Bogoliubov sound speed in periodically modulated Bose-Einstein condensates

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We study the Bogoliubov excitations of a Bose-condensed gas in an optical lattice. Of primary interest is the long wavelength phonon dispersion for both current-free and current-carrying condensates. We obtain the dispersion relation by carrying out a systematic expansion of the Bogoliubov equations in powers of the phonon wave vector. Our result for the current-carrying case agrees with the one recently obtained by means of a hydrodynamic theory.

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I. INTRODUCTION

The possibility of creating optical lattices in trapped Bose-condensed gases has provided an opportunity to study superfluids in novel situations. The presence of the lattice leads to a variety of solid state effects associated with the coherent motion of the atoms in a periodic potential. For example, the oscillation frequency of the centre of mass motion of the condensate is reduced as a result of the enhanced effective mass of the atoms tunnelling between potential wells. Furthermore, when subjected to a uniform force, as provided by gravity or alternatively by accelerating the optical lattice itself, Bloch oscillations of the condensate have been observed. Reducing the amplitude of the lattice potential leads to a breakdown of these oscillations as a result of Landau-Zener tunnelling between bands. All of these observations are essentially a manifestation of the superfluidity of the Bose condensate in an optical lattice. Another aspect of equal interest is the breakdown of superfluidity as recently observed in a study of the centre of mass motion of a trapped condensate moving through an optical lattice. When the amplitude of the oscillation exceeded a critical value, dissipation was seen to set in.

In this paper we study a Bose-condensed gas subjected to a uniform optical lattice in a regime where the dynamics of the condensate wave function is well described by the time-dependent Gross-Pitaevskii (GP) equation. In particular, we are concerned with small amplitude collective modes which at long wavelength are phonon-like excitations. The relevant physical parameters determining the properties of the excitation are the optical potential amplitude, \( V_0 \), the lattice constant, \( d \), the mean density, \( \bar{n} \), of the gas, and the magnitude of the supercurrent. The problem has been addressed theoretically in a number of papers using a variety of techniques and approximations.

Berg-Sørensen and Mølmer were the first to investigate phonon excitations within an optical lattice. They solved the Bogoliubov equations numerically for a onedimensional model and established that the long wavelength excitations are phonon-like, having an energy dispersion that is linear in the wave vector of the mode. They also obtained an analytic expression for the sound speed, \( s \), which is based on a combined weak potential and slowly varying approximation. These calculations were extended by Wu and Niu to the case in which the condensate carries a current. This work is noteworthy for having pointed out that the modes exhibit both energetic and dynamic instabilities for sufficiently large currents. The former instability is associated with the Landau criterion for the breakdown of superfluidity, while the latter is related to the onset of dissipation as observed in.

The recent paper by Machholm et al. explores these instabilities further. Similar results were obtained by Bronski et al. by considering a special form of the lattice potential, while Konotop and Salerno used a different approach to establish that the dynamic (or modulational) instability leads to the generation of solitons.

When the potential wells are sufficiently deep, the condensate is well-localized on each lattice site and a tight-binding description becomes useful. Javanainen used this picture within a many-body formulation to derive the phonon dispersion throughout the Brillouin zone for a one dimensional lattice. This calculation is in fact equivalent to one based on the Bogoliubov equations or the discrete version of the time-dependent GP equation. The virtue of these methods is that they provide analytical expressions for the dispersion relation, although an accurate a priori determination of the tight-binding parameters involves further numerical calculation. Smerzi et al. extended the results of Javanainen by deriving the phonon dispersion for a current-carrying state and found a dynamic instability that is responsible for a so-called ‘superfluid-insulator’ transition.

The phonon dispersion at long wavelengths was addressed by deriving an energy functional involving density and phase fluctuations which vary slowly in space. The approach is closely allied to the effective mass approximation used in solid state physics and recently applied to Bose gases in optical lattices, and to multiple-scale analysis. The phonon sound speed is found to be

\[
s = \sqrt{\frac{n \partial \mu}{m^* \partial \bar{n}}}
\]

where \( m^* \) is an effective mass and \( \mu \) is the chemical potential. The precise definition of the effective mass as...
part we restrict ourselves to a cubic lattice for which \( R \) is a Bravais lattice vector. For the most part we restrict ourselves to a cubic lattice for which the effective mass appearing in both the effective mass and multiple-scale theories is that corresponding to the bare optical potential. In other words, the effect of the interactions on this parameter is not included, and therefore the use of the dynamical equations obtained in these theories will not in general give the correct Bogoliubov sound speed.

Our purpose in this paper is to obtain the long-wavelength phonon dispersion directly from the Bogoliubov equations defining the collective modes. This is achieved by developing a systematic expansion of these equations in powers of the phonon wave vector \( q \). We do this first for the current-free state (Sec. III), confirming the result for the sound speed given above. We then consider a current-carrying state (Sec. IV) and obtain the analogous phonon dispersion in this case, reproducing the result obtained by means of a hydrodynamic analysis. Our expansion technique can be viewed as a justification of the assumptions on which the hydrodynamic approach is based. Furthermore, it provides explicit perturbative expressions for the various physical quantities that appear in the theory (for example, the effective mass).

In Sec. II we present the theoretical background required for the calculation of small amplitude collective excitations in an optical lattice. For the most part we consider a three dimensional optical potential with cubic symmetry, although we also touch on systems with one dimensional modulation as well as radially confined condensates. The underlying periodicity of the optical potential implies that the Bogoliubov equations admit solutions having a Bloch function form. This aspect accounts for the use of a Bloch function basis in solving these equations in both the current-free (Sec. III) and current-carrying (Sec. IV) states. However, different calculational methods are used in the two cases and these are therefore presented separately. We also examine various physical limits (Thomas-Fermi, weak potential, weak coupling and tight-binding) in order to make contact with previous work. As stated previously, our main result for the phonon dispersion affirms the result which follows from the insightful use of hydrodynamic equations to describe the dynamics of long wavelength fluctuations.

II. BASIC THEORY

We consider an extended 3D BEC subjected to standing wave light fields that give rise to a periodic external potential having the property \( V_{opt}(r + R) = V_{opt}(r) \), where \( R \) is a Bravais lattice vector. For the most part we restrict ourselves to a cubic lattice for which \( R = d(n_1\hat{x} + n_2\hat{y} + n_3\hat{z}) \), with \( n_i \) an integer.

We base our analysis on the time-dependent Gross-Pitaevskii (GP) equation for the condensate wave function, \( \Psi(r,t) \),

\[
    i\hbar \frac{\partial}{\partial t} \Psi(r,t) = \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{opt}(r) + g|\Psi(r,t)|^2 \right) \Psi(r,t).
\]

This equation admits stationary solutions of the form \( \Psi(r,t) = \Phi(r)e^{-i\mu t/\hbar} \) where \( \Phi(r) \) satisfies the time-independent GP equation

\[
    \frac{-\hbar^2}{2m} \nabla^2 \Phi + V_{opt}\Phi + g|\Phi|^2\Phi = \mu\Phi \tag{2}
\]

with the normalization \( \int_V d^3r |\Phi(r)|^2 = N \), where \( N \) is the total number of particles in the volume \( V \). Also of interest is the total energy of the system given by

\[
    E_{tot} = \int_V d^3r \Phi^* \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{opt} \right) \Phi + \frac{g}{2} \int_V d^3r |\Phi|^4. \tag{3}
\]

The energy parameter \( \mu \) is the chemical potential and is related to \( E_{tot} \) by \( \mu = \partial E_{tot}/\partial N \).

Often the ground state solution of the GP equation is of interest but we shall also consider states which have a superfluid flow. These states have a Bloch function form

\[
    \Phi_{nk}(r) = \sqrt{n} e^{ik \cdot r} w_{nk}(r) \tag{4}
\]

where \( n \) is a band index and \( k \) is a wave vector restricted to the first Brillouin zone. The factor \( \sqrt{n} \), where \( \bar{n} \) is the mean density, is introduced in the definition of \( w_{nk} \) so as to give the normalization

\[
    \frac{1}{\Omega} \int_\Omega d^3r |w_{nk}(r)|^2 = 1, \tag{4}
\]

where \( \Omega \) is the Wigner-Seitz volume. The condensate density is then \( n_c(r) = |\Phi_{nk}(r)|^2 = \bar{n}|w_{nk}(r)|^2 \). The Bloch function \( w_{nk}(r) \) is in general complex and is the self-consistent solution of

\[
    \left( -\frac{\hbar^2 (\nabla + i\mathbf{k})^2}{2m} + V_{opt} + g\bar{n}|w_{nk}|^2 \right) w_{nk} = \mu_{nk} w_{nk}. \tag{5}
\]

We assume that \( w_{nk} \) has the periodicity of the lattice, \( w_{nk}(r+R) = w_{nk}(r) \), although it should be noted that period-doubled states also exist. The chemical potential, \( \mu_{nk}(\bar{n}) \), is implicitly a function of the mean density and depends on the particular Bloch state being considered.
The superfluid current density in this state is
\[ j_s(r) = \frac{\hbar}{2im} (\Phi_{nk}^* \nabla \Phi_{nk} - \nabla \Phi_{nk}^* \Phi_{nk}) \]
\[ = \frac{\hbar}{2m} n k |w_{nk}(r)|^2 + \frac{\hbar n}{2m} [w_{nk}^* \nabla w_{nk} - (\nabla w_{nk}^*) w_{nk}] \]
and has the property \( \nabla \cdot j_s(r) = 0 \). Introducing the superfluid velocity according to the relation
\[ j_s(r) = n_s(r) v_s(r), \]
we have
\[ v_s(r) = \frac{\hbar}{m} (k + \nabla \theta_{nk}(r)) \]
where \( \theta_{nk}(r) \) is the phase of the Bloch function \( w_{nk} \). The spatially-averaged superfluid velocity is
\[ \langle v_s \rangle = \frac{1}{\Omega} \int_{\Omega} d^3r \ n_s(r) = \frac{\hbar}{m} (k + \langle \nabla \theta_{nk} \rangle). \]
In one dimension, the periodicity of \( w_{nk}(x) \) implies \( \langle d\theta_{nk}/dx \rangle = 2\pi l/d \), where \( l \) is an integer. By continuity of the phase with \( k \), we expect \( l \) to have a fixed value for a given band, and \( \langle v_s \rangle = (\hbar/m)(k + G) \) where \( G \) is some reciprocal lattice vector. For the lowest band, we show in Appendix A that \( G = 0 \). Thus, we arrive at the somewhat surprising conclusion that \( \langle v_s \rangle = h \pi/m \). We suspect that similar results apply in higher dimensions but have not been able to show this explicitly.

