

# Collective excitations of a periodic Bose condensate in the Wannier representation

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**Abstract.** We study the dispersion relation of the excitations of a dilute Bose-Einstein condensate confined in a periodic optical potential and its Bloch oscillations in an accelerated frame. The problem is reduced to one-dimensionality through a renormalization of the  $s$ -wave scattering length and the solution of the Bogolubov-de Gennes equations is formulated in terms of the appropriate Wannier functions. Some exact properties of a periodic one-dimensional condensate are easily demonstrated: (i) the lowest band at positive energy refers to phase modulations of the condensate and has a linear dispersion relation near the Brillouin zone centre; (ii) the higher bands arise from the superposition of localized excitations with definite phase relationships; and (iii) the wavenumber-dependent current under a constant force in the semiclassical transport regime vanishes at the zone boundaries. Early results by Slater [Phys. Rev. **87**, 807 (1952)] on a soluble problem in electron energy bands are used to specify the conditions under which the Wannier functions may be approximated by on-site tight-binding orbitals of harmonic-oscillator form. In this approximation the connections between the low-lying excitations in a lattice and those in a harmonic well are easily visualized. Analytic results are obtained in the tight-binding scheme and are illustrated with simple numerical calculations for the dispersion relation and semiclassical transport in the lowest energy band, at values of the system parameters which are relevant to experiment.

**PACS.** 67.40.Db Quantum statistical theory; ground state, elementary excitations

## 1 Introduction

The dynamics of cold atomic vapours trapped in a periodic external potential, as created by means of a far-detuned standing wave of light, has become an active area of research. Studies of ultracold atoms in such a confinement have revealed a number of behaviours which are well-known in solid state physics: Wannier-Stark ladders [1, 2], Bloch oscillations [3, 4] and Landau-Zener tunneling [5]. More recently, the observation of interference between macroscopic quantum states of Bose-Einstein-condensed vapours of <sup>87</sup>Rb atoms confined in a vertical array of optical traps has been reported [6]. Interference between the condensates in different lattice wells manifests itself in falling drops, which are emitted with a period determined by the Bloch oscillations induced by the gravitational field and are interpreted as coherent matter-wave pulses.

The properties of a Bose-Einstein condensate (BEC) in a regular array of optical wells have been studied theoretically and numerically by a number of authors [7–13]. Especially relevant for our present purposes is the work on an interacting BEC in an infinitely extended lattice potential by Berg-Sørensen and Mølmer [7], who demonstrated band structure and Bloch oscillations by solving numerically the Bogolubov-de Gennes equations for the

excitations and the time-dependent Gross-Pitaevskii equation for motion under a constant applied force. They also gave analytic results for the excitation spectrum in the limit where the periodic potential can be treated as a perturbation.

From solid state theory a tight-binding (TB) approach offers the possibility of an analytic study of the same phenomena in the opposite limit, when the lattice potential is so strong compared with all other energy scales as to allow the use of on-site orbitals for the approximate construction of the Bloch states. In fact, the proper theoretical tools are the so-called Wannier functions, which are defined through the Fourier transform of the Bloch eigenfunctions in the momentum representation. In the particular case of one-dimensional (1D) motion, the energy bands are non-degenerate and the states in any given one of them are described from a single Wannier function, by repeating it at each lattice site with the appropriate phase relationship between different sites. The TB scheme may then be realized by replacing the Wannier function by an on-site “atomic” orbital, under suitable limiting conditions which may be valid for the low-lying energy bands.

While the Wannier functions for motion in a generic periodic potential are usually not easy to calculate, it turns out that for the specific problem of 1D periodicity posed by the confinement of a BEC in an array of optical

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wells one can take advantage of the results contained in a classic paper by Slater [14] on a soluble problem in energy bands for electrons. Slater's work also discusses the conditions under which the Wannier functions for the low-lying energy bands can be accurately approximated by on-site orbitals, which in this case are the harmonic-oscillator wave functions associated with the parabola describing the bottom of each well.

The plan of the paper is as follows. In Section 2 we first model a dilute BEC confined in a periodic optical potential as a 1D dynamical system via inclusion of the transverse size into a renormalized contact interaction. We then formulate the problem of 1D band structure in terms of Wannier functions, the only conceptual difference from the analogous problem of 1D motion of electrons in a periodic potential being that for condensed bosons there is no gap between the condensate ground state and the excitation spectrum. In the same section we also formulate the problem of Bloch oscillations of the condensate in a single band in terms of the Fourier transform of the corresponding Wannier function.

The reduction of the general formalism to the TB approximation is effected in Section 3, after recalling Slater's conditions for its validity and extending them to an interacting BEC. The TB scheme displays in an explicit manner how the energy levels of a BEC in a single well are shifted and spread into bands by the periodic replica of the well potential. We give special attention to (i) the lowest-lying energy band of the BEC, which contains its wave-like phase excitations, and (ii) the connection that the TB approximation exhibits between the excitations in the next two higher bands and the dipole ("sloshing") and quadrupole excitations in an effectively 1D harmonic well. The discussion suggests how excitations in these two bands may be observed. We conclude this section by simple numerical illustrations of the dispersion relation in the lowest band and of the current induced by a constant external force, for values of the system parameters which are relevant to the experiments of Anderson and Kasevich [6]. Finally, Section 4 ends the paper with some concluding remarks.

