Bogoliubov speed of sound for a dilute Bose–Einstein condensate in a 3d optical lattice

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We point out that the velocity of propagation of sound wavepackets in a Bose–Einstein condensate filling a three-dimensional cubic optical lattice undergoes a maximum with increasing lattice depth. For a realistic choice of parameters, the maximum sound velocity in a lattice condensate can exceed the sound velocity in a homogeneous condensate with the same average density by 30%. The maximum falls into the superfluid regime, and should be observable under currently achievable laboratory conditions.

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There have been vigorous activities, and impressive achievements, concerning Bose–Einstein condensates in optical lattice potentials recently, both experimentally [1, 2, 3, 4, 5, 6] and theoretically [7, 8, 9, 10, 11, 12, 13, 14, 15], culminating in the observation of the quantum phase transition from a superfluid to a Mott insulator with a condensate of ^{87}Rb atoms [5].

On the theoretical side, substantial effort has been devoted to calculating the low-lying excitations of a condensate in an optical lattice, and thus the speed of sound, within the Bogoliubov theory [16, 17, 18]. In particular, it has been predicted that in a one-dimensional optical lattice the velocity of propagation of sound wavepackets decreases monotonically with increasing lattice depth [19, 20]. In this letter, we argue that the situation is different for condensates in three-dimensional lattices: In this case the velocity of sound undergoes a pronounced maximum when the lattice is made successively deeper, which falls into the superfluid regime, and should be observable under currently achievable experimental conditions.

We consider a 3d Bose–Einstein condensate subjected to a simple d-dimensional optical cosine lattice ($d = 1, 3$) of depth V_0,

$$V(\boldsymbol{r}) = \frac{V_0}{2} \sum_{i=1}^{d} \cos(2k_{\mathrm{L}} x_i) \; , \tag{1}$$

where $k_{\mathrm{L}} = 2\pi/\lambda$ denotes the wavenumber associated with the lattice-generating laser radiation of wavelength λ. For $d = 1$ we study the propagation of sound in the direction of the lattice, while assuming that the condensate remains homogeneous in the orthogonal plane. We also assume that the depth V_0 of the lattice be sufficiently deep so that only the lowest Bloch band needs to be taken into account.

The velocity of sound propagation in a Bose–Einstein condensate filling the lattice then is given by the standard expression [19, 20]

$$c = \sqrt{\frac{U}{m^*}} \; , \tag{2}$$

where m^* is the effective mass pertaining to the lowest band, and U is the inverse compressibility of the condensate in the lattice.

In principle, also the effective mass m^* appearing in eq. (2) does depend on the density of the condensate, and has to be determined by solving the Gross–Pitaevskii equation for the condensate in the lattice [7, 11, 13, 18]. This is particularly pertinent if one considers a 1d lattice filled with an effectively 1d condensate, strongly confined by restoring potentials orthogonal to the lattice direction, so that the transversal degrees of freedom are frozen out entirely. If then each lattice site carries a comparatively large number of particles, nonlinear effects due to the mean-field interaction play a decisive role. In contrast, we focus here on truly 3d condensates, with an average density N/V of presently achievable magnitude. Taking the moderate value $N/V = 10^{13}$ cm^{-1}, say, and a lattice constant $\lambda/2 = 426$ nm, one obtains an average occupancy of about 0.8 atoms per unit cell in a 3d lattice. Thus, we define the site occupancy N_s by writing

$$\frac{N}{V} = \frac{N_s}{(\lambda/2)^3} \; , \tag{3}$$

and consider values of N_s which are on the order of unity. In this case, the density dependence of m^* is negligible, as wittnessed by numerical calculations for $d = 1$ [19, 20], so that we obtain quite accurate predictions by invoking the effective mass, and the band structure, of the single-particle problem.