The average superfluid velocity should be distinguished from the velocity determining the average current density
\[ \langle j_s \rangle = \frac{1}{V} \int_V d^3r \ n_s(r) \frac{\hbar}{m} \nabla \Phi_{nk} \]
\[ = \frac{\hbar}{m \Omega} \int_{\Omega} d^3r w_{nk}^* (p + i\hbar) w_{nk} \]
\[ \equiv \bar{n} v_{nk}. \]
This velocity is given by \[ v_{nk} = \frac{1}{\bar{n}} \nabla \bar{n} \bar{\varepsilon}(\bar{n}, k), \]
where \( \bar{\varepsilon}(\bar{n}, k) = \epsilon_{\text{tot}}/N \) is the energy per particle in the state characterized by the mean density \( \bar{n} \) and quasimomentum \( k \).

In one dimension, the average current density vanishes at the zone boundary \( k = \pi/d \) if the mean density is below a critical value \( \bar{n}_c \). On the other hand, the average superfluid velocity is \( \langle v_s \rangle = h \pi/md \). This is not a contradiction since the local superfluid velocity in \[ v_{nk} \] is averaged differently when calculating the average current density.

Dynamical states of the condensate are determined by the time-dependent GP equation \[ \Psi(r, t) = [\Phi_{nk}(r) + \delta \Phi(r, t)] e^{-i\omega_{nk} t/\hbar} \]
and the GP equation is expanded to first order in the deviation \( \delta \Phi(r, t) \). By writing
\[ \delta \Phi(r, t) = u_i(r) e^{-iE_i t/\hbar} - v_i(r) e^{iE_i t/\hbar}, \]
where \( E_i \) is allowed to be complex, one obtains the following Bogoliubov equations for the quasiparticle amplitudes \( u_i \) and \( v_i \),
\[ \hat{L} u_i(r) - g \Phi_{nk}^2(r) v_i(r) = E_i u_i(r) \]
\[ \hat{L} v_i(r) - g \Phi_{nk}^2(r) u_i(r) = -E_i v_i(r) \]
where the operator \( \hat{L} \) is defined as
\[ \hat{L} \equiv -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{opt}} + 2g|\Phi_{nk}|^2 - \mu_{nk}. \]
Each distinct solution labelled by the index \( i \) corresponds to a collective excitation of the condensate and \( E_i \) represents the excitation energy of the mode. The orthonormality of the quasiparticle amplitudes is specified by
\[ \int_V d^3r [u_i^* u_j - v_i^* v_j] = \delta_{ij}. \]

Since the operator \( \hat{L} \) has the translational symmetry of the lattice, the Bogoliubov equations admit solutions of the form
\[ u_i(r) = e^{i(q+k) \cdot r} \tilde{u}_i(r) \]
\[ v_i(r) = e^{i(q-k) \cdot r} \tilde{v}_i(r) \]
where \( \tilde{u}_i(r) \) and \( \tilde{v}_i(r) \) have the periodicity of the lattice. These functions satisfy
\[ \hat{L}_{q,k} \tilde{u}_i(r) - g \bar{n} \tilde{w}_{nk}^2(r) \tilde{v}_i(r) = E_i \tilde{u}_i(r) \]
\[ \hat{L}_{q,-k} \tilde{v}_i(r) - g \bar{n} \tilde{w}_{nk}^2(r) \tilde{u}_i(r) = -E_i \tilde{v}_i(r) \]
with
\[ \hat{L}_{q,k} \equiv -\frac{\hbar^2}{2m} (\nabla + i q + i k)^2 + V_{\text{opt}} + 2g\bar{n}|w_{nk}|^2 - \mu_{nk}. \]
Our notation emphasizes that \( q \) and \( k \) play distinct roles in the Bogoliubov equations: the former characterizes the Bloch-like character of the quasiparticle amplitudes while the latter corresponds to the quasimomentum of the condensate wave function.

In the following, we shall also make use of the Hamiltonian
\[ \hat{h}_k(q) \equiv -\frac{\hbar^2}{2m} (\nabla + i q + i k)^2 + V_{\text{opt}} + g\bar{n}|w_{nk}|^2 - \mu_{nk} \]
which for \( q = 0 \) is just the Hamiltonian determining the time-independent condensate wave function \( w_{nk} \).
III. PHONON DISPERSION FOR A STATIONARY CONDENSATE

We begin by considering the simpler situation in which there is no superfluid flow \((\mathbf{k} = 0)\). In this case, the ground state solution of the time-independent GP equation can be taken to be real, and \(\hat{\mu}_n = \hat{\mu}_n (\mathbf{r}) = \hat{\mu}_n (\mathbf{r}) = n \psi (\mathbf{r})\). It is then convenient to introduce the functions \(\psi_i^\pm = \hat{u}_i \pm \hat{v}_i\) and to combine the Bogoliubov equations into a single equation for \(\psi_i^+\)

\[
\hat{h}_0 \psi_i^+ + 2 g n_c \hat{h}_0 \psi_i^+ = E_i^2 \psi_i^+ \tag{19}
\]

where \(\hat{h}_0\) is the Hamiltonian

\[
\hat{h}_0 (q) = -\frac{\hbar^2}{2m} (\nabla + i q)^2 + V_{\text{opt}} + g \bar{n} |w_{0,0}|^2 - \mu_{0,0}, \quad (20)
\]

in which the mean field, \(g \bar{n} |w_{0,0}|^2\), of the current-free condensate appears.

To solve (19), we introduce a complete set of Bloch states which are solutions of the equation

\[
\hat{h}_0 (q) w_{nq} = \varepsilon_n (q) w_{nq}. \tag{21}
\]

This is a linear Schrödinger equation but the solution for \(q = 0\) and \(n = 0\) coincides with the self-consistent GP solution \(w_{0,0}\). By definition, the band energies, \(\varepsilon_n (q)\), are referred to \(\mu_{0,0}\), so that \(\varepsilon_0 (0) = 0\). The functions \(w_{nq}\) satisfy the periodicity property \(w_{nq} (\mathbf{r} + \mathbf{R}) = w_{nq} (\mathbf{r})\) and the orthonormality relation

\[
\frac{1}{\Omega} \int_{\Omega} d^3 r w^*_{nq} w_{n'q} = \delta_{nn'} . \tag{22}
\]

In addition, at \(q = 0\) they are chosen to be real.

Since \(\psi_i^+\) is itself a Bloch function, it can be expanded as

\[
\psi_i^+ (\mathbf{r}) = \sum_n c_n (q) w_{nq} (\mathbf{r}). \tag{23}
\]

The label \(i\) represents a band index \(m\) and the Bloch wave vector \(q\). However in the following, we will only be interested in the lowest excitation band and will therefore drop the label for convenience. Substituting this expansion into (19) we obtain

\[
\sum_{n'} M_{nn'} (q) \varepsilon_{n'} (q) c_{n'} (q) = E^2 (q) c_n (q) \tag{24}
\]

where

\[
M_{nn'} (q) = \frac{1}{\Omega} \int_{\Omega} d^3 r w^*_{nq} (\mathbf{r}) 2 g n_c (\mathbf{r}) w_{n'q} (\mathbf{r}) + \varepsilon_n (q) \delta_{nn'}. \tag{25}
\]

We have displayed explicitly the \(q\)-dependence of all the variables.

For a cubic lattice, we anticipate a particular eigenvalue \(E(q)\) which has a linear dispersion of the form

\[
E(q) = \hbar s q + \cdots \tag{26}
\]

Our objective is to derive an explicit expression for the Bogoliubov sound speed \(s\). From Eq. (19) it is clear that in the \(q \to 0\) limit, the eigenvector corresponding to this particular eigenvalue will be

\[
c_n (0) = \delta_{n0}, \tag{27}
\]

where \(n = 0\) labels the lowest Bloch band, since only this band has a vanishing energy \(\varepsilon_0 (0) = 0\). As a function of \(q\), the lowest band energy behaves as

\[
\varepsilon_0 (q) = \frac{\hbar^2 q^2}{2m_0} + \mathcal{O}(q^4) \tag{28}
\]

which defines the effective mass \(m_0\) of this band. We emphasize that this band mass is determined by the linear Schrödinger equation (21). More will be said about this later. The phonon eigenvector is a continuous function of \(q\) and, as we shall see, behaves as \(c_n (q) = \delta_{n0} + \mathcal{O}(q^2)\) for small \(q\).

To obtain an expression for \(s\) we separate the \(n = 0\) equation in (24)

\[
E^2 c_0 (q) = M_{00} (q) \varepsilon_0 (q) c_0 (q) + \sum_{n' \neq 0} M_{0n'} (q) \varepsilon_{n'} (q) c_{n'} (q)
\]

from the \(n \neq 0\) equations

\[
E^2 c_n (q) = M_{nn} (q) \varepsilon_n (q) c_0 (q) + \sum_{n' \neq 0} M_{nn'} (q) \varepsilon_{n'} (q) c_{n'} (q).
\]

Since \(\varepsilon_0 (q)\) and \(E^2\) are both proportional to \(q^2\), the latter equation shows that \(c_n (q) \propto q^2\) for \(n \neq 0\), as claimed. Thus, to order \(q^2\), these equations can be replaced by

\[
E^2 c_0 (0) = M_{00} (0) \varepsilon_0 (0) c_0 (0) + \sum_{n' \neq 0} M_{0n'} (0) \varepsilon_{n'} (0) c_{n'} (0)
\]

\[
0 = M_{n0} (0) \varepsilon_0 (0) c_0 (0) + \sum_{n' \neq 0} M_{nn'} (0) \varepsilon_{n'} (0) c_{n'} (q) \tag{29}
\]

Solving for \(E^2\), we obtain

\[
E^2 = \varepsilon_0 (q) \left[ M_{00} - \sum_{n'n'} M_{0n'} (\tilde{M}^{-1})_{nn'} M_{n0} \right] \tag{30}
\]

where all quantities within the square brackets are understood to be the \(q = 0\) values. The prime on the summation indicates that the terms \(n = 0\) and \(n' = 0\) are excluded from the sum. The matrix \(\tilde{M}_{nn'}\) is the matrix obtained by deleting the first row and first column of \(M_{nn'}\). We note that this combination of matrix elements can in fact be written as

\[
M_{00} - \sum_{n'n'} M_{0n'} (\tilde{M}^{-1})_{nn'} M_{n0} = \frac{1}{(M^{-1})_{00}}. \tag{31}
\]
Thus we find that the square of the sound speed is given by

\[ s^2 = \frac{1}{2m_0(M^{-1})_{00}}. \] (32)

We next relate the sound speed to variations of the chemical potential with mean density. Writing for simplicity \( w_0 \equiv w_{0,0} \) and \( \mu_0 \equiv \mu_{0,0} \), we have

\[ -\frac{k^2}{2m} \nabla^2 w_0 + V_{\text{opt}} w_0 + g n w_0^3 = \mu_0 w_0. \] (33)

