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Quantum fluctuations and Collective Oscillations of a Bose-Einstein Condensate in a 2D Optical Lattice

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We use Bogoliubov theory to calculate the beyond mean field correction to the equation of state of a weakly interacting Bose gas in the presence of a tight 2D optical lattice. We show that the lattice induces a characteristic 3D to 1D crossover in the behavior of quantum fluctuations. Using the hydrodynamic theory of superfluids, we calculate the corresponding shift of the collective frequencies of a harmonically trapped gas. We find that this correction can be of the order of a few percent and hence easily measurable in current experiments. The behavior of the quantum depletion of the condensate is also discussed.

Recently, the group of Ketterle at MIT reported [1] the first measurements of the quantum depletion in a condensate of ^{23}Na atoms in tight optical lattices. The condensate fraction corresponds to the population of the interference peaks observed in the time-of-flight images, whereas the remaining diffusive background is interpreted as the quantum depletion.

From the theoretical point of view, the quantum depletion of a weakly interacting Bose gas can be calculated from Bogoliubov theory. Another closely related quantity is the beyond mean field correction to the equation of state. In free space (no lattice) this is known as the Lee-Huang-Yang (LHY) correction [2]. In Ref. [3], Pitaevskii and Stringari suggested to observe the LHY correction through the measurements of the collective frequencies which are sensitive to changes in the equation of state. However, for typical values of the atom density and scattering length, this correction remains very small and difficult to measure. First experimental signatures of these corrections have been recently observed in a superfluid Fermi gas on the Bose-Einstein condensate side of the Feshbach resonance [4]. The inclusion of the lattice is expected to enhance the role of correlations, and therefore effects beyond mean field might become visible in such configurations. Previous experimental [5] and theoretical [6,7] attempts to investigate beyond mean field effects in the collective frequencies of trapped Bose gases have focused on 1D systems, where the gas undergoes a crossover from a weakly interacting Bose-Einstein condensate to a Tonks gas by decreasing the atomic density in the tube.

In this Letter, we investigate a Bose-Einstein condensates in a tight 2D periodic potential forming a 2D array of weakly coupled tubes. For a fixed atom density, the gas is in an anisotropic 3D regime at small values of the laser intensity and it undergoes a dimensional crossover to a 1D regime when the lattice depth is increased. We calculate the beyond mean field correction to the ground state energy due to quantum fluctuations along the crossover. We then include the harmonic trapping and apply the hydrodynamic theory of superfluids to calculate the corresponding frequency shift of the lowest compressional mode along the axial direction, where atoms are free to oscillate subject to the harmonic potential and two-body interactions. We show that for values of physical parameters available in current experiments, this shift becomes large enough to be detected. Our results in the asymptotic 1D regime are consistent with those obtained in Ref. [7].

Let us first consider a Bose-Einstein condensate in the presence of a 2D optical lattice:

$$V_{opt}(x, y) = sE_R[\sin^2(q_B x) + \sin^2(q_B y)], \qquad (1)$$

where s is the laser intensity and $E_R = \hbar^2 q_B^2/2m$ is the recoil energy, with $\hbar q_B$ the Bragg quasimomentum and m the atomic mass. The lattice period is fixed by $d = \pi/q_B$. Atoms are unconfined in the axial direction. The role of the additional harmonic trapping will be discussed later.

The interparticle interaction is described by an s-wave contact potential with coupling constant $g = 4\pi\hbar^2 a/m$, a being the 3D scattering length. We will discuss the situation where the laser intensity is sufficiently large ($s \gtrsim 5$) and the chemical potential μ is small compared to the interband gap. We thus restrict ourselves to the lowest Bloch band, where the physics is governed by the ratio between the chemical potential and the bandwidth $8t$, where t is the tunneling rate between neighboring wells. For $\mu \ll 8t$, the system retains an anisotropic 3D behavior, whereas for $\mu \approx 8t$, the system undergoes a dimensional crossover to a 1D regime. Experimentally, this crossover can be realized by either increasing the laser intensity (t decreases) or increasing the atom density n (μ increases).