Moreover, for low site occupancies it is not necessary to solve the Bogoliubov–de Gennes equations in order to obtain the elementary excitations, but we may perform the Bogoliubov transformation directly on the basis of the single-particle Bloch waves $u_{\boldsymbol{k}}(\boldsymbol{r})$. We then find for the inverse compressibility the convenient expression

$$U = U_0 \frac{1}{\Omega} \int_{\text{unit cell}} \mathrm{d}^d\boldsymbol{r} \, |u_{\boldsymbol{0}}(\boldsymbol{r})|^4 \;, \tag{4}$$

where $\Omega = (\lambda/2)^d$ is the volume of the unit cell, and $u_{\boldsymbol{0}}(\boldsymbol{r})$ is the Bloch function corresponding to zero quasimomentum, normalized such that $\int \mathrm{d}^d\boldsymbol{r} \, |u_{\boldsymbol{0}}(\boldsymbol{r})|^2 = \Omega$, with the integral again extending over one unit cell. The factor

$$U_0 = \frac{4\pi a\hbar^2}{m} \frac{N}{V} \tag{5}$$

coincides with the customary interaction energy parameter characterizing a homogeneous Bose–Einstein condensate with a density of N particles per volume V, which consists of atoms with (bare) mass m possessing the s-wave scattering length a.

One can intuitively capture the physics expressed by eq. (4) by imagining an initially homogeneous 3d condensate within which a d-dimensional optical lattice is errected adiabatically; the particles then gradually get concentrated around the local minima of the lattice potential. This is described by the fact that the Bloch function $u_{\boldsymbol{0}}(\boldsymbol{r})$ develops a maximum within each well; the integral over the fourth power of this function, taken over one unit cell, increases slowly with increasing lattice depth. Obviously, the density reached at the potential minima becomes the higher, the larger the lattice dimension d; as a consequence, the compressibility U^{-1} of the gas within the lattice also exhibits a significant d-dependence. It is this feature which translates itself into a dependence of the velocity of sound on the lattice depth which is markedly d-dependent.

Before presenting numerical data for the velocity of sound in one- and three-dimensional lattices, it is useful to consider the analytically tractable limiting case of a deep optical lattice. Introducing the single-photon recoil energy $E_{\mathrm{R}} = \hbar^2 k_{\mathrm{L}}^2/(2m)$, and the associated recoil velocity $v_{\mathrm{R}} = \hbar k_{\mathrm{L}}/m$, we rewrite eq. (2) in terms of convenient dimensionless ratios, obtaining

$$\frac{c}{v_{\mathrm{R}}} = \sqrt{\frac{U}{2E_{\mathrm{R}}} \frac{m}{m^*}} \;. \tag{6}$$

Expanding the lattice potential quadratically around the minima of the cosine wells, the Bloch function $u_{\boldsymbol{0}}(\boldsymbol{r})$ can be approximated by a superposition of the groundstate wave functions of the corresponding harmonic oscillators, if the lattice is sufficiently deep. This harmonic approximation immediately leads to the estimate

$$\frac{1}{\Omega} \int_{\text{unit cell}} \mathrm{d}^d\boldsymbol{r} \, |u_{\boldsymbol{0}}(\boldsymbol{r})|^4 \sim \left(\frac{\pi^2}{4} \frac{V_0}{E_{\mathrm{R}}}\right)^{d/4} \qquad \text{for } V_0/E_{\mathrm{R}} \gg 1 \;, \tag{7}$$

where here and in the following the "$\sim$"-sign means asymptotic equality. By comparison with exact numerical data, we infer that for $d = 1$ and $V_0/E_{\mathrm{R}} = 10$ this approximation is about 12% too high; the error decreases to 5% when $V_0/E_{\mathrm{R}} = 25$.

This estimate now allows us to specify the condition for the validity of our approach more precisely: Since the gap between the lowest two single-particle Bloch bands amounts to $V_0/2$, and that gap has to be large in comparison with the interaction energy per particle in order to justify the restriction to the lowest band, we require $V_0 \gg U$. Using the above approximation in eq. (4) for U, together with the expression (3) for the density, this gives for $d = 3$ the condition

$$\left(\frac{V_0}{E_{\mathrm{R}}}\right)^{1/4} \gg 4\sqrt{2\pi} \, N_s \frac{a}{\lambda} \;. \tag{8}$$

Since the ratio a/λ of the s-wave scattering length a to the laser wavelength λ usually is of the order of $1/100$, this condition indeed limits the validity of our reasoning to occupancies N_s of a few atoms per site, a "site" corresponding to the volume $(\lambda/2)^3$.