## 2 Band structure and Bloch oscillations of a BEC from Wannier orbitals

We consider a dilute vapour of atoms of mass  $m$  in a Bose-condensed state at zero temperature, which interact *via* elastic collisions described by an  $s$ -wave scattering length  $a$  and are confined in the optical lattice created by a laser field. The lattice can be modelled as a transverse Gaussian potential times a periodic potential along the  $z$ -direction, namely the confining potential is

$$U_1(r, z) = U_0 \exp(-r^2/r_{\text{lb}}^2) \sin^2(kz). \quad (1)$$

Here  $U_0$  is the well depth, scaling linearly with the intensity of the laser beam,  $r_{\text{lb}}$  is the transverse size of the beam and  $k = 2\pi/\lambda$  its wavenumber. The lattice period is  $d = \lambda/2$ .

In this work we reduce the above problem in cylindrical symmetry to an effective 1D problem. To this end we freeze the transverse motions of the BEC and renormalize the interactions by a method proposed by Jackson *et al.* [15] to treat an elongated BEC, in which the coherence length as introduced by Baym and Pethick [16] is much larger than the transverse size. This reduction will evidently be inapplicable to high-energy excitations, when the excitation energy becomes comparable with the transverse confinement energy and transverse motions can therefore be induced. Its quantitative accuracy for low-energy excitations is under numerical study.

Under the conditions indicated just above, the transverse confinement modifies the mean-field interactions by a factor depending on the axial density  $\sigma(z)$ , the factor being  $\int dx dy |G(x, y; \sigma(z))|^4$  where  $G$  is the transverse part of the wave function in the  $xy$ -plane. Using a harmonic approximation for the radial part of the optical potential, we obtain in the present problem an effective scattering length per unit area given by

$$\tilde{a} = \frac{an_0}{r_{\text{lb}}d} \sqrt{\frac{2|U_0|}{E_R}}, \quad (2)$$

where  $n_0$  is the number of atoms per lattice well and  $E_R = \hbar^2/(md^2)$ . Notice that the energy  $E_R$  differs by a factor eight from the recoil energy  $E_{\text{recoil}} = \hbar^2 k^2/2m$ . A similar renormalization of  $U_0$  in equation (1) is negligible, since  $r_{\text{lb}} \gg \lambda$ .

The effective 1D Hamiltonian  $H$  that we treat thus is

$$H = \int dz \psi^\dagger(z) \Lambda(z) \psi(z) + \frac{1}{2} g \int dz \psi^\dagger(z) \psi^\dagger(z) \psi(z) \psi(z) \quad (3)$$

where  $\psi(z)$  is the field operator,  $g = 4\pi\hbar^2\tilde{a}/m$  and  $\Lambda(z) = -(\hbar^2/2m)\nabla^2 + U_p(z) - \mu$ , with  $\mu$  the chemical potential and  $U_p(z) = U_0 \sin^2(kz)$ . In the following all energies are referred to the bottom of the lattice potential.

### 2.1 Lattice symmetry and Bose statistics

Let us summarily go through the standard Bogolubov procedure [17] for treating the boson Hamiltonian (3). We make the Ansatz  $\psi(z) = \phi(z) + \tilde{\psi}(z)$ , which separates the coherent condensate function  $\phi(z)$  from the fluctuating part  $\tilde{\psi}(z)$  in the field operator. Upon substituting this Ansatz in equation (3) and requiring that linear terms in  $\tilde{\psi}(z)$  vanish, one obtains the Gross-Pitaevskii equation for  $\phi(z)$ :

$$[\Lambda(z) + g\phi^2(z)] \phi(z) = 0. \quad (4)$$

We are taking  $\phi(z)$  as real without loss of generality, with normalization to unity over the lattice period.

To quadratic terms the Hamiltonian in the fluctuation operators is diagonalized by the canonical transformation

$$\begin{aligned} \tilde{\psi}(z) &= \sum_{\alpha} [u_{\alpha}(z)a_{\alpha} - v_{\alpha}(z)a_{\alpha}^{\dagger}], \\ \tilde{\psi}^{\dagger}(z) &= \sum_{\alpha} [u_{\alpha}^*(z)a_{\alpha}^{\dagger} - v_{\alpha}^*(z)a_{\alpha}]. \end{aligned} \quad (5)$$

In equation (5) the suffix  $\alpha$  denotes an appropriate set of quantum numbers and the functions  $\{u_\alpha, v_\alpha\}$  satisfy the Bogolubov-de Gennes equations,

$$\begin{aligned} L(z)u_\alpha(z) - H_I(z)v_\alpha(z) &= E_\alpha u_\alpha(z), \\ L(z)v_\alpha(z) - H_I(z)u_\alpha(z) &= -E_\alpha v_\alpha(z). \end{aligned} \quad (6)$$

Here,  $H_I(z) = g\phi^2(z)$ ,  $L(z) = \Lambda(z) + 2H_I(z)$  and the  $E_\alpha$ 's are the (real) excitation energies that we aim to determine. We explicitly point out that with this form of  $H_I(z)$  the interactions enter the determination of the excited-state wave functions only through the density distribution of the condensate ground state. The same assumption has been made in dealing with the excitations of condensates in harmonic traps [18] and has led to good agreement with experiment for the eigenfrequencies of the quadrupolar surface modes.