In tight-binding approximation the states of the lowest Bloch band can be written in terms of Wannier functions as $\phi_{k_x}(x)\phi_{k_y}(y)$, where $\phi_k(u) = \sum_\ell e^{i\ell k u} w(u - \ell d)$ and $w(u) = \exp[-u^2/2\sigma^2]/\pi^{1/4}\sigma^{1/2}$ is a variational Gaussian ansatz. By minimizing the free energy functional with respect to σ, one finds $d/\sigma \simeq \pi s^{1/4} \exp(-1/4\sqrt{s})$.

The system Hamiltonian takes the form

$$H' = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{\tilde{g}}{2V} \sum_{\mathbf{k},\mathbf{q},\mathbf{k}'} a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'-\mathbf{q}}^\dagger a_{\mathbf{k}'} a_{\mathbf{k}}, \quad (2)$$

where $\epsilon_{\mathbf{k}}^0 = \hbar^2 k_z^2/2m + 2t[2 - \cos k_x - \cos k_y]$ is the energy dispersion of the noninteracting model, V is the volume, and $\tilde{g} = C^2 g$ is an effective coupling constant, with $C = d \int_{-d/2}^{d/2} w^4(u)du \simeq d/\sqrt{2\pi}\sigma$.

In the following we assume that the number of atoms per tube is sufficiently large. Under this assumption, we can neglect the Mott insulator phase transition which would occur only for extremely large values of the laser intensity. Applying Bogoliubov theory to the Hamiltonian (2), the energy spectrum $E_{\mathbf{k}}$ of the elementary excitations is given by $E_{\mathbf{k}}^2 = \epsilon_{\mathbf{k}}^0(\epsilon_{\mathbf{k}}^0 + 2\tilde{g}n)$ [8]. The ground state energy of the system can be obtained from the relation $E = n^2 \tilde{g}V/2 - \sum_{\mathbf{k}\neq 0}(\epsilon_{\mathbf{k}}^0 + \tilde{g}n - E_{\mathbf{k}})/2$, where the second term corresponds to the beyond mean field correction due to quantum fluctuations. This correction can be shown to be always negative (in free space this formula would contain an ultraviolet divergence to be cured by a proper renormalization of the coupling constant).

Replacing the sum with integrals and performing the integration over the axial momentum k_z, we find

$$\frac{E}{V} = \frac{1}{2}\tilde{g}n^2 - \frac{1}{4\pi}\frac{\tilde{g}n}{d^2}\sqrt{2m\tilde{g}n}f\left(\frac{2t}{\tilde{g}n}\right), \quad (3)$$

where the function $f(x)$ is defined as

$$f(x) = \frac{\pi}{2\sqrt{x}} \int_{-\pi}^{\pi} \frac{d^2\mathbf{k}}{(2\pi)^2} \frac{{}_2F_1(1/2, 3/2, 3, -\frac{2}{x\gamma(\mathbf{k})})}{\sqrt{\gamma(\mathbf{k})}}, \quad (4)$$

with $\gamma(\mathbf{k}) = 2 - \cos k_x - \cos k_y$. Here ${}_2F_1(a, b, c, d)$ is the hypergeometric function and the integration over the transverse quasimomenta is restricted to the first Brillouin zone $|k_x|, |k_y| \leq \pi$. Equation (4) has been integrated numerically and the result is shown in Fig. 1 (left panel). For vanishing x, $f(x)$ saturates to the value $4\sqrt{2}/3 \simeq 1.89$. In this limit, corresponding to $8t \ll \mu$, we can neglect the Bloch dispersion and Eq. (3) yields the ground state energy of a 1D Bose gas:

$$\frac{E}{L} = \frac{1}{2}g_{1D}n_{1D}^2 - \frac{2}{3\pi}\sqrt{m}(n_{1D}g_{1D})^{3/2}, \quad (5)$$

with linear density $n_{1D} = nd^2$ and coupling constant $g_{1D} = \tilde{g}/d^2$. Here L is the length of the tube. Result (5) is in agreement with the exact Lieb-Liniger solution [9] of the 1D model expanded in the weak coupling regime $mg_{1D}/\hbar^2 n_{1D} \ll 1$.