The theory of the Mathieu equation now allows one to state an approximate expression for the width Δ of the lowest energy band when the cosine lattice is sufficiently deep, namely [21, 23]

$$\frac{\Delta}{E_{\mathrm{R}}} \sim \frac{16}{\sqrt{\pi}} \left(\frac{V_0}{E_{\mathrm{R}}}\right)^{3/4} \exp\left(-2\sqrt{V_0/E_{\mathrm{R}}}\right) \;. \tag{9}$$

For $V_0/E_R = 10$, this estimate still is about 18.5% too high; the error becomes less than 5% only if $V_0/E_R > 90$. Since a quadratic expansion of the tight-binding cosine energy dispersion relation readily connects the band width with the effective mass,

$$\frac{m^*}{m} = \frac{4}{\pi^2} \frac{1}{\Delta/E_R} \ , \tag{10}$$

we obtain

$$\frac{m^*}{m} \sim \frac{1}{4\pi^{3/2}} \left(\frac{V_0}{E_R}\right)^{-3/4} \exp\left(2\sqrt{V_0/E_R}\right) \qquad \text{for } V_0/E_R \gg 1 \ . \tag{11}$$

Combining now the deep-lattice estimates (7) and (11), the velocity of sound (6) takes the form

$$\frac{c^{d=1}}{v_R} \sim 2^{1/4} \pi \sqrt{\frac{U_0}{E_R}} \left(\frac{V_0}{E_R}\right)^{1/2} \exp\left(-\sqrt{V_0/E_R}\right) \tag{12}$$

for $d = 1$, while for $d = 3$ we find

$$\frac{c^{d=3}}{v_R} \sim \frac{\pi^{3/2}}{2^{1/4}} \sqrt{\frac{U_0}{E_R}} \left(\frac{V_0}{E_R}\right)^{3/4} \exp\left(-\sqrt{V_0/E_R}\right) \ , \tag{13}$$

assuming $V_0/E_R \gg 1$ in both cases. The exponential decrease of these velocities with increasing lattice depth is due to the increase of the effective mass (11), or, equivalently, the reduction of the tunneling contact between the wells, while the different exponents appearing in the prefactors can be traced to the d-dependent inverse compressibilities (4).

In needs to be kept in mind, however, that when the lattice depth V_0 exceeds a critical magnitude, the transition from the superfluid to the Mott insulator state occurs [5, 8, 22, 23]. Since the Bogoliubov theory treats the interaction only approximately, it is incapable of describing large depletions of the condensate, and thus does not incorporate the transition [16]. Hence, the Bogoliubov speed of sound (2), and the above estimates, are meaningful only in the superfluid regime, sufficiently remote from the transition point. Within the tight-binding approximation, and assuming unit occupancy $N_s = 1$, in a three-dimensional lattice the transition takes place if the ratio of the on-site interaction energy per particle,

$$\widetilde{U} = \frac{4\pi a \hbar^2}{m} \int d^3 \boldsymbol{r} \, |w(\boldsymbol{r})|^4 \ , \tag{14}$$

and the hopping matrix element $\Delta/4$ adopts the critical value

$$\left(\frac{4\widetilde{U}}{\Delta}\right)_c \approx z \times 5.8 \ , \tag{15}$$

where $z = 6$ is the number of nearest neighbours of each site. (For high N_s, the critical ratio approaches $4N_s z$ [23].) The function $w(\boldsymbol{r})$ appearing in eq. (14) is the Wannier function for the lowest band. Approximating this Wannier function once again by the groundstate wave function of the harmonic oscillator corresponding to a quadratically approximated cosine well [24], we find

$$\frac{\widetilde{U}}{E_R} \sim 4\sqrt{2\pi} \frac{a}{\lambda} \left(\frac{V_0}{E_R}\right)^{3/4} \ . \tag{16}$$

In conjunction with the approximate relation (9) for the band width, the criterion (15) then allows us to estimate the critical lattice depth for $d = 3$ as

$$\frac{V_c}{E_R} \approx \frac{1}{4} \ln^2 \left(7.83 \frac{\lambda}{a}\right) \ . \tag{17}$$

Actually, this simple estimate appears to be quite reliable: Considering ^{87}Rb atoms, one has an s wave scattering length of $a = 6$ nm. Choosing $\lambda = 852$ nm then gives $V_c/E_R \approx 12.3$, in perfect agreement with what has been observed in the experiment [5].

