Macroscopic dynamics of a trapped Bose-Einstein condensate in the presence of 1D and 2D optical lattices

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The hydrodynamic equations of superfluids for a weakly interacting Bose gas are generalized to include the effects of periodic optical potentials produced by stationary laser beams. The new equations are characterized by a renormalized interaction coupling constant and by an effective mass accounting for the inertia of the system along the laser direction. For large laser intensities the effective mass is directly related to the tunneling rate between two consecutive wells. The predictions for the frequencies of the collective modes of a condensate confined by a magnetic harmonic trap are discussed for both 1D and 2D optical lattices and compared with recent experimental data.

The experimental realization of optical lattices\textsuperscript{[1–6]} is stimulating new perspectives in the study of coherence phenomena in trapped Bose-Einstein condensates. A first direct measurement of the critical Josephson current has been recently obtained in\textsuperscript{[3]} by studying the center of mass motion of a magnetically trapped gas in the presence of a 1D periodic optical potential. Under these conditions the propagation of collective modes is a genuine quantum effect produced by the tunneling through the barriers and by the superfluid behaviour associated with the coherence of the order parameter between different wells. The effect of the optical potential is to increase the inertia of the gas along the direction of the laser giving rise to a reduction of the frequency of the oscillation.

The purpose of the present work is to investigate the collective oscillations of a magnetically trapped gas in the presence of 1D and 2D optical lattices taking into account the effect of tunneling, the role of the mean field interaction and the 3D nature of the sample. Under suitable conditions these effects can be described by properly generalizing the hydrodynamic equations of superfluids\textsuperscript{[7]}. Let us assume that the gas, at $T = 0$, be trapped by an external potential given by the sum of a harmonic trap of magnetic origin $V_{\text{ho}}$ and of a stationary optical potential $V_{\text{opt}}$ modulated along the $z$-axis. The resulting potential is given by

$$V_{\text{ext}} = \frac{1}{2} m \left( \omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right) + s E_R \sin^2 q z$$

(1)

where $\omega_x, \omega_y, \omega_z$ are the frequencies of the harmonic trap, $q = 2\pi/\lambda$ is fixed by the wavelength of the laser light creating the stationary 1D lattice wave, $E_R = \hbar^2 q^2 / 2m$ is the so called recoil energy and $s$ is a dimensionless parameter providing the intensity of the laser beam. The optical potential has periodicity $d = \pi/q = \lambda/2$ along the $z$-axis. The case of a 2D lattice will be discussed later. In the following we will assume that the laser intensity be large enough to create many separated wells giving rise to an array of several condensates. Still, due to quantum tunneling, the overlap between the wave functions of two consecutive wells can be sufficient to ensure full coherence. In this case one is allowed to use the Gross-Pitaevskii (GP) theory for the order parameter to study both the equilibrium and the dynamic behaviour of the system at zero temperature\textsuperscript{[8]}. Eventually, if the tunneling becomes too small, the fluctuations of the relative phase between the condensates will destroy the coherence of the sample giving rise to new quantum configurations associated with the transition to a Mott insulator phase\textsuperscript{[9]}. In the presence of coherence it is natural to make the ansatz

$$\Psi(r) = \sum_k \Psi_k(x, y) f_k(z) e^{i S_k(x,y)}$$

(2)

for the order parameter in terms of a sum of many condensate wave-functions relative to each well. Here $S_k(x,y)$ is the phase of the $k$-component of the order parameter, while $\Psi_k$ and $f_k$ are real functions. We will make the further periodicity assumption $f_k(z) = f_0(z - kd)$ where $f_0$ is localized at the origin. The above assumptions for $\Psi$ and $f_k$ are justified for relatively large values of $s$ where the interwell barriers are significantly higher than the chemical potential. In this case the condensate wave functions of different sites are well separated (tight binding approximation).

