destroyed decreases with the value of \( t_2 \). This correlates with the increasing shallowness of the kinetic energy dispersion as \( t_2 \) approaches \(-0.5\), where the dispersion becomes a pair of flat valley intercepting one another in a cruciform centered at the \( \Gamma \) point. This homogeneous-inhomogeneous transition occurs well below the critical value of \( u_{00} \approx 16 - 23 \) required for the superfluid-Mott insulator transition on a commensurate lattice \[9, 10, 11, 12, 13\], and so is a property of the superfluid state. There are different irregular patterns in the inhomogeneous phase depending also on the intersite interaction \( u_{01} \), which are reminiscent but not identical to transformations of a homogeneous Bose condensate into a density wave superfluid \[14, 15\] with a tendency to the phase separation \[16\].

Can one increase the magnitude of \( t_2 \) further? In a conventional optical lattice, one cannot, as a result of the textbook theorem to the effect that the ground state wave-function of a single particle must not contain any nodes \[17, 18\]. This places limits on the values of hopping parameters that are physically meaningful, since they cannot take values that give rise to additional minima in the kinetic dispersion of the lowest band of the Hamiltonian. However, there are a number of feasible situations where the theorem is not applied due to many-body effects \[19, 20\] or through the effects of internal degrees of freedom \[21, 22\]. Recent experimental \[23, 24\] and theoretical work \[25\] has also suggested that condensation may be induced in an excited but metastable p-band state. Also, this concern does not arise with composite bosons such as bipolarons \[4\], since the single polaron band, where the condensation is occurring, is rarely the ground state band due to the Pauli exclusion principle. In this case the hopping parameters are determined by the symmetries of the wavefunctions of two components of the boson, so that there is no constraint on variation of any hopping parameter.

With these considerations we turn to the results presented in Figures 2 and 3. Fig. 2 represents a shallow square lattice, where the magnitude of \( t_3 \) is comparable with \( t_1 \). At some value of \( t_3 \) the minimum of the single-particle band shifts from the \( \Gamma \) point with \( k = 0 \) to 4 finite wave-vectors within the first Brillouin zone, \( k_1 = k(1, 1), \ k_2 = k(-1, 1), \ k_3 = k(-1, -1), \) and \( k_4 = k(1, -1) \) where Bose condensation takes place, Fig. 2 (the value of \( k \) is calculated below). The four minima are degenerate. A small repulsion removes the degeneracy, so that the true condensate wave function in the Wannier space is one of the superpositions respecting the parity and time-reversal symmetry, \( f_m \propto \cos(k_1 \cdot m) \), \( f_m \propto \cos(k_2 \cdot m) \), or \( f_m \propto \cos(k_1 \cdot m) \pm \cos(k_2 \cdot m) \), depending on the repulsion. In our example with the on-site repulsion only the order parameter and the density of condensed bosons is stripped along a diagonal direction, Fig. 2. Here the on-site repulsion \( u_{00} = 0.02 \), and the nearest-neighbor interaction \( u_{01} = 0.01 \).

FIG. 3: Energy band dispersion in a shallow square lattice potential with \( t_1 = -1, t_2 = -0.6 \) and \( t_3 = 0 \) (a), the real space order parameter (b), and the checkerboard particle density (c) on a section of a \( 50 \times 50 \) lattice. Here the weak on-site repulsion is \( u_{00} = 0.02 \), and the nearest-neighbor interaction \( u_{01} = 0.01 \).
of a single boson on the lattice. With the positive $t_1 = 1$, zero $t_2$ and a negative $t_3$ the dispersion law is given by $E(k) = -2[\cos(k_x) + \cos(k_y)] - 2t_3[\cos(2k_x) + \cos(2k_y)]$, where the lattice constant is taken as $a = 1$. Expanding in powers of $k_{xy}$ one obtains $E(k) \approx -4 - 4t_3 + \hbar^2 k^2/2m^*$ with the effective mass $m^* = \hbar^2/(1 + 4t_3)$, so that QPT appears at $t_{3c} = -0.25$ when $m^* = \infty$. The QPT order parameter is the wave-vector (or inverse period of the modulation), which above $t_{3c}$ is given by $k = \cos^{-1}(1/4|t_3|)$. It changes continuously from zero at the transition up to $k = \pi/2$ at large $|t_3|$, so that QPT is of the second order. The transition is driven entirely by the kinetic energy dispersion, rather than by the repulsion, so that it could be named a kinetic quantum phase transition (KQPT). A similar calculation for the case where $t_2$ is varied and $t_3$ held fixed at zero shows that there is a phase transition at $t_{2g} = -0.5$ to a state with 4 degenerate minima located at $k = (\pi,0), (-\pi,0), (0,\pi)$ and $(0,-\pi)$, and is discussed in relation to Fig.3. Due to the discontinuous nature of this phase transition, it is first order.

Quite generally, if the boson band dispersion has its minima at finite $k$ the Bose condensate is nonuniform. Another example is the center-of-mass band dispersion $k_{minima}$ at finite $t$. An interesting example is the case of a small bipolaron composed of two holes on neighboring oxygen ions proposed as an explanation of the $p$-symmetry of oxygen orbitals, so that the minima of the bipolaronic band are found at the Brillouin zone boundaries. Minimizing the energy functional with negative $t_3 = -1$ yields different patterns of the order parameter and the density depending on the interaction matrix elements and longer range hopping terms. In this case we observe the relocation of 4 minima initially located at $k = (\pm\pi, \pm\pi)$ to new positions within the first Brillouin zone, rather than a change from 1 to 4 minima. An interesting example is the case of $t_2 < -0.5$ and $t_3 = 0$, where a weak nearest-neighbor repulsion $u_{10}$ can stabilize the d-wave checkerboard order parameter (see Fig.3) – as anticipated in Ref.21 – provided that $u_{00}$ is not too strong. Intriguingly, the same values of $t_2$, $t_3$ and the repulsions also typically give a checkerboard state for the positive $t_1 = 1$.

Cold atoms in optical lattices have provided an excellent tool for investigating quantum phase transitions, but finding a reliable diagnostic criterion for superfluidity is not straightforward. Our prediction of QPTs in dilute bosonic superfluids, which is strongly affected or even driven by the kinetic energy dispersion, opens up new perspectives on the unique diagnostic criteria of superfluidity. These states can most likely be detected through the use of optical probe spectroscopy and/or phase sensitive experiments.

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