Bloch function description of a Bose-Einstein condensate in a finite optical lattice

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(November 10, 2021)

We consider stationary and propagating solutions for a Bose-Einstein condensate in a periodic optical potential with an additional confining optical or magnetic potential. Using an effective mass approximation we express the condensate wavefunction in terms of slowly-varying envelopes modulating the Bloch modes of the optical lattice. In the limit of a weak nonlinearity, we derive a nonlinear Schrödinger equation for propagation of the envelope function which does not contain the rapid oscillation of the lattice. We then consider the ground state solutions in detail in the regime of weak, moderate and strong nonlinear interactions. We describe the form of solution which is appropriate in each regime, and place careful limits on the validity of each type of solution.

I. INTRODUCTION

There have now been a large number of experiments and an enormous quantity of theory devoted to the properties of the trapped Bose-Einstein condensates (BEC) \[1\]. Motivated by the existing experiments, the bulk of the theoretical work so far assumes a harmonic trap in one, two or three dimensions. Lately, a few papers have considered the consequences of exposing a BEC to an optical periodic potential \[2–4\]. While not yet observed experimentally, such a situation could easily be produced by applying counter-propagating optical beams along one or more axes to produce a standing-wave optical lattice. Indeed, the directional output coupler of the BEC demonstrated by Leng et al. \[3\] uses such counter-propagating beams to induce Raman transitions into untrapped states. In this paper, we consider the special case of a BEC confined in a finite optical lattice, and develop theory to describe the properties of the lattice BEC.

Subjecting a BEC to a periodic potential opens the way for a number of new phenomena. Sørenberg and Mølmer \[2\] assumed an infinite lattice potential and showed as one would expect, that the quasi-particle excitation spectrum exhibits a band-structure. Zobay et al. \[3\] considered a propagating field of three internal levels connected by Raman transitions. They showed that if the center wavenumber is tuned close to the band gap induced by the optical lattice, one can derive a pair of coupled mode equations \[1\] for forward and backward propagating waves. These equations are well-known to support the interesting class of solitary waves known as “gap solitons” \[6\]. Gap solitons have been observed when a periodic structure in an optical fiber is subjected to high intensity light \[7\] but have not been observed in an atom optics context. Finally, Jaksch et al. \[4\] have demonstrated an equivalence between the system of a condensate trapped in an optical lattice and the Bose-Hubbard model of condensed-matter physics. At very low site-occupation numbers, they predict the occurrence of phase transitions between a Mott insulating state and coherent superfluid flow. Jaksch et al. also considered a complication not present in the other two papers—the inclusion of a weak harmonic trap in addition to the rapidly oscillating lattice.

It is this complication that we pursue in the present paper. As the eigenstates or “Bloch functions” of a pure lattice potential are of infinite extent, any real system must always include some form of additional confining potential. (In any case, a real optical lattice is always finite.) Thus we consider the case of an infinite periodic potential combined with a weak confining potential. While we will allow the form of this potential to be rather general, in many cases a harmonic oscillator form may be appropriate. For example, one might use optical beams to generate the lattice and provide the ultimate confinement with a weak magnetic trap in the standard way. In fact, red-detuned counter-propagating focussed Gaussian beams would effectively create both a lattice and a harmonic-like axial trap due to the reduced intensity away from the beam focus. In this case, however, the lattice potential would also be modulated by a Gaussian envelope. We shall restrict to the case where the periodic part of the potential is uniform.

Our aim is to describe in detail the properties of the condensate wave function in such a potential in both stationary and propagating regimes. We assume the condensate may be described by the standard Gross-Pitaevskii equation (GPE) with the addition of a periodic potential. Numerically at least, finding the exact ground-state wavefunction is then a straight-forward application of one’s favorite method—imaginary time propagation, shooting or relaxation. Similarly, propagation problems may be solved by an appropriate split-step algorithm for example. However, these procedures are computationally very intensive as compared to the analogous problems in the absence of the lattice for the following reason. Typically, we are interested in cases for which the period or “lattice constant” is relatively short compared to the extent of the wave function when just the trapping potential is present. (If that is not the case, one is really not dealing with a lattice at all, but a small set of coupled non-identical wells.) Thus we are concerned with...
the case of a rapidly varying periodic potential superposed on the slowly-varying background of the trap potential. Hence as the wave function samples many wells of the potential, it possesses a detailed structure on the same scale as the lattice and a large number of grid points is necessary for accurate calculations. A time-dependent propagation of the field in a two-dimensional potential say, represents a formidable calculation. While such calculations are certainly possible [3], it is desirable to find a method that would circumvent the computational burden as well as highlight the underlying physics of the system.

Consider first the stationary problem, where it is clear what the general form of the ground-state solution must be: to minimize the energy, the atoms pile up in the lattice wells, and the relative density in each well is determined by the local value of the confining part of the potential. The natural way to treat such a problem is to capture the rapid variation on the scale of the lattice using the Bloch functions of the periodic potential. If the nonlinearity is not too strong, the solution may be represented as a sum of a small number of slowly-varying envelope functions modulating appropriate Bloch functions. These envelope functions obey simpler equations from which all the rapid variation has been removed. For propagating problems, one may proceed in the same fashion but using different Bloch functions. In the language of solid state physics, this approach is essentially an effective mass representation with the addition of the nonlinear perturbation of the atomic collisions. We should remark that the work of Zobay et al. [3] also uses an envelope function approach, but their work does not include a confining potential and is restricted to solutions close to a band edge. In addition, they use plane waves rather than Bloch functions as a basis, which limits the treatment to only relatively weak lattices.

The paper is structured as follows. In section II we derive simple approximate equations for stationary and propagating BECs in a finite optical lattice. In section III we present solutions for the stationary ground state, comparing exact numerical solutions with our Bloch function approach. Section IV discusses extensions to treat fields near a band gap before we conclude.