Using the ansatz (2) for the order parameter one finds the following result for the mean field expectation value of the effective Hamiltonian $H = \sum_j (p_j^2 / 2m + V_{\text{ext}}(r_j)) + g \sum_{j<k} \delta(r_j - r_k)$:

$$E = \langle H \rangle = \left[ \int dz \frac{\hbar^2}{2m} (\partial_z f_0)^2 + f_0^2 V_{\text{opt}} \right] \sum_k \int dx dy \Psi_k^2$$

$$+ \frac{g}{2} \left[ \int dz f_0^4 \right] \sum_k \int dx dy \Psi_k^4$$
various terms of the energy. Through such a procedure we obtain the following macroscopic expression for the energy

\[ E = \int dV n_M \left[ \frac{\hat{g} n_M}{2} + V_{\text{ho}} + \frac{\hbar^2}{2m} (\partial_{x_L} S)^2 - \delta \cos [d \partial_z S] \right], \]  

where we have introduced the renormalized coupling constant \( \hat{g} = g \int f^0_0 dz \), we have neglected quantum pressure terms originating from the radial term in the kinetic energy and we have set \( \Psi_k \Psi_{k+1} \sim \Psi_k^2 = dn_M \). We have also omitted some constant terms (first two terms in eq. (6)) which do not depend on \( n_M \) or on \( S \).

With respect to the functional characterizing a trapped Bose gas in the absence of optical confinement, one notices two important differences: first the interaction coupling constant is renormalized due to the presence of the optical lattice. This is the result of the local compression of the gas produced by the tight optical confinement which increases the repulsive effect of the interactions. Second the kinetic energy term along the \( z \)-direction has no longer the classical quadratic form as in the radial direction, but exhibits a periodic dependence on the gradient of the phase. By expanding this term for small gradients, which is the case in the study of small amplitude oscillations, one derives a quadratic term of the form \( (\hbar^2/2m^*) \int dV n_M (\partial_z S)^2 \) characterized by the effective mass

\[ \frac{m}{m^*} = \frac{m \delta d^2}{\hbar^2} = \frac{\delta \pi^2}{E_R 2}, \]  

where \( \delta \) is defined by eq. (3). Notice that within the employed approximation the value of \( \delta \), and hence of \( m^* \), does not depend on the number of atoms, nor on the mean field interaction.

The equilibrium density profile, obtained by minimizing eq. (7) with \( S = 0 \) has the typical form of an inverted parabola [10]

\[ n_M^0 = \left( \mu - \frac{1}{2} m (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) / \hat{g} \right), \]  

which conserves the aspect ratio of the original magnetic trapping. The size of the condensate has instead increased since \( \hat{g} > g \). For large \( s \) the increase of the coupling constant can be large (\( \hat{g} \sim 4^{1/4} \)). However, since the radius of the sample scales like the 1/5-th power of \( \hat{g} \) the resulting increase in the size of the system is not very spectacular (for \( s = 15 \) we find an increase of the size by \( \sim 20\% \) for the experimental setting of [3]).

The functional (7) can be used to carry out dynamic calculations. In this case one needs the action \( A = \int dt \left( H - i \hbar \langle \frac{\delta}{\delta t} \rangle \right) \), with the second term given by \( i \hbar \langle \frac{\delta}{\delta t} \rangle = - \int dV n_M \dot{S} \). The resulting equations of motion are obtained by imposing the stationarity condition on the action with respect to arbitrary variations of the density \( n_M \) and of the phase \( S \). The equations take the form

\[ \dot{n}_M + \frac{\hbar}{m} \partial_{x_L} \left( n_M \partial_{x_L} S \right) + \frac{\delta d}{\hbar} \partial_z \left( n_M \sin [d \partial_z S] \right) = 0, \]  

