CHIN. PHYS. LETT. Vol. 31, No. 3 (2014) 030302

Collective Excitation and Quantum Depletion of a Bose–Einstein Condensate in a Periodic Array of Quantum Wells *

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(Received 13 December 2013)

With the help of a set of exact closed-form solutions to the stationary Gross–Pitaevskii (GP) equation, we calculate the collective excitation and quantum depletion of a weakly interacting Bose gas in the presence of a periodic array of quantum wells. The excitation spectrum (Bogoliubov spectrum) is obtained from the solution of the linearized time-dependent GP equation, which develops energy bands $\hbar\omega_j(p)$ periodic in quasi-momentum space. Moreover, we calculate the excitation strengths $Z_j(p)$ relative to the density operator and then the dynamic structure factor $S(p,\omega)$. Accordingly, the analytical expressions of quantum depletion of the system are obtained. We find that the quantum depletion is enhanced when the interatomic interactions become larger and the potential is sufficiently deep. The conditions for the possible experimental realization of our scenario are also proposed.

PACS: 03.75.Kk, 67.10.−j, 03.75.Lm DOI: 10.1088/0256-307X/31/3/030302

Loading the ultracold atomic gases into an optical lattice has provided a versatile and powerful toolbox to study many physical problems due to their abilities to accurately implement various lattice models without impurities, lattice phonon and other complications.[1−3] In such cases, the resulting standard and exotic many-body Hamiltonians can be used to simulate otherwise untractable systems in condensed matter physics. For example, the cornerstone along this research line consists of the experimental realization of quantum transitions from superfluid to Mott insulator.[4]

So far, almost all theoretical investigations have been primarily focused on BECs in a sinusoidal optical lattice with the period of d, which is induced by the ac Stark shift in optical standing waves and is therefore composed of a single Fourier component.[2,5,6] On the other hand, the state-of-the-art technology[7,8] allows us to Fourier-synthesize arbitrarily periodic potentials for atoms with the help of a higher order multiphoton Raman process, where a $2N$th order multiphoton process can yield a spatial periodicity of $d/2N$. Therefore, we reasonably expect that, if the more Fourier components that are multiples of the fundamental are added, the potential would become a lattice of well-separated wells. In the limit that the width of these wells becomes much smaller than the lattice period, the potential virtually can be treated as a periodic array of quantum wells (see Eq. (2)). Now, it is clear that the experimental progress in lattice physics makes the study of BECs in a periodic array of quantum wells highly interesting, which previously seems to only be academic.

In this Letter, we are motivated to launch a comprehensive investigation on a BEC in a periodic array of quantum wells. Based on a set of exact Bloch-state solutions, we analytically calculate the collective excitation, dynamic structure factor and quantum depletion of a BEC in a periodic array of quantum wells. Our results show convincingly that the fundamental properties of a BEC in a periodic potential do not depend on the shape of a lattice potential. As a result, theorists are at liberty to choose the form of a periodic potential for the convenience of their study. On the other hand, our results root into the exact solutions and therefore can be treated as a standard of testing the various other theoretical approaches.

We consider that a BEC is subjected to a periodic potential in the x-direction and tightly confined along the transverse directions. Then the dynamics of such

*Supported by the International Science and Technology Cooperation Program of China under Grant Nos 2013DFR10150 and 2012DFA10680, the National Natural Science Foundation of China under Grant Nos 61127015, 11004200 and 11274315, and the International Science and Technology Cooperation Program of Shanxi under Grant No 2012081029.

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a system of a BEC is governed by the one-dimensional stationary Gross–Pitaevskii (GP) equation[9]

$$\Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V_{\rm pot}(x)+gnd|\psi|^2\Big)\psi=\mu\psi, \tag{1}$$

where $g=4\pi\hbar^2 a_{\rm s}/m$ is the 1D reduced coupling constant and n is the 3D average density; $a_{\rm s}>0$ is the s-wave scattering length, m is the atomic mass, μ is the chemical potential and the order parameter ψ is normalized according to $\int_0^d dx|\psi|^2=1$.

The periodic potential $V_{\rm pot}(x)$ is assumed to be a periodic array of quantum wells,

$$V_{\rm pot}(x)=\sum_{n=-\infty}^{+\infty}V_q(x-ld), \tag{2}$$

with

$$V_q(x)=\begin{cases}0, & 0<x\le a,\\ V_0E_{\rm R}, & a<x\le a+b,\end{cases} \tag{3}$$

where a is the well width and b is the barrier width. In Eq. (2), $V_{\rm pot}(x)$ has a periodicity of $d=a+b$. In Eq. (3), V_0 is a dimensionless parameter that denotes the strength of the $V_{\rm pot}(x)$ in units of the recoil energy $E_{\rm R}=\hbar^2q_{\rm B}^2/2m$, with $q_{\rm B}=\pi/d$ being the Bragg momentum.