For a BEC in a 1D periodic potential the quantum numbers  $\alpha$  are the band index  $n$  and the lattice quasi-momentum  $q$ . From symmetry under time reversal we have that, if  $\{u_{nq}, v_{nq}\}$  is a solution of equations (6) corresponding to energy  $E_{nq}$ , then  $\{v_{nq}, u_{nq}\}$  is a solution corresponding to energy  $-E_{nq}$  [19, 20]. We may for convenience call these the particle-like and the hole-like solution, respectively, and limit ourselves to calculate the spectrum at positive energy. As for the homogeneous Bose fluid we expect gaplessness, since in its ground state the whole condensate is in a single energy level placed at the chemical potential. Therefore, the excitations of lowest energy (referred to the chemical potential) are phonons, *i.e.* they have a linear dispersion relation.

It is convenient to introduce solutions  $Z_{nq\pm}(z)$  which have definite symmetry under time reversal [7], by setting  $Z_{nq\pm}(z) = [u_{nq}(z) \pm v_{nq}(z)]/\sqrt{2}$ . From equations (6) we have

$$L_-(z)Z_{nq+}(z) = E_{nq}Z_{nq-}(z) \quad (7)$$

and

$$L_+(z)Z_{nq-}(z) = E_{nq}Z_{nq+}(z), \quad (8)$$

where  $L_\pm(z) = L(z) \pm H_I(z)$ . Hence,

$$L_\pm(z)L_\mp(z)Z_{nq\pm}(z) = E_{nq}^2 Z_{nq\pm}(z). \quad (9)$$

This equation shows that the functions  $Z_{nq+}(z)$  and  $Z_{nq-}(z)$  are the right and left eigenvectors of the non-Hermitian product operator  $L_+(z)L_-(z)$ .

The ground state of the condensate can be taken at  $q = 0$  in the lowest band ( $n = 0$ , say) and special care is needed in handling the functions  $Z_{00\pm}(z)$ , in order to ensure gaplessness. This point is discussed for a periodic condensate in Appendix A, following the arguments given in references [19, 20]. Here we only need to note that an evaluation of the functions  $Z_{nq-}(z)$  is not necessary for the determination of the excitation energy eigenvalues. These are calculated by solving equation (9) for  $Z_{nq+}(z)$ , which reads

$$L_+(z)L_-(z)Z_{nq+}(z) = E_{nq}^2 Z_{nq+}(z). \quad (10)$$

This equation applies also to the state  $Z_{00+}(z)$  at zero energy (relative to the chemical potential). Of course, the function  $Z_{00+}(z)$  is simply proportional to the function  $\phi(z)$  introduced in equation (4). The solutions of equation (10) must have the Bloch symmetry, which imposes definite  $q$ -dependent phase relationships between different wells.

## 2.2 Expansion in terms of Wannier functions

It is well known from solid state theory [21] that any Bloch orbital can be expressed as a superposition of the so-called Wannier functions centred on the lattice sites. We thus write

$$Z_{nq\pm}(z) = \frac{1}{\sqrt{N}} \sum_l \exp(ilqd)w_{n\pm}(z - ld) \quad (11)$$

where the index  $l$  runs over all  $N$  sites of the lattice. Of course, the Wannier functions  $w_{n\pm}(z)$  have the same parity under time reversal as the corresponding Bloch orbitals  $Z_{nq\pm}(z)$ . We may also recall that the Wannier functions form a complete orthonormal set, *i.e.* they satisfy the relation  $\int dz w_{n\pm}^*(z - ld)w_{n'\pm}(z - l'd) = \delta_{nn'}\delta_{ll'}$ . Orthogonality between different wells implies oscillatory tails, falling off more rapidly as overlap decreases.

Equation (11) expresses a Fourier-transform relationship between Bloch orbitals and Wannier functions, embodying the Bloch translational symmetry. The  $q$ -dependent Bloch orbitals emphasize the extended nature of the lattice states and the periodicity of their energy eigenvalues in momentum space. The representation in terms of Wannier functions emphasizes instead that the lattice is a periodic assembly of identical wells. The Bloch symmetry of the Fourier series in equation (11) is ensured by the fact that the Fourier coefficients do not involve a separate dependence on position  $z$  and on lattice site index  $l$ .