II. BEC IN A FINITE OPTICAL LATTICE

We consider a BEC in an infinite optical lattice with an additional confining potential. To avoid incoherent heating from spontaneous emission, the laser beams creating the lattice are detuned far from the atomic resonance. In this case, the atomic field for the internal excited state may be adiabatically eliminated and the optical lattice acts as an external potential for the ground state field \( \hat{\psi}_g(x) \) [10,11]. Then the macroscopic wavefunction \( \psi(x) = \langle \hat{\psi}_g(x) \rangle \) satisfies the GPE

\[
i \hbar \frac{\partial \psi(x,t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + U(x) + V(x) + \Gamma |\psi(x,t)|^2 \right] \psi(x,t),
\]

where the optical dipole potential \( U(x) \) is periodic in one or more dimensions. For simplicity we assume that the beams are aligned along the coordinate axes and have wave vectors \( \hat{k}_x, \hat{k}_y \) and \( \hat{k}_z \). Thus dropping an unimportant constant in the potential we may write

\[
U(x) = - \sum_{\mu} \kappa_{\mu} \cos(k_{\mu}x_{\mu})
\]

where \( x_{\mu} \) runs over the coordinates \( x, y, \) and \( z \), and \( k_{\mu} = 2\hat{k}_{\mu} = 2\pi/d_{\mu} \), where \( d_{\mu} \) is the period of the lattice along axis \( \mu \). Also, \( V(x) \) is the magnetic trap potential and \( \Gamma = 4\pi\hbar^2 a/m \) is the interatomic interaction strength, with \( a \) the s-wave scattering length.

We now seek solutions to Eq. (1) using an expansion in terms of suitable Bloch functions of the optical potential. It will be helpful to begin by stating a few results.

A. Band structure and Bloch functions

We consider stationary solutions to the linear Schrödinger equation

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(x) \right] \phi(x) = E\phi(x).
\]

Bloch’s theorem [12] states that the solutions take the form

\[
\phi(x) = \phi_{n,k}(x) = e^{ik \cdot x} u_{nk}(x),
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where the functions $u_{nk}(x) = u_{nk}(x + R_s)$ share the periodicity of the lattice potential $U$, i.e., $R_s$ is any “lattice vector”, translation by which maps the potential onto itself. The energy eigenvalues $E = E_{nk}$ form a series of bands indexed by the quantum number $n$, with an infinite number of bands for each value of the wavevector $k$. It is also shown in any solid-state physics textbook, that the wavevectors are unique only up to the addition of an arbitrary “reciprocal lattice vector”. One can then restrict consideration to wavevectors lying within the “first Brillouin zone” [12]. In the one-dimensional case, this corresponds to the range $|k| < \pi/d$. We shall use a Dirac notation in which the wavefunction $\phi_{nk}(x)$ is denoted by $|nk\rangle$. In the usual way we restrict the wavevector to $N$ discrete values with $N$ large, so that the Bloch functions are normalized as

$$\langle mk|nk\rangle = \int_N d^3x \phi^*_m(x) \phi_{nk}(x) = N \Omega \delta_{mn} \delta_{kk'},$$

(5)

where the integral is taken over $N$ unit cells of volume $\Omega$.

For the potential in Eq. (2), Eq. (3) is separable and the well-known solutions are given by Mathieu functions [3]. In practice, the solutions and eigenvalues are probably found most simply by solving Eq. (3) directly.

B. Equations of motion

1. Bloch function expansion

Using the properties of the Bloch functions, we now develop an envelope function approach for an atomic field $\psi(x, t = 0)$ in a finite lattice. Certainly any wave function $\psi(x, t)$ may be expanded in terms of the complete Bloch modes as

$$\psi(x, t) = \sum_n \sum_k A_{nk}(t) |nk\rangle e^{-iE_{nk}t/\hbar}.$$  

(6)

One could easily write down evolution equations for the amplitudes $A_{nk}$ but such a procedure is of little use for finite systems in which the wave function does not have the infinite extent of the Bloch modes. A very large number of the $A_{nk}$ would be required to accurately describe the dynamics. Instead it is more natural to use the Bloch functions to capture the rapid oscillations in the wave function but describe the localization of the field through slowly varying envelopes. We thus suppose that the atomic field is characterized by a central wave vector $k_0$ and try an expansion of the form

$$\psi(x) = \sum_n f_{nk_0}(x, t) |nk_0\rangle e^{-iE_{nk_0}t/\hbar}.$$  

(7)

where the envelope functions $f_{nk_0}(x, t)$ are assumed to vary slowly on the scale of the lattice period. This is just the case for atomic BECs or an atom laser, as the momentum distribution is always distributed narrowly about some central wave vector. We defer the question of the choice of $k_0$ and the calculation of the initial envelopes $f_{nk_0}(x, t = 0)$ for a moment and concentrate on the dynamics.

Substituting Eq. (7) into the governing Eq. (1) gives a complicated equation involving sums over all the envelope functions and still involving the rapidly oscillating periodic potential. To obtain a simpler description, one insists that the variation of the $f_{nk_0}$ with $x$ occurs on slower scales than that of the Bloch functions $|nk_0\rangle$. Such a condition may be applied using the effective mass formalism of solid state theory [12], or equivalently, using “multiple scales” techniques as has been demonstrated in the context of nonlinear optics in a series of papers by de Sterke, Sipe and co-workers [8,14]. Essentially, one obtains an equation for each envelope by dotting from the left with each Bloch function $\langle nk|$. Essentially, one obtains an equation for each envelope by dotting from the left with each Bloch function $\langle nk|$. In fact, if more than two envelopes are included the resulting equations remain quite complicated. For a start, all the bands are coupled by the nonlinearity, but there are also linear couplings that occur between bands with a small energy separation [14]. However, for many problems of interest, it may be sufficient to consider just one or two bands. For example, the stationary ground state solution must attain the lowest energy possible. Providing the nonlinearity is not too large, the dominant contribution to the solution is then provided by the lowest band at $k_0 = 0$. If the nonlinearity is very large, coupling to the higher bands can not be ignored and either more bands must be included or a different approach adopted. We return to this point in section IV. A one band approach can also be acceptable for time-dependent problems. A natural experiment might be to form a condensate in the stationary ground state of the lattice and then apply a weak momentum kick via a momentary change in the potential. In this case, we would expect the solution to be well represented by an expansion on the lowest band but concentrated around a nonzero value $k_0$. If the system is tuned close to a band gap, however, there is strong coupling between the Bloch modes above and below the gap, and a two-mode approach is necessary [3]. We consider this situation in section IV. 