Despite non-linearity, Eq. (1) permits solutions in the form of Bloch waves[10,11]

$$\psi_k(x)=e^{ikx}\phi_k(x), \tag{4}$$

where k is the Bloch wave vector and $\phi_k(x)$ is a periodic function with the same periodicity as $V_{\rm pot}(x)$. The GP Eq. (1), in terms of the function $\phi_k(x)$, can be rewritten as

$$\Big[\frac{(-i\hbar\partial_x+k)^2}{2m}+V_{\rm pot}+gnd|\phi_k|^2\Big]\phi_k=\mu(k)\phi_k. \tag{5}$$

Note that the chemical potential $\mu(k)$, which is derived from Eq. (5),

$$\mu(k)=\int_0^d dx\phi_k^*\Big[\frac{(-i\hbar\partial_x+k)^2}{2m}+V_{\rm pot}+gnd|\phi_k|^2\Big]\phi_k, \tag{6}$$

usually does not coincide with the energy $\varepsilon(k)$ of the BEC system defined by

$$\varepsilon(k)=\int_0^d dx\phi_k^*\Big[\frac{(-i\hbar\partial_x+k)^2}{2m}+V_{\rm pot}+\frac{1}{2}gnd|\phi_k|^2\Big]\phi_k. \tag{7}$$

To find the solution of a Bloch state in the lowest band, we substitute an ansatz of $\psi(x)=r(x)\exp(-i\Theta(x))$ into Eq. (1), yielding,

$$\Big(\frac{\partial\rho(x)}{\partial x}\Big)^2=2\eta\rho(x)^3+4(\mu-V_{\rm pot})\rho(x)^2-\beta\rho(x)-4\alpha^2, \tag{8}$$

and

$$\Theta=\int dx\frac{\alpha}{\rho(x)}, \tag{9}$$

with $\rho(x)=r^2(x)$ being the density of the state and α, β being two integral constants. In Eq. (8), the length scale is d/π and the $\eta=gnd/E_{\rm R}$ represents the nonlinear interaction. As shown in Refs. [12–14] the exact solutions to Eq. (8) can be analytically expressed in terms of the Jacobi Elliptic functions (SN, CN, and NC). Moreover, in our recent work,[15,16] we have pointed out that there exist two different classes of exact solutions of Eq. (8), depending on the relation of the chemical potential μ and the barrier height V_0. (i) For $\mu>V_0$, we have $\rho_1(x)=A/8K^2-(A/8K^2-128K^4\alpha^2/A(16K^4+A\eta))SN^2(Kx+\delta,n_1)$. (ii) For $\mu<V_0$, we have two different kinds of exact solutions of Eq. (8), corresponding to there existing zero or only one node within the barrier region. For the case without a node in the barrier region, the exact solution reads $\rho_2(x)=B/8Q^2+(B/8Q^2+128Q^4\alpha^2/B(16Q^4-B\eta))SC^2(Qx+\gamma,n_2)$. However, for the case of there being only one node in the barrier region, we have $\rho_2(x)=-B/8Q^2+(Q^2/\eta+B/8Q^2-Q\sqrt{BQ^2-16\alpha^2\eta}/\sqrt{B}\eta)NC^2(Qx+\gamma,n_2)$. Here the free parameters of A, B, K, Q, δ, γ, and α can be totally determined by imposing the continuity of the wave function and the first derivative of the wave function at $x=a$, and the Bloch periodic condition.[15]

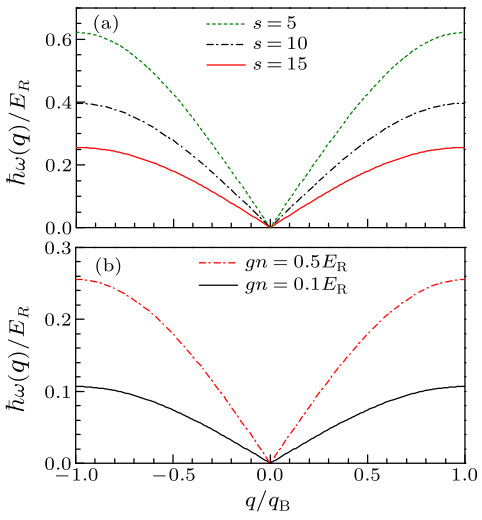


Fig. 1. (a) Elementary excitation spectrum $\hbar\omega(q)$ as a function of q for $s=5$, 10, 15 when $gn=0.1E_{\rm R}$. (b) Elementary excitation spectrum $\hbar\omega(q)$ as a function of q for $gn=0.1E_{\rm R}$ and $0.5E_{\rm R}$ when $s=15$.