In the case of a BEC in a lattice, a general consequence of the Wannier-function description is immediately evident from equation (11). Since the ground state is at the chemical potential and has been taken to lie at  $q = 0$  in the bottom of the lowest band, the excitations in this band are wave-like modulations of the condensate phase and their energy vanishes linearly in the limit  $q \rightarrow 0$ . This fact can be traced back to the existence of a Goldstone phonon – a collective mode without restoring force [19] resulting from spontaneous symmetry breaking (see the discussion in Appendix A).

Similarly, for the higher excitation bands equation (11) shows that each of them is a superposition of localized excitations (described by  $w_{n+}(z)$ ), which is constructed by imposing definite phase relationships between the various sites as dictated by the translational lattice symmetry. This theorem is valid, of course, within the Bogolubov approach and has been derived through the reduction to one-dimensionality.

In practice, the calculation of Wannier functions is in general not an easy task. In the limit in which the Wannier

functions become almost confined inside each lattice well (which may be true for low-lying states), they can be expanded in a limited number of “atomic” orbitals. We shall discuss in the next section the conditions under which one may replace the Wannier functions for a BEC in a periodic optical potential by single-well orbitals and thereby obtain explicit solutions in the TB limit.

### 2.3 Semiclassical transport in band states

We proceed to express through the Wannier functions the current carried by a periodic Bose-condensed system subject to a constant force  $F$  in the semiclassical regime. We restrict ourselves to Bloch oscillations in the lowest band, described by the Wannier function  $w_{0+}(z)$ . Through equation (11) taken at  $q = 0$ , this function is immediately related to the ground state  $\phi(z)$  of the condensate.

The quantity of interest is the expectation value  $\bar{p}(t)$  of the momentum operator  $p = -i\hbar d/dz$  in the state  $Z_{0q(t)+}(z)$ , where  $q(t) = Ft/\hbar$ . We introduce the Fourier transform  $f_0(k)$  of  $w_{0+}(z)$ ,

$$f_0(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dz w_{0+}(z) \exp(-ikz). \quad (12)$$

Hence,

$$Z_{0q+}(z) = \frac{1}{\sqrt{2\pi N}} \sum_l \int_{-\infty}^{\infty} dk f_0(k) \exp[i(q-k)ld + ikz] \quad (13)$$

and a straightforward calculation yields

$$\bar{p}(q(t)) = \frac{\hbar \sum_l \int_{-\infty}^{\infty} dk k |f_0(k)|^2 \cos[ld(q(t) - k)]}{\sum_l \int_{-\infty}^{\infty} dk |f_0(k)|^2 \cos[ld(q(t) - k)]}. \quad (14)$$

This is an exact expression, which holds independently of the confining periodic potential and of the interaction between the particles.

It is easily seen from equation (14) that (i)  $\bar{p}(t)$  is a periodic function of time with the Bloch period  $T_B = \hbar/(Fd)$  and (ii)  $\bar{p}(t)$  vanishes at the Brillouin zone edges, *i.e.* at  $q = \pm\pi/d$  or  $t = \pm T_B/2$ .

### 3 Tight-binding approximation

The aim of the TB approximation is to relate the properties of the periodic system in a lattice potential to the solution of the single (isolated) well problem. The results of the method are quantitative as long as the single-well solutions at adjacent sites do not overlap much with each other. Namely, the validity of the TB approximation is limited by the condition that the band-width be smaller than the height of the lattice potential.

Slater [14] has studied the Wannier functions of the “Mathieu problem” defined by the Schrödinger equation for non-interacting electrons moving in the periodic potential  $U_p(z) = U_0 \sin^2(kz)$  of present interest. He showed

that for the first five low-lying energy bands the Wannier functions are well approximated by Hermite polynomials under the condition  $U_0 > 2E_R$ , relaxing to  $U_0 > E_R/4$  if only the lowest energy band is of interest. Slater’s argument is summarized in Appendix B and extended there to an interacting BEC. In essence the mean-field interactions may be viewed in the present context as effecting a renormalization in the height of the external potential, accompanied by a spread of the wave functions. Slater’s thresholds are thereby shifted by the amount

$$\Delta U_0 = \frac{\tilde{a}dE_R}{\pi}. \quad (15)$$

If the threshold conditions are satisfied, the Wannier functions  $w_{n+}(z)$  at positive energy could be approximately replaced by the eigenfunctions of the harmonic approximation to the single-well potential  $\bar{U}_p^{(s)}(z) = \bar{U}_0 \sin^2(kz)$  with  $z \in [-d/2, d/2]$  and  $\bar{U}_0 = U_0 + \tilde{a}dE_R/\pi$ .