The derivative of this equation with respect to \( \bar{n} \) is

\[ \hat{h}_0(0) w_{0,\bar{n}} + g w_0^3 + 2 g \bar{n} w_0^2 w_{0,\bar{n}} = \mu_0 \bar{n} w_0 \] (34)

where we use the notation \((\cdots)_{\bar{n}}\) to denote a derivative with respect to \( \bar{n} \). Taking the inner product of (34) with \( w_0 \) and noting that \( \hat{h}_0 w_0 = 0 \), we find

\[ \mu_{0,\bar{n}} = \frac{g}{\Omega} \int d^3 r w_0^4 + \frac{2 \bar{n}}{\Omega} \int d^3 r w_0^3 w_{0,\bar{n}}. \] (35)

To solve (34) for \( w_{0,\bar{n}} \), we note that the normalization condition in (32) implies

\[ \int d^3 r w_{0,\bar{n}} w_0 = 0. \] (36)

Thus, \( w_{0,\bar{n}} \) is orthogonal to \( w_0 \) and has the expansion

\[ w_{0,\bar{n}} = \sum_{n \neq 0} a_n w_n \] (37)

in terms of the (real) \( q = 0 \) Bloch functions \( w_n = w_{n,q=0} \). Substituting this expansion in (34) yields

\[ \sum_{n'} M_{n'n} a_{n'} = -\frac{1}{2\bar{n}} M_{00}. \] (38)

Using the expansion (37) for \( w_{0,\bar{n}} \) in (35), with the expansion coefficients defined by (38), we find

\[ \mu_{0,\bar{n}} = \frac{1}{2\bar{n}} \left( M_{00} - \sum_{n'n} M_{nn'} \bar{M}^{-1}_{n'n'} M_{00} \right). \] (39)

Comparing this with (34), we see that (34) is equivalent to

\[ s = \sqrt{\frac{\bar{n} \mu_{0,\bar{n}}}{m_0}} = \sqrt{\frac{\bar{n}}{m_0} \frac{\partial \mu_{0,0}}{\partial \bar{n}}} \] (40)

This result for an optical lattice was first given by Menotti et al. [17] on the basis of general dynamical considerations. We see here that it follows directly from the Bogoliubov equations and also applies in the case of a 3D lattice with cubic symmetry. The small-\( q \) expansion can be viewed as a systematic way of implementing the slowly varying ansatz used by Krämer et al. [13]. The expression for \( s \) has the same form as for a homogeneous gas, with \( m_0 \) replacing the bare mass \( m \) and the density derivative of the chemical potential, \( \mu_{0,\bar{n}} \), replacing the interaction parameter \( g \). In other words, at long wavelengths the condensate behaves as a gas of particles of mass \( m_0 \) with a compressibility, \( \kappa \), given by \( \kappa^{-1} = \bar{n} \left( \partial \mu_{0,0} / \partial \bar{n} \right) \).

### A. Thomas-Fermi Limit

The Thomas-Fermi (TF) approximation is valid when the density varies in space on a length scale much larger than the local coherence length \( \xi = \sqrt{\hbar^2 / 2m gn} \). In this situation, the density is well-approximated by

\[ n_0(r) = \frac{1}{g} (\mu_0 - V_{\text{opt}}(r)) \] (41)

except in regions where \( V_{\text{opt}} \approx \mu_0 \). This does not occur if \( \mu_0 > [V_{\text{opt}}]_{\text{max}} \), and we then have

\[ \mu_0 = g \bar{n} + \nabla_{\text{opt}}, \] (42)

where \( \nabla_{\text{opt}} \) is the mean value of the optical potential in the unit cell. Thus, \( \mu_{0,\bar{n}} = g \) as for a homogeneous gas. Since the effective potential, \( V_{\text{opt}} + gn_0 \), in the GP equation is a constant in the TF limit, we would expect the band mass, \( m_0 \), to be close to the free particle mass, \( m \). One can in fact show that the deviation of \( m_0 \) from \( m \) is proportional to \( V_{\text{opt}}^2 (\xi / d)^4 \), where \( V_0 \) is the amplitude of the potential modulation. Since we are assuming that \( \xi / d \ll 1 \), \( m_0 \approx m \) and the TF sound velocity is

\[ s_{\text{TF}} \approx \sqrt{\frac{gn}{m}}, \] (43)

as for a uniform gas. It should be noted that this result is valid even when the amplitude of the density modulation is of order the mean density \( \bar{n} \), provided only that the inequality \( \xi / d \ll 1 \) is everywhere satisfied.

If \( \mu_0 < [V_{\text{opt}}]_{\text{max}} \), the Thomas-Fermi density develops 'holes' in regions where \( V_{\text{opt}} > \mu_0 \). For a one-dimensional modulation the density is disjoint, as is the case in two or three dimensions for sufficiently small density. In this situation long wavelength propagating phonon excitations cannot exist within the TF approximation since the necessary fluctuations in the number of atoms from one lattice cell to the next cannot occur. In reality, the GP density in regions where \( V_{\text{opt}} > \mu_0 \) is small but finite and phonon-like excitations continue to exist. However, increasing the localization of the density in the potential minima leads to larger effective masses and eventually the sound speed \( s \) tends to zero. This behaviour cannot be described within the TF approximation.

### B. Weak-Coupling Limit

The \( g \)-dependence of \( \mu_{0,\bar{n}} \) appears explicitly in (38) and implicitly through the wave function \( w_0 \) which satisfies (34). To extract the dependence in the limit \( g \to 0 \), we expand the wave function as \( w_0 = w_0^{(0)} + g(\partial w_0 / \partial g)_{g=0} + \cdots \). Since \( w_0 \) depends on \( g \) through the combination \( gn \), we see that \( g(\partial w_0 / \partial g) = \bar{n} (\partial w_0 / \partial \bar{n}) \). Thus, the combination \( gn w_{0,\bar{n}} \) appearing in (34) is proportional to \( g \) in the small-\( g \) limit and the second term on the right
hand side of (35) is of order $g^2$. We then have
\[ \mu_{0,\tilde{n}} = \frac{g}{\Omega} \int d^3 r (w_0^{(0)})^4 \]
\[ + \frac{6g^2}{\Omega} \int d^3 r (w_0^{(0)})^3 (\tilde{n}w_{0,\tilde{n}}/g)_{g=0} + \cdots \quad (44) \]
As discussed in Ref. [13], the first term accounts for the effect of the lattice on the compressibility, $\kappa$, which decreases with increasing localization of the wave function $w_0^{(0)}$. The two-dimensional potential is the case of a weak optical potential.

Consider a weak one-dimensional periodic potential where perturbation theory applies. For simplicity we consider a weak onedimensional periodic potential $V_{\text{opt}} = V_0 \cos(Gz)$, where $G = 2\pi/d$, applied to an otherwise three-dimensional system. The relevant GP equation is now one-dimensional,
\[ -\frac{\hbar^2}{2m} \frac{d^2 w_0}{dz^2} + V_0 \cos(Gz)w_0 + g\tilde{n}w_0^3 = \mu_0 w_0. \quad (46) \]
In treating the optical potential as a perturbation, we expand the wave function as $w_0 = w_0^{(0)} + w_0^{(1)} + w_0^{(2)} + \cdots$, and chemical potential as $\mu_0 = \mu_0^{(0)} + \mu_0^{(1)} + \mu_0^{(2)} + \cdots$, where the superscript here denotes the order in $V_0$. The properly normalized wave function in the absence of the potential is $w_0^{(0)} = 1$ and $\mu_0^{(0)} = g\tilde{n}$. To first order in $V_0$, $\mu_0^{(1)} = 0$ and
\[ w_0^{(1)} = -\frac{V_0}{\varepsilon_G^{(0)} + 2g\tilde{n}} \cos(Gz), \quad (47) \]
where $\varepsilon_G^{(0)} = \hbar^2 G^2/2m$. In calculating the second order contribution, $\mu_0^{(2)}$, to the chemical potential, the second order wave function $w_0^{(2)}$, need not be determined, but the normalization condition $\int d^3 r dz w_0^{(0)} w_0^{(2)} = -(1/2) \int d^3 r dz (w_0^{(1)})^2$ is required. Thus, the chemical potential correct to second order in $V_0$ is found to be
\[ \mu_0 = g\tilde{n} - \frac{\varepsilon_G^{(0)} V_0^2}{2(\varepsilon_G^{(0)} + 2g\tilde{n})^2} + \cdots \quad (48) \]
Taking the derivative with respect to $\tilde{n}$, we have
\[ \mu_{0,\tilde{n}} = g + \frac{2g V_0^2 \varepsilon_G^{(0)}}{(\varepsilon_G^{(0)} + 2g\tilde{n})^3}. \quad (49) \]
The weak-coupling limit of this result to lowest order in $g$ is $\mu_{0,\tilde{n}} = g(1 + 2(V_0/\varepsilon_G^{(0)}))^2$. This can be shown to agree with the expansion of the first term in (35) in second order in $V_0$.

To complete the calculation of the sound speed, we require an equivalent expression for the effective mass. This can be obtained by solving
\[ -\frac{\hbar^2}{2m} \left( \frac{d}{dz} + iq \right)^2 w_{0q} + V_0 \cos(Gz)w_{0q} + (g\tilde{n}w_0^2 - \mu_0)w_{0q} = \varepsilon_0(q)w_{0q}, \quad (50) \]
where $w_0$ is the solution of (47). Since the correction to the effective mass is second order in $V_0$, it is sufficient to consider the mean-field potential ($g\tilde{n}w_0^2 - \mu_0$) to first order in $V_0$. We must then solve
\[ -\frac{\hbar^2}{2m} \left( \frac{d}{dz} + iq \right)^2 w_{0q} + V_0' \cos(Gz)w_{0q} = \varepsilon_0(q)w_{0q}, \quad (51) \]
Inserting (51) and (49) into (40), and discarding the quartic term in $V_0$, we arrive at the following expression for the sound speed
\[ s = \frac{g\tilde{n}}{m} \left( 1 - \frac{4g\tilde{n}V_0^2}{(\varepsilon_G^{(0)} + 2g\tilde{n})^3} \right). \quad (52) \]
When $\varepsilon_G^{(0)} \ll g\hbar$ (or $\xi/d \ll 1/2\pi$), this expression reduces to

$$s = \sqrt{\frac{g\hbar}{m} \left(1 - \frac{V_0^2}{2(g\hbar)^2}\right)}$$  \hspace{1cm} (53)$$

in agreement with the approximation to the sound speed obtained by Berg-Sørensen and Mølmer [3].