The knowledge of a linear response of a complex system gives crucial information about its many-body behavior.[17] For the system of BEC, the superfluid properties are intimately related to the linear part of the phononic dispersion relation at low momenta. The presence of a periodic potential enriches the excitation spectrum of BEC in a remarkable way. First,

the lattice increases the local atomic density, which enhances the interactions. The increase of density leads to the effective interaction coupling constant $\widetilde{g}(s) = g\int_0^a \rho_1^2(x)dx + g\int_a^T \rho_2^2(x)dx$, where $\rho_1(x)$ and $\rho_2(x)$ are solutions respectively in well and barrier.[15] The second effect of the lattice is to modify the dispersion $T(q)$, which is simply $T(q) = \hbar^2 q^2/2m$ for free atoms. The effect of the periodic potential can be accounted by an increased effective mass m^*, where the effective mass is defined by $1/m^* = \partial^2\varepsilon/\partial k^2$,[9,11,15] reading $T'(q) = 2\hbar^2 \sin^2(dq/2)/(m^* d^2)$. According to the above physical picture, the dispersion of the elementary excitations can be well approximated in the tight-binding limit[18]

$$\hbar\omega(q) = \sqrt{\frac{2\hbar^2}{m^* d^2}\sin^2\left[\frac{dq}{2}\right]\left[\frac{2\hbar^2}{m^* d^2}\sin^2\left(\frac{dq}{2}\right) + 2\kappa^{-1}\right]}, \tag{10}$$

where q is the quasi-momentum. As expressed in Eq. (10), just knowing information of the effective mass m^* and the compressibility κ is enough to study the excitation energy in the tight-binding limit. In our case, the compressibility κ is given by $\kappa^{-1} = n\partial\mu/\partial n$.[9,11,15] In Fig. 1, the elementary excitation spectrum of the BEC system as functions of two-body interaction and potential depth is comprehensively investigated. It is clear that all the excitations in the lowest band acquire the linear phonon dispersion with a finite slope at small quasi-momenta and the role of two-body interactions is strongly enhanced with the increase of the potential depth. Experimentally, Bragg spectroscopy represents an excellent experimental tool to investigate the linear response of BECs.[19] It has allowed us to measure the dispersion relation of BECs in the mean-filed regime[21–23] to the deep Mott insulator.[24] Theoretically, the capability of the system to an external density 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[9]

$$S(p,\omega) = \sum_j Z_j(p)\delta(\omega - \omega_j(p)), \tag{11}$$

where $Z_j(p)$ are the excitation strength relative to the jth band and $\hbar\omega_j(p)$ are the excitation energy. We only calculate $Z_1(p)$, i.e., the excitation strength relative to the lowest Bloch band, due to the fact that we are mainly interested in the ground state of Eq. (5). The analytical expression of $Z_1(p)$ can be written in the tight-binding limit

$$\frac{Z_1(p)}{N_{\rm tot}} = \frac{\varepsilon(p)}{\hbar\omega(p)}\left|\int_0^d dx(|\psi(x)|^2 e^{ip/q_{\rm B}x})\right|^2, \tag{12}$$

where

$$\varepsilon(p) = \frac{m}{m^*}\frac{4}{\pi^2}\sin^2\left(\frac{\pi}{2}p\right), \tag{13}$$

and

$$\hbar\omega(p) = \sqrt{\frac{m}{m^*}\sin^2\left(\frac{\pi}{2}p\right)\left[\frac{m}{m^*}\sin^2\left(\frac{\pi}{2}p\right) + 2\kappa^{-1}\right]}. \tag{14}$$

In Fig. 2, we plot the excitation strength Z_1 relative to the lowest Bloch band via the transfer momentum p with different interactions $gn/E_{\rm R}$. It is found that for an interacting system, the strength towards the first band develops an oscillating behavior as a function of the momentum transfer, vanishing at even multiples of the Bragg momentum due to the presence of a phononic regime.

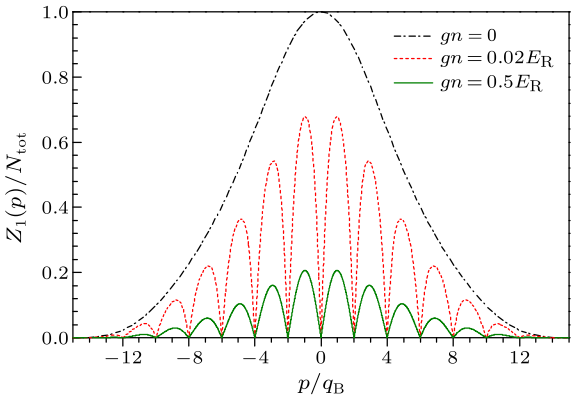


Fig. 2. Excitation strength $Z_1(p)$ at lattice depth $s = 10$ for $gn = 0$ (dash-dotted line), $gn = 0.02E_{\rm R}$ (shot dashed line) and $gn = 0.5E_{\rm R}$ (solid line).

