Dynamic structure factor of a Bose-Einstein condensate in a one-dimensional optical lattice

C. Menotti,[1,2] M. Krämer,[1] L. Pitaevskii,[1,3] and S. Stringari[1]
[1]*Dipartimento di Fisica, Università di Trento and BEC-INFM, I-38050 Povo, Italy*
[2]*Dipartimento di Matematica e Fisica, Università Cattolica del Sacro Cuore, I-25121 Brescia, Italy*
[3]*Kapitza Institute for Physical Problems, 117334 Moscow, Russia*
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We study the effect of a one-dimensional periodic potential on the dynamic structure factor of an interacting Bose-Einstein condensate at zero temperature. We show that, due to phononic correlations, the excitation strength toward the first band develops a typical oscillating behavior as a function of the momentum transfer, and vanishes at even multiples of the Bragg momentum. The effects of interactions on the static structure factor are found to be significantly amplified by the presence of the optical potential. Our predictions can be tested in stimulated photon scattering experiments.

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When a Bose-Einstein condensate is loaded into an optical lattice, its properties change in a very marked way [1]. For deep potential wells, it even happens that the coherence of the sample is lost and one observes the transition to the Mott-insulator phase [2,3]. Interesting phenomena also occur for low optical potential depth. For instance, Bloch oscillations [4], tunneling effects [5–7], and swallowtail features of the band structure [8] can be investigated in this regime. In one-dimensional (1D) optical lattices, the transition to the insulator phase is expected to take place for very large intensities of the optical lattice, so that there is a very extended range of parameters where the gas can be described as a fully coherent system.

In this paper, we study the elementary excitations of an interacting Bose gas in the presence of a periodic potential and discuss how these states can be excited via inelastic processes using, for example, Bragg spectroscopy [9,10]. To this purpose we develop the formalism of the dynamic structure factor, a quantity directly related to the linear response of the system.

We will restrict ourselves to the case of a system in the presence of a one-dimensional optical potential

$$V(z)=sE_R\sin^2\left(\frac{\pi z}{d}\right) \tag{1}$$

created by two counterpropagating laser beams. In Eq. (1), d is the lattice spacing and s is a dimensionless parameter which denotes the intensity of the laser in units of the recoil energy $E_R=q_B^2/2m$. Here $q_B=\hbar\pi/d$ is the Bragg momentum denoting the boundary of the first Brillouin zone and m is the atomic mass. The inclusion of an additional harmonic potential produced, for example, by magnetic trapping does not modify the excitation spectrum in a profound way, unless the wavelength of the excitation is comparable with the size of the sample. Along the tranverse directions we assume uniform confinement, so that the 3D Gross-Pitaevkii (GP) equation for the ground state order parameter $\varphi(z)$ takes the 1D form

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}+sE_R\sin^2\left(\frac{\pi z}{d}\right)+gnd|\varphi(z)|^2\right]\varphi(z)=\mu\varphi(z), \tag{2}$$

where n is the *average* 3D density and the order parameter φ is normalized according to $\int_{-d/2}^{d/2}|\varphi(z)|^2dz=1$. As usual, $g=4\pi\hbar^2a/m$ is the interaction coupling constant fixed by the scattering length a.

The elementary excitations correspond to solutions of the linearized time-dependent GP equation and are described by the Bogoliubov equations

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}+sE_R\sin^2\left(\frac{\pi z}{d}\right)-\mu+2gnd|\varphi|^2\right]u_{jq}+gnd\varphi^2v_{jq}=\hbar\omega_j(q)u_{jq}, \tag{3}$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}+sE_R\sin^2\left(\frac{\pi z}{d}\right)-\mu+2gnd|\varphi|^2\right]v_{jq}+gnd\varphi^{*2}u_{jq}=-\hbar\omega_j(q)v_{jq}, \tag{4}$$