[12]
2. Single band approach

In calculating solutions we shall concentrate on the stationary ground state of the BEC in the finite lattice, and hence a single envelope function is sufficient. We emphasize that for the envelope function approach to be valid, the nonlinearity must be considered a perturbation. We discuss the regime of applicability imposed by this constraint when we examine results in section 3A.

By applying the effective mass or multiple scales methods, we simply obtained the reduced GPE for the envelope function \( f_{n_{k_0}} \),

\[
\tag{8}
\hat{h} \left( \frac{\partial f_{n_{k_0}}}{\partial t} + \mathbf{v}_g \cdot \nabla f_{n_{k_0}} \right) = -\frac{\hbar^2}{2m^{*\mu\nu}} \frac{\partial^2}{\partial x_\mu \partial x_\nu} f_{n_{k_0}} + V(x)f_{n_{k_0}} + \Gamma^* |f_{n_{k_0}}|^2 f_{n_{k_0}},
\]

where

\[
\mathbf{v}_g = \mathbf{v}_{n_{k_0}}(k_0), \\
\frac{1}{m^{*\mu\nu}} = \frac{1}{m} + \sum_{p \neq n} \frac{\delta_{p_{n_{k_0}}}(k_0)\nu_p(k_0) + \nu_{p_{n_{k_0}}}(k_0)\nu_p(k_0)}{(E_{n_{k_0}} - E_{p_{k_0}})},
\]

\[
\Gamma^* = \frac{\Gamma}{\Omega} \int_{\text{cell}} d^3\mathbf{x} |u_{n_{k_0}}(\mathbf{x})|^4,
\]

and the velocity matrix elements are defined as

\[
\mathbf{v}_{ij}(k_0) = \frac{\langle k_0 | \hat{p}_j k_0 \rangle}{m} = \frac{1}{m} \left( \hbar \delta_{ij} + \int_{\text{cell}} d^3\mathbf{x} u_{n_{k_0}}(\mathbf{x})^{*} \frac{\mathbf{p} u_{j_{k_0}}(\mathbf{x})}{m} \right).
\]

Equation (8) is valid provided that the maximum nonlinear “detuning” \( \Gamma^* |f_{n_{k_0}}|^2 \) at the point where \( |f_{n_{k_0}}| \) attains its largest value is small compared to the energy separation to the nearest adjacent band at wave vector \( k_0 \). If this is not the case we must use a two band model as discussed in section 3B. We now have a significant advance in that the periodic potential does not appear explicitly in Eq. (8). Its action is effectively represented through the three parameters in Eqs. (9) which we now discuss. The envelope \( f_{n_{k_0}} \) moves with a group velocity \( \mathbf{v}_g \) which is simply the gradient of the band \( n \) at wavevector \( k_0 \). Note that at particular points of symmetry the group velocity vanishes, notably at the band edges, and of course at the bottom of the lowest band for \( n = 0, k = 0 \). The bare atomic mass \( m \) has been replaced by the effective mass tensor \( m^{*\mu\nu} \) which is determined by the interaction of the other bands with the band of interest [Eq. (10)]. The term involving the effective mass in Eq. (8) acts as a source of dispersion on the atomic field. Taken together the group velocity and effective mass constitute a quadratic expansion of the band \( n \) around the point \( k_0 \). Finally, the parameter \( \Gamma^* \) describes the change in the effective nonlinearity due to the shape of the Bloch function. With a weak potential, for which \( u_{n_{k_0}}(\mathbf{k}) \) is almost a constant function, \( \Gamma^* \approx \Gamma \). However with a strong lattice, for which the Bloch functions become peaked within or between the wells, the magnitude of the effective nonlinearity increases significantly.

The wavevector \( k_0 \) is chosen in the first Brillouin zone and may be known from the nature of the problem—say an atom laser pulse of known momentum incident on the optical lattice—or might be calculated using an appropriate definition such as

\[
\mathbf{k}_0 = \int d\mathbf{k}^3 |\hat{\psi}(\mathbf{k}, t = 0)|^2 \mathbf{K}(\mathbf{k})
\]

where \( \hat{\psi}(\mathbf{k}) \) is the Fourier transform of \( \psi(\mathbf{x}) \) and \( \mathbf{K}(\mathbf{k}) \) is the vector in the first Brillouin zone equivalent to \( \mathbf{k} \). If a stationary state is sought we of course have \( \mathbf{k}_0 = 0 \).

3. Soliton solutions

Equation (8) is a nonlinear Schrödinger equation (NLSE) describing the evolution of the envelope field as it propagates through the lattice under the influence of the atomic interactions and the external potential \( V(x) \). Note that for one-dimensional geometries in the limit of vanishing \( V(x) \) we can obtain soliton solutions for the envelope. It must be emphasized that it is the envelope function that has soliton solutions, hence these are not the same objects as the standard atomic solitons found when the field operator or wave function itself satisfies a NLSE. The
envelope soliton propagates at a velocity determined by the local gradient of the band structure and with a width
determined by a balance between the nonlinearity and the effective mass, rather than the bare mass. Such “Bragg
grating solitons” have been observed in recent years in optical fiber gratings at extremely high laser powers [1,2].
In the present case, the nonlinearity is much stronger and BEC grating solitons should be easier to generate.
For example, our calculations suggest that for sodium atoms in a weak lattice generated by a diode laser of wavelength
985 nm (see section III A), a condensate of 500 atoms could produce a Bragg soliton extending over 30 periods of the
lattice.

