Dynamic structure factor of a Bose Einstein condensate in a 1D optical lattice

1,2C. Menotti, 1M. Krämer, 1,3L. Pitaevskii and 1S. Stringari

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, ul. Kosygina 2, 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 towards the first band develops a typical oscillating behaviour 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.

When a Bose-Einstein condensate is loaded into an optical lattice, its properties change in a very strong 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 occur also for low optical potential depth, for instance Bloch oscillations [4] and tunneling effects [5–7] can be investigated in this regime. In 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 Letter, 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 [8,9]. 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 1-dimensional optical potential

\[ V(z) = s E_R \sin^2 \left( \frac{\pi z}{d} \right) \]

for the ground state order parameter \( \varphi(z) \) takes the 1D form

\[
\left[ \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + s E_R \sin^2 \left( \frac{\pi z}{d} \right) + gn d |\varphi(z)|^2 \right] \varphi(z) = \mu \varphi(z), \quad (2)
\]

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

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

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

\[
\left[ \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + s E_R \sin^2 \left( \frac{\pi z}{d} \right) - \mu + 2 gn d |\varphi|^2 \right] v_{jq} + gn d \varphi^2 u_{jq} = -\hbar \omega_j(q) v_{jq}, \quad (4)
\]

where \( \varphi \) is the ground state solution of Eq.(2) and the amplitudes \( u_{jq} \) and \( v_{jq} \) satisfy the normalization condition \( \int \frac{d^3q}{(2\pi)^3} [u_{jq}(z)]^2 = 1 \). 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 quasi-momentum \( q \), Eqs.(3,4) provide an infinite set of solutions \( \omega_j(q) \), forming a band structure labelled with \( j \) (“Bogoliubov bands”). Due to the periodicity of the problem, the solutions of Eqs.(3,4) 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 quasi-momentum space with period \( 2QB \) (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 behaviour of the system. First numerical solutions of Eqs.(3,4) in the presence of a periodic potential were obtained in [10].

The capability of the system to respond to an excitation probe transferring momentum \( p \) and energy \( \hbar \omega \) is
As we will see later the dynamic structure factor obeys the Feynman relation

\[ S(p,\omega) = \int S(p,\omega)d\omega. \]

(5)

where \( Z_j(p) \) are the excitation strengths relative to the \( j^{th} \) band (see Eq.(11) below) and \( \hbar \omega_j(p) \) are the corresponding excitation energies, defined by the solutions of Eqs.(3,4). 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)

\[ S(p) = \int S(p,\omega)d\omega. \]

(6)

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

A second important sum-rule obeyed by the dynamic structure factor is the model independent \( f \)-sum rule

\[ \int \hbar \omega S(p,\omega)d\omega = \frac{p^2}{2m}. \]

(7)

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

\[ \frac{1}{\hbar \omega} \int S(p,\omega)d\omega \bigg|_{p \to 0} = \frac{\kappa}{2}, \]

(8)

where \( \kappa = [n(\partial^2\varphi/\partial n)]^{-1} \) is the thermodynamic compressibility. The density dependence of the chemical potential, and hence \( \kappa \), can be obtained by solving the GP equation (2) [11]. The compressibility \( \kappa \) is naturally expressed in terms of the sound velocity \( c \), characterizing the low \( q \) phononic behaviour of the dispersion law \( (\hbar \omega = cq) \), through the relation

\[ \kappa = \frac{1}{m^* c^2}, \]

(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 been recently calculated in [12].

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

\[ S_B(p) = \frac{p^2}{2m^* \hbar \omega_B(p)} \]

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 dotted lines in Figs.2). Notice that in the absence of two-body interactions, \( S(p) = 1 \) for any value of \( p \).
values of $p$ outside the first Brillouin zone. In Figs. 2(a,b), we show our results for two different choices of the interaction at $s = 10$.

\[ u_q(z) = U_q \sum_k e^{i q k d / \hbar} f(z - k d) \]  

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 $\varphi(z) = \sum_k f(z - k d)$.

In the tight binding approximation the dispersion law of the lowest band takes the Bogoliubov-like form [14]

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

where

\[ \varepsilon(p) = 2 \delta \sin^2 \left(\frac{pd}{2\hbar}\right). \]

In the above equations $\delta$ is 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 by increasing the laser intensity $s$. The parameter $\kappa$ is the compressibility of the gas as emerges from the low momentum behaviour of the dispersion law (13): $\hbar \omega = \sqrt{\kappa^{-1}/m^*p}$. In the tight binding limit, one finds $\kappa^{-1} = gn \int_{-d/2}^{d/2} f^4(z)dz$ [15].

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

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

for the strength relative to the first band, where the width $\sigma$ can be calculated numerically by minimization of the ground state energy and behaves like $\sigma \sim s^{-1/4}d/\pi$ for $s \gg 1$. 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 behaviour 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 ($\kappa \to 0$) and by increasing the optical potential ($\delta \to 0$). In the cases of Figs. 1(a,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 $Z_1(p) = \exp \left(-\pi^2 \sigma^2 p^2 / 2d^2q_B^2\right)$. The comparison then clearly shows that the oscillating behaviour 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 towards the higher bands, provided $gn \ll \sqrt{5}E_R$. 

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**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).

Let us first discuss the dynamic structure factor in the low energy region and in particular the behaviour of the contribution $Z_1(p)$ arising from the first band (dashed line). We find that $Z_1(p)$ exhibits characteristic oscillations whose amplitude is suppressed at large $p$. The zeros of $Z_1(p)$ at $p = 2\ell q_B$ ($\ell$ integer) reflect directly the phonon behaviour of the excitation spectrum which vanishes at the same values (see Fig. 1).

The behaviour 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. (3,4) in the lowest band by
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 $h\omega$ corresponding to the first Bogoliubov band. In order to detect a sizeable signal at large $p$ and to point out the corresponding oscillating behaviour of $Z_1(p)$ (see Figs.2), the intensity $s$ of the optical lattice potential should be neither too small, nor too large. In fact for $s \to 0$ 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 Figs.2 we also report the results for the static structure factor (full line) corresponding to the sum $S(p) = \sum_\jmath Z_\jmath(p)$. One finds that for weak interactions (Fig.2(a)) also the static structure factor 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 behaviour of $S(p)$ in the uniform gas (10) (dotted lines in Figs.2).

The behaviour 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 $p$ behaviour 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 the low $p$ behaviour of the static structure factor is entirely determined by phonon correlations and behaves like

$$S(p) \xrightarrow{p \to 0} \frac{|p|}{2m^*c}$$

(16)

consistently with the phononic dispersion law and Eqs.(8,9) for the compressibility sum-rule. It is worth noticing that result (16) holds for any value of $s$ and $gn$. In the absence of the 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 $\kappa^{-1}$ 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 Figs.2.

Let us conclude by recalling that in Bragg scattering experiments one actually measures the imaginary part of the response function $\chi$ rather than the dynamic structure factor. The two quantities are related by the equation $\text{Im}(\chi) = -\pi (S(p,\omega) - S(-p, -\omega))$. The subtraction between the two terms can be crucial also at low temperatures. Actually, due to thermal excitation of phonons, the dynamic structure factor exhibits a strong temperature dependence when $h\omega < k_BT$, 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 $\text{Im}(\chi)$ provides reliable information on the zero temperature behaviour of the dynamic structure factor [18].

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