In the opposite 3D regime $x \gg 1$, the function (4) approaches the asymptotic law $f(x) \simeq 1.43/\sqrt{x} - 16\sqrt{2}/15\pi x$. This is shown in Fig. 1 (left panel) with the dashed line. Introducing the notation $\tilde{a} = C^2 a$, Eq. (3) takes the asymptotic form
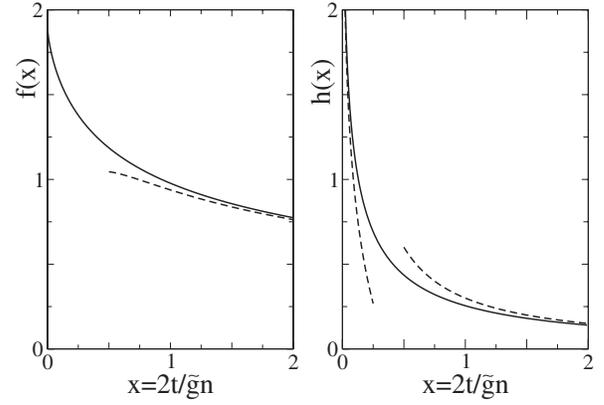

FIG. 1. Left panel: scaling function $f(x)$ [see Eq. (4)] (solid line) and its asymptotic behavior (dashed line). Right panel: scaling function $h(x)$ [see Eq. (7)] (solid line) and its asymptotic behavior (dashed lines).

$$\frac{E}{V} = \frac{2\pi}{m}n^2\tilde{a}\left[1 + \frac{\tilde{a}}{\tilde{a}_{cr}} + \frac{128}{15}\left(\frac{n\tilde{a}^3}{\pi}\right)^{1/2}\frac{m^*}{m}\right], \quad (6)$$

where $m^* = \hbar^2/2td^2$ is the effective mass associated with the band and $\tilde{a}_{cr} = -0.24d\sqrt{m/m^*}$. The last term in the right-hand side of Eq. (6) corresponds to the generalized LHY correction in the presence of the optical lattice. We see that with respect to the free case, the LHY correction is magnified by the renormalization of both the coupling constant ($\tilde{a} > a$) and the effective mass ($m^* > m$). It is worth noticing that Eq. (6) is valid only for $\mu \ll 8t$, a condition which, for large s, requires ultralow atomic densities.

The term $\tilde{a}/\tilde{a}_{cr} < 0$ in Eq. (6) is more subtle and amounts to a further renormalization of the scattering length due to the optical lattice. In particular, the correct value for the scattering length for low-energy ($E \ll 8t$) two-body collisions is given by $1/a_{eff} = 1/\tilde{a} - 1/\tilde{a}_{cr}$ [10]. In Eq. (6) a_{eff} is replaced by the linear expansion $a_{eff} \simeq \tilde{a}(1 + \tilde{a}/\tilde{a}_{cr})$.

The equation of state $\mu = \partial E/\partial N$ can be obtained by differentiating Eq. (3). We find it convenient to write it as $\mu = \tilde{g}n[1 + k(n)]$, where the term proportional to $k(n)$ accounts for the effects of quantum fluctuations. In the 1D limit $k(n) = -1/(\pi d^2)\sqrt{m\tilde{g}/n}$, whereas in the opposite 3D regime we find $k(n) = \tilde{a}/\tilde{a}_{cr} + \beta(m^*/m)\sqrt{\tilde{a}^3 n}$, with $\beta = 32/3\sqrt{\pi}$.