For time-dependent problems, the term in $V(x)$ in Eq. (3) describes the response of the soliton to slow changes in
the non-periodic potential. For example a broad laser beam incident from the side could be used to produce a local
“hill” in the optical lattice. Gradients in this potential of course generate spatial oscillations in the field, which is to
say, they induce wave vector shifts. For modest wave vector shifts, Eq. (8) correctly describes the resulting changes in
the non-periodic potential. For example a broad laser beam incident from the side could be used to produce a local

III. STATIONARY SOLUTIONS

While the possibility of Bragg solitons in BEC’s is interesting, it is the properties of the ground state solution of a
BEC in a lattice which are initially likely to be of most importance for experiments, and it is on these that we focus.
We shall concentrate on the one-dimensional geometry which is perhaps the most pertinent experimentally. The
harmonic trap potential $V\equiv \frac{1}{2}m\omega^2 r^2$ of the lattice is unity. We shall find it useful to use both at different t
imes. The sets are introduced by choosing natural choices of dimensionless variables: the usual set of harmonic
oscillator units and a set in which the period $\omega_0$ and the velocity and shape of the soliton. However, if the shift becomes too large, the quadratic expansion of the Bloch band
say, they induce wave vector shifts. For modest wave vector shifts, Eq. (8) correctly describes the resulting changes in

The wave function is written $\psi(z) = a(\xi)\phi_0(\xi)$ where $\phi_0(\xi)$ is the lowest energy Bloch function ($k = 0$ in the lowest
band) for a lattice of depth $\kappa$ and period 1, and has eigenvalue $E_{k=0}(\kappa) = E_{n=0,k=0}/\epsilon_0$. In the lattice units, Eq. (8)
becomes

$$Ea(\xi) = \left[ -\frac{1}{2}\frac{d^2}{d\xi^2} + \frac{1}{2}\bar{\Omega}_0^2\xi^2 + C^*|a(\xi)|^2 \right] a(\xi). \quad (14)$$

$$\mu\psi(z) = \left[ -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} - \kappa\cos(k_z z) + \frac{1}{2}m\omega_z^2 z^2 + N\bar{\Gamma}|\psi(z)|^2 \right] \psi(z), \quad (12)$$

where $\bar{\Gamma} = \Gamma/A_{\text{eff}} = 2\hbar\omega_{\text{eff}} a$ is the effective nonlinearity taking account of the transverse mode profile. There are two
canonical choices of dimensionless variables: the usual set of harmonic oscillator units and a set in which the period of the
lattice is unity. We shall find it useful to use both at different times. The sets are introduced by choosing
appropriate energy and distance scales. For the oscillator case, these are $\epsilon_0 = \hbar\omega_z$ and $Z_0 = \sqrt{\hbar/(m\omega_z)}$ respectively.
For the lattice case we instead have $\epsilon_l = \hbar^2/(md^2)$ and $Z_l = d$. We will use an overbar to denote quantities in
oscillator units and a caret for quantities in lattice units. Thus in oscillator units we have $\zeta = z/Z_0$, $f(\zeta) = \sqrt{Z_0}\psi(z)$,
$\hat{\Lambda} = \lambda Z_0$, $\hat{\kappa} = \kappa/\epsilon_0$, $\hat{\mu}_0 = \mu/\epsilon_0$, $\Omega_0 = \hbar\omega_z/\epsilon_0 = 1$ and $\hat{C} = N\bar{\Gamma}/(\epsilon_0 Z_0)$. Similarly for the lattice case, we have $\xi = z/Z_l$, $g(\xi) = \sqrt{Z}\psi(z)$ and $\hat{\Lambda} = \lambda Z_l = 2\pi$, while the other parameters are defined in the obvious fashion, replacing
the subscripts $l$ by $l$ and the overbars by carets.

We have included the number of atoms $N$ in the nonlinear constants $\hat{C}$ and $\hat{C}$ and so the wave functions are
normalized to unity. We now turn to finding the ground state solutions of Eq. (12), identifying a number of regimes
depending on the relative strength of the interactions and the lattice.

A. Weak nonlinearity

The regime of a weak nonlinearity is handled well by the effective mass envelope function approach introduced in
section 4. In this case the nonlinearity and the harmonic trap both act as perturbations to the dominant lattice
potential and it is convenient to use lattice units. Thus we seek solutions to

$$\hat{\mu}g(\xi) = \left[ -\frac{1}{2}\frac{d^2}{d\xi^2} - \hat{\kappa}\cos(2\pi\xi) + \frac{1}{2}\bar{\Omega}_0^2\xi^2 + \hat{C}|g(\xi)|^2 \right] g(\xi). \quad (13)$$

The wave function is written $g(\xi) = a(\xi)\phi_0(\xi)$ where $\phi_0(\xi)$ is the lowest energy Bloch function ($k = 0$ in the lowest
band) for a lattice of depth $\kappa$ and period 1, and has eigenvalue $E_{k=0}(\kappa) = E_{n=0,k=0}/\epsilon_1$. In the lattice units, Eq. (8)
becomes

$$\hat{E}a(\xi) = \left[ -\frac{1}{2}\frac{d^2}{d\xi^2} + \frac{1}{2}\bar{\Omega}_0^2\xi^2 + C^*|a(\xi)|^2 \right] a(\xi). \quad (14)$$
As the lattice period in Eq. (12) is unity, the shape of the Bloch function \( \phi_0(\xi) \) is specified by the single parameter \( \hat{\kappa} \), as are the values of the nonlinearity \( \hat{C}^* = \gamma(\hat{\kappa}) \hat{C} \), with

\[
\gamma(\hat{\kappa}) = \int_0^1 d\xi |\phi_0(\xi)|^4,
\]

and the (now scalar) effective mass given by

\[
\frac{1}{\hat{m}^*} = 1 + 2 \sum_{\rho>0} \frac{\left| \langle \phi_\rho(\xi) | -i\partial/\partial\xi | \phi_0(\xi) \rangle \right|^2}{E_{\rho 0} - E_{\rho 0}},
\]

where the Bloch functions \( \phi_\rho(\xi) \) and energies \( E_{\rho 0} \) are of course normalized in lattice units. If we did not use lattice units, we would be forced to consider the dependence of these quantities on the lattice period as well. The effective quantities for the cosine potential are plotted in Fig. 1 as a function of \( \hat{\kappa} \). Note that in the limit of a vanishing lattice potential, \( \hat{m}^* = 1 \) and \( \gamma(\hat{\kappa}) = 1 \). For large \( \hat{\kappa} \), the Bloch function tends to a sequence of harmonic oscillator ground state wave functions and \( \gamma(\hat{\kappa}) \to \hat{\kappa}^{1/4} \).

