Dispersive law for a one-dimensional weakly interacting Bose gas with zero boundary conditions

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From the time-dependent Gross equation, we find the quasiparticle dispersion law for a one-dimensional weakly interacting Bose gas with a non-point interatomic potential and zero boundary conditions (BCs). The result coincides with the dispersion law for periodic BCs, i.e., the Bogolyubov law
\[
E_B(k) = \sqrt{\left(\frac{\hbar^2 k^2}{2m}\right)^2 + n_0 \nu(k) \frac{\hbar^2 k^2}{m}}.
\]
In the case of periodic BCs, the dispersion law can be easily derived from Gross’ equation. However, for zero BCs, the analysis is not so simple.

1 Introduction

The quasiparticle dispersion law is usually derived under periodic boundary conditions (BCs), because under such BCs the analysis is the simplest [1–6]. In nature, however, BCs are typically close to zero ones. An analysis under zero BCs is of independent interest from a mathematical point of view. From a physical point of view, it is interesting to ascertain whether the boundaries affect the dispersion law \( E(k) \) of the quasiparticles. Another interesting point is that under zero BCs, the wave functions of the system are not eigenfunctions of the momentum operator. Therefore, the value of \( k \) in the quasiparticle dispersion law \( E(k) \) is a quasimomentum (instead of momentum).

The dispersion law \( E(k) \) for a one-dimensional (1D) system of weakly interacting bosons with zero BCs has already been found using the Bethe ansatz [7] (for a point interaction) and by a generalization of Bogoliubov’s method [8] (for a non-point interaction). Both solutions coincide with the Bogoliubov law [1, 2]
\[
E_B(k) = \sqrt{\left(\frac{\hbar^2 k^2}{2m}\right)^2 + n_0 \nu(k) \frac{\hbar^2 k^2}{m}}.
\] (1)

It was also found within Haldane’s harmonic-fluid approach that the sound velocity in a 1D Bose system with zero BCs is the same as that in a similar system with periodic BCs [9].
The dispersion law (1) is in approximate agreement with the experiment \[10, 17\] (true, all experiments except \[17\] were performed with a nonuniform gas in a trap). The results in \[7\] hint that in the case of zero BCs, quasimomentum seems to be an additional (non-additive) integral of motion instead of an additive momentum. However, we do not know whether there exists an operator that corresponds to the quasimomentum of the system and commutes with the Hamiltonian of the system.

In the present work, we determine the dispersion law of a 1D system of weakly interacting bosons under zero BCs and in the absence of an external field. The interatomic potential is assumed to be in its general form. We use Gross’ approach \[3, 18, 19\] which is the simplest method of describing a weakly interacting Bose system. In this case, we obtain new solutions of Gross’ equation \[2\]. Such an approach complements the methods in \[7–9\] and helps to better understand the properties of quasiparticles under zero BCs, including the nature of the quasimomentum of the quasiparticle.

## 2 Solutions of Gross’ equation

For simplicity, we restrict ourselves to a 1D case. Consider a weakly interacting Bose gas placed in a vessel with zero BCs in the absence of an external field. Let the temperature be extremely low, \(T \rightarrow 0\) K. Such a gas can be described by the time-dependent Gross equation \[3, 19\]

\[
i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + \Psi(x,t) \int_0^L dx' U(|x-x'|)|\Psi(x',t)|^2
\]

(2)

with the normalization

\[
\int_0^L dx |\Psi(x,t)|^2 = N,
\]

(3)

where \(N\) is the total number of particles. Let the system be in interval \(x \in [0, L]\). Zero BCs mean that

\[
\Psi(x = 0, t) = \Psi(x = L, t) = 0.
\]

(4)

Gross’ equation \[2\] follows from the Heisenberg operator equation if we set \(\hat{\psi}(x,t) = \Psi(x,t)\) in the latter \[3, 19\]. In this case, \(N\) must be large \((N \gg 1)\), and \(\Psi(x,t)\) can be regarded as the wave function (WF) of a nonuniform quasicondensate. Later, equation (2) was derived by three other methods \[20–22\].

If we replace the interatomic potential \(U(|x-x'|)\) by a point-like one \(2c\delta(x-x')\), then Eq. \(2\) passes into the Gross–Pitaevskii equation \[23, 24\]

\[
i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi(x,t) + 2c|\Psi(x,t)|^2 \Psi(x,t).
\]

(5)

In what follows we consider the general case of a non-point potential \(U(|x-x'|)\).
Note that condensate \( N_{k=0} \sim N \) for an infinite 1D uniform system is forbidden at \( T > 0 \) and even at \( T = 0 \). However, all systems in nature are finite. For a finite 1D uniform system at \( T \geq 0 \), the lowest macroscopically occupied state is permitted, although its properties correspond to a quasicondensate rather than a condensate. For our approach, the distinction between condensate and quasicondensate is inessential; both can be described by WF \( \Psi(x,t) \).