### 3.1 Band structure for a periodic BEC

More generally, the evaluation of the energy bands for a periodic condensate in the TB approximation would require a preliminary solution of the on-site problem. To this end, we separate the on-site parts  $L_{\pm}^{(s)}(z)$  out of the operators  $L_{\pm}(z)$  entering equation (9) by writing  $L_{\pm}(z) = L_{\pm}^{(s)}(z) + \Delta L_{\pm}(z)$ . The detailed definitions of these operators are given in Appendix C. The on-site operators  $L_{\pm}^{(s)}(z)$  determine the single-well orbitals  $\varphi_{n\pm}(z)$  corresponding to single-well energy eigenvalues  $\epsilon_n$ , according to

$$\begin{aligned} L_-^{(s)}(z)\varphi_{n+}(z) &= \epsilon_n \varphi_{n-}(z), \\ L_+^{(s)}(z)\varphi_{n-}(z) &= \epsilon_n \varphi_{n+}(z). \end{aligned} \quad (16)$$

Again, the condensate in a single well lies at the chemical potential  $\mu_s$  (see the definitions of  $L_{\pm}^{(s)}(z)$  in Appendix C). Conjugation between fluctuations in the particle number and in the phase must also be taken care of, as shown in references [19, 20].

We define the overlap integrals

$$\mathcal{I}_n(l) = \int dz \varphi_{n-}^*(z) \varphi_{n+}(z - ld)$$

and the interaction integrals

$$\mathcal{J}_n(l) = \int dz \varphi_{n-}^*(z) \Delta [L_+(z)L_-(z)] \varphi_{n+}(z - ld)$$

(see the definitions of the  $\Delta L_{\pm}(z)$  operators given in Appendix C). By exploiting equations (16) one easily finds from equation (9) the dispersion relation

$$E_{nq}^2 = \epsilon_n^2 + \frac{\sum_l \mathcal{J}_n(l) \exp(ildq)}{\sum_l \mathcal{I}_n(l) \exp(ildq)}. \quad (17)$$

An adiabatic argument regarding the switching-on of the (spatial-symmetry conserving) mean-field interactions shows that the product  $\varphi_{n-}^*(z)\varphi_{n+}(z')$  is even under space inversion. Both series in equation (17) are therefore real quantities.

Equation (17) displays the two main changes induced by lattice periodicity on the single-well energy levels, namely (i) a shift of each level relative to the single-well value  $\epsilon_n$  and (ii) the broadening of the level into a band. In particular, for the lowest band the shift corresponds to a renormalization of the chemical potential from the single-well value  $\mu_s$  to the value  $\mu$ , which has to be evaluated self-consistently from the condition  $E_{00} = \mu$ . The resulting gaplessness introduces in equation (17) for  $n = 0$  the linear, acoustic-phonon-like dispersion of the excitation energies in the long wavelength limit  $q \rightarrow 0$ .

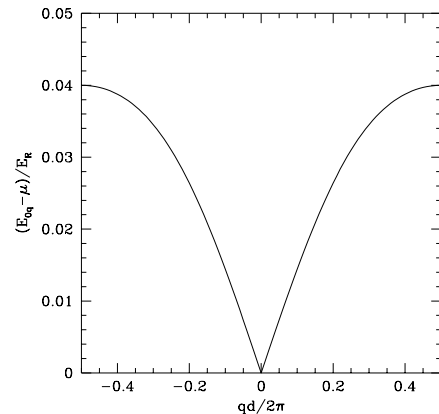
We can now see how the excitations in the bands with  $n = 1$  and  $n = 2$  may be related to single well excitations. We make use of the present replacement of Wannier functions by on-site orbitals, which are approximately described by the eigenfunctions of the 1D harmonic oscillator. Evidently, this allows us to identify the on-site excitation leading to the  $n = 1$  band with the dipolar sloshing mode of the condensed particles within the well. The construction of Bloch orbitals from these localized sloshing motions simply amounts to fixing, for each value of the wavenumber  $q$ , their relative phases according to the lattice translational symmetry (see the discussion already given near the end of Sect. 2.2). Similarly, the excitations in the  $n = 2$  band may be viewed as resulting from localized, single-well quadrupolar modes with relative phases depending on  $q$  as imposed by lattice symmetry. Of course, the approximate validity of such a visualization of the collective low-lying modes of a periodic BEC is subject not only to conditions relating to effective one-dimensionality in a mean-field approach, but also to the restrictions associated with the TB scheme.

The above discussion also suggests how these collective band modes may become accessible to experimental or computational observation. Clearly, at  $q = 0$  the dipolar mode can be excited by a rigid shaking of the lattice and the quadrupolar one by a modulation of the width of all the wells. Excitation of dipolar and quadrupolar band modes at finite  $q$  would require similar probes at given wavelengths.

### 3.2 Dispersion relation and Bloch oscillations in the lowest band

We conclude this section by presenting some illustrative numerical results for the lowest band in the TB approximation. According to equation (15), in the case of repulsive interactions the inequality  $U_0 > (0.25 + \tilde{a}d/\pi)E_R$  must be satisfied for the appropriate Wannier function to be approximated by the Gaussian function

$$\varphi_{0+}(z) = \frac{1}{(\sqrt{\pi}\sigma)^{1/2}} \exp(-z^2/2\sigma^2). \quad (18)$$



**Fig. 1.** An example of the dispersion relation of phase excitations in a BEC confined in an optical potential. We plot the lowest-lying energy band as a function of the wave number  $q$  (in units of  $2\pi/d$ ) within the 1D Brillouin zone, for values of the system parameters given by  $a = 110a_0$ ,  $r_{1b} = 80 \mu\text{m}$ ,  $n_0 = 10^3$ ,  $U_0/E_R = 0.25$  and  $\sigma/d = 0.27$ .