The importance of Eq. (14) is that the problem including the lattice has now been reduced to the usual GPE for a condensate in just a harmonic trap with no lattice. All the physics involving the lattice is contained in the effective parameters and we are left with an equation whose properties are well understood. Equation (14) may naturally be solved in identical fashion to the standard GPE—numerically in general, or using Gaussian or Thomas-Fermi approximations (TFA) in appropriate limits. In particular, the TFA solution has the form

\[
|\alpha(\xi)|^2 = \max \left\{ \frac{\hat{E} - \hat{\Omega}_0 \hat{\kappa}^2/2}{\hat{C}^*}, 0 \right\}.
\]

Note that as the effective mass grows rapidly with \( \hat{\kappa} \) (see Fig. 1), the TFA to Eq. (14) is valid for quite modest values of \( \hat{\kappa} \). It must be emphasized though, that physically, this “effective mass TFA” (EMTFA) is a rather different approximation to the standard TFA which applies when the total kinetic energy is negligible. Here it is only the kinetic energy associated with the oscillation in the Bloch function but this of course has been removed from Eq. (14). It must be realized that even if Eq. (14) is solved numerically, this represents a significant gain over a direct numerical solution of the complete GPE with the lattice potential included. From a practical point of view, the numerical routine is much faster as it requires a small fraction of the grid points required to simulate the whole lattice. This advantage is most obvious when one considers time-dependent problems using Eq. (14) rather than Eq. (1). Less prosaically, the separation of scales allows a clearer physical insight into the expected general shape of the ground state condensate, with the precise details of the rapid oscillation subsumed into a few parameters, that need only be calculated once.

Let us now consider the regime of validity for the effective mass approach as a whole and the EMTFA. To justify an expansion in terms of the linear Bloch modes of the lattice, the effect of the nonlinearity in Eq. (13) must be small compared to that of the lattice potential, on the scale of a single period. This is the sense in which the nonlinearity is to be regarded as a perturbation. Thus if \( \rho = g(\xi)^2 \) is the density of the envelope function, we require

\[
\hat{C}\rho \ll \hat{\kappa}.
\]

Assuming that this is so, it may be checked that the EMTFA to Eq. (14) is valid if

\[
\hat{C}^* \gg 2\sqrt{\hat{\Omega}_0/(\hat{m}^*)^{3/4}},
\]

Using the EMTFA expression for the peak envelope density at the origin, Eq. (18) may then be expressed as

\[
\hat{\Omega}_0 \hat{C} \ll \frac{2}{3} \sqrt{\gamma(\hat{\kappa})(2\hat{\kappa})^3}.
\]

Note that due to its weak dependence on \( \hat{\kappa} \), the dependence on \( \gamma(\hat{\kappa}) \) may usually be ignored. If the EMTFA is not valid, we can obtain a different bound on \( \hat{C} \) by noting that the peak density of the envelope will certainly be lower than for the associated linear system for which \( a(\xi) = 1/\sqrt{2r_0 \pi} \exp(-\xi^2/(2r_0^2)) \), with \( r_0 = 1/\sqrt{\hat{\Omega}_0 \hat{m}^*} \). Thus we obtain the condition

\[
\hat{C} \ll \hat{\kappa} \sqrt{\frac{\hat{\Omega}_0 \hat{m}^*}{\pi}}.
\]
But as Eq. (19) is not true, Eq. (21) is satisfied provided only that \( \hat{\Omega}_0 \ll \sqrt{\pi \hat{\kappa}} \). These conditions are summarized in Table I along with the chemical potential which is given by \( \tilde{\mu} = \tilde{E}_0(\hat{\kappa}) + \tilde{E} \rightarrow \hat{E}_0 + (\tilde{3C}C^\ast\hat{\Omega}_0/2)^{2/3}/2 \), where the second relation holds when the EMTFA is valid. To demonstrate that these conditions could be satisfied by current experiments we consider Na\(^{23}\) atoms with a lattice produced by counter propagating beams from a diode laser at 985 nm \([21]\) so that \( d = 0.49 \mu \text{m} \). Taking a detuning of \( \Delta = 10^{10} \text{s}^{-1} \) and a maximum Rabi frequency of \( \Omega_s = 0.01\Delta \) we obtain a maximum lattice depth of \( \hat{\kappa}_{\text{max}} = \kappa_{\text{max}}/\epsilon_1 = \hbar\Omega_s^2/(\epsilon_1\Delta) \approx 90 \). Assuming \( \omega_r/(2\pi,50) = \omega_z/(2\pi) = 20 \text{ Hz} \) and a scattering length \( a = 5 \text{ nm} \) gives \( \hat{\Omega}_0 = 0.01 \) and \( \hat{C} = 0.013N \). Choosing \( \hat{\kappa} = 90 \), we could satisfy Eq. (20) with condensates of up to a few million atoms.