The quasicondensate WF reads
\[
\Psi(x,t) = R(x,t) e^{iS(x,t)/\hbar},
\]
where \( R \) and \( S \) are real functions. Let the quasicondensate in the ground state be described by the WF
\[
\Psi_0(x,t) = R_0(x) e^{iS_0/\hbar}, \quad S = -\epsilon t,
\]
which satisfies the equation
\[
e\Psi_0 = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_0}{\partial x^2} + \Psi_0(x,t) \int_0^L dx' U(|x - x'|) |\Psi_0(x',t)|^2.
\]
The BCs are \( R_0(x = 0, t) = R_0(x = L, t) = 0 \). Such a quasicondensate is uniform everywhere except in a very narrow region near the walls, and the particle number density is \( n_0(x) = R_0^2(x) \). In the presence of small oscillations, we obtain:
\[
R(x,t) = R_0(x) + \delta R(x,t), \quad S(x,t) = -\epsilon t + s_0(x,t),
\]
and \( n(x) \equiv R^2(x) = n_0(x) + \tilde{n}_0(x,t) \). Because \( R, n \) and \( S \) are real, the quantities \( \tilde{n}_0(x,t) \) and \( s_0(x,t) \) must also be real. By substituting function (6) with \( R(x,t), S(x,t) \) into Eq. (2) and separating the real and imaginary parts, we obtain the following equations for the small quantities \( \tilde{n}_0(x,t) \) and \( s_0(x,t) \):
\[
\frac{\partial \tilde{n}_0}{\partial t} = -\frac{1}{m} \nabla [(n_0 + \tilde{n}_0) \nabla s_0],
\]
\[
-\frac{\partial s_0}{\partial t} = -\frac{\hbar^2}{2m} \frac{\nabla^2 [(n_0 + \tilde{n}_0)^{1/2} - n_0^{1/2}]}{(n_0 + \tilde{n}_0)^{1/2}} + \frac{(\nabla s_0)^2}{2m} + \frac{\hbar^2 \delta R}{2m R_0 R_0 + \delta R} \int_0^L dx' \tilde{n}_0(x',t) U(|x - x'|).
\]
To simplify these equations, we neglect the nonuniformity of \( R_0(x) \) near the walls by setting \( \nabla n_0 = 0 \) and \( \nabla R_0 = 0 \). In this case \( n_0(x) = n_0 = N/L \). If \( N \gg 1 \) and the coupling is not too weak, the values of \( \nabla n_0 \) and \( \nabla R_0 \) are significantly different from zero only at a distance from the wall, which is less than or of the order of the mean interatomic distance \( \bar{R} = L/N \). Therefore, we may expect that consideration of the nonuniformity of \( R_0(x) \) near the wall will
affect only the solution for the ground state, but not the dispersion law, because the latter is a bulk property.

Furthermore, we consider the oscillations of the density and the phase to be so weak that their smallness exceeds the smallness of the potential. In this case we can restrict ourselves by a linear approximation. Thus, we obtain

\[
\frac{\partial \tilde{n}_0}{\partial t} = -\frac{n_0}{m} \nabla^2 s_0, \tag{12}
\]

\[
-\frac{\partial s_0}{\partial t} = -\frac{\hbar^2}{4 mn_0} \nabla^2 \tilde{n}_0 + \int_0^L dx' \tilde{n}_0(x', t) U(|x - x'|), \tag{13}
\]

and the zero BCs take the form

\[
\tilde{n}_0(x = 0, t) = 0, \quad \tilde{n}_0(x = L, t) = 0. \tag{14}
\]

Because only standing waves can be stationary in the presence of boundaries, we seek solutions in the form

\[
\tilde{n}_0(x, t) = \tilde{n}(x) T_n(t), \quad s_0(x, t) = s(x) T_s(t). \tag{15}
\]

Substituting these functions into Eqs. (12) and (13) and separating the variables, we obtain:

\[
\frac{1}{T_s(t)} \frac{\partial T_n(t)}{\partial t} = C_1, \tag{16}
\]

\[
-\frac{1}{T_n(t)} \frac{\partial T_s(t)}{\partial t} = C_2, \tag{17}
\]

\[
C_1 \tilde{n}(x) = -\frac{n_0}{m} \nabla^2 s(x), \tag{18}
\]

\[
C_2 s(x) = -\frac{\hbar^2}{4 mn_0} \nabla^2 \tilde{n}(x) + \int_0^L dx' \tilde{n}(x') U(|x - x'|). \tag{19}
\]