where φ is the ground state solution of Eq. (2) and the amplitudes u_{jq} and v_{jq} satisfy the normalization condition $\int_{-d/2}^{d/2}[|u_{jq}(z)|^2-|v_{jq}(z)|^2]dz=1$. The solutions $u_{jq}(z)$ and $v_{jq}(z)$ are Bloch waves: $u_{jq}(z)=\exp(iqz/\hbar)\tilde{u}_{jq}(z)$ where $\tilde{u}_{jq}$ is periodic in space with period d, and analogously for v_{jq}. For each value of the quasimomentum q, Eqs. (3) and (4) provide an infinite set of solutions $\omega_j(q)$, forming a band structure labeled with j ("Bogoliubov bands"). Due to the periodicity of the problem, the solutions of Eqs. (3) and (4) with q restricted to the first Brillouin zone and j varying over all the bands exhaust the elementary excitations of the system. Still, it is often convenient to consider values of q outside the first Brillouin zone and to treat the energy spectrum and the functions u_{jq} and v_{jq} as periodic in quasimomentum space with period $2q_B$ (see Fig. 1). The intensity s of the optical potential and ratio gn/E_R between the interaction and the recoil energy are the relevant dimensionless parameters in terms of which we will discuss the physical behavior of the system. Numerical solutions of Eqs. (3) and (4) in the presence of a periodic potential were, for example, obtained in [11].

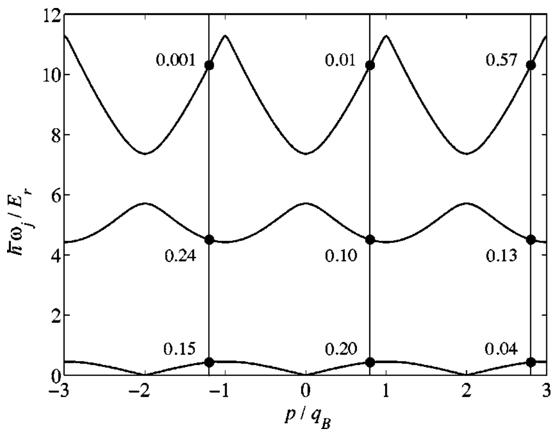

FIG. 1. Bogoliubov bands for $s=10$ and $gn=0.5E_R$; excitation strengths Z_j toward the states in the first three bands for $p=-1.2q_B$, $p=0.8q_B$, and $p=2.8q_B$.

The capability of the system to respond to an excitation probe transferring momentum p and energy $\hbar\omega$ is described by the dynamic structure factor. In the presence of a periodic potential the dynamic structure factor takes the form

$$S(p,\omega)=\sum_j Z_j(p)\,\delta(\omega-\omega_j(p)), \tag{5}$$

where $Z_j(p)$ are the excitation strengths relative to the jth band [see Eq. (11) below] and $\hbar\omega_j(p)$ are the corresponding excitation energies, defined by the solutions of Eqs. (3) and (4). Note that p, here assumed to be along the optical lattice (z axis), is not restricted to the first Brillouin zone, being the momentum transferred by the external probe. In this respect, it is important to point out that, while the excitation energies $\hbar\omega_j(p)$ are periodic as a function of p, this is not true for the excitation strengths Z_j.

The dynamic structure factor satisfies important sum rules. The integral of the dynamic structure factor provides the static structure factor (non-energy-weighted sum rule)

$$S(p)=\int S(p,\omega)d\omega. \tag{6}$$

As we will see later, $S(p)$ is strongly affected by the combined presence of two-body interactions and the optical lattice.