\[ \hbar \dot{S} + \hat{g} n_M + V_{\text{mag}} + \frac{\hbar^2}{2m} (\partial_{x_L} S)^2 - \delta \cos [d \partial_z S] = 0. \]
In particular, at equilibrium these equations reproduce result (3) for the equilibrium density. Furthermore, Josephson-type oscillations are among those captured by eqns. (4) and (11). To see this consider the case of a uniform gradient of the phase along \( z \), \( \partial_z S = P_Z(t) / \hbar \), where \( P_Z \) is a time-dependent parameter. From eqs. (4) and (11) one can then derive equations of motion for the center of mass \( Z(t) = \int dV n_m(t) / N \) and for the conjugate momentum variable \( P_Z \):

\[
\hbar \dot{Z} - \delta s \frac{d}{d \hbar} \left[ \frac{d P_Z}{d \hbar} \right] = 0, \tag{12}
\]

\[
\dot{P}_Z + m \omega^2 Z = 0, \tag{13}
\]

which have the typical Josephson form.

In the limit of small oscillations the solutions of eqs. (4) and (11) have the form \( n = n^0_M + \delta n(r) e^{i \omega t} \) with \( \delta n \) obeying the hydrodynamic equations:

\[
-\omega^2 \delta n = \partial_r \left[ \frac{\mu - V_{ho}}{m} \partial_r \delta n \right] + \partial_z \left[ \frac{\mu - V_{ho}}{m^*} \partial_z \delta n \right], \tag{14}
\]

where \( \mu = \tilde{g} n^0_M(0) \) is the chemical potential of the sample and \( n^0_M(0) \) is the equilibrium density (3) evaluated at the center. The solutions of (14) provide the low energy excitations of the system. In the absence of magnetic trapping these solutions of (14) do not depend on the value of the coupling constant. By applying the transformation \( z \rightarrow \sqrt{m^*/m} z \), one actually finds that the new frequencies are simply obtained from the results of (4) by replacing \( \omega \rightarrow \omega \sqrt{m/m^*} \). (15)

For an elongated trap (\( \omega_\perp = \omega_y = \omega_z \gg \omega_x \)) the lowest solutions are given by the center-of-mass motion \( \omega_D = \sqrt{m/m^*} \omega_z \) and by the quadrupole mode \( \omega_Q = \sqrt{3/2} \sqrt{m/m^*} \omega_z \). The center-of-mass frequency coincides with the value obtained from eqs. (12) and (13) in the limit of small oscillations. Concerning the quadrupole frequency we note that the occurrence of the factor \( \sqrt{3/2} \) is a non-trivial consequence of the mean field interaction predicted by the hydrodynamic theory of superfluids in the presence of harmonic trapping (3). In addition to the low-lying axial motion the system exhibits radial oscillations at high frequency, of the order of \( \omega_\perp \). The most important ones are the transverse breathing and quadrupole oscillations occurring at \( \omega = 2 \omega_\perp \) and \( \omega = \sqrt{2} \omega_\perp \) respectively. For elongated traps the frequencies of these modes should not be affected by the presence of the optical potential. Different scenarios are obtained for disc-shaped traps (\( \omega_z \gg \omega_\perp \)). The above results apply to the linear regime of small oscillations. Eqns. (12) and (13) show that in the case of center-of-mass oscillations, the linearity condition is achieved for initial displacements \( \Delta x \) of the trap satisfying \( \Delta x \ll \sqrt{2 \hbar / m \omega_e^2} \), which becomes more and more severe as the laser intensity increases. For larger initial displacements the oscillation is described by the pendulum equations. For very large amplitudes the motion is however dynamically unstable (3).