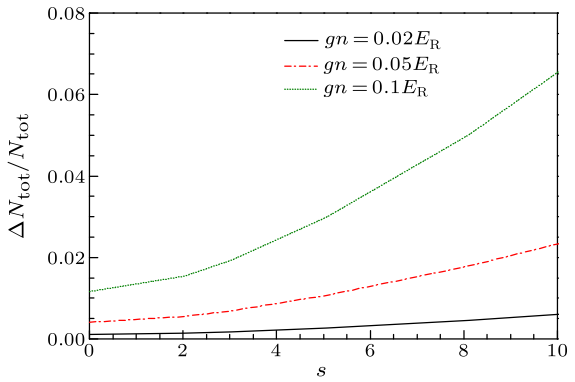


Fig. 3. Quantum depletion as a function of potential depth s for $gn = 0.02E_{\rm R}$, $0.05E_{\rm R}$ and $0.1E_{\rm R}$.

Also, it is important to study the effect of the lattice on the quantum depletion of the condensate. The presence of the optical potential may introduce phase fluctuations which reduce the degree of coherence of the sample. This effect is known to yield spectacular consequences in 3D periodic lattices, giving rise to a transition from the superfluid to the Mott insulator phases. Also in the presence of a 1D periodic lattice, one can predict interesting effects. The quantum depletion of the condensate increases as a consequence of the increase of the effective coupling constant and of the effective mass. Depending on the parameters of

the problem, we distinguish among different configurations which show 1D features. The quantum depletion of the condensate can be calculated by using the Bogoliubov result[9]

$$\frac{\Delta N_{\rm tot}}{N_{\rm tot}} = \frac{1}{N_{\rm tot}} \sum_{j} \sum_{q,p_x,p_y} \int dz \int dx \int dy |v_{j,q,p_x,p_y}(r)|^2, \tag{15}$$

where $N_{\rm tot}$ denotes the total number of atoms and $\Delta N_{\rm tot}$ is the number of non-condensed particles. We sum over all bands j, over the quasi-momenta q in the first Brillouin zone and the momenta of elementary excitations in the transverse directions p_x and p_y allowed by the periodic boundary conditions. In the thermodynamic limit, the depletion can be calculated by replacing the sum with an integral in Eq. (15), the quantum depletion takes the generalized Bogoliubov form[9]

$$\frac{\Delta N_{\rm tot}}{N_{\rm tot}} = \frac{8}{3} \frac{1}{\pi^{1/2}} \sqrt{\frac{m^*}{m}} \left(\frac{\pi}{8}\right)^{3/2} \left(\frac{\kappa^{-1}}{E_{\rm R}}\right)^{3/2}. \tag{16}$$

We find that the quantum depletion of the condensate increases as a consequence of the increase of the effective coupling constant and of the effective mass. According to Eq. (16), we can calculate the quantum depletion of condensates in a 1D periodic potential. However, Eq. (16) is valid in the cases of weak interactions and relatively low values of the lattice depth.

We plot the quantum depletion as a function of the potential depth s for $gn = 0.02E_{\rm R}$, $gn = 0.05E_{\rm R}$ and $gn = 0.1E_{\rm R}$ in Fig. 1. When $gn = 0.02E_{\rm R}$, the quantum depletion increases slowly with the potential depth s. With the increase of the interatomic interactions gn, the quantum depletion is enhanced remarkably. The quantum depletion increases rapidly with the increase of potential depth s.

In summary, with the help of a set of exact closed-form solutions, we have investigated the collective excitation and quantum depletion of a Bose-Einstein condensate in a periodic array of quantum wells. Using m^* and κ, the interaction effects on collective excitations, the dynamic structure factor and quantum depletion of the system of BEC are comprehensively studied. The excitations in the lowest band are strongly enhanced with the increase of interactions and potential depth. In the cases of weak interactions and relatively low values of the lattice depth, we can obtain the analytical expressions for quantum depletion, which can be rewritten as a function of the compressibility and effective mass of a system of BEC. We can see that the increase of the quantum depletion relates to the potential depth s and the interatomic interactions gn. The quantum depletion is enhanced when the interatomic interactions become larger and the potential is sufficiently deep.

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