We show two examples of the envelope approach in Fig. 3 comparing the condensate density as a function of position according to the various models discussed above. For both plots the nonlinearity \( \hat{C} = 1 \) and trap frequency \( \Omega_0 = 0.05 \). Fig. 3a shows a case for a weak lattice with \( \hat{\kappa} = 10 \), while in Fig. 3b, the lattice strength is \( \hat{\kappa} = 100 \). The results of exact numerical calculations using Eq. (13) are shown by the solid line in each figure. For clarity, we show only the positive \( \xi \) part of the solution; the negative part is an exact mirror of this. The overall extent of the wave function is similar in the weak and strong lattices with the weak lattice case appearing to have a longer tail in the condensate density. In the stronger lattice, the oscillations are clearly more pronounced with the density confined more closely to the center of each well.

Turning to the accuracy of our approximate descriptions, for the weak case in Fig. 3a, the effective mass description of Eq. (14) is shown with a dotted line which is barely distinguishable from the exact result. The dashed line indicates the EMTFA solution which provides reasonable agreement with the exact solution near the center of the trap but fails towards the edge where the neglect of the envelope’s kinetic energy with respect to the nonlinear part is invalid. For the strong lattice (Fig. 3b), the effective mass and EMTFA results are now perfectly superposed and are both indicated by the dashed line which has excellent agreement with the exact case for all but the last two peaks of the distribution. These results concur with the validity regime calculations above: due to the difference in effective masses, Eq. (19) predicts that the EMTFA should be valid for the strong lattice but not for the weak.

An additional dot-dashed line in each figure indicates the exact solution of Eq. (12) when the nonlinearity vanishes (\( \hat{C} = 0 \)). Comparing the two linear solutions shows how in the absence of a nonlinearity, the condensate shrinks with increasing lattice strength due to the increase in effective mass. In both figures, the exact solution is clearly broader than the linear result, despite the repulsive effect of the kinetic energy being reduced through the effective mass. This reduction is of course outweighed by the dominant repulsive nature of the nonlinearity. In spite of this, the linear Bloch function is perfectly adequate to represent the rapid oscillation—the nonlinearity is not strong enough to distort the wave function on the scale of a single period.

Finally we consider the relative density distributions for the two exact solutions. Increasing the lattice strength produces two competing effects—the increase effective mass reduces the repulsion due to the kinetic energy, while the increase in effective nonlinearity increases the interatomic repulsion. For large enough effective mass, however, the kinetic energy plays essentially no role and any further increase in the mass makes no difference, whereas the effective nonlinearity and therefore the nonlinearly-induced repulsion grows slowly but without bound. Hence, we should expect that the condensate spreads out with increasing lattice strength. In Fig. 3, we plot the cumulative density \( \int_{-rac{\pi}{2}}^{\frac{\pi}{2}} d\xi' |g(\xi')|^2 \) as a function of \( \xi \) for several values of the lattice strength \( \hat{\kappa} \). From this plot it is clear that in spite of the weakening kinetic energy, the condensate slowly expands as the lattice strength ranges over \( \hat{\kappa} = 0 \) (dot-dashed line), 10 (solid), 50 (dotted) and 100 (dashed), due to the increase in the effective nonlinearity [see Eq. (15)]. The second dot-dashed line indicates the cumulative density according to the EMTFA envelope for \( \hat{\kappa} = 100 \). Note that the exact solution in the weak lattice appears to have a longer tail than for the strong lattice (solid lines in Figs. 3).

Figure 3 shows that the structure of the tail is not indicative of the global density distribution.

### B. Strong nonlinearity

As the nonlinearity increases or the trap tightens, the assumption that the nonlinearity plays no role over a single period [Eq. (18)] breaks down. While one may use additional envelope functions each with their own Schrödinger equation, the utility of such an approach decreases quickly. However, if the nonlinearity is sufficiently large, we may abandon the Bloch function approach altogether, instead using the standard Thomas-Fermi approximation (TFA) by neglecting the kinetic energy term in Eq. (12). Sørenberg and Mølmer \([22]\) have used this approximation for the infinite uniform lattice. Here, we examine the more complicated system including the trap potential in the Thomas-Fermi regime. In this regime, the lattice is effectively a perturbation to the dominant harmonic trap, and it is natural to
invoke oscillator units, so that Eq. (12) becomes
\[
\bar{\mu} f(\zeta) = \left[ -\frac{1}{2} \frac{d^2}{d\zeta^2} - \bar{\kappa} \cos(\bar{\Lambda}\zeta) + \frac{1}{2} \zeta^2 + \bar{C}|f(\zeta)|^2 \right] f(\zeta).
\]
(22)

In estimating the boundary point \(\zeta_0\) of the condensate we may neglect the effect of the lattice, and take the usual value \(\zeta_0 = \sqrt{2\bar{\mu}}\). This is consistent with the nature of the approximation which is poor at the boundary anyway. Moreover, to the same degree of approximation the dependence of the chemical potential on atom number is unchanged from the lattice free result \(\bar{\mu} = (3\bar{C}/2)^{2/3}/2\).

The regime of applicability for the TFA is analyzed as follows. We must certainly have \(\bar{\mu} > \bar{\kappa}\) which prevents the solution from attaining zero density regions in every lattice well. The standard TFA condition that the total kinetic energy be negligible compared to the total potential and nonlinear energies is given by \(\bar{C} \gg 1\) as for the lattice-free case. However, if the oscillatory part of the solution is to be accurately represented by the factor \(\bar{\kappa} \cos(\bar{\Lambda}\zeta)/\bar{C}\) in Eq. (23) we must also consider the relative energies associated with just the oscillatory part. An approximate condition may be found by evaluating these energies over a single lattice period at the center of the trap and insisting as usual that the resulting kinetic energy be small compared to the potential and nonlinear energies. Assuming \(\bar{\kappa} \ll \bar{\mu}\) we eventually arrive at the additional condition
\[
\bar{\mu} \gg \bar{\Lambda}^2/4,
\]
(24)
or
\[
\bar{C} \gg 0.24\bar{\Lambda}^3.
\]
(25)

Note that in the lattice units, this has the slightly odd form \(\bar{\mu} \gg \pi^2\). We see below that this new condition is genuinely necessary.

