Influence of trapping potentials on the phase diagram of bosonic atoms in optical lattices

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We study the effect of external trapping potentials on the phase diagram of bosonic atoms in optical lattices. We introduce a generalized Bose-Hubbard Hamiltonian that includes the structure of the energy levels of the trapping potential, and show that these levels are in general populated both at finite and zero temperature. We characterize the properties of the superfluid transition for this situation and compare them with those of the standard Bose-Hubbard description. We briefly discuss similar behaviors for fermionic systems.

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1) Introduction. - Exciting progress in the manipulation of neutral atoms in optical lattices has recently led, in a series of beautiful experiments, to the first verification in atomic systems of a quantum phase transition from a superfluid to a Mott insulator phase [1,2]. From a more general perspective, the physics of ultracold neutral atoms in discrete structures has become an ideal testing ground for the study and the realization of complex systems of condensed matter physics [3,4,5].

Because of the great current interest in the physics of atomic systems in optical lattices, much theoretical effort has been devoted to the characterization of the different quantum phases arising in these structures. Most of the studies have been restricted to situations in which the atoms are assumed to be confined in the lowest Bloch band of the periodic lattice potential, and to the ground state of the trapping harmonic oscillator potential, so that the description is given in terms of the standard Bose-Hubbard model [3,5]. However, one observes that often, in practical situations, the atoms (either fermions or bosons), while remaining confined in the lowest band of the periodic lattice potential (for sufficiently low temperatures), nevertheless may occupy large bundles of excited levels of the harmonic confining potential. This is an indication that the description in terms of the standard Hubbard and Bose-Hubbard models is not always fully adequate, even at very low temperatures.

In the present work we aim to characterize the physics of neutral atoms in single-band optical lattices, but including the energy structure due to the presence of the trapping potential. This leads to the introduction of generalized Hubbard and Bose-Hubbard models that are able to explain in a natural way the occupation of the excited levels of the trapping potential. We discuss how such an energy structure affects the phase diagram of the system and the nature of the superfluid phase. The problem is rather trivial if one considers identical fermions, but becomes more interesting in the case of bosons. We will comment in more detail about fermions in the conclusions. In the following, we consider a dilute ensemble of identical, spinless neutral bosonic atoms subject both to a 3-D anisotropic harmonic trapping and a 1-D optical lattice potential. We derive a generalized Bose-Hubbard Hamiltonian and we evaluate, both numerically and analytically, the free energies of the system. We show that, taking into account the possibility to populate the excited levels of the harmonic trapping potential, allows the superfluid to become distributed among the different energy levels. This effect of distributed superfluidity is realized in a single, stable superfluid state, and therefore should not be confused with the concept of multiple (fragmented), unstable superfluid states [7]. This fact allows to define suitable renormalized quantities that establish a precise mapping between the generalized and the standard Bose-Hubbard model.

II) General setting. - The microscopic Hamiltonian for an ensemble of bosonic atoms subject to an optical lattice potential and confined by an additional, slowly varying, external harmonic trapping reads \( \hat{H} = \hat{T} + \hat{V} + \hat{W} \), where \( \hat{T} \) is the kinetic energy term, \( \hat{V} \) represents the external potential energy term and \( \hat{W} \) is the local two-body interaction with coupling constant \( g_{BB} = 4\pi\hbar^2a_{BB}/2m \), where \( m \) is the mass of the atoms and \( a_{BB} \) is the s-wave scattering length. In the following, we will always assume boson-boson repulsion \( a_{BB} > 0 \). The potential energy \( \hat{V} \) is made up by two different contributions. The first contribution is an harmonic potential \( \hat{V}_H \) representing the effects of the quadrupolar trapping magnetic field, \( \hat{V}_H = m\omega^2(x^2 + \lambda y^2 + \lambda^2 z^2)/2 \). Here \( \lambda \) denotes the anisotropy coefficient and \( \omega \) is the frequency associated to the harmonic trap in the \( x \) direction. We consider the situation \( \lambda \ll 1 \), representative of the so-called “pancake-shaped” configuration. The ground state harmonic oscillator length in the \( x \) direction is \( L_x = \sqrt{\hbar/(m\omega)} \), while for \( L_y \) and \( L_z \) we have that \( L_y = L_z = L_x/\sqrt{\lambda} \), i.e. \( L_y, z \gg L_x \). The second contribution to the potential energy is a 1-D periodic optical lattice \( V_{opt} = V_0 \sin^2(\pi z/a) \), where \( V_0 \) is the maximum amplitude of the light shift associated to the intensity of the laser beam and \( a \) is the lattice spacing related to the wave vector \( k \) of the standing laser light by \( k = \pi/a \). This choice of the geometrical setting, which is not the one commonly used in experiments, is merely due to the numerical simplification of the energy spectra, and does not affect the general phenomenological features, as we will discuss in the following.