In order to obtain numerical data for the speed of sound which are not restricted to the deep-lattice regime, we calculate the exact Bloch waves for the cosine lattice numerically and perform the Bogoliubov transformation,
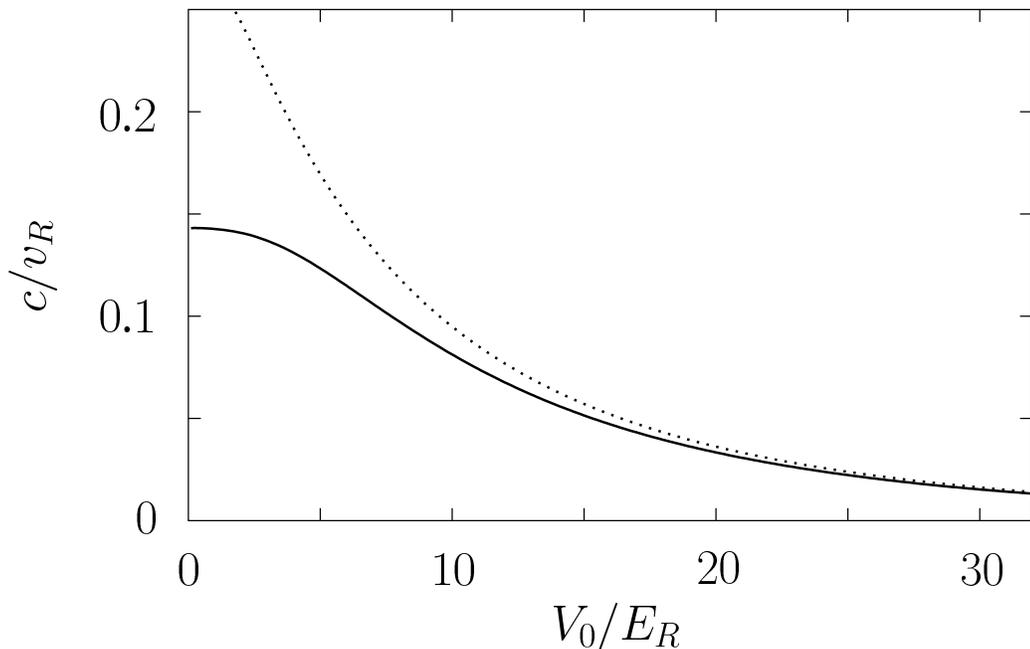
FIG. 1: Velocity of sound for a dilute Bose–Einstein condensate with $U_0/E_R = 0.036$ in a 1d optical lattice, as function of the lattice depth. The full line is the result of the Bogoliubov theory, evaluated numerically; the dotted line indicates the asymptotic prediction (12).

assuming the lowest Bloch state $u_0(\boldsymbol{r})$ to be macroscopically occupied; the speed of sound then is extracted directly from the slope of the quasiparticle energies $\varepsilon(k)$ for low wavenumbers k. Figure 1 shows the result for $d = 1$, as function of the lattice depth, for $U_0/E_R = 0.036$, as corresponding, according to eq. (5), to the Rubidium data $a = 6$ nm, $\lambda = 852$ nm, and $N_s = 1$. Comparison with the deep-lattice formula (12) shows that this estimate describes the numerical data quite well for $V_0/E_R > 20$. Here the speed of sound decreases monotonically with increasing lattice depth; the perfect agreement of our numerically calculated curve with the ones obtained before by Krämer $et\ al.$ [19], and by Menotti $et\ al.$ [20], clearly underlines the correctness of our reasoning.