The solution of Eqs. (16) and (17) can be written as

\[
T_n(t) = \cos \omega t, \quad T_s(t) = \sin \omega t, \quad C_1 = C_2 = -\omega \tag{20}
\]

in the real form or

\[
T_n(t) = T_s(t) = e^{i\omega t}, \quad C_1 = -C_2 = i\omega \tag{21}
\]

in the complex form. The real values of \(\tilde{n}_0(x, t)\) and \(s_0(x, t)\) are only obtained for the solution (20), which is used in the following. Then the equations for \(\tilde{n}(x)\) and \(s(x)\) take the form:

\[
\omega \tilde{n}(x) = \frac{n_0}{m} \nabla^2 s(x), \tag{22}
\]

\[
-\omega s(x) = -\frac{\hbar^2}{4 mn_0} \nabla^2 \tilde{n}(x) + \int_0^L dx' \tilde{n}(x') U(|x - x'|). \tag{23}
\]
These are the two basic equations that we will study here. They are simple enough but are generally not easily solvable.

Let us try to find a solution as a single harmonic:

\[ \hat{n}(x) = n_0 a_{2l} \sin(k_{2l}x), \quad s(x) = b_{2l} \sin(k_{2l}x), \quad k_{2l} = 2\pi l/L. \]  

(24)

Under periodic BCs, the potential can be expanded in a Fourier series

\[ U(|x_1 - x_2|) = \frac{1}{L} \sum_{j=0,\pm 1,\pm 2,...} \nu(k_j) e^{ik_j(x_1 - x_2)}, \]  

(25)

\[ \nu(k) = \int_{-L}^{L} U_1(|x|) e^{-ikx} dx, \]  

(26)

where \( x = x_1 - x_2 \), and \( k_j = 2\pi j/L \). In this case, the potential is

\[ U(|x_1 - x_2|) = U_1(|x_1 - x_2|) + U_1(L - |x_1 - x_2|), \]  

(27)

because one particle acts on the other particle from both sides. Note that Eq. (26) contains namely \( U_1(x) \), rather than \( U(x) \). The formulae (25) and (26) follow from Fourier analysis if we consider that the argument(s) of the function \( U(|x_1 - x_2|) \) is (are) [i] \( x_1 - x_2 \) or [ii] \( x_1 \) and \( x_2 \) independently. In the thermodynamic limit, the addition \( U_1(L - |x_1 - x_2|) \) into (27) is usually omitted. By substituting (24) and (25) into (22) and (23), we can easily obtain the Bogoliubov dispersion law (1).

If we take boundaries into account and try to solve the problem in a similar way, we will fail. This is due to the fact that, because of the different expansion of the potential, substituting the harmonic (24) into Eqs. (22) and (23) generates many other harmonics. According to the rules of Fourier analysis, for a system with zero BCs, the potential \( U(|x_1 - x_2|) \) can be expanded into the following series:

\[ U(|x_1 - x_2|) = \sum_{j=0,\pm 1,\pm 2,...} \frac{\nu(k_j)}{2L} e^{ik_j(x_1 - x_2)} \]

\[ = \frac{\nu(0)}{2L} + \sum_{j=1,2,...} \frac{\nu(k_j)}{L} \cos[k_j(x_1 - x_2)], \]  

(28)

\[ \nu(k) = \int_{-L}^{L} U(|x|) e^{-ikx} dx, \]  

(29)

where \( k_j = \pi j/L \). This series exactly reproduces the initial function over the entire domain \( x_1, x_2 \in [0, L] \). The expansions for periodic and zero BCs were analyzed in detail in [40].

From equations (22), (23), and (28), we now find the dispersion law under zero BCs

\[ \hat{n}(0) = 0, \quad \hat{n}(L) = 0. \]  

(30)
We represent $\tilde{n}(x)$ and $s(x)$ in the form of expansions in the complete set of sines:

$$\tilde{n}(x) = n_0 \sum_{l=1,2,\ldots} a_l \sin (k_l x), \quad (31)$$

$$s(x) = \sum_{l=1,2,\ldots} b_l \sin (k_l x), \quad (32)$$

where $k_l = \pi l / L$. Then the BCs (30) are satisfied, and the expansions (31) and (32) contain all possible wavelengths ($\lambda = 2L/l$) corresponding to the zero BCs. Therefore, the expansions (31) and (32) ensure a correct and complete description of the system.