Using the same formalism it is possible to calculate the quantum depletion given by $N - N_0 = \sum_{\mathbf{k}\neq 0}(\epsilon_{\mathbf{k}}^0 + \tilde{g}n - E_{\mathbf{k}})/2E_{\mathbf{k}}$. Taking the continuum limit, we find

$$\frac{N - N_0}{N} = \frac{1}{4\pi}\frac{1}{d^2}\sqrt{\frac{2m\tilde{g}}{n}}h\left(\frac{2t}{\tilde{g}n}\right), \quad (7)$$

with

$$h(x) = \int_{-\pi}^{\pi} \frac{d^2\mathbf{k}}{(2\pi)^2} \int_{x\gamma(\mathbf{k})}^{\infty} \frac{dt}{\sqrt{t - x\gamma(\mathbf{k})}}\left[\frac{t+1}{\sqrt{t^2 + 2t}} - 1\right]. \quad (8)$$

Differently from the beyond mean field correction to the ground state energy (5), the quantum depletion diverges for vanishing tunneling as $h(x) \simeq -\ln(2.7x)/\sqrt{2}$. This signals that in the absence of tunneling there is no real Bose-Einstein condensation in agreement with the general theorems in one dimension [11]. In the opposite 3D regime $x \gg 1$ the function $h(x)$ decays as $4/(3\pi\sqrt{2}x)$, and from Eq. (7) we find $(N - N_0)/N = (8m^*/3m)(\tilde{a}^3 n/\pi)^{1/2}$, which generalizes the standard 3D result in free space [11].

In the second part of the Letter we apply the hydrodynamic theory of superfluids to investigate the effects of quantum correlations on the collective frequencies of a trapped gas. Expanding the atom density as $n(\mathbf{r}, t) = n(\mathbf{r}) + \delta n(\mathbf{r}, t)$, the hydrodynamic equations in the presence of the lattice can be written in the useful form [12]

$$m \frac{\partial^2 \delta n}{\partial t^2} - \tilde{\nabla} \left[n \tilde{\nabla} \left(\frac{\partial \mu}{\partial n} \delta n \right) \right] = 0, \qquad (9)$$

where we have introduced the notation $\tilde{\nabla} \equiv (\nabla_\perp \sqrt{m/m^*}, \nabla_z)$. For trapped configurations, the ground state density $n(\mathbf{r})$ entering Eq. (9) has to be calculated by imposing the local equilibrium condition $\mu_0 = \mu(n(\mathbf{r})) + V_{\text{ext}}(\mathbf{r})$, where μ_0 is the ground state value of the chemical potential, fixed by the proper normalization of $n(\mathbf{r})$, and $V_{\text{ext}}(\mathbf{r}) = (\omega_\perp^2 \mathbf{r}_\perp^2 + \omega_z z^2)/2m$ is the external trapping potential, here assumed of axial symmetry.

By substituting $\mu = \tilde{g}n[1 + k(n)]$ into Eq. (9) and retaining only terms linear in $k(n)$, we obtain

$$m\omega^2 \delta n + \tilde{\nabla}(gn_{\text{TF}} \tilde{\nabla} \delta n) = -\tilde{\nabla}^2 \left(\tilde{g} n_{\text{TF}}^2 \frac{\partial k}{\partial n_{\text{TF}}} \delta n \right), \quad (10)$$

where $n_{\text{TF}}(\mathbf{r}) = [\mu_0 - V_{\text{ext}}(\mathbf{r})]/\tilde{g}$ is the Thomas-Fermi density profile. Equation (10) can be solved by treating its right-hand side as a small perturbation, following the procedure of Ref. [3]. To this purpose one first solves the associated zeroth order hydrodynamic equation setting the right-hand side of Eq. (10) equal to zero [13]. The corresponding solution can then be used to calculate the frequency shift induced by the perturbation. One finds

$$\frac{\delta\omega}{\omega} = -\frac{\tilde{g}}{2m\omega^2} \frac{\int d^3\mathbf{r}\, \delta n(\tilde{\nabla}^2 \delta n^*) n_{\text{TF}}^2 \partial k/\partial n_{\text{TF}}}{\int d^3\mathbf{r}\, \delta n^* \delta n}, \quad (11)$$

where the integrals extend to the region where the Thomas-Fermi density is positive. We see from Eq. (11) that the shift in the frequency is not proportional to $k(n)$ but rather to its derivative $\partial k/\partial n$, so that the *density-independent* term $\tilde{a}/\tilde{a}_{\text{cr}}$ does not contribute to the frequency shift (11). Furthermore, the shift can be positive even if $k(n)$ is negative, as happens in the 1D regime.