The bosonic field operators can be expanded in the basis of the single-particle Wannier wave functions localized at each lattice site \( z_i \). The presence of the optical lattice and the strong anisotropy define different energy scales along the different spatial directions. The energy gap between different
eigenstates along the $y$ direction is much smaller than the gap along the other ones. Because the typical interaction energies involved are normally not strong enough in order to excite higher vibrational states in the $x$ and $z$ directions, we can retain only the the lowest vibrational state at each lattice potential well. In the harmonic approximation, the Wannier wave functions $\Psi(\vec{r})$ factorize in the product of harmonic oscillator states $w(\vec{r})$: $\Psi(\vec{r}) = \sum_{i,\alpha} \hat{a}_{i,\alpha} w(z_i) w^\dagger(y) w(x)$, where $z_i$ is the center of the $i$th lattice site and $\hat{a}_{i,\alpha}$ is the bosonic annihilation operator acting on the $\alpha$-th harmonic oscillator level at the $i$-th lattice site. Considering different geometries such as a cigar-shaped or a fully isotropic potential will introduce extra indices in the orthogonal ($x$, $z$) directions, thus complicating the numerical evaluations but not changing the basic physical phenomena. The local ground state spatial extension $l_z$ for each lattice potential well is $l_z = (a^4 E_R/\hbar^2)^{1/4}$, where $E_R = (\pi \hbar)^2/2a^2m$ is the lattice recoil energy.

The condition of anisotropy $\lambda \ll 1$, implies that one can neglect in the Hamiltonian all terms proportional to powers of $\lambda$ higher than one. Moreover, in the presence of a slowly varying harmonic potential, we may neglect both next-to-nearest neighbor hopping and nearest-neighbor interaction terms that are of order of magnitude smaller than, respectively, nearest-neighbor hopping and on-site interaction terms. The harmonic Wannier scheme thus leads to the following multi-band Bose-Hubbard Hamiltonian

$$\hat{H} = \hat{H}_l - \sum_{i,j,\geq \alpha} J_{\alpha}^2 \hat{a}_{i,\alpha}^+ \hat{a}_{j,\alpha} ,$$

$$\hat{H}_l = \sum_{i,\alpha} \left( E_0 + \lambda \alpha \hbar \omega \right) \hat{n}_{i,\alpha} + \sum_{i,\alpha,\beta,\gamma,\delta} d_{\alpha,\beta,\gamma,\delta} \hat{a}_{i,\alpha}^+ \hat{a}_{i,\beta} \hat{a}_{i,\gamma} \hat{a}_{i,\delta} .$$

Here $\hat{H}_l$ stands for local terms. We see that neglecting the terms proportional to $\lambda^2$ (and higher powers of $\lambda$) makes the Hamiltonian homogeneous. Thus, in this setting (which is experimentally realistic), homogeneity is a consequence of strong anisotropy. The nonlocal term in Eq. (1) is the nearest-neighbor hopping contribution with amplitude $J_{\alpha}$ for a fixed harmonic energy level $\alpha$. In standard experimental situations we have $J_0 > 0$, and from the analytical expression of the hopping amplitude one finds that $J_{\alpha+1} < J_{\alpha}$ for every $\alpha > 0$. The first local term in Eq. (1) is the sum of local, level-dependent energies proportional to the on-site number operators $\hat{n}_{i,\alpha}$ on the $\alpha$th harmonic level on site $i$. This term has two contributions: a zero-point energy ($E_0$) and an excitation energy ($\lambda \alpha \hbar \omega$) that a boson needs to occupy the $\alpha$th harmonic energy level. The second local term in the Hamiltonian is the boson-boson on-site interaction with coupling constant $U = g_B/\sqrt{L_x L_y \pi (2\pi)^{3/2}}$. The numerical coefficients $d_{\alpha,\beta,\gamma,\delta}^{\alpha,\beta}$ read $d_{\alpha,\beta,\gamma,\delta}^{\alpha,\beta} = L_\beta \sqrt{2\pi} \int_{-\infty}^{\infty} w(\gamma) w(\delta) w(\gamma) w(\delta) d\gamma d\delta$. It is easy to prove that $d_{\alpha,\beta,\gamma,\delta}^{\alpha,\beta} = 1$, with the exception $d_{\alpha,\beta,\gamma,\delta}^{\alpha,\beta} = 0$. Contrary to what happens in the standard Bose-Hubbard setting, we see that the local interaction term involves both inter-level interactions and inter-level hoppings which do not commute with the on-site number operators $\hat{n}_{i,\alpha}$ for a given harmonic oscillator level. As a consequence, the two local terms of the generalized Bose-Hubbard Hamiltonian (11) do not in general commute. We then introduce the total on-site number operator $\hat{N}_i = \sum_{\alpha} \hat{n}_{i,\alpha}$. It is straightforward to verify that $[\hat{N}_i, \hat{H}_l] = 0$, so that there exists a complete set of states that are simultaneous eigenstates of $\hat{H}_l$ and $\hat{N}_i$. Therefore, the eigenstates of $\hat{H}_l$ can be arranged in classes characterized by a fixed eigenvalue of $\hat{N}_i$, with each class possessing a lowest eigenvalue.