We show examples in Fig. 4 with exact numerical solutions to Eq. (22) in solid lines, and the TFA in dotted lines. In all three plots we have \(\bar{C} = 3000\). In Fig. 4a the lattice strength \(\bar{\kappa} = 10\), and \(\bar{\Lambda} = 2\pi\). The exact chemical potential is \(\bar{\mu} = 136.2\). The requirements for the TFA are thus satisfied and there is good agreement between the exact and approximate solutions except near the boundary of the condensate. Figure 4b shows the solutions where the lattice strength is increased to \(\bar{\kappa} = 50\), for which the exact chemical potential is \(\bar{\mu} = 133.8\). The region of disagreement near the boundary is now of course larger, but there is still good agreement near the center of the condensate despite \(\bar{\kappa}\) approaching 50% of the chemical potential. In Fig. 4c, we have \(\bar{\kappa} = 50\) with a reduced lattice period such that \(\bar{\Lambda} = 5\pi\). The chemical potential is \(\bar{\mu} = 134\). As the ratio \(\bar{\mu}/(\bar{\Lambda}^2/4) = 0.54\), Eq. (24) indicates the TFA is invalid, in accord with the poor agreement between the TFA and exact curves. We emphasize that if the lattice were not present, the TFA would certainly be valid in this case because \(\bar{C} \gg 1\). The condition given by Eq. (24) is indeed important. The dashed lines in Fig. 4c indicate the extent of oscillations in the solution predicted by the single band Bloch function description used in the previous section for weak nonlinearity. This is clearly unsuccessful in this regime as we would expect. Comparing it to the exact solution indicates that the repulsive nature of the nonlinearity tends to reduce the amplitude of the oscillations as compared to the linear regime. Note that despite the range in shapes of the three exact solutions in Figs. 4a-c, the chemical potential varies by only a few per cent from the lattice free value \(\bar{\mu} = 136.2\). The parameter values used here would be easily obtained experimentally. Using the same trap frequencies \(\omega_t/(2\pi 50) = \omega_z/(2\pi) = 20\) Hz, we find a maximum lattice strength of \(\bar{\kappa}_{\text{max}} \approx 8000\) and an effective nonlinearity of \(\bar{C} \approx 0.1N\). Hence, a condensate of about \(N = 30000\) atoms would correspond to the predictions in Figs. 4. Note that when expressed in equivalent units, the lattice strength here is around 1% of that in section 11A, which explains why condensates of a million atoms could be considered to be weakly nonlinear in that section.

It is worth noting that in the TFA regime, an envelope function approach is not appropriate, because the amplitude of the oscillations in the condensate density due to the lattice are of the same size across the whole condensate. In contrast, we expect an envelope function approach to be appropriate if the rapid oscillations in the density scale linearly with the envelope density. This difference is clearly apparent if the exact solutions in Figs. 2 and 4 are compared.
Finally, we return to the propagation problem and briefly discuss the rather different physics involved for condensates with a center wave vector tuned close to a band gap. In this case, unless the gap is very large and the field is tuned close to one edge, then neither of the two bands surrounding the gap can be regarded as remote and the field should be expanded using a Bloch function from each band. As our primary interest has been in the ground state stationary solution which is always far from any gap, we shall not explore this case in detail. For the sake of completeness, however, we state the dynamical equations that correctly describe such a situation using a method of de Sterke et al. [14].

We label the two bands $u$ (upper) and $l$ (lower) and expand around a frequency $\omega_0 = (\omega_{uk} + \omega_{lk})/2$:

$$
\psi(x, t) = [f_{uk}(x, t) | uk] + f_{lk}(x, t) | lk] e^{-i\omega_0 t}.
$$

(26)

Again one insists that both $f_{uk}$ and $f_{lk}$ are slowly-varying functions and using the effective mass or multiple scales techniques obtains two coupled nonlinear equations for $f_{uk}$ and $f_{lk}$. In coupled mode theory of periodic structures it is often found convenient to work with envelopes modulating forward and backward going amplitudes as opposed to Bloch functions as these envelopes correspond closely to the field incoming and outgoing from the periodic structure. It can be shown that the amplitudes $G_\pm = (f_{lk} \mp i f_{uk})/2$ correspond to such amplitudes. In the limit of a weak potential where the Bloch functions at the band edge are cosine functions, the amplitudes $G_\pm$ simply modulate forward and backward-going plane waves. In terms of these variables the final dynamical equations are [14]

$$
\begin{align}
  i \frac{\partial G_+}{\partial t} &+ \bar{\nabla} G_+ + \sigma G_+ + V(x)G_+ + \Gamma_0(|G_+|^2 + 2|G_-|^2)G_+ + \Gamma_1(|G_+|^2 + |G_-|^2)G_- + \Gamma_2 G_+^2 G_-^* = 0, \\
  i \frac{\partial G_-}{\partial t} &- \bar{\nabla} G_- + \sigma G_- + V(x)G_- + \Gamma_0(|G_-|^2 + 2|G_+|^2)G_- + \Gamma_1(|G_+|^2 + |G_-|^2)G_+ + \Gamma_2 G_-^2 G_+^* = 0.
\end{align}

(27a)

(27b)

The linear coupling parameter $\sigma = \Delta/2$, the group velocity $\bar{v}_g = |\langle uk | \hat{p} | lk \rangle|$, while the nonlinear coefficients are found from overlaps of the (real) Bloch functions:

$$
\begin{align}
  \Gamma_0 &= \frac{\alpha_{llll} + 2\alpha_{ulul} + \alpha_{uuuu}}{2}, \\
  \Gamma_1 &= \frac{\alpha_{llll} - \alpha_{uuuu}}{2}, \\
  \Gamma_2 &= \frac{\alpha_{llll} - 6\alpha_{ulul} + \alpha_{uuuu}}{2},
\end{align}

(28)

(29)

(30)

where

$$
\alpha_{ijkl} = \frac{1}{\Omega} \int_{\text{cell}} d^3x \phi_i(x) \phi_j(x) \phi_k(x) \phi_l(x)
$$