In order to observe effects beyond mean field, we focus on the lowest compressional mode along the axial direction. For simplicity we assume an *effective* disc-shaped trap $\omega_\perp/\sqrt{m^*} \ll \omega_z$. In this case the zeroth order dispersion is given by $\omega = \sqrt{3}\omega_z$ with density oscillations of the form $\delta n(\mathbf{r}) \sim z^2 - Z_{\text{TF}}^2/3$, where $Z_{\text{TF}}^2 = 2\mu_0/m\omega_z^2$ is the

square of the Thomas-Fermi radius along the axial direction. Calculating $k(n)$ from Eq. (3) and inserting it into Eq. (11), after integration over coordinates, we find

$$\frac{\delta\omega}{\omega} = \frac{21}{512} \sqrt{\frac{m\tilde{g}}{n(0)}} \frac{1}{d^2} Y\left(\frac{2t}{\tilde{g}n(0)} \right), \qquad (12)$$

where $n(0) = n_{\text{TF}}(0)$ is the density evaluated in the center of the trap and

$$Y(x) = \frac{16\sqrt{2}}{\pi} \sqrt{x} \int_0^1 dr\, r^2 (r^2 - 1) G\left(\frac{x}{1 - r^2} \right). \qquad (13)$$

Here $x = 2t/\tilde{g}n(0)$ is the parameter controlling the dimensional crossover for *trapped* gases and $G(y) = y^{3/2} f''(y) - 3f(y)/4\sqrt{y}$. The function (13) satisfies $Y(0) = 1$ and decreases monotonically as x increases, reaching the asymptotic law $Y(x) = 5/6\pi x$ for large values of x.

Equations (12) and (13) are the key results of this Letter. In the 1D regime, corresponding to large values of the laser intensity, $\delta\omega/\omega = (21/512)\sqrt{m\tilde{g}/n(0)d^4}$, showing that the shift increases by decreasing the central density. In the opposite 3D regime of small values of s, the frequency shift is instead given by $\delta\omega/\omega = (35\sqrt{\pi}m^*/128m) \times \sqrt{\tilde{a}^3 n(0)}$, and hence increases by increasing the central density. This latter equation provides the lattice generalization of the frequency shift due to the LHY correction investigated in Ref. [3].

In Fig. 2 we show the calculated frequency shift as a function of the laser intensity for atomic samples of ^{23}Na (3D scattering length $a = 2.75$ nm) in a 2D optical lattice with period $d = 297.3$ nm (generated by a dye laser) for different values of the central density. We see that the
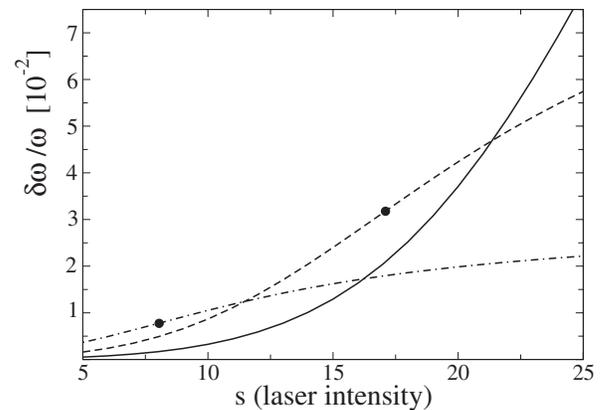