A second important sum rule obeyed by the dynamic structure factor is the model-independent f-sum rule [18]

$$\int \hbar\omega S(p,\omega)d\omega=\frac{p^2}{2m}. \tag{7}$$

Another important sum rule is the compressibility sum rule (inverse-energy-weighted sum rule)

$$\int \frac{S(p,\omega)}{\hbar\omega}d\omega\bigg|_{p\to 0}=\frac{\kappa}{2}, \tag{8}$$

where $\kappa=[n(\partial\mu/\partial n)]^{-1}$ is the thermodynamic compressibility. The density dependence of the chemical potential, and hence κ, can be obtained by solving the GP equation (2) [12]. The compressibility κ is naturally expressed in terms of the sound velocity c, characterizing the low q phononic behavior of the dispersion law in the lowest band ($\hbar\omega=cq$), through the relation

$$\kappa=\frac{1}{m^*c^2}, \tag{9}$$

where the effective mass m^* differs from the bare mass because the Hamiltonian is not translationally invariant. The effective mass in the presence of the external potential (1) has recently been calculated in [13].

In a uniform Bose gas, the sum (5) is exhausted by a single mode with energy $\hbar\omega_B(p)=\sqrt{p^2/2m(p^2/2m+2gn)}$. In this case the static structure factor obeys the Feynman relation

$$S_B(p)=\frac{p^2}{2m\hbar\omega_B(p)}, \tag{10}$$

where we have used the f-sum rule (7). For $p\to 0$ the static structure factor (10) behaves like $|p|/2mc_B$, while the compressibility sum rule (8) becomes $1/2mc_B^2$, where $c_B=\sqrt{gn/m}$ is the Bogoliubov sound velocity. The suppression of $S_B(p)$ at small momenta is a direct consequence of the phononic correlations. For large momenta, instead, the static structure factor (10) approaches unity (see the dotted lines in Fig. 2). Notice that in the absence of two-body interactions $S(p)=1$ for any value of p.

In the presence of the optical lattice the behavior of the dynamic structure factor changes in a drastic way. In particular, for a given value of momentum transfer p, it is possible to excite several states, corresponding to different bands [see Eq. (5) and Fig. 1]. An important consequence is that on one hand it is possible to excite high energy states with small values of p, and on the other hand one can excite low energy states, belonging to the lowest band, also with high momenta p outside the first Brillouin zone. This behavior introduces additional possibilities in Bragg spectroscopy experiments.

In general, the dynamic structure factor has to be calculated numerically. Starting from the solution of Eqs. (3) and (4), the excitation strengths Z_j can be evaluated using the standard prescription (see, for example, [14])

$$Z_j(p)=\left|\int_{-d/2}^{d/2}[u_{jq}^*(z)+v_{jq}^*(z)]e^{ipz/\hbar}\varphi(z)dz\right|^2, \tag{11}$$

where q belongs to the first Brillouin zone and is fixed by the relation $q=p+2\ell q_B$ with ℓ integer. This equation shows that, by solving Eqs. (3) and (4) within the first Brillouin zone, one can calculate the strength $Z_j(p)$ for values of p outside the first Brillouin zone also. In Figs. 2(a) and 2(b), we show our results for two different choices of the interaction at $s=10$.

Let us first discuss the dynamic structure factor in the low energy region and in particular the behavior of the contribution $Z_1(p)$ arising from the first band (dashed line). We find that $Z_1(p)$ exhibits characteristic oscillations whose ampli-