The width  $\sigma$  of this Gaussian is determined in a first approximation by the curvature of the bottom of the single well. A more accurate estimate of  $\sigma$ , which takes account of the interactions between the particles in the BEC, is given in Appendix C.

In fact, for the calculation of the dispersion relation it is more convenient to revert back to equation (10) and directly evaluate the integrals

$$K(l) = \int dz \varphi_{0+}(z) [L_+(z)L_-(z)] \varphi_{0+}(z - ld) \quad (19)$$

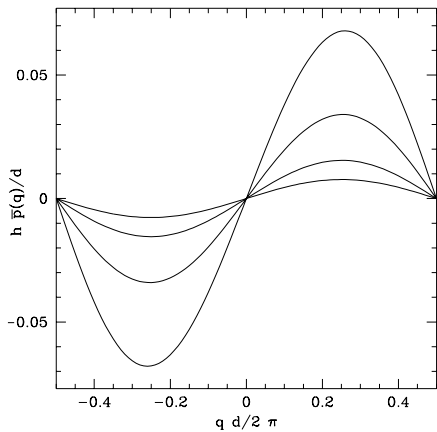
and  $I(l) = \int dz \varphi_{0+}(z)\varphi_{0+}(z - ld)$ . This procedure has the advantage of involving only the known symmetric function  $\varphi_{0+}(z)$  given in equation (18). We estimate  $I_0(0) \simeq 0.99$  and hence we obtain

$$E_{0q}^2 = \mu^2 + 2K(1) [\cos(qd) - 1] \quad (20)$$

where  $\mu^2 = K(0) + 2K(1)$ . We recall that the energies in equation (20) are referred to the bottom of the lattice potential.

We have calculated the integrals entering equation (20) with the wave function in equation (18) for  $U_0/E_R = 0.25$ , which corresponds to a value of  $\sigma/d = 0.27$ , in the case  $a = 110a_0$ ,  $r_{1b} = 80 \mu\text{m}$  and  $n_0 = 10^3$ . These values are relevant to the experiment of Anderson and Kasevich [6]. The results are  $K(1) \simeq -4 \times 10^{-4} E_R^2$  and  $\mu \simeq 0.1 E_R$ , yielding the value  $c_s \simeq 0.02 E_R d/\hbar$  for the speed of phonon-like excitations. Figure 1 shows the corresponding dispersion curve over the whole Brillouin zone.

Using equation (18) in equations (12, 14) we find the following expression for the current induced by a constant



**Fig. 2.** Average momentum of the BEC in the lowest-lying energy band, in units of  $\hbar/d$ , as a function of the wave number inside the 1D Brillouin zone, for the case  $a = 110a_0$ ,  $r_{1b} = 80 \mu\text{m}$ ,  $n_0 = 10^3$  and for various values of the parameter  $U_0/E_R$ . From top to bottom on the RHS of the drawing:  $U_0/E_R = 0.25, 0.4, 0.8$  and  $1.2$ .

external force in states of the lowest band,

$$\bar{p}(q(t)) = \frac{\hbar d}{\sigma^2} \frac{\sum_{l=1}^{\infty} l \sin(lqd) \exp\left[-(ld/2\sigma)^2\right]}{1 + 2 \sum_{l=1}^{\infty} \cos(lqd) \exp\left[-(ld/2\sigma)^2\right]}. \quad (21)$$

In practice, in the TB limit the leading term in the numerator is dominant and the denominator can be replaced by unity. Namely,

$$\bar{p}(q) \simeq \frac{\hbar d}{\sigma^2} \sin(qd) \exp\left[-(d^2/4\sigma^2)\right]. \quad (22)$$

Figure 2 shows the behaviour of  $\bar{p}(q)$  over the Brillouin zone for various values of the parameter  $\alpha = U_0/2E_R$  in the case  $a = 110a_0$ ,  $r_{1b} = 80 \mu\text{m}$  and  $n_0 = 10^3$ .

## 4 Concluding remarks

In summary, and as already discussed in the work of Berg-Sørensen and Mølmer [7], the properties which derive from lattice symmetry for the wave functions and the energy eigenvalues of electrons moving in a periodic 1D potential also hold for a Bose-condensed system. However, Bose statistics and spontaneous symmetry breaking imply that there is no gap between the condensate ground state and the excitation spectrum. This latter property can be met in the energy spectra of electrons in semiconductors only as a consequence of accidental degeneracies induced by specific space symmetries, a well-known instance being provided by graphite [22]. For a periodic Bose condensate the gaplessness property, together with the quadratic structure of the energies as expressed in equations (9) (see Sect. 2.1), yields on general grounds the linear dispersion relation  $E_{0q} = c_s(|qd|) + O(q^2d^2)$  for the lowest energy band.