FIG. 2. Calculated frequency shift of the axial mode for a bosonic cloud of ^{23}Na atoms in a disc trap as a function of the laser intensity for different values of the central density $n(0) = 10^{12}$ cm^{-3} (solid line), 10^{13} cm^{-3} (dashed line), and 10^{14} cm^{-3} (dash-dotted line). The circles correspond to $x = 0.25$, when the chemical potential in the center of the trap is equal to the bandwidth [for $n(0) = 10^{12}$ cm^{-3} the 1D regime is achieved for larger values of s]. Parameters used: $a = 2.75$ nm; $d = 297.3$ nm.
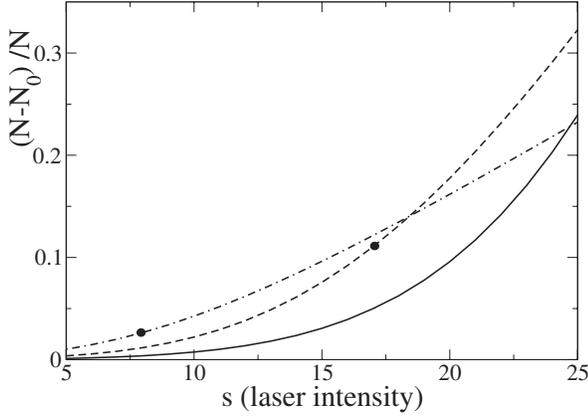
FIG. 3.   Calculated quantum depletion for a bosonic cloud of
^{23}Na atoms in a disc trap as a function of the laser intensity for
different values of the central density $n(0) = 10^{12}$ cm^{-3} (solid
line), 10^{13} cm^{-3} (dashed line), and 10^{14} cm^{-3} (dash-dotted
line). Parameters as in Fig. 2.

frequency shift can be of the order of a few percent for
values of s easily accessible in experiments.

It is interesting to compare the frequency shift with the
quantum depletion in the presence of the trap. Starting
from Eqs. (7) and (8), and inserting the external potential
via a local density approximation, we find

$$\frac{N - N_0}{N} = \frac{15\sqrt{2}}{8\pi} \sqrt{\frac{m\tilde{g}}{n(0)}} \frac{1}{d^2} Q\left(\frac{2t}{\tilde{g}n(0)}\right), \qquad (14)$$

where the function $Q(x)$ is defined as

$$Q(x) = \int_0^1 dr r^2 (1 - r^2)^{1/2} h\left(\frac{x}{1 - r^2}\right). \qquad (15)$$

For vanishing x, $Q(x)$ diverges logarithmically as $Q(x) = -0.26 - \pi \ln x / 16\sqrt{2}$, whereas in the 3D regime $x \gg 1$ we
find $Q(x) = 1/24\sqrt{2}x$, yielding the known result $(N - N_0)/N = (5\sqrt{\pi}m^*/8m)\sqrt{\tilde{a}^3 n(0)}$ [11]. In Fig. 3 we plot
the quantum depletion evaluated from Eq. (14) as a func-
tion of the laser intensity for the same parameters used in
Fig. 2. The comparison with Fig. 2 shows that the effects of
the lattice on the quantum depletion are larger than on the
frequency shifts [14]. However, one should recall that the
measurement of the collective frequencies can be obtained
with much higher precision.

Let us finally discuss the conditions of applicability of
our results. First, the effects of the trap are taken into
account via local density approximation. This requires
that the trapping frequencies $\omega_\perp$, ω_z are small compared
to the chemical potential μ and the bandwidth $8t$. In
particular, the condition $\omega_z \ll 8t$ ensures that the gas

oscillating along the tubes retains the 3D coherence.
Second, the mean-field value $\omega = \sqrt{3}\omega_z$ for the frequency
of the collective oscillation is valid only for a strongly
anisotropic trap $\omega_\perp / \sqrt{m^*} \ll \omega_z$. For a finite value of the
anisotropy, one should start from the more general formula
obtained in Ref. [13] and valid in the absence of the lattice.
We see from Eq. (9) that in the hydrodynamic theory the
lattice enters through the renormalization of the effective
mass $m \to m^*$ along the confined directions. From
Ref. [13] we then obtain $(\delta\omega/\omega)_{\text{ani}} = (m/9m^*)\omega_\perp^2/\omega_z^2$,
showing that the correction *decreases* by increasing the
laser intensity, being proportional to m/m^*.

In conclusions, our results show that the measurement of
the collective frequencies in the presence of 2D optical
lattices can provide an efficient tool to investigate beyond
mean field effects along the dimensional crossover.

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[14] The fact that the quantum depletion becomes larger and
larger as s increases does not necessarily invalidate the use
of Bogoliubov theory for the calculation of the frequency
shift. Even in the deep 1D regime, where the condensate is
fully depleted, the perturbative expansion (5) is still valid,
provided $mg_{1D}/\hbar^2 n_{1D} \ll 1$.