To make contact with Ref. [15], we introduce the recoil energy $E_R = \hbar^2\pi^2/2md^2 = \varepsilon_G^{(0)}/4$ and define $2V_0 = \sigma E_R$ (the parameter $\sigma$ is called ‘$s$’ in Ref. [15]). Eq. (52) can then be rewritten as

$$\frac{s}{s_0} = 1 - \frac{\gamma\sigma^2}{128(1 + \gamma/2)^3}$$  \hspace{1cm} (54)$$

where $s_0 = \sqrt{g\hbar/m}$ is the sound speed for the homogeneous gas and $\gamma$ is the ratio $g\hbar/E_R = (d/\pi\xi)^2$. This shows that $s$ decreases quadratically with the strength of the optical potential, which is consistent with the numerical results in Ref. [15]. This expression is valid if $2V_0 \ll \varepsilon_G^{(0)}$, or $\sigma \ll 4$, however, this constitutes a rather limited range of the values of $\sigma$ of physical interest.

### D. Radially Confined Condensates

As a final application of the results derived in this section we consider a condensate that is confined in the radial direction. To be specific, we assume a potential of the form

$$V(r) = V_{\text{opt}}(z) + V_\perp(\rho)$$  \hspace{1cm} (55)$$

where $V_\perp(\rho) = m\omega_\perp\rho^2/2$, that is, harmonic confinement in the radial ($\rho$) direction. The optical potential is periodic in the axial direction with periodicity $d$. This potential approximates the situation of a long cigar-shaped trap with an axial standing light wave.

Although the geometry is quite different from that considered earlier, the previous analysis can be carried over with minor modification. The ground state GP solution has the property $\Phi_0(\rho, z + d) = \Phi_0(\rho, z)$, and has the normalization

$$\frac{1}{d} \int_{-d/2}^{d/2} dz \int d^2r_\perp |\Phi_0(r)|^2 = \bar{\lambda},$$  \hspace{1cm} (56)$$

which defines the mean linear density $\bar{\lambda}$ along the length of the condensate. As before, it is convenient to define $\Phi_0(r) \equiv \lambda w_0(r)$.

The Bogoliubov excitations in the present situation have a Bloch wave character along the axis and are obtained from (159) with the Hamiltonian

$$\hat{h}_0(q) = -\frac{\hbar^2}{2m} \left[\nabla_\perp^2 + \left(\frac{\partial}{\partial z} + iq\right)^2\right] + V + g\bar{\lambda}|w_0|^2 - \mu_0.$$  \hspace{1cm} (57)$$

The eigenstates of $\hat{h}_0(q)$ are now labelled by the set of quantum numbers $\{q, n, m, \nu\}$, where $n$ is a one-dimensional band index, $m$ is the azimuthal quantum number associated with the $z$-component of angular momentum, and $\nu$ labels the different radial excitations. Of interest here are axially symmetric solutions ($m = 0$) since these have the character of the phonon mode of interest.

The analysis after (119) is followed step by step, the only change being the integration volume used in the normalization of the states. We thus find that the sound speed is given by

$$s = \sqrt{\frac{\lambda}{m_0}} \frac{\partial\mu_0}{\partial\lambda}$$  \hspace{1cm} (58)$$

where $m_0$ is the effective mass of the lowest band ($n = 0$ and $\nu = 0$).

Eq. (58) is of course valid in the absence of the optical potential. Treating the condensate in the TF approximation, we find $\lambda = \pi\mu_0^2/gm_\perp^2$ and $\partial\mu_0/\partial\lambda = gm_\perp^2/2\pi\mu_0$. This gives a sound speed

$$s = \sqrt{\frac{g\mu_0(0)}{2m}}$$  \hspace{1cm} (59)$$

where $\mu_0(0) = \mu_0/g$ is the density at the centre of the trap. This result was first obtained in Ref. [24] using a different method. In the weak coupling limit, (55) applies. In this case, the condensate wave function is a gaussian,

$$w_0^{(0)} = \frac{m\omega_\perp}{\sqrt{2\pi}\hbar} \exp\left(-\frac{m\omega_\perp}{\hbar}r^2\right),$$

and one again obtains the result in (59) for the sound speed, as found previously [24].

When the optical potential is strong the condensate becomes localized on each site. In this situation, the tight-binding approximation is a useful method for dealing with the system [10, 11, 24]. Approximating the condensate wave function as $\Phi(r) = \sum_i c_if_i(r)$ where $f_i(r)$ is a function localized on the $i$-th site and normalized to unity, the energy of the system is given approximately by

$$E_{\text{tot}} \approx \sum_i \varepsilon_0|c_i|^2 - t \sum_{i,i'} (c_i^\ast c_{i+1} + c_i c_{i+1}^\ast) + \frac{1}{2} \tilde{g} \sum_i |c_i|^4,$$

where $\varepsilon_0$ is an on-site energy, $t$ is a hopping matrix element connecting the amplitudes on nearest-neighbour sites and $\tilde{g}$ is an effective interaction strength. For the ground state, $|c_i|^2 = \nu$, where $\nu$ is the number of atoms per site. We then have

$$E_{\text{tot}} = (\varepsilon_0 - 2t)N + \frac{1}{2} \tilde{g} \nu N.$$

Assuming that the parameters $\varepsilon_0$, $t$ and $\tilde{g}$ are density independent in the extreme tight-binding limit, we
have \( \mu_0 = \partial E_{\text{tot}} / \partial N = (\varepsilon_0 - 2t) + \dot{q} \nu \) and \( \partial \mu_0 / \partial \lambda = \dot{g} d \). Within the same approximation the band energy is 
\( \varepsilon(q) = \varepsilon_0 + \dot{q} \nu - 2t \cos(qd) \), which gives an effective mass 
\( m_0 = h^2 / 2td^2 \). Thus the Bogoliubov sound speed from (55) is 
\( \nu_b \simeq \sqrt{2 \dot{q} \nu / d^2} \), which is the result obtained 
by Javanainen [10].

**IV. PHONON DISPERSION FOR A MOVING CONDENSATE**

We turn next to the derivation of the phonon dispersion 
relation for the case where the condensate is “flowing” 
through the optical lattice. We address this problem 
by directly solving the Bogoliubov equations in (16) 
for a specific condensate wave function \( w_{nk} \) in the limit of 
small wave vectors \( q \). The structure of these equations 
is quite different when \( k \neq 0 \) and the method used in 
the previous section to determine the dispersion relation 
can no longer be applied. In fact, the analysis is much 
more intricate as will soon become apparent. The 
results we obtain confirm the more intuitive hydrodynamic 
approach presented recently [7], which describes the 
dynamics of the system in terms of slowly varying hydro-
dynamic variables (density and momentum). By includ-
ing small length scale variations, our approach in a sense 
provides a “microscopic” derivation of the hydrodynamic 
equations that one would expect to be valid in the long 
wavelength limit.

Since the solution in the small-\( q \) limit is required, we 
rewrite (16) so as to display the \( q \)-dependent terms 
explicitly:

\[
\begin{align*}
(\sqrt{h} \mathbf{p} + \mathbf{h}k) + \frac{h^2 q^2}{2m} + g\nu |w_{0k}|^2 \right) \tilde{u} & = -g\nu w_{0k}^2 \tilde{v} = E\tilde{u} \\
\left(\sqrt{h} \mathbf{p} - \mathbf{h}k + \frac{h^2 q^2}{2m} + g\nu |w_{0k}|^2 \right) \tilde{v} & = -g\nu w_{0k}^2 \tilde{u} = -E\tilde{v},
\end{align*}
\]

where \( \mathbf{p} = (h/i) \nabla \) is the momentum operator. The GP 
Hamiltonian here is \( \mathbf{h}k (q = 0) \) as defined in [8]. In 
these equations, we have adopted the index \( n = 0 \) for 
the condensate wave function. We will usually think of 
this state as the lowest Bloch state solution of the GP 
equation, although it in principle could correspond to an 
arbitrary excited band. For simplicity we have dropped 
the index on the quasiparticle amplitudes \( \tilde{u} \) and \( \tilde{v} \) 
and the excitation energy \( E \) as we will only be considering 
the phonon-like excitation.

It is clear that for \( q = 0 \) \( \tilde{u} \) admits a solution with 
\( \tilde{u} \propto w_{0k}, \tilde{v} \propto w_{0k}^* \) and \( E = 0 \). For finite \( q \) we seek 
solutions in the form of an expansion in eigenfunctions 
of \( \mathbf{h}k \), namely,

\[
\tilde{v} = \sum_n a_n(q) w_{nk}
\]

where

\[
\hat{h}_k w_{nk} = \varepsilon_{nk} w_{nk}
\]

According to this definition, \( \varepsilon_{ok} = 0 \). The functions \( w_{nk} \) 
are an orthonormal set with normalization given by \( \langle 0 | 0 \rangle = 1 \). 
Although we use the same notation, it should be noted 
that these functions are distinct from those defined in 
(21). In addition, we may assume \( w_{n-k} = w_{nk}^* \) 
and \( \varepsilon_{n-k} = \varepsilon_{nk} \).

Substituting these expansions into (60), we obtain the matrix equations

\[
\begin{align*}
\varepsilon_{nk} k^2 &+ \frac{h^2 q^2}{2m} \right) a_n + \sum_{n'} \frac{h}{m} q \cdot \mathbf{P}_{nn'} a_{n'} \\
+ \sum_{n'} (A_{nn'} a_{n'} - B_{nn'} b_{n'}) & = E a_n, \\
\varepsilon_{nk} &\frac{h^2 q^2}{2m} b_n - \sum_{n'} \frac{h}{m} q \cdot \mathbf{P}^*_{nn'} b_{n'} \\
+ \sum_{n'} (A_{nn'} b_{n'} - B_{nn'} a_{n'}) & = -E b_n,
\end{align*}
\]

where we have defined the matrices

\[
\begin{align*}
A_{nn'}(k) & = \int \Omega \frac{w_{nk}^* g \nu w_{0k}^* w_{n'k}^* d^3r,} \\
B_{nn'}(k) & = \int \Omega \frac{w_{nk}^* g \nu w_{0k}^* w_{n'k}^* d^3r,} \\
P_{nn'}(k) & = \int \Omega \frac{w_{nk}^* (p + h\mathbf{k}) w_{n'k}^* d^3r.}
\end{align*}
\]

Due to the inversion symmetry of the lattice, the Bloch 
states at the zone centre \( k = 0 \) can be chosen to be 
simultaneous eigenstates of parity. Although parity is 
not a good quantum number for states with nonzero \( k \), 
each band can nevertheless be assigned a parity index 
\( \eta_n = \pm 1 \) such that

\[
w_{n-k}(-r) = \eta_n w_{nk}(r),
\]

This property is proved explicitly in one dimension in 
Appendix A and can also be shown to follow to lowest 
order in \( k \) by means of \( k \cdot p \) perturbation theory. Together 
with the conjugation (time-reversal) property \( w_{nk}^*(r) = 
\]

\[
w_{n-k}(r),
\]

we have

\[
w_{nk}^*(r) = \eta_n w_{nk}(-r).
\]

This important property is used throughout the following 
discussion. For example, it can be used to show that the 
matrices in (65) satisfy the following relations

\[
\begin{align*}
A_{nn'}(k) & = A_{n'n}(k) = A_{nn'}(-k) = \eta_n \eta_{n'} A_{nn'}(k) \\
B_{nn'}(k) & = B_{nn'}(-k) = \eta_n \eta_{n'} B_{nn'}(k) = \eta_n \eta_{n'} B_{n'n}(k) \\
P_{nn'}(k) & = P_{n'n}(k) = -P_{nn'}(-k) = \eta_n \eta_{n'} P_{nn'}(k)
\end{align*}
\]

(70)
Note that $A$ and $P$ are hermitian while $B$ is not. In addition, we see that $A_{nn'}(0)$ and $B_{nn'}(0)$ are real and nonzero only for pairs of states having the same parity index, while $P_{nn'}(0)$ is purely imaginary and only couples states with opposite parity.