We have seen that the specific form of the optical potential acting on a BEC from a laser field admits two important simplifications in the band-structure problem. Firstly, the problem for the low-lying bands can be mapped into a one-dimensional one by accounting for the transverse cross-section of the BEC through a renormalization of the  $s$ -wave scattering length. This mapping has been shown to be useful in relation to the experiments performed by Anderson and Kasevich [12]. Secondly, the 1D problem away from the weak-confinement limit is most naturally formulated in terms of the Wannier functions, which have already been studied for the Mathieu problem by Slater [14]. The use of Wannier functions, as demonstrated in Section 2.2, provides an exact formulation of the lattice problem and immediately shows that (i) the lowest excitations of a condensate in a periodic potential are wave-like phase modulations, and (ii) the higher bands arise from the superposition of localized excitations with definite phase relationships.

An analytic study of semiclassical transport in a periodic condensate subject to a constant external force becomes straightforward with the use of Wannier functions. The expectation value of the momentum operator is periodic with the Bloch period and vanishes at the Brillouin zone edges, as shown in Section 2.3.

The work of Slater [14] allows one to specify the conditions under which the Wannier functions for the low-lying bands of the BEC in an optical periodic potential, and in particular that for the lowest band containing its phase excitations, can be accurately approximated by harmonic-oscillator wave functions. These functions are simply described by the curvature of the on-site well as renormalized by the interactions in the BEC and allow an explicit, though approximate, connection to be made between band modes and single-well modes. They also allow very simple calculations on a periodic BEC, as illustrated in Section 3 for the dispersion relation in the lowest energy band and for the average wavenumber-dependent momentum in correspondence to a particular set of system parameters which is relevant to experiment.

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## Appendix A: The zero-energy solutions for the lattice problem

The equation obeyed by the wave function  $Z_{0q+}(z)$  at  $q = 0$ , that is  $Z_{00+}(z) \propto \phi(z)$ , is

$$L_-(z)Z_{00+}(z) = 0. \quad (23)$$

We have chosen  $E_{00} = 0$  relative to the chemical potential  $\mu$  of the condensate (see the definition of  $\Lambda(z)$  immediately below Eq. (4)).

In view of the macroscopic occupation of this quantum state, one must allow for fluctuations in the number of particles and for the accompanying shifts of the phase of the condensate. This is accounted for by adding in the Hamiltonian a “kinetic energy” term  $\alpha P^2/2$ , where  $P = \int dz Z_{00+}(z)[\tilde{\psi}(z) + \tilde{\psi}^\dagger(z)]$  is the number operator generating such a “translation” and  $1/\alpha$  plays the role of a mass. The canonically conjugate operator  $Q = i \int dz Z_{00-}(z)[\tilde{\psi}(z) - \tilde{\psi}^\dagger(z)]$  is easily seen to be the phase operator. It satisfies the appropriate commutation relation provided that the weighting function  $Z_{00-}(z)$  obeys the equation

$$L_+(z)Z_{00-}(z) = \alpha Z_{00+}(z), \quad (24)$$

with the condition  $\int dz Z_{00-}(z)Z_{00+}(z) = 1/2$ .

From a more formal viewpoint [19,20], the Bogolubov equations (6) at zero energy admit the eigenvector  $\{Z_{00+}, Z_{00+}\}$ . A second solution is provided by the eigenvector of the squared Bogolubov operator with zero eigenvalue. This implies that the result of applying the Bogolubov operator to the second solution is proportional to  $\{Z_{00+}, Z_{00+}\}$  through a constant to be determined, leading to equation (24). In fact, upon differentiation of the Gross-Pitaevskii equation with respect to the total number of particles  $n$  one is led again to equation (24), with  $Z_{00-}(z) = 2\sqrt{n}\partial(\sqrt{n}Z_{00+}(z))/\partial n$  and  $\alpha = 2m\partial\mu/\partial n$ . Clearly, the constant  $\alpha$  is related to the change induced in the chemical potential  $\mu$  by a fluctuation in the number of particles.

## Appendix B: Wannier functions for low-lying bands

For the 1D Mathieu problem (non-interacting particles moving in the potential  $U_p(z) = U_0 \sin^2(kz)$ ), Slater [14] shows that the eigenfunctions  $f_n(k)$  in the momentum representation obey the adimensional finite-difference equation

$$\left(p^2 + \frac{1}{2}s - \epsilon\sqrt{s}\right) f_n(p) - \frac{1}{4}s [f_n(p+2) + f_n(p-2)] = 0, \quad (25)$$

where  $p = kd/\pi$ ,  $s = 8U_0/E_R$  and  $\epsilon = E_R\sqrt{s}/U_0$ . In the low-lying energy bands  $f_n(p)$  is a slowly varying function of its argument, so that equation (25) is reduced to the differential equation

$$-s \frac{d^2 f_n(p)}{dp^2} + (p^2 - \epsilon\sqrt{s}) f_n(p) = 0. \quad (26)$$

Evidently, this is the Schrödinger equation for a harmonic oscillator, with energy levels  $\epsilon_n = 2n + 1$  and eigenfunctions  $f_n(\kappa) \propto \exp(-\kappa^2/2)H_n(\kappa)$  where  $\kappa = s^{-1/4}p$  and  $H_n(\kappa)$  are the Hermite polynomials.