III) Mean field theory and superfluid structure. - The above analysis suggests to divide the problem of finding the eigenstates of $\hat{H}_l$ in different problems in which one determines only the eigenstates characterized by a fixed eigenvalue $\hat{N}_i$. For ease of numerical evaluation it is convenient to adopt the grand canonical description $\hat{K} = \hat{H} - \mu \sum_i \hat{N}_i$, where $\mu$ is the chemical potential. We can analyze this problem by a mean field approach that corresponds to the approximation in which the hopping term is fully decoupled, in analogy with the standard Bose-Hubbard problem [8]: $\hat{a}_{i,\alpha}^+ \hat{a}_{j,\alpha} = (\hat{a}_{i,\alpha}^+ + \hat{a}_{j,\alpha}) \phi_{\alpha} - \phi_{\alpha}^2$, where $\phi_{\alpha} = \langle a_{i,\alpha}^+ \rangle = \langle a_{i,\alpha} \rangle$ is the real (without loss of generality), homogeneous superfluid order parameter for the $\alpha$th harmonic energy level. The introduction of a homogeneous superfluid parameter is justified by the homogeneity of the generalized Bose-Hubbard Hamiltonian, which, in the mean-field approximation reads

$$\hat{K}_{MF} = \hat{H}_l - \mu \sum_i \hat{N}_i - \sum_{i,\alpha} J_{\alpha} (a_{i,\alpha}^+ + a_{i,\alpha}) \phi_{\alpha} + \sum_{i,\alpha} \frac{J_{\alpha}}{2} \phi_{\alpha}^2 .$$

At fixed values of both the chemical potential and the temperature, we obtain the eigenvalues of $\hat{H}_l - \mu \sum_i \hat{N}_i$ associated to the eigenvectors of $\hat{H}_l$. To achieve this goal we proceed by truncating at a number $n_{max}$ of harmonic oscillator levels, and then diagonalizing the $n_{max} \times n_{max}$ matrix elements of $\hat{K}_{MF}$ obtaining the eigenvalues and, hence, the free energy. We then iterate the process by increasing $n_{max}$. Convergence is reached when the difference between the iterated free energies is lower than a given control parameter. This is a generalization of the Sheshadri approach to the standard Bose-Hubbard problem [8]. A first physical consequence is that the mean value of the local occupation number of the $\alpha$th level is in general nonvanishing, thus explaining the possible occupation of the excited levels of the harmonic trapping potential, even at zero temperature. In general, the procedure outlined above leads to consider several eigenvectors of $\hat{H}_l$ and the large matrices so obtained require thorough numerical evaluations. However, with suitable choices of the physical parameters only the two lowest eigenstates give non negligible contributions, and in this case the analytical diagonalization of $\hat{K}_{MF}$ is possible. In particular, this situation is realized when $J_0 \ll \lambda \hbar \omega$ and the chemical potential $\mu$ is chosen in such a way that the state $|\phi_{\alpha}(\lambda)\rangle$, i.e. the eigenstate with the lowest energy in the set of eigenstates of $\hat{H}_l$ with $\hat{N}_i = n$, and the
state \( |\psi_0^{(n+1)}\rangle \), i.e. the eigenstate with the lowest energy in the set of eigenstates of \( \hat{H}_I \) with \( N_i = n + 1 \), are nearly degenerate (i.e., the difference between the local eigenvalues of these two states is comparable in magnitude with \( J_0 \)). Let us introduce the quantity \( 2\Delta \), the small energy gap between these two states. The diagonal terms of the matrix Hamiltonian read