In solving (68) and (69), it is convenient to define the following linear combinations: $c_n = \frac{1}{2}(a_n + \eta_nb_n)$ and $d_n = \frac{1}{2}(a_n - \eta_nb_n)$. Introducing these variables into (63) and (64), and making use of the relations in (70), we obtain the equations:

$$
(\varepsilon_{nk} + \frac{\hbar^2q^2}{2m})c_n + \sum_{n'}(A_{nn'} - B_{nn'})c_{n'}
+ \sum_n \frac{\hbar}{m}q \cdot P_{nn'}d_n = Ed_n,
$$

$$
(\varepsilon_{nk} + \frac{\hbar^2q^2}{2m})d_n + \sum_{n'}(A_{nn'} + B_{nn'})d_{n'}
+ \sum_n \frac{\hbar}{m}q \cdot P_{nn'}c_n = Ec_n,
$$

where we have defined the hermitian matrix $\tilde{B}_{nn'} = B_{nn'}\eta_{nn'}$. As in our earlier analysis, we anticipate that $E(q)$ will depend linearly on $q$ for $q \to 0$, but due to the quasimomentum $k$ of the condensate, it no longer depends simply on the magnitude $q$. To extract this dependence we systematically expand the coefficients $c_n(q)$ and $d_n(q)$ as a series in powers of $q$. Specifically, we write

$$
c_n(q) = h(q)c_n^{(0)} + c_n^{(1)} + c_n^{(2)} + \ldots
$$

$$
d_n(q) = h(q)d_n^{(0)} + d_n^{(1)} + d_n^{(2)} + \ldots
$$

where the superscript indicates the order of $q$ in the respective terms (here, order signifies similar powers of the vector magnitude $q$). The factor $h(q)$ contains the nonanalytic behaviour of the coefficients which is required in order to satisfy the normalization condition in (15). For a homogeneous system, $h(q) \propto q^{-1/2}$, and we expect a similar dependence in the case of a lattice. In the following, it is sufficient to note that this factor is the same for both coefficients and can therefore be ignored in developing a systematic $q$-expansion.

We noted earlier that $\tilde{a} \propto w_{0k}$ and $\tilde{b} \propto w_{0k}$ for $q \to 0$ which, according to (15), implies that $a_n(q) \propto \delta_{n0}$ and $b_n(q) \propto \delta_{n0}$ in this limit. If the state $w_{0k}$ is an even parity state ($\eta_0 = +1$), as we assume in the following, we must then have $c_n^{(0)} = d_n^{(0)} = 0$. With this information, (71) gives to $O(q^3)$ the equation

$$
\varepsilon_{0k} + (A_{00} - \tilde{B}_{00}) = 0
$$

which is satisfied since $\varepsilon_{0k} = 0$ and $\tilde{B}_{00} = A_{00}$. To $O(q^5)$, (71) gives

$$
\varepsilon_{nk}c_n^{(1)} + \sum_{n'}(A_{nn'} - \tilde{B}_{nn'})c_{n'}^{(1)} = 0.
$$

Similarly, (72) gives

$$
\sum_{n'} N_{nn'}d_{n'}^{(1)} = E\delta_{n0} - \frac{\hbar}{m}q \cdot P_{n0},
$$

where we have defined the hermitian matrix

$$
N_{nn'}(k) = A_{nn'}(k) + \hat{B}_{nn'}(k) + \varepsilon_{nk}\delta_{nn'}.
$$

Eq. (77) is homogeneous and indicates that $c_n^{(1)} = 0$. On the other hand, (76) can be solved for $d_{n}^{(1)}$ in terms of the unknown excitation energy $E$. To determine the latter, we must consider (77) to $O(q^7)$, obtaining

$$
\varepsilon_{nk}c_n^{(2)} + \frac{\hbar^2q^2}{2m}\delta_{n0} + \sum_{n'}(A_{nn'} - \tilde{B}_{nn'})c_{n'}^{(2)}
+ \sum_n \frac{\hbar}{m}q \cdot P_{nn'}d_n^{(1)} = Ed_n^{(1)}.
$$

Setting $n = 0$ in this equation, and noting that $\varepsilon_{0k} = 0$ and that $A_{00} = \hat{B}_{00}$, we find

$$
\frac{\hbar^2q^2}{2m} + \sum_n \frac{\hbar}{m}q \cdot P_{0n}d_{n}^{(1)} = Ed_{0}^{(1)}.
$$

Since $d_{0}^{(1)}$ is itself linear in $E$ according to (76), we see that (79) is implicitly a quadratic equation for $E$ which can be solved to determine the excitation energy to lowest order in $q$. However, to do so directly would not reveal the interesting dependences on various physical parameters that in fact emerge. As seen in the $k = 0$ analysis, the excitation energy could be related to the variation of the chemical potential with mean density $\bar{\eta}$. This remains a quantity of interest in the present case, but we must also consider variations of the chemical potential with $k$. We thus turn next to the determination of $\mu_{0k,\bar{\eta}} \equiv \partial \mu_{0k} / \partial \bar{\eta}$ and $\mu_{0k,i} \equiv \partial \mu_{0k} / \partial k_i$.

### A. Determination of $\mu_{0k,\bar{\eta}}$

The chemical potential $\mu_{0k}$ is determined by the self-consistent solution of the GP equation, $\tilde{h}_kw_{0k} = 0$, with $\tilde{h}_k$ given by (15) with $q = 0$. The variation of this equation with respect to $\bar{\eta}$ gives

$$
\tilde{h}_kw_{0k,\bar{\eta}} + g|w_{0k}|^2w_{0k} + g\bar{\eta}(w_{0k,\bar{\eta}}w_{0k} + w_{0k}^*w_{0k,\bar{\eta}})w_{0k} = \mu_{0k,\bar{\eta}}w_{0k},
$$

where $w_{0k,\bar{\eta}} \equiv \partial w_{0k} / \partial \bar{\eta}$. Taking the derivative of the normalization (22) with respect to $\bar{\eta}$, and using (90), we find that

$$
\int_{\Omega} w_{0k,\bar{\eta}}^*w_{0k,\bar{\eta}}d^3r = 0.
$$

Thus, $w_{0k,\bar{\eta}}$ is orthogonal to $w_{0k}$ and has the expansion

$$
w_{0k,\bar{\eta}} = \sum_n \alpha_n w_{nk},
$$
where as before, the prime on the summation indicates that the \( n = 0 \) term is excluded from the sum. Inserting this expansion into (80), and taking the inner product with respect to \( w_{n k} \), we obtain
\[
\frac{1}{2\hbar} \tilde{N} n_0 + \sum_n' N_{nn'} \alpha_{n'} - \mu_{0 k, \tilde{n}} \delta_{n0} = 0,
\] (83)
where we have noted that \( \alpha^*_n = \eta_n \alpha_n \) as a result of the symmetry property (68). Setting \( n = 0 \) in (83), we find
\[
\mu_{0 k, \tilde{n}} = \frac{1}{2\hbar} \tilde{N}_{00} + \sum_n' \tilde{N}_{0n} \alpha_n.
\] (84)
The set of equations for \( n \neq 0 \) has the solution
\[
\alpha_n = -\frac{1}{2\hbar} \sum_n' (\tilde{N}^{-1})_{nn'} N_{n'0},
\] (85)
where \( \tilde{N} \) is the reduced matrix obtained by deleting the first row and first column from \( N \). Thus we find that
\[
\mu_{0 k, \tilde{n}} = \frac{1}{2\hbar} \left( \tilde{N}_{00} - \sum_n' \tilde{N}_{0n} (\tilde{N}^{-1})_{n0} N_{n'0} \right).
\] (86)
This is analogous to (59) and reduces to it in the \( k = 0 \) limit since the \( M \) and \( N \) matrices are then the same (note that \( w_{n0} \) are defined to be real).

### B. Determination of \( \mu_{0 k, i} \)

We follow a similar method to obtain \( \mu_{0 k, i} \). Taking the derivative of \( \hbar k w_0 k = 0 \) with respect to \( k_i \), we have
\[
\left[ \frac{\hbar}{m} \left( p_i + \hbar k_i \right) + g \tilde{n} \left( w_{0 ki, i} w_{0 k} + w_{0 ki}^* w_{0 k} \right) - \mu_{0 k, i} \right] w_0 k + \hbar k w_{0 ki, i} = 0,
\] (87)
where \( w_{0 ki, i} = \partial w_{0 k} / \partial k_i \). Noting the orthogonality of each vector component \( w_{0 ki, i} \) with \( w_{0 k} \), we have the following expansion
\[
w_0 k_i = \sum_n' \beta_{in} w_{n k},
\] (88)
where the expansion coefficients, \( \beta_{in} \), define the Cartesian components of a vector \( \beta_n \). Inserting (88) into (57), and taking the inner product with \( w_{n k} \), we obtain
\[
\frac{\hbar}{m} (P_i)_{n0} + \sum_n' N_{nn'} \beta_{in'} - \mu_{0 k, i} \delta_{n0} = 0.
\] (89)
where, as before, we have used \( \beta^*_n = \eta_n \beta_n \). An expression for \( \mu_{0 k, i} \) can be found by setting \( n = 0 \) in (88):
\[
\mu_{0 k, i} = \frac{\hbar}{m} (P_i)_{00} + \sum_n' N_{0n'} \beta_{in'}.
\] (90)

The set of equations for \( n \neq 0 \) yield the solution vector,
\[
\beta_{in} = -\frac{\hbar}{m} \sum_n' (\tilde{N}^{-1})_{nn'} (P_i)_{n'0},
\] (91)
and thus,
\[
\mu_{0 k, i} = \frac{\hbar}{m} \left( (P_i)_{00} - \sum_n' N_{0n} (\tilde{N}^{-1})_{n0} (P_i)_{n'0} \right).
\] (92)

### C. Excitation Energy

These results will now be used to obtain an expression for the excitation energy \( E \) from (16) and (70). Setting \( n = 0 \) in (70) we have
\[
\sum_n' N_{0n'0} d_{n0}^{(1)} = E - \frac{\hbar}{m} q \cdot P_{00} - N_{00} d_0^{(1)}
\] (93)
while for \( n \neq 0 \) we see that
\[
d_{n0}^{(1)} = -\sum_n' (\tilde{N}^{-1})_{nn'} \left( \frac{\hbar}{m} q \cdot P_{n0} + N_{n'0} d_0^{(1)} \right)
\] (94)
The quantities on the right hand side of this equation are in fact related to the expansion coefficients \( \alpha_n \) in (58) and \( \beta_{in} \) in (91). We find the simple relation
\[
d_{n0}^{(1)} = 2\bar{n} d_0^{(1)} \alpha_n + q \cdot \beta_n.
\] (95)
Using this result in (16), we have
\[
\left( \tilde{N}_{00} + 2\bar{n} \sum_n N_{0n} \alpha_n \right) d_0^{(1)} = E - \frac{\hbar}{m} q \cdot P_{00} - \sum_n' N_{0n} q \cdot \beta_n
\] (96)
which with (51) and (50) can be written as
\[
2\bar{n} \mu_{0 k, i} d_0^{(1)} = E - q \cdot \nabla_{k\mu} \phi_{0k}.
\] (97)
We see that \( d_0^{(1)} \) and \( E \) are now related to each other through physically meaningful and calculable parameters.