The corresponding data for $d = 3$ are displayed in fig. 2. Now the numerical data for comparatively shallow lattices, for which the estimate (13) does not apply, show a well-developed maximum at $V_0/E_R \approx 6.1$, the speed of sound in a lattice of this depth being roughly 30% higher than in a homogeneous condensate with the same average density. Since the superfluid/Mott insulator-transition occurs, for the parameters considered, only when $V_0/E_R \approx 12.3$, as discussed above, this maximum falls well into the superfluid regime, where the simple Bogoliubov approach is still reliable. (For $d = 2$, one finds a rather weak maximum at an even lower V_0/E_R.)

The appearance of a pronounced maximum of the velocity of sound wavepackets reflects the competition between the slowly decreasing compressibility U^{-1}, and the exponentially increasing effective mass m^*, with increasing lattice depth. For $d = 1$, the decrease of compressibility is so weak that the increasing effective mass wins this competition right from the outset, resulting in a monotonically decreasing speed of sound. However, for $d = 3$ the stronger decrease of compressibility, resulting from the enhanced concentration of the condensate at the lattice sites, can over-compensate the increase of m^* at least in shallow lattices, giving rise to a substantial enhancement of the speed of sound before the increasing effective mass again diminishes that speed when the lattice is made deeper. An experimental observation of this maximum, which should be possible under presently accessible laboratory conditions, would constitute an important confirmation of our present understanding of the dynamics of Bose–Einstein condensates in optical lattices.
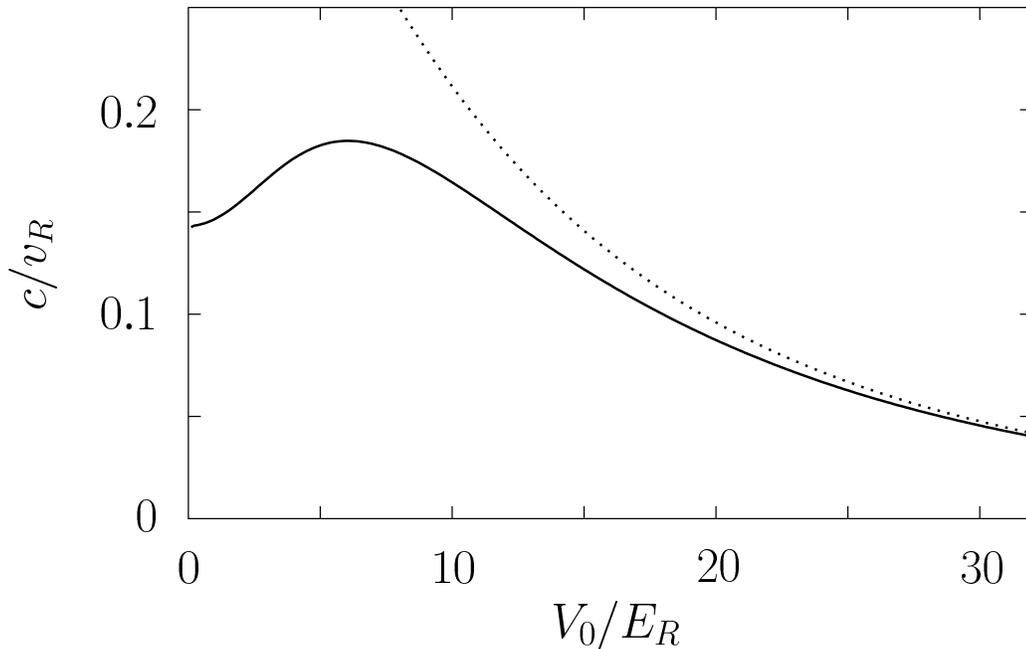
FIG. 2: Velocity of sound for a dilute Bose–Einstein condensate with $U_0/E_R = 0.036$ in a 3d optical lattice, as function of the lattice depth. The full line is the result of the Bogoliubov theory, evaluated numerically; the dotted line indicates the asymptotic prediction (13). The Mott insulator state, for which the Bogoliubov theory does not apply, occurs for values of V_0/E_R higher than about 12.3. The maximum of the velocity of sound lies at $V_0/E_R \approx 6.1$, well in the superfluid regime.

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