\[
\langle \psi_0^{(n)} | (\hat{H}_I - \mu \sum_i \hat{N}_i) | \psi_0^{(n)} \rangle = \Delta ,
\]

\[
\langle \psi_0^{(n+1)} | (\hat{H}_I - \mu \sum_i \hat{N}_i) | \psi_0^{(n+1)} \rangle = -\Delta ,
\]

while the off-diagonal terms due to the hopping are

\[
\langle \psi_0^{(n)} \mid \sum_{i,\alpha} J_{\alpha} \phi_{\alpha} (\hat{a}_{i,\alpha}^{\dagger} + \hat{a}_{i,\alpha}) | \psi_0^{(n+1)} \rangle = \sum_{\alpha} J_{\alpha} \phi_{\alpha} c_{\alpha} ,
\]

where \( c_{\alpha} \) stands for \( \langle \psi_0^{(n)} | \hat{a}_{\alpha} | \psi_0^{(n+1)} \rangle \). The eigenvalues \( \lambda \) of the energy matrix are \( \lambda_{1,2} = \pm \sqrt{\Delta^2 + (\sum_{\alpha} J_{\alpha} \phi_{\alpha} c_{\alpha})^2} \). Knowing the eigenvalues, we may write the free energy of the system \( F = -\beta^{-1} \ln |2 \cosh(\beta \lambda)| + (\sum_{\alpha} J_{\alpha} \phi_{\alpha}^2) / 2 \), with \( \beta = (k_B T)^{-1} \), \( T \) the absolute temperature, and \( k_B \) the Boltzmann constant. The free energy is a functional of the whole set of order (superfluid) parameters \( \phi_{\alpha} \) determined self-consistently through the minimization conditions

\[
\frac{\partial F}{\partial \phi_{\alpha}} = 0 \Rightarrow \phi_{\alpha} = \frac{c_{\alpha}}{\lambda} \tanh(\beta \lambda) \left( \sum_{\alpha} J_{\alpha} \phi_{\alpha} c_{\alpha} \right) .
\]

Obviously, this set of self-consistent equations allows for the existence of a disordered phase in which all the superfluid order parameters vanish identically. The crucial question arising from Eq. (5) is whether ordered phases are possible and the superfluid can be distributed among the different harmonic levels. To have the whole superfluid concentrated on a single level, the set of equations (5) should allow a solution in which only one order parameter, say \( \phi_k \) with \( k \) fixed, is nonvanishing. Hence the question is whether a solution of this kind is allowed. Let us first consider the case of filling factor \( n = 1 \), when the states considered are \( | \psi_0^{(1)} \rangle \) and \( | \psi_0^{(2)} \rangle \).

In the state \( | \psi_0^{(1)} \rangle \), due to the presence of exactly one atom per lattice site, the boson-boson local interaction vanishes and hence \( | \psi_0^{(1)} \rangle \) simply factorizes in the product of single-particle ground states \( | 1 \rangle_0 \), each containing one boson. On the other hand, \( | \psi_0^{(2)} \rangle \) is not an eigenstate of \( \hat{n}_{i,\alpha} \) for any \( \alpha \), but it may be written as a linear combination \( | 1,1 \rangle_{\gamma,\delta} \), characterized by having a boson in the \( \gamma \)th level and a boson in the \( \delta \)th level:

\[
| \psi_0^{(2)} \rangle = \sum_{\delta \leq \gamma} u_{\gamma,\delta} | 1,1 \rangle_{\gamma,\delta} .
\]

The coefficients \( u_{\gamma,\delta} \) are functions of the relative intensity of the two-body interactions and of the gap between the different harmonic levels. Taking into account the expression of \( | \psi_0^{(2)} \rangle \), the coefficients \( c_{\alpha} \) that appear in the off-diagonal terms of the truncated energy matrix Eq. (4) become equal to \( u_{0,\gamma} \) for \( \gamma \neq 0 \) and \( \sqrt{2} u_{0,0} \) otherwise. From these expressions and from the form of Eqs. (5), we see that the solution with the superfluid confined in a single band is allowed if and only if the coefficients \( u_{0,\gamma} \) are zero for each \( \gamma \) except at a single fixed value \( \gamma = k \). However, this condition is inconsistent with the requirement that \( | \psi_0^{(2)} \rangle \) be an eigenstate of \( \hat{H}_I \), because this latter constraint implies, for every coefficient \( u_{0,\gamma'} \),