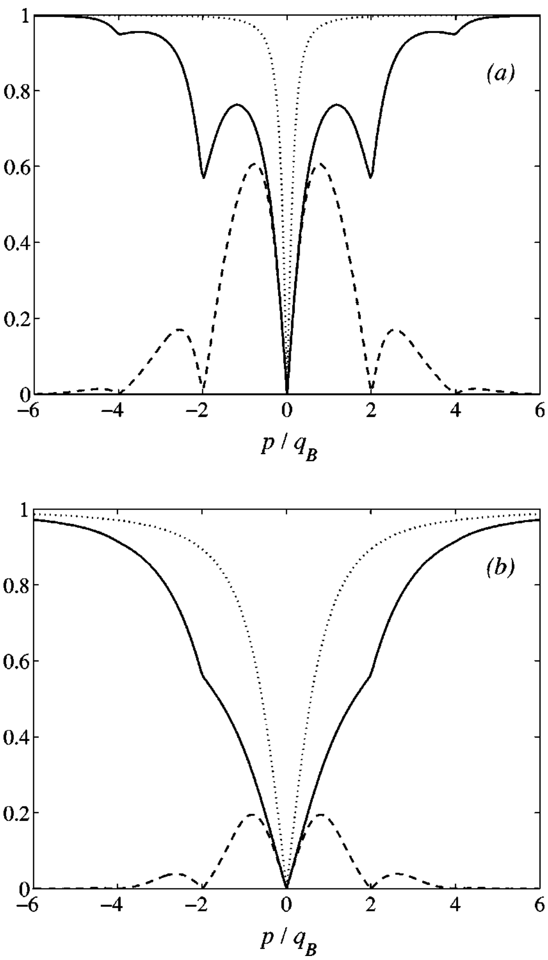

FIG. 2. Static structure factor (full line), $Z_1(p)$ (dashed line) for $s=10$, and static structure factor in the uniform gas ($s=0$, dotted line); for $gn=0.02E_R$ (a) and $gn=0.5E_R$ (b).

tude is suppressed at large p. The zeros of $Z_1(p)$ at $p=2\ell q_B$(ℓ integer) directly reflect the phonon behavior of the excitation spectrum, which vanishes at the same values (see Fig. 1).

The behavior of $Z_1(p)$ can be studied analytically in the large s limit where the tight binding approximation applies. In this limit one can approximate the solutions of Eqs. (3) and (4) in the lowest band by

$$u_q(z)=U_q\sum_k e^{iqkd/\hbar}f(z-kd), \tag{12}$$

and analogously for $v_q(z)$, where $f(z)$ is a function localized near the bottom of the optical potential V at $z=0$, and k labels the potential wells. Within this approximation the function f also characterizes the ground state order parameter, which reads $\varphi(z)=\Sigma_k f(z-kd)$.

In the tight binding approximation the dispersion law of the lowest band takes the Bogoliubov-like form [15]

$$\hbar\omega(p)=\sqrt{\varepsilon(p)[\varepsilon(p)+2\kappa^{-1}]}, \tag{13}$$

where

$$\varepsilon(p)=2\,\delta\sin^2\left(\frac{pd}{2\hbar}\right). \tag{14}$$

In the above equations, $\varepsilon(p)$ is the lowest Bloch band, describing the energy per particle of a condensate with quasimomentum p, δ being the tunneling rate of particles between two consecutive wells. The tunneling rate is related to the effective mass entering the compressibility sum rule (8),(9) by $\delta=2mE_R/\pi^2m^*$ and decreases on increasing the laser intensity s. The parameter κ is the compressibility of the gas as emerges from the low momentum behavior of the dispersion law (13): $\hbar\omega=\sqrt{\kappa^{-1}/m^*}p$. In the tight binding limit, one finds $\kappa^{-1}=gnd\int_{-d/2}^{d/2}f^4(z)dz$ [16].

By approximating the function $f(z)$ with the Gaussian $f(z)=\exp[-z^2/2\sigma^2]/(\pi^{1/4}\sqrt{\sigma})$, one finds, after some straightforward algebra, the result

$$Z_1(p)=\frac{\varepsilon(p)}{\hbar\omega(p)}\exp\left(-\frac{\pi^2\sigma^2p^2}{2d^2q_B^2}\right) \tag{15}$$