The Wannier functions appropriate to the low-lying energy bands of the 1D Mathieu problem are, therefore, single-well orbitals with the same functional form

as for the harmonic oscillator. From his study of the exact Wannier functions of the same problem Slater [14] then showed that these single-well orbitals provide an accurate description of the first five bands under the restriction  $s > 16$  *i.e.*  $U_0 > 2E_R$ . The condition of validity for the first Wannier function in equation (18) can be estimated from Slater’s numerical results as  $U_0 > E_R/4$ .

To extend this argument to the Wannier functions of an interacting BEC, we view the mean-field interactions as equivalent to a renormalization in the height of the external potential, by an amount that we may estimate as the average value of  $g\phi^2(z)$  over a lattice cell. From the normalization condition satisfied by  $\phi(z)$ , in the case of repulsive interactions the height of the periodic potential is then *lowered* by an amount  $g/d$ . This leads to equation (15) in the main text.

## Appendix C: Details on the on-site problem

### C.1 On-site Bogolubov operators

The operators  $L_\pm$  entering the Bogolubov equations (7, 8) can be split into an on-site part and a residual part as  $L_\pm(z) = L_\pm^{(s)}(z) + \Delta L_\pm(z)$ , where

$$L_-^{(s)} = -\nabla^2/2m + U_p^{(s)} + H_1^{(s)} - \mu_s, \quad (27)$$

$$L_+^{(s)} = L_-^{(s)} + 2H_1^{(s)} \quad (28)$$

and

$$\Delta L_- = \Delta U_p + \Delta H_1 - \Delta\mu, \quad (29)$$

$$\Delta L_+ = \Delta L_- + 2\Delta H_1. \quad (30)$$

In equations (27-30)  $U_p^{(s)}$  is the single-well potential  $U_p^{(s)} = U_p(z)\theta(1 - 4z^2/d^2)$ ,  $\theta(x)$  being the step function,  $H_1^{(s)}$  is the on-site mean-field potential  $H_1^{(s)} = gw_{0+}^2(z)$  and  $\mu_s$  is the on-site chemical potential, while the  $\Delta$ ’s are differences between lattice and single-well values. Namely,

$$\Delta U_p(z) = U_0 \sin^2(kz)\theta\left(\frac{4z^2}{d^2} - 1\right) \quad (31)$$

and

$$\Delta H_1(z) = g(|Z_{00+}(z)|^2 - |w_{0+}(z)|^2). \quad (32)$$

### C.2 Variational calculation of Gaussian width

A crucial quantity in the calculations reported in Section 3.2 is the width  $\sigma$  of  $\varphi_{0+}(z)$ , since the integrals entering equation (20) are determined by the overlap in adjacent wells. A first estimate of  $\sigma$  can be obtained from the curvature of the bottom of the well: this determines a frequency  $\omega = (U_0 E_R/2\hbar^2)^{1/2}$  such that  $\sigma = (\hbar/m\omega)^{1/2}$ . A more refined variational estimate can be based on a method first proposed by Baym and Pethick [16], including the effect of interactions in the condensate.

We construct the energy functional

$$E[\phi] = \frac{\hbar^2}{2m} \int dz \left| \frac{d\phi(z)}{dz} \right|^2 + \int dz W(z) |\phi(z)|^2 + \frac{1}{2} g \int dz |\phi(z)|^4 \quad (33)$$

and require that it be minimized by  $\varphi_{0+}(z)$  when we set  $W(z) = m\omega^2 z^2/2$ . This yields the energy function

$$E(\sigma) = \frac{\hbar^2}{4m\sigma^2} + \frac{1}{4} m\omega^2 \sigma^2 + \frac{g}{2\sigma\sqrt{2\pi}}, \quad (34)$$

which is minimized when  $\sigma$  obeys the condition

$$\sigma^4 = \left( \frac{\hbar}{m\omega} \right)^2 + \frac{g\sigma}{\sqrt{2\pi}m\omega^2}. \quad (35)$$

Evidently, repulsive interactions broaden the Wannier function. A similar estimate of  $\sigma$  for the  $n = 1$  band states shows that the role of the interactions is decreasing with increasing energy.

#### Note added in proof

An optimized reduction to one-dimensionality for an interacting Bose condensate in an optical potential has been proposed by two of us [M.L. Chialfalo, M.P. Tosi, Phys. Lett. A **268**, 406 (2000)].

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