From the previous discussion it emerges that the effective mass is the crucial parameter needed to predict the value of the small amplitude collective frequencies. An estimate of \( m/m^* \) can be made by neglecting the magnetic trapping as well as the role of the mean field interaction. Within this approximation the effective mass is easily obtained from the excitation spectrum of the Schrödinger equation for the 1D Hamiltonian \( H = -\hbar^2 / 2 m d^2 / d z^2 + s E_0 \sin^2 z \), avoiding the explicit determination of the tunneling parameter (4). One looks for solutions of the form \( e^{ipz/\hbar} f_p(z) \) where \( p \) is the quasi-momentum of the atom and \( f_p(z) \) is a periodic function of period \( d \). The resulting dispersion law \( \epsilon(p) \) provides, for small \( p \), the effective mass according to the identification \( \epsilon(p) \approx \epsilon_0 + p^2 / 2 m^* \). The value of \( m/m^* \), which turns out to be a universal function of the intensity parameter \( s \), has been evaluated for a wide range of values of \( s \) (see fig. 3). These results for \( m^* \) can be used to estimate the actual value of the collective frequencies. The method described here to calculate \( m^* \) is expected to be reliable not only for very large laser intensities \( s \) when the tight binding approximation applies and the effective mass can be expressed in terms of the tunneling rate (see eqs. (3), (4)), but also for smaller values of \( s \). Of course for very small laser intensities, as in the experiment (4), the determination of \( m^* \) requires the inclusion of the mean field interaction and of the magnetic trapping through the explicit solution of the GP-equation.

In fig. 2 we compare our predictions for the frequencies of the center-of-mass motion with the recent experimental data obtained in (3). The comparison reveals good agreement with the experiments. Our results also agree well with those obtained from the numerical solution of the time-dependent GP-equation (12).

The above formalism is naturally generalized to include a 2D optical lattice where the optical potential is \( V_{opt} = s E_0 \sin^2 qx + s E_0 \sin^2 qy \). The actual potential now generates an array of 1D condensates which has already been the object of experimental studies (4). For a 2D-lattice the ansatz for the order parameter is (15)

\[
\Phi(r) = \sum_{k_x, k_y} \Psi_{k_x, k_y}(z) f_{k_x, k_y}(x, y) e^{i S_{k_x, k_y}(z)}. \tag{16}
\]

In the TF-limit the groundstate smoothed density \( n_M = \Psi_{k_x, k_y}^2 / d^2 \) still has the familiar form \( n_M^0 = (\mu - V_{ho}) / \tilde{g} \) with the redefined coupling constant \( \tilde{g} = g (d \int dx f^2) \), where \( f_0 \) is still given by the solution of eq. (3) and we
have used the same approximations as in the 1D case.

Also with regard to dynamics, one can proceed as for the 1D lattice. One finds that the equations of motions, after linearization, take the form

$$\dot{\delta n} = \partial_z \left[ \frac{\mu - V_{ho}}{m} \partial_z \delta n \right] + \partial_{k_z} \left[ \frac{\mu - V_{ho}}{m} \partial_{k_z} \delta n \right]. \tag{17}$$

The frequencies of the low energy collective modes are then obtained from those in the absence of the lattice \(k\) by simply replacing \(\omega_{k} \rightarrow \sqrt{m/m^*} \omega_{k}\) and \(\omega_y \rightarrow \sqrt{m/m^*} \omega_y\). For large laser intensities the value of \(m^*\) coincides with the one calculated for the 1D array. If \(\omega_y >> \omega_x \sqrt{m/m^*, \omega_y \sqrt{m/m^*}}\), the lowest energy solutions involve the motion in the \(x-y\) plane. The oscillations in the \(z\)-direction are instead fixed by the value of \(\omega_z\). These include the center-of-mass motion \(\omega = \omega_z\) and the lowest compression mode \(\omega = \sqrt{3} \omega_z\) \([\text{3}]\). The frequency \(\omega = \sqrt{3} \omega_z\) coincides with the value obtained by directly applying the hydrodynamic theory to 1D systems \([\text{15}]\) and reveals the 1D nature of the tubes generated by the 2D lattice. If the radial trapping generated by the lattice becomes too strong the motion along the tubes can no longer be described by the mean field equations and one jumps into more correlated 1D regimes \([\text{18}]\).

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