for the strength relative to the first band, where the width σ can be calculated numerically by minimization of the ground state energy and behaves like $\sigma\sim s^{-1/4}d/\pi$ for $s\gg1$. Equation (15) reproduces with good accuracy the numerical results obtained by solving the Bogoliubov equations for relatively large values of s. It accounts for both the suppression of the strength at large p through the Gaussian term, and the oscillating behavior through the Feynman-like term $\varepsilon(p)/\hbar\omega(p)$. The strength Z_1 has a maximum close to the edge of the first Brillouin zone, where it takes approximately the value $Z_1(q_B)\approx\sqrt{\kappa\delta/(\kappa\delta+1)}$. This simple expression shows that Z_1 is quenched both by increasing interactions $(\kappa\to0)$ and by increasing the optical potential $(\delta\to0)$. In the cases of Figs. 2(a) and 2(b) one has $\kappa\delta=0.95$ and 0.056, respectively. In the noninteracting case $(\kappa^{-1}=0)$ one has $\varepsilon(p)=\hbar\omega(p)$ and the strength (15) reduces to $Z_1(p)=\exp(-\pi^2\sigma^2p^2/2d^2q_B^2)$. The comparison then clearly shows that the oscillating behavior of $Z_1(p)$ as well as its quenching at large s are a direct consequence of two-body interactions. On the other hand, two-body interactions scarcely affect the strengths toward the higher bands, provided $gn\ll\sqrt{s}E_R$.

The quantity $Z_1(p)$ could be measured in Bragg spectroscopy experiments by tuning the momentum and the energy transferred by the scattering photon to the values of p and $\hbar\omega$ corresponding to the first Bogoliubov band. In order to detect a sizable signal at large p and to point out the corresponding oscillating behavior of $Z_1(p)$ (see Fig. 2), the intensity s of the optical potential should be neither too small nor too large. In fact, for $s\to0$ the strength to the lowest band becomes weaker and weaker if p is outside the first Brillouin zone. For large s the strength is instead quenched for all values of p because of the presence of two-body interactions.

In Fig. 2 we also report the results for the static structure factor (full line) corresponding to the sum $S(p)=\Sigma_jZ_j(p)$. One finds that for weak interactions [Fig. 2(a)] the static structure factor also exhibits characteristic oscillations, reflecting the contribution from the first band. This effect is less pronounced for larger values of gn [Fig. 2(b)] due to the quenching of $Z_1(p)$. In both cases one observes an important difference with respect to the behavior of $S(p)$ in the uniform gas (10) (dotted lines in Fig. 2).

The behavior of $S(p)$ at small momenta can be described exactly using sum-rule arguments. In fact, phonons exhaust both the non-energy- and inverse-energy-weighted sum rules when $p \to 0$, high energy bands giving rise to contributions of order p^2. As a consequence, high energy bands contribute to the *f*-sum rule (7) but cannot affect the low *p* behavior of the non-energy-weighted moment (6), which behaves like $|p|$, nor the inverse-energy-weighted moment (8), which approaches a constant value when $p \to 0$. The result is that in the presence of two-body interactions the low *p* behavior of the static structure factor is entirely determined by phonon correlations and behaves like

$$S(p) \sim \frac{|p|}{2m^*c}, \tag{16}$$

for $|p| \to 0$, consistently with the phononic dispersion law and Eqs. (8) and (9) for the compressibility sum rule. It is worth noticing that the result (16) holds for any value of *s* and gn. In the absence of an optical lattice one has $m^* = m$ and *c* coincides with the Bogoliubov sound velocity c_B. Since one can write $m^* c = \sqrt{m^* \kappa^{-1}}$ and both m^* and κ^{-1} increase with *s*, one finds that the presence of the lattice results in a suppression of the static structure factor at low values of *p*, as clearly shown in Fig. 2.

The presence of the optical potential may introduce phase fluctuations which reduce the degree of coherence of the sample. The amount of such fluctuations depends explicitly on the geometry of the system. For example, if the radial size is much smaller than the axial one, the fluctuations are determined by the 1D nature of the sample. In this case, at $T = 0$, the off-diagonal one-body density exhibits the power law decay $n^{(1)}(|\mathbf{r}-\mathbf{r}'|) \to |\mathbf{r}-\mathbf{r}'|^{-\nu}$ at large distances. For a superfluid, the value of ν is fixed by the hydrodynamic fluctuations of the phase and is given by the expression $\nu = m^* c d/(2\pi\hbar N_0)$ [19], where N_0 is the number of atoms per site. One can easily check that, unless N_0 is of the order of unity or m^* is extremely large, the value of ν always remains very small. Hence, coherence survives at large distances and the application of the Bogoliubov theory is justified.