\[
0 = \left( \gamma' \lambda \hbar \omega - E_0^{(2)} \right) u_{0,\gamma'} + 4 \sum_{\delta < \gamma} u_{\gamma,\delta} d_{\gamma,\delta}^{0,\gamma'} + 2 \sqrt{2} \sum_{\gamma} u_{\gamma,\delta} d_{\gamma,\delta}^{0,\gamma'} ,
\]

where \( E_0^{(2)} \) is the eigenvalue of \( \hat{H}_I \) associated to \( | \psi_0^{(2)} \rangle \). For any \( \gamma' \) such that \( k + \gamma' \) is even (this assumption is important because if \( k + \gamma' \) is odd, then \( d_{0,\gamma'}^{0,0} = 0 \)), solving for \( u_{0,k} \) yields

\[
| \psi_0^{(2)} \rangle = \frac{1}{4d_{0,\gamma'}^{0,0}} \left( 4 \sum_{\gamma < \delta < \gamma} u_{\gamma,\delta} d_{\gamma,\delta}^{0,\gamma'} + 2 \sqrt{2} \sum_{\gamma < \delta} u_{\gamma,\delta} d_{\gamma,\delta}^{0,\gamma'} \right) ,
\]

We thus arrive at a set of equations with a number of variables less than the number of equations. Because the extra equations are linearly independent from each other it is impossible to find a set of hamiltonian parameters that allows \( u_{0,\gamma} = 0 \) for any \( \gamma \neq k \). Numerical evidence shows that qualitatively similar results hold for \( n > 1 \). In the case \( n = 0 \) (hard core limit), the superfluid is confined to the harmonic oscillator ground state. This result may be explained by observing that in this case the local interactions do not play any role.

\section*{IV) Results and discussion}

- In Fig. 1 we show the behavior of the superfluid order parameters associated to different harmonic oscillator energy levels as functions of the temperature for different values of the energy gap between the states \( | \psi_0^{(2)} \rangle \) and \( | \psi_0^{(1)} \rangle \). (In all figures the quantities plotted are dimensionless). From Fig. 1 we see that the ratio of superfluid in the different levels is fixed and independent of the temperature. This is clear evidence that, although the superfluid is distributed among the different levels, the superfluid state is...
unique, and therefore stable [7]. From Eq. (5) the ratios are simply: \( r_\alpha = c_\alpha / \sqrt{\sum_\alpha c_\alpha^2} \), where \( r_\alpha \) is the fraction of superfluid in the level \( \alpha \). The fact that the superfluid state is unique leads naturally to the existence of a unique critical temperature \( T_c \). The latter depends on the energy gap \( \Delta \) and on the different hopping amplitudes \( J_\alpha \), and may be obtained from the set of Eqs. (5): it is the temperature for which there exists a double solution at \( \phi_\alpha = 0 \) for every \( \alpha \):

\[
\beta_c \Delta = \text{arctanh} \left( \frac{\Delta}{\sum_\alpha c_\alpha^2 J_\alpha} \right). \tag{8}
\]

In Fig. 3 we show the behavior of \( T_c \) for varying \( \lambda \hbar \omega \) at fixed \( J_\alpha \). As far as \( T_c \) is concerned, one can see from this figure and Eq. (5) that the transition is analogous to that of a standard Bose-Hubbard model with renormalized hopping amplitude \( J_R = \sum_\alpha c_\alpha^2 J_\alpha \). In Fig. 3 we show the behavior of the critical temperature as a function of the filling factor \( n \) both for the analytical solution with only the two lowest-lying local states and the numerical solution obtained after full convergence is reached. The zero-temperature quantum phase transition from a superfluid to a Mott-insulator phase is recovered for the value \( \Delta_c \) at which \( T_c = 0 \). From Eq. (8) one has \( \Delta_c = \sum_\alpha c_\alpha^2 J_\alpha \).

In conclusion, we have studied the properties of an ensemble of neutral bosonic atoms in an optical lattice, including the energy structure due to the presence of a superimposed trapping potential. We have shown that the system possesses an ordered phase in which the superfluid is distributed among the different harmonic energy levels. Our analysis holds in a similar way in the much simpler instance of spin-polarized fermions and thus provides the physical mechanism explaining the population of the excited levels of the harmonic trapping potential. Work is in progress for the case of interacting fermions, and will be reported elsewhere. An interesting possibility for future research lies also in the study of the energy structure for multicomponent systems and mixtures of bosonic and fermionic atoms in optical lattices. We thank INFN, INFM, and MIUR under national project PRIN-COFIN 2002 for financial support.

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