We now substitute (95) into (79) to obtain
\[
\frac{\hbar^2 q^2}{2m} + \sum_n' \frac{\hbar}{m} (q \cdot P_{0n}) (q \cdot \beta_n) = \left( E - \frac{\hbar}{m} q \cdot P_{00} - \sum_n' \frac{\hbar}{m} q \cdot P_{0n} 2\bar{n} \alpha_n \right) d_0^{(1)}.
\] (98)
With (58), the sum on the right hand side becomes
\[
\sum_n' \frac{\hbar}{m} P_{0n} 2\bar{n} \alpha_n = -\sum_m' \frac{\hbar}{m} P_{0m} (\tilde{N}^{-1})_{nm} N_{n'0}
\] (99)
In going from the first to the second line, we have used the fact that all the matrices have the transposition property \( M_{n'n} = \eta_n \eta_{n'} M_{nn'} \). With the expression for \( \mu_{0,k,i} \) in \((98)\), thus becomes

\[
\frac{h^2q^2}{2m} + \sum_n \frac{h}{m} (q \cdot P_{0n}) (q \cdot \beta_n) = (E - q \cdot \nabla_k \mu_{0,k}) d_0^{(1)}
\]

Eliminating \( d_0^{(1)} \) from \((97)\) and \((100)\), we finally obtain

\[
E = q \cdot \nabla_k \mu_{0,k} + \sqrt{2 \mu_{0,k}} \left[ \frac{h^2q^2}{2m} + \frac{h}{m} \sum_n (q \cdot P_{0n})(q \cdot \beta_n) \right].
\]

The sign of the square root is chosen to be positive to give a positive excitation energy in the \( k \to 0 \) limit. The final quantity to interpret is the summation within the square root.

\[\text{D. Effective Mass Tensor}\]

The square bracket in \((101)\) involves the tensor

\[
\left( \frac{1}{m} \right)_{ij} = \frac{1}{m} \delta_{ij} + \frac{2}{mn} \sum_{n'} (P_i)_{0n}(\beta_j)_{n'}
\]

\[
= \frac{1}{m} \delta_{ij} - \frac{2}{mn} \sum_{n'} (P_i)_{0n}(\tilde{N})_{nn'} (P_j)_{n0}. \tag{102}
\]

This expression is similar to the usual effective mass tensor defined on the basis of \( k \cdot p \) perturbation theory, although the structure of the summation is different. To make contact with the \( k \cdot p \) expression we consider the \( N_{nn'} \) matrix in the \( k \to 0 \) limit. Quite generally, this matrix has the block structure

\[
N(k) = \begin{pmatrix}
A_{++} + B_{++} + D_+ & A_{+-} - B_{-+} \\
A_{-+} + B_{+-} & A_{--} - B_{-+} + D_-
\end{pmatrix}
\]

(103)

where the blocks are defined according to the parity index of the various states. For example, the block in the upper-left corner contains matrix elements between states with a positive parity index, \( \eta = +1 \). The diagonal matrix \( D \) contains the energy eigenvalues \( \varepsilon_{nk} \) on its diagonal. In the limit \( k \to 0 \), we have \( B(k = 0) = A(k = 0) \) and \( A_{nn'} = 0 \) if \( \eta_n \neq \eta_{n'} \). Thus, in this limit we have

\[
N(k = 0) = \begin{pmatrix} 2A_{++} + D_+ & 0 \\ 0 & D_-
\end{pmatrix}
\]

that is, \( N(k = 0) \) is block-diagonal, which of course is also true of its inverse. Since, \( P_i \) only connects states of \textit{opposite} parity in the \( k = 0 \) limit, we thus see that

\[
\lim_{k \to 0} \left( \frac{1}{m} \right)_{ij} = \frac{1}{m} \delta_{ij} - \frac{2}{m^2} \sum_n (P_i)_{0n}(P_j)_{n0} \varepsilon_{n0}. \tag{105}
\]

This is precisely the effective mass tensor obtained by means of \( k \cdot p \) perturbation theory as applied to the Hamiltonian \( \hat{h}_0(q) \) in \((20)\). The tensor defined in \((102)\) is a generalized effective mass tensor in that it depends on the presence of a superfluid flow (\( k \neq 0 \)). Also because of this, it is no longer diagonal despite the cubic symmetry of the optical lattice.

To complete the identification of \((m^{-1})_{ij}\), we consider variations of the GP equation with respect to the condensate wave vector \( k \). The second derivative of \( \hat{h}_k w_{0k} = 0 \) yields the equation

\[
\hat{h}_{k,i} w_{0k} + \hat{h}_{k,j} w_{0k,j} + \hat{h}_{k,i} w_{0k,i} + \hat{h}_{k,j} w_{0k,i} = 0. \tag{106}
\]

Here,

\[
\hat{h}_{k,i} = \frac{\hbar}{m} (p_i + \hbar k_i) + gn_{c,i} - \mu_{0,k},
\]

\[
\hat{h}_{k,j} = \frac{\hbar^2}{m} \delta_{ij} + gn_{c,ij} - \mu_{0,k}. \tag{107}
\]

The inner product of \((106)\) with \( w_{0k} \) gives

\[
\frac{1}{\Omega} \int_{\Omega} \overline{w_{0k}^* (\hat{h}_{k,i} w_{0k} + \hat{h}_{k,j} w_{0k,j} + \hat{h}_{k,i} w_{0k,i} + \hat{h}_{k,j} w_{0k,i})} d^3 r = 0. \tag{109}
\]

The first integral is

\[
\frac{1}{\Omega} \int_{\Omega} \overline{w_{0k}^* \hat{h}_{k,i} w_{0k,j} + \hat{h}_{k,j} w_{0k,i}} d^3 r
\]

while the integral of the next two terms gives the result

\[
\frac{1}{\Omega} \int_{\Omega} \overline{w_{0k}^* (\hat{h}_{k,i} w_{0k,j} + \hat{h}_{k,j} w_{0k,i})} d^3 r
\]

\[
= \frac{\hbar}{m} \sum_n [(P_i)_{0n}(\beta_j)_{n} + (P_j)_{0n}(\beta_i)_{n}]
\]

\[
+ \frac{g}{\Omega} \int_{\Omega} n_{c,i} n_{c,ij} d^3 r. \tag{111}
\]

We thus find

\[
\mu_{0,k} = \frac{\hbar^2}{m} \delta_{ij} + \frac{2\hbar}{m} \sum_n (P_i)_{0n}(\beta_j)_{n} + \frac{g}{2\Omega} \int_{\Omega} (n_{c}^2)_{ij} d^3 r. \tag{112}
\]

With this result we see that the effective mass tensor defined in \((102)\) can be expressed as

\[
\left( \frac{1}{m} \right)_{ij} = \frac{1}{\hbar^2} \frac{\partial^2}{\partial k_i \partial k_j} (\mu_{0k} - \frac{g}{2\Omega} \int_{\Omega} n_{c}^2 d^3 r). \tag{133}
\]

\[\text{E. Relation to Energy Density}\]

This last result can be related to the total energy \( E_{\text{tot}} \) in the state \( \Phi_{0k} \). Defining the energy per particle as \( E_{\text{opt}} \equiv N \varepsilon (\bar{n},k) \), we have

\[
\varepsilon (\bar{n},k) = \frac{1}{\Omega} \int_{\Omega} w_{0k}^* \left( -\frac{\hbar^2}{2m} (\nabla + ik)^2 + V_{\text{opt}} \right) w_{0k} d^3 r
\]

\[
+ \frac{g\bar{n}}{2\Omega} \int_{\Omega} |w_{0k}|^4 d^3 r. \tag{114}
\]
Comparing this with \( \mu_{0k} \), we see that

\[
\tilde{\epsilon}(\vec{n}, k) = \mu_{0k} - \frac{g\vec{n}}{2\Omega} \int_{\Omega} |w_{0k}|^4 d^3r
\]  

(115)

which is the expression in brackets in (113). Thus the effective mass tensor is given by

\[
\left( \frac{1}{m} \right)_{ij} = \frac{1}{h^2} \frac{\partial^2 \tilde{\epsilon}}{\partial k_i \partial k_j}.
\]

(116)

For a cubic lattice, \( \mu_{0k} \) has an expansion of the form

\[ \mu_{0k} = \mu_{00} + h^2 k^2/2m_k + \cdots. \]

Similarly, \( \tilde{\epsilon}(\vec{n}, k) = \epsilon(\vec{n}, 0) + h^2 k^2/2m_e + \cdots \). However, as proved by (105), the parameter \( m_e \) is in fact the band mass \( m_0 \) defined by the Hamiltonian (20). In other words, the correct effective mass parameter can be extracted without solving the GP equation for \( w_{0k} \) (with \( k \neq 0 \)) self-consistently. We note in passing that direct differentiation of (115) establishes the relation \( (\langle j_\perp \rangle) = \nabla_k (\overline{n} \tilde{\epsilon})/h \).

With these results, the phonon energy (101) can be given in a compact form. Defining the mean energy density as \( e \equiv \bar{n} \tilde{\epsilon} \), the Bogoliubov excitation energy at long wavelengths is given by

\[
E = e,_{\bar{n}} q_i t_i + \sqrt{e,_{\bar{n}} e,_{ij} q_i q_j}
\]

(117)

where we use a repeated summation convention on the Cartesian indices \( i \) and \( j \). This is precisely the expression given by Machholm et al. [9] who argued that the dynamics of the system at long wavelengths could be based on a hydrodynamic analysis. Since their approach arrives at (117) in a more economical fashion, it is useful to summarize the essential assumptions on which it is based.