(31)

for $\{i, j, k, l\} \in \{u, l\}$. In these equations, we have dropped the kinetic energy terms involving the effective mass altogether. The coupling between the bands through the parameter $\sigma$ itself produces a dispersive behavior which is much larger than the intrinsic dispersion within each band. In the limit of a weak potential, the coefficients $\Gamma_1$ and $\Gamma_2$ vanish and one obtains the well-known coupled mode equations for propagation in nonlinear periodic systems. Such equations were recently obtained in the BEC context by Zobay et al. [3] and used to predict the occurrence of gap solitons in condensates with multiple internal levels. Their system differs from ours in that it involves a Raman coupling between two magnetic ground states whereas we have used a strictly scalar field interacting with an external potential. The fact that both systems can be reduced to identical equations is an indication of the underlying physical consequences of combining a nonlinearity with a periodic system—properties such as gap solitons and switching appear ubiquitously. The full “deep grating” equations [27] with $\Gamma_1, \Gamma_2 \neq 0$ (but $V(x) = 0$ were first derived by Salinas et al. [22] to describe optical propagation in Bragg gratings with large index variation between the two media. The additional terms in these equations lead to predictions that depart from the shallow grating results for index variations of 10% or more. In the atomic case, the analogous situation is when the lattice potential is deep and the Bloch functions at the band edge depart from simple plane waves. The exposure of condensates to such deep lattices is certainly a realistic goal in the laboratory and the use of the deep grating equations may thus be important.
in modeling propagation in lattices in the future. These arguments hold equally for the Raman geometry used by Zobay et al.

We should remark that the use of a two band model as described here is not always possible. In the case of extremely deep potentials the band gap widths may broaden so much they become comparable to the original separations between the gaps. In that case, the existence of two bands that are significantly closer to the center frequency than all the others is doubtful. However, if the desired center frequency is closer to one band edge than the other, a one band model may again become feasible.

V. CONCLUSION

We have introduced a Bloch function analysis of a BEC trapped in a finite optical potential. The approach describes both pulse propagation and stationary solutions providing a single Schrödinger like equation for the envelope function provided the nonlinearity is not too large. If the physical parameters lie within the constraints we have given, the envelope function solution agrees extremely well with the exact numerical results. For very strong nonlinearities, the standard Thomas-Fermi approximation is the correct description for the ground state, but its application requires a stronger condition than in the absence of the lattice.

ACKNOWLEDGMENTS

We thank C. Martijn de Sterke and Karl-Peter Marzlin for useful discussions. This research was supported by the Australian Research Council.

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FIG. 1. Effective nonlinearity $\Gamma^*$ (solid) and mass $m^*$ (dotted) for a one-dimensional cosine potential of strength $\kappa$. 
FIG. 2. Wave function $\psi(\xi)$ as a function of $\xi$ for a) $\hat{\kappa} = 10$ and b) $\hat{\kappa} = 100$. Other parameters are $\hat{\Omega}_0 = 0.05$ and $\hat{C} = 1$. Line styles indicate models as exact numerical (solid), effective mass (dotted), EMTFA (dashed) and linear (dot-dashed). In b), the effective mass and EMTFA models are both represented by the dashed curve.

FIG. 3. Cumulative density $\int_{-\xi}^{\xi} d\xi' |g(\xi')|^2$ as a function of $\xi$ for values of the lattice depth $\hat{\kappa} = 10$ (solid line), 50 (dotted) and 100 (dashed). The dot-dashed lines indicate the cumulative density of the exact solution for $\hat{\kappa} = 0$, and of the EMTFA envelope for $\hat{\kappa} = 100$.

FIG. 4. Exact wave function $f(\zeta)$ (solid line) and Thomas-Fermi estimate (dotted) with nonlinearity $\bar{C} = 3000$ and a) $\bar{\kappa} = 10$, $\bar{A} = 2\pi$, b) $\bar{\kappa} = 50$, $\bar{A} = 2\pi$ and c) $\bar{\kappa} = 50$, $\bar{A} = 5\pi$. The dashed line in c) denotes the prediction of the envelope function approach.

| Regime                      | Conditions                                                                 | Chemical potential                                                                 |
|-----------------------------|-----------------------------------------------------------------------------|-----------------------------------------------------------------------------------|
| Weak: $\hat{C}_\rho \ll \hat{\kappa}$, (EMTF) | $C^* \gg 2\sqrt{\hat{\Omega}_0/\hat{m}^*}^{3/4}$, $\hat{\Omega}_0 \hat{C} \ll \frac{2}{3} \hat{\gamma} (\hat{\kappa}) (2\hat{\kappa})^3$ | $\bar{\mu} = \bar{E}_{00}(\hat{\kappa}) + (3\bar{C}^*/2)^{2/3}/2$ |
| Weak: $\hat{C}_\rho \ll \hat{\kappa}$, (non-EMTF) | $\hat{C} \ll \hat{\kappa} \sqrt{\hat{\Omega}_0 \hat{m}^*}/\pi$                 | $\bar{\mu} = \bar{E}_{00}(\hat{\kappa}) + \bar{E}$                                |
| Thomas-Fermi:               | $\bar{\mu} \gg \bar{A}^2/4$, $\bar{C} \gg 0.24\bar{A}^3$                 | $\bar{\mu} \approx (3\bar{C}/2)^{2/3}/2$                                        |

**TABLE I.** Validity criteria and chemical potential for ground state solutions in different regimes.
Steel and Zhang, Figure 3

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3}
\caption{Cumulative density function for different values of $\hat{\kappa}$.}
\end{figure}
Steel and Zhang, Figure 4b
Steel and Zhang, Figure 2a

The graph shows the function $g(\xi)$ plotted against $\xi$. The x-axis represents $\xi$ ranging from 0 to 14, and the y-axis represents $g(\xi)$ ranging from 0 to 0.6. The graph includes multiple curves, indicating variations in $g(\xi)$.