Let us conclude by recalling that in Bragg scattering experiments one actually measures the imaginary part of the response function χ rather than the dynamic structure factor. The two quantities are related by the equation $\mathrm{Im}(\chi) = -\pi[S(p,\omega) - S(-p,-\omega)]$. The subtraction between the two terms can also be crucial at low temperatures. Actually, due to thermal excitation of phonons, the dynamic structure factor exhibits a strong temperature dependence when $\hbar\omega < k_B T$, even if *T* is much smaller than the critical temperature for Bose-Einstein condensation. However, the difference $S(p,\omega) - S(-p,-\omega)$ cancels out most of this temperature dependence so that the measurement of $\mathrm{Im}(\chi)$ provides reliable information on the zero-temperature behavior of the dynamic structure factor [20].

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[1] J. H. Denschlag, J. E. Simsarian, H. Haffner, C. McKenzie, A. Browaeys, D. Cho, K. Helmerson, S. L. Rolston, and W. D. Phillips, J. Phys. B **35**, 3095 (2002).
[2] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).
[3] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature (London) **415**, 39 (2002).
[4] O. Morsch, J. H. Muller, M. Cristiani, D. Ciampini, and E. Arimondo, Phys. Rev. Lett. **87**, 140402 (2001).
[5] B. P. Anderson and M. A. Kasevich, Science (Washington, DC, U.S.) **282**, 1686 (1998).
[6] A. Trombettoni and A. Smerzi, Phys. Rev. Lett. **86**, 2353 (2001).
[7] F. S. Cataliotti, S. Burger, C. Fort, P. Maddaloni, F. Minardi, A. Trombettoni, A. Smerzi, and M. Inguscio, Science (Washington, DC, U.S.) **293**, 843 (2001).
[8] B. Wu and Q. Niu, Phys. Rev. A **61**, 023402 (2000); B. Wu, R. B. Diener, and Q. Niu, *ibid.* **65**, 025601 (2002); D. Diakonov, L. M. Jensen, C. J. Pethick, and H. Smith, *ibid.* **66**, 013604 (2002); M. Machholm, C. J. Pethick, and H. Smith, Phys. Rev. A (to be published), e-print cond-mat/0301012.
[9] J. M. Vogels, K. Xu, C. Raman, J. R. Abo-Shaeer, and W. Ketterle, Phys. Rev. Lett. **88**, 060402 (2002).
[10] J. Steinhauer, R. Ozeri, N. Katz, and N. Davidson, Phys. Rev. Lett. **88**, 120407 (2002).
[11] K. Berg-Sorensen and K. Molmer, Phys. Rev. A **58**, 1480 (1998); see also M. L. Chiofalo, M. Polini, and M. P. Tosi, Eur. Phys. J. D **11**, 371 (2000).
[12] M. Krämer, C. Menotti, L. Pitaevskii, and S. Stringari (unpublished).
[13] M. Krämer, L. Pitaevskii, and S. Stringari, Phys. Rev. Lett. **88**, 180404 (2002).
[14] W.-C. Wu and A. Griffin, Phys. Rev. A **54**, 4204 (1996).
[15] J. Javanainen, Phys. Rev. A **60**, 4902 (1999).
[16] In deriving Eq. (13) we have assumed $n\partial\delta/\partial n \ll \kappa^{-1}$. The most general form of the dispersion law, whose derivation goes beyond the scope of this paper [12,17], does not affect the conclusions of the present discussion.
[17] A. Smerzi and A. Trombettoni, Chaos (to be published).
[18] D. Pines and P. Noziéres, *The Theory of Quantum Liquids* (Benjamin, New York, 1966), Vol. I.
[19] L. Pitaevskii and S. Stringari, *Bose-Einstein Condensation* (Oxford University Press, Oxford, 2003).
[20] F. Zambelli, L. Pitaevskii, D. M. Stamper-Kurn, and S. Stringari, Phys. Rev. A **61**, 063608 (2000).