The central assumption is the existence of an average phase fluctuation, \( \langle \theta(r, t) \rangle \), that varies slowly in space and time. Expanding this average phase as

\[
\langle \theta(r + \Delta r, t + \Delta t) \rangle = \langle \theta(r, t) \rangle + \nabla \langle \theta(r, t) \rangle \cdot \Delta r + \frac{\partial \langle \theta(r, t) \rangle}{\partial t} \Delta t + \cdots,
\]

(118)

one identifies \( \nabla \langle \theta \rangle \) with the local wave vector, \( (k) \), and \( \partial \langle \theta \rangle / \partial t \) with \( -\mu/h \) where \( \mu \) is the local chemical potential. The equation of motion for the local wave vector is thus

\[
h \frac{\partial \langle k \rangle}{\partial t} = -\nabla \langle \nu \rangle.
\]

(119)

The second hydrodynamic equation is the continuity equation

\[
\frac{\partial \langle n \rangle}{\partial t} + \nabla \cdot \langle j_\perp \rangle = 0,
\]

(120)

where \( \langle j_\perp \rangle \) is the local current density. The current density and chemical potential are then assumed to be given by the usual expressions for a uniform system, namely,

\[
\langle j_\perp \rangle = \frac{1}{h} \nabla \langle k \rangle e, \quad \langle \mu \rangle = \frac{\partial e}{\partial \langle n \rangle}
\]

(121)

where \( e(\langle n \rangle, \langle k \rangle) \) is the average energy density for a uniform optical lattice, viewed as a function of the local density \( \langle n \rangle \) and wave vector \( k \).

By expanding the variables as \( \langle n \rangle = \bar{n} + \delta n \) and \( \langle k \rangle = k + \delta k \), one obtains a pair of equations for the fluctuations which admits wave-like solutions with frequency \( \omega = E/h \) and wave vector \( q \). The dispersion relation found is identical to (117).

It is clear that the assumptions made in the hydrodynamic approach are completely justified. The average energy density \( e \) is the fundamental quantity determining the excitation energy at long wavelengths, as confirmed by our systematic \( q \)-expansion. The additional information provided by the expansion technique are the perturbative expressions for \( \partial \mu_{0k} / \partial \bar{n}, \nabla_k \mu_{0k} \) and \( (1/m)_{ij} \) as given by (88), (92) and (102), respectively.

\[ \text{F. Discussion} \]

For small \( k \), \( e(\bar{n}, k) \approx e(\bar{n}, 0) + n \hbar^2 k^2/2m_0 + \cdots \), and the Bogoliubov excitation energy is

\[
E/h \approx \hbar q \cdot k \frac{\partial}{\partial n} \left( \frac{\bar{n}}{m_0} \right) + sq
\]

(122)

where \( s \) is the sound speed for the condensate at rest. This result was given previously by Krämer et al. [18].

The energy first becomes negative when the superfluid flow satisfies \( k > m_0 s/h \), where \( 1/m_0 = \partial (\bar{n}/m_0) / \partial \bar{n} \) which defines the Landau criterion for energetic instability at long wavelengths in an optical lattice. The region of energetic instability was mapped out for arbitrary \( q \) by Wu and Niu [6, 28] and Machholm et al. [9]. In this region the energy of the superfluid state is no longer a local maximum. As a result, transitions to lower energy states can occur spontaneously provided a means of conserving energy and quasimomentum is available.

The excitation energy given by (117) becomes imaginary when the argument of the square root is negative. This signals a dynamic instability whereby the amplitude of the condensate fluctuation grows (or decays) in time. Of the two factors in the square root, \( e_{ij} \), or equivalently the effective mass tensor, \( (1/m)_{ij} \), is the most physically relevant.

It is instructive to examine the latter in the weak potential limit. We consider for simplicity the one-dimensional situation discussed in Sec. III C. Repeating the perturbative analysis in Sec. III C for the case \( k \neq 0 \), we find

\[
\tilde{\epsilon}(n, k) = \frac{1}{2} g\bar{n} + \epsilon^{(0)}_k - \frac{V_0^2}{2 \left( \epsilon^{(0)}_G + 2g\bar{n} - 4\epsilon^{(0)}_k \right)} + \cdots
\]

(123)

We note that this expression becomes singular at a wave vector \( k_c \) satisfying \( \epsilon^{(0)}_G + 2g\bar{n} - 4\epsilon^{(0)}_k = 0 \), which gives

\[
k_c = \sqrt{k_0^2 + G^2/4}
\]

(124)
where \( k_0 = m s_0 / \hbar \). The singularity is indicating the breakdown of nondegenerate perturbation theory, but provided \( k \) is not too close to \( k_c \), we can use (128) to evaluate the effective mass. To second order in \( V_0 \) we have

\[
\frac{1}{m_0(k)} = \frac{1}{m} \left[ 1 - \frac{2V_0^2}{(\varepsilon_G(0) + 2g\bar{n} - 4\varepsilon_k(0))^2} \right] - \frac{32\varepsilon_k(0)V_0^2}{(\varepsilon_G(0) + 2g\bar{n} - 4\varepsilon_k(0))^3} + \cdots
\]

(125)

At \( k = 0 \) we recover the result found in Sec. C. For \( m_0^{-1} \) to go to zero, \( k \) must be close to \( k_c \). With \( \Delta k = k_c - k \), we find

\[
\frac{\Delta k}{k_c} \simeq \left( \frac{V_0}{\varepsilon_G + 2g\bar{n}} \right)^{2/3},
\]

(126)

that is, the wave vector \( k \) approaches \( k_c \) as \( V_0 \to 0 \). We note that at \( k = k_c - \Delta k \), the perturbative correction to the energy in (128) is still small so that the perturbation theory estimate of where \( m_0^{-1} \) goes to zero is reasonable. We thus expect a dynamic instability to set in when \( k \simeq k_c \) in the weak potential limit.

This condition for the dynamical instability is the \( q = 0 \) limit of the result given in Refs. [2] and [3]. The Bogoliubov excitations of wave vector \( q \) in an homogeneous gas with current \( \langle j_x \rangle = \bar{n} \hbar k / m \) have the energies

\[
E_{\pm}(q) = \frac{\hbar^2 k q}{m} \pm \sqrt{\frac{\bar{n} g \hbar^2 q^2}{m} + \frac{\hbar^4 q^4}{4m^2}}.
\]

(127)

We follow Wu and Niu [6] in referring to the modes with the plus (minus) sign as phonons (anti-phonons). The former correspond to physical excitations in that their normalization is given by (15). The effect of an optical potential is to couple an anti-phonon mode with wave vector \( q \) to a phonon mode with wave vector \( q - G \). The condition that \( E_{\pm}(q) = E_{\pm}(q - G) \) implies that the two modes are resonantly coupled and gives the critical wave vector

\[
k_c = \frac{1}{G} \left( \sqrt{k_0^2 q^2 + \frac{1}{4} q^4} + \sqrt{k_0^2 (G - q)^2 + \frac{1}{4} (G - q)^4} \right).
\]

(128)

For \( q = 0 \), this gives the critical wave vector in (123). The expression in (128) was shown in [6] to account for the boundary of the dynamically unstable region in the weak potential limit. In fact, it can be shown by means of degenerate perturbation theory (Appendix B) that imposing a weak optical potential indeed gives rise to complex Bogoliubov eigenvalues.

Alternatively, the condition \( E_{\pm}(q) = E_{\pm}(q - G) \) can be written as \( E_+(q) + E_+(q - G) = 0 \). This was interpreted by Machholm et al. as a Landau criterion for the emission of two phonon excitations with zero total energy. Although this physical interpretation is appealing, it is not clear how it can be used to actually determine the rate at which the excitations are being produced, short of performing the perturbation analysis carried out in Appendix B in terms of phonon and anti-phonon modes.

We thus see that the phonon-anti-phonon resonance condition, or alternatively the two-phonon Landau criterion, is consistent with the effective mass condition for a dynamical instability in the \( q \to 0 \) limit. A similar statement can be made in the weak coupling limit (\( g \to 0 \)). Wu and Niu [6] noted from their numerical analysis that one boundary of the dynamically unstable region is given by the condition \( \varepsilon_0(q + k) - \varepsilon_0(k) = \varepsilon_0(k) - \varepsilon_0(k - q) \) where \( \varepsilon_0(k) \) is the band energy for the optical potential by itself. In the small-\( q \) limit, this condition becomes

\[
\frac{\partial^2 \varepsilon_0(k)}{\partial k^2} = 0.
\]

Thus the onset of dynamical instability at \( q = 0 \) in the weak coupling limit is again given by the point at which the inverse effective mass goes to zero.

\section{V. Conclusions}

We have studied the long wavelength phonon excitations in a three dimensional optical lattice. By making use of a systematic expansion of the Bogoliubov equations in terms of the phonon wave vector \( q \), we obtain the phonon dispersion in the long wavelength limit. Our result for the current-free state defines the sound speed in terms of the effective mass \( m_0 \) and variations of the chemical potential with \( \bar{n} \) and agrees with the result given by Menotti et al. [17]. The effective mass is defined quite generally in terms of the energy per particle, \( \varepsilon(\bar{n}, k) \), but can also be calculated using the current-free GP Hamiltonian in the \( k \to 0 \) limit. We present analytic expressions for the sound speed in the Thomas-Fermi, weak potential, weak coupling and tight-binding limits.

For the current-carrying case, we rederive the dispersion relation obtained by means of a hydrodynamic analysis (see also [13]). Our approach confirms that the dynamics at long wavelengths is defined by the local energy density \( \epsilon(\bar{n}, k) \) viewed as a function of the slowly varying local density, \( \langle n(r) \rangle \), and local condensate wave vector, \( \langle k(r) \rangle \). At long wavelengths, dynamical instabilities arise at the point where the generalized effective mass tensor has a vanishing eigenvalue.

\appendix

\section{A. Reflection Symmetry of Bloch Functions}

In this Appendix we give a proof of the symmetry property used throughout our analysis. We do this for the one-dimensional case for which the wave function is
a solution of
\[ -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x), \quad (A1) \]
where the potential is periodic, \( V(x + d) = V(x) \), and is assumed to have inversion symmetry, \( V(-x) = V(x) \). In the context of the GP equation, \( V(x) = V_{\text{opt}}(x) + gn_c(x) \) and the inversion property is valid if the condensate density also satisfies \( n_c(-x) = n_c(x) \). This is ensured if the wave function has the property we wish to prove.

We seek solutions of the Bloch form, \( \psi(x + d) = e^{ikd}\psi(x) \). Due to the inversion symmetry, the linearly independent solutions of (A1) can be chosen to be even \((\psi_e)\) or odd \((\psi_o)\) functions of \( x \) and \( \psi(x) \) can be expressed as the linear combination
\[ \psi(x) = a\psi_e(x) + b\psi_o(x). \quad (A2) \]
The periodic part of the Bloch function is then
\[ w_k(x) = e^{-ikx}(a\psi_e(x) + b\psi_o(x)). \quad (A3) \]
The two independent solutions at energy \( E \) are chosen to have the normalization
\[ \frac{1}{d} \int_{-d/2}^{d/2} |\psi_{e/o}(x)|^2 \, dx = 1. \quad (A4) \]
Imposing the Bloch condition, we obtain the relation
\[ \frac{\psi'_e}{\psi_e} = \frac{\psi'_o}{\psi_o} \tan \left( \frac{kd}{2} \right) \quad (A5) \]
where all the functions are evaluated at \( x = d/2 \). Since \( \psi_e \) and \( \psi_o \) are functions of the energy, \( E \), this equation determines the band energy \( E_k \). Clearly \( E_{-k} = E_k \). If \( E_0 \) is the band energy at the zone centre \((k = 0)\), we must have either \( \psi'_e(d/2; E_0) = 0 \) or \( \psi_o(d/2; E_0) = 0 \). The former defines what we shall refer to as an even-parity band, while the latter defines an odd-parity band. The small-\( k \) behaviour of \( E \) is thus readily obtained from these properties. For example, for an odd-parity band we have
\[ \psi_o(d/2; E) = \psi_o(E - E_0) + \cdots \quad (A6) \]
where \( \psi'_o \equiv d\psi_o(d/2; E)/dE|_{E=E_0} \). We then have
\[ E_k = E_0 + \frac{\psi'_o\psi'_e}{\psi_o\psi_e} \left( \frac{dk}{2} \right)^2 + \cdots \quad (A7) \]
The coefficient of \( k^2 \) defines the effective mass of the band. A similar result applies in the case of the even-parity bands.

Once the energy eigenvalue for a given \( k \) is known, the coefficients \( a \) and \( b \) are related by
\[ \frac{b}{a} = i \frac{\psi_e}{\psi_o} \tan \left( \frac{kd}{2} \right). \quad (A8) \]
For a given band, \( n \), the ratio \( b/a \) is a continuous function of \( k \). At \( k = 0 \) we choose \( w_{e/o}(x) \) to be real and assume that it is a parity eigenstate. In this situation, we must have either \( b(k = 0) = 0 \) (even-parity bands) or \( a(k = 0) = 0 \) (odd-parity bands).

The normalization of \( w_k \) leads to the expressions
\[ |a|^2 = \frac{1}{1 + \lambda^2}, \quad |b|^2 = \frac{\lambda^2}{1 + \lambda^2} \quad (A9) \]
where
\[ \lambda(k) = \frac{\psi_e}{\psi_o} \tan \left( \frac{kd}{2} \right). \quad (A10) \]
For an even-parity band \( \lambda \to 0 \) as \( k \to 0 \), so that \( a(k) \to 1 \) and \( b(k) \to 0 \). In this case,
\[ w_k(x) = e^{-ikx} \left( \frac{\psi_e(x)}{\sqrt{1 + \lambda^2}} + i \frac{\lambda \psi_o(x)}{\sqrt{1 + \lambda^2}} \right). \quad (A11) \]
Since \( \lambda(-k) = -\lambda(k) \), we see that \( w_{-k}(-x) = w_k(x) \). On the other hand, for an odd-parity band, \( \lambda(k) \to \infty \) as \( k \to 0 \), and \( b(k) \to 1 \). As a result, we have
\[ w_k(x) = e^{-ikx} \left( -i \frac{\text{sgn}(\lambda)\psi_e(x)}{\sqrt{1 + \lambda^2}} + \frac{|\lambda|\psi_o(x)}{\sqrt{1 + \lambda^2}} \right), \quad (A12) \]
which implies \( w_{-k}(-x) = -w_k(x) \). We have thus shown that the Bloch functions have the property
\[ w_{-k}(-x) = \pm w_k(x) \quad (A13) \]
where the positive (negative) sign corresponds to the even (odd) parity bands. Together with the conjugation property \( w_k^*(x) = w_{-k}(x) \), we have \( w_k^*(x) = \pm w_k(x) \).

For an even-parity band, the real and imaginary parts of \( w_k \) are
\[ \Re w_k(x) = \frac{1}{\sqrt{1 + \lambda^2}} \cos(kx)\psi_e(x) + \lambda \sin(kx)\psi_o(x) \]
\[ \Im w_k(x) = \frac{1}{\sqrt{1 + \lambda^2}} \left( -\sin(kx)\psi_e(x) + \lambda \cos(kx)\psi_o(x) \right). \]
Thus the real part is an even function of \( x \) with the property \( d\Re w_k/\text{d}x|_{x=d/2} = 0 \), while the imaginary part is odd and \( \Im w_k(\pm d/2) = 0 \). The opposite is true of an odd-parity band. One can show for an arbitrary \( k \) in the lowest band that there is no net change in the phase \( \theta_k(x) = \tan^{-1}(\Im w_k(x)/\Re w_k(x)) \) as \( x \) varies between \(-d/2 \) and \( d/2 \). We make use of this result in Sec. 11.

The method described above cannot be used in three dimensions, but perturbation theory allows one to infer the same symmetry property. We write the Schrödinger equation for the Bloch function \( w_k(r) \) as
\[ (\hat{h}_0 + \delta V)w_k(r) \quad (A14) \]
where \( \hat{h}_0 = -(\hbar^2/2m)\nabla^2 + \hbar^2k^2/2m + V(r) \) and \( \delta V = (\hbar k/m) \cdot \nabla \). The eigenfunctions of \( \hat{h}_0 \), \( w_n(r) \), with
APPENDIX B: DYNAMIC INSTABILITY IN THE WEAK POTENTIAL LIMIT

As pointed out by Wu and Niu [2], the boundary of the dynamically unstable region in the weak potential limit is given by the condition \( E_-(q) = E_+(q - G) \) where \( E_\pm(q) \) is given by (127). These energies are the eigenvalues of the Bogoliubov equations

\[
\hat{B}_0 \begin{pmatrix} u_+ \\ v_+ \end{pmatrix} = E_\pm \begin{pmatrix} u_+ \\ -v_\mp \end{pmatrix}
\]

(B1)

with

\[
\hat{B}_0 = \begin{pmatrix} -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + g\tilde{n} - \varepsilon_k^{(0)} & -g\tilde{n}e^{2ikz} \\ -g\tilde{n}e^{-2ikz} & -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + g\tilde{n} - \varepsilon_k^{(0)} \end{pmatrix}
\]

(B2)

The phonon mode of interest is

\[
\begin{pmatrix} u_+ \\ v_+ \end{pmatrix} = \begin{pmatrix} a_+e^{i(q-G-k)z} \\ b_+e^{i(q-G-k)z} \end{pmatrix}
\]

(B3)

with \( a_+ = \sqrt{\tilde{\varepsilon}_q - \tilde{\varepsilon}_G + E_+} / 2\tilde{E}_+ \) and \( b_+ = \sqrt{\tilde{\varepsilon}_q - \tilde{\varepsilon}_G} / 2\tilde{E}_+ \) where \( \tilde{\varepsilon}_q = \varepsilon_k^{(0)} + g\tilde{n} \) and \( E_+ = E_+(q - G) - \hbar^2k(q - G)/m \). The normalization of the mode is \( a_+^* a_+ - b_+^* b_+ = 1 \). The anti-phonon mode which is coupled to the phonon mode by a weak optical potential, \( V_{\text{opt}} = V_0 \cos(Gz) \), is

\[
\begin{pmatrix} u_- \\ v_- \end{pmatrix} = \begin{pmatrix} a_-e^{i(q+k)z} \\ b_-e^{i(q+k)z} \end{pmatrix}
\]

(B4)

with \( a_- = \sqrt{\tilde{\varepsilon}_q - \tilde{\varepsilon}_G} / 2\tilde{E}_- \) and \( b_- = \sqrt{\tilde{\varepsilon}_q + \tilde{\varepsilon}_G} / 2\tilde{E}_- \), where \( \tilde{E}_- = E_+(q) - \hbar^2kq/m \).

We note that in this case the mode has normalization \( a_+^*a_+ - b_+^*b_+ = -1 \).

The degeneracy of the phonon and anti-phonon modes \( (E_-(q) = E_+(q - G) \equiv \equiv E_0) \) suggests that we seek a solution of the Bogoliubov equations

\[
\hat{B} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ -v \end{pmatrix}
\]

in the form

\[
\begin{pmatrix} u \\ v \end{pmatrix} = A \begin{pmatrix} u_+ \\ v_+ \end{pmatrix} + B \begin{pmatrix} u_- \\ v_- \end{pmatrix} \]

(B6)

Expanding the operator \( \hat{B} \) to first order in the optical potential, we have \( \hat{B} = \hat{B}_0 + \hat{B}_1 \) with

\[
\hat{B}_1 = \begin{pmatrix} V_{\text{opt}} + 2g\tilde{n}(w_1 + w_1^*) & -2g\tilde{n}e^{2ikz}w_1 \\ -2g\tilde{n}e^{-2ikz}w_1^* & V_{\text{opt}} + 2g\tilde{n}(w_1 + w_1^*) \end{pmatrix}
\]

(B7)

Here we have written the condensate wave function as \( \Phi_k(x) = \sqrt{\tilde{n}}e^{ikx}(1 + w_1 + \cdots) \) where the first order correction is \( w_1(x) = \alpha_+ e^{iGx} + \alpha_- e^{-iGx} \) with

\[
\alpha_\pm = \frac{-\sqrt{\varepsilon_G^{(0)}} + \sqrt{4\varepsilon_G^{(0)}\varepsilon_k^{(0)}}V_0}{2 \left[ (\varepsilon_G^{(0)})^2 + 2g\tilde{n}\varepsilon_G^{(0)} - 4\varepsilon_G^{(0)}\varepsilon_k^{(0)} \right]}
\]

(B8)

Taking the inner product of \( \alpha_\pm \) with \( (u_+^* \ v_+^*) \) and \( (u_-^* \ v_-^*) \), and noting the different normalizations of the two modes, we obtain the matrix equation

\[
\begin{pmatrix} E_0 - E \\ \Delta \end{pmatrix} = \begin{pmatrix} \alpha_+ a_+ + b_+ b_- \\ -2g\tilde{n}\alpha_- a_- b_- + \alpha_+ a_- b_+ \end{pmatrix} \]

(B10)

A nontrivial solution to the matrix equation is obtained if

\[
E = E_0 \pm i|\Delta|.
\]

(B11)

Thus, the line in the \( k,q \) plane defined by \( \varepsilon_k^{(0)} \) lies within the region of dynamical instability when \( V_0 \) is finite. As emphasized by Wu and Niu [2], the dynamical instability in the weak potential limit arises from a resonant coupling between phonon and anti-phonon modes.

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