Let us substitute these series into Eq. (22). Because the sines $\sin (k_l x)$ are independent basis functions, the equations for the coefficients $a_l$, $b_l$ and frequency $\omega$ can be obtained if the sum of the coefficients of each of $\sin (k_l x)$ is set to zero. In this way, equation (22) yields

$$b_l = -\frac{\omega m}{k_l^2} a_l, \quad l = 1, 2, \ldots, \infty. \quad (33)$$

Using (28), (31), and (32) and the expansions

$$\cos(k_j x) = \sum_{p=1,2,3,\ldots} c^p_j \sin(k_p x), \quad (34)$$

$$1 = \sum_{p=1,2,3,\ldots} c^p_0 \sin(k_p x) \quad (35)$$

with

$$c^p_j = \begin{cases} 0 & \text{for even } p - j, \\ \frac{2}{\pi} \left( \frac{1}{p-j} + \frac{1}{p+j} \right) & \text{for odd } p - j, \end{cases} \quad (36)$$

we find after some algebra:

$$\int_0^L dx' \tilde{n}(x')U(|x - x'|) = \frac{n_0 \nu(0)}{2L} \sum_{p=1,2,\ldots} \frac{a_p}{k_p} [1 - (-1)^p] \sum_{l=1,2,\ldots} c^0_l \sin (k_l x) \quad (37)$$

Subject to (31), (32), (33), and (37), equation (23) is reduced to:

$$\sum_{l=1,2,\ldots} a_l \sin (k_l x) \frac{E^2_{M}(k_l) - \hbar^2 \omega^2}{\hbar^2 k_l^2 / m} + \sum_{l=1,2,\ldots} c^l_0 \sin (k_l x) \sum_{p=1,2,\ldots} \frac{n_0 \nu(0)}{2\pi p} a_p [1 - (-1)^p]$$

$$+ \sum_{j,p=1,2,\ldots} \frac{c^j_p n_0 \nu(k_j)}{2\pi} a_p [1 - (-1)^p+j] \left( \frac{1}{p-j} + \frac{1}{p+j} \right) = 0. \quad (38)$$
Because the functions \( \sin(k_l x) \) are independent, from (38) we obtain the system of equations for the unknown coefficients \( a_l \) and frequency \( \omega \):

\[
(E^2_M(k_l) - \hbar^2\omega^2)a_l + c^l_0 \sum_{p=1,2,\ldots} \frac{\varepsilon^2_q(0)}{\pi p} [1 - (-1)^p]a_p
\]

\[
+ \sum_{j,p=1,2,\ldots} j \neq p \frac{\varepsilon^p_q(0)}{\pi} [1 - (-1)^{p+j}] \left( \frac{1}{p - j} + \frac{1}{p + j} \right) a_p = 0, \quad l = 1, 2, \ldots, \infty,
\]

where

\[
\varepsilon^2_q(0) = n_0 \nu_q \frac{\hbar^2 k_l^2}{2m}.
\]

Because the factor \( c^l_0 \) is zero for all even \( l \)'s and non-zero for all odd \( l \)'s, the system of equations (40) splits into two independent systems of equations, one for \( a_l \)'s with even \( l \)'s and the other for \( a_l \)'s with odd \( l \)'s. These systems of equations can be written as follows:

\[
a_{2l}(E^2_M(k_{2l}) - \hbar^2\omega^2) + 4 \sum_{j=0,\pm 1,\pm 2,\ldots} \frac{\varepsilon^2_{2l}(k_{2j+1})}{2l - 2j - 1}
\]

\[
\times \sum_{p=1,2,\ldots} a_{2p} \left[ \frac{1}{2p - 2j - 1} + \frac{1}{2p + 2j + 1} \right] = 0, \quad l = 1, 2, \ldots, \infty,
\]

\[
a_{2l-1}(E^2_M(k_{2l-1}) - \hbar^2\omega^2) + 4 \sum_{j=0,\pm 1,\pm 2,\ldots} \frac{\varepsilon^2_{2l-1}(k_{2j})}{2l - 2j - 1}
\]

\[
\times \sum_{p=1,2,\ldots} a_{2p-1} \left[ \frac{1}{2p - 2j - 1} + \frac{1}{2p - 1 + 2j} \right] = 0, \quad l = 1, 2, \ldots, \infty.
\]

We now take into account that, for any integer \( l \),

\[
\frac{4}{\pi^2} \sum_{j=0,\pm 1,\pm 2,\ldots} \frac{1}{(2l - 2j - 1)^2} = 1.
\]

For a large \( N \) the function \( \varepsilon^2_{2l}(q_{2j+1}) \) varies slightly as \( j \) changes by one. The main contribution to sum (44) is made by the terms with \( j = l, l - 1 \) and the nearest ones. Therefore, we have

\[
\frac{4}{\pi^2} \sum_{j=0,\pm 1,\pm 2,\ldots} \frac{\varepsilon^2_{2l}(k_{2j+1})}{(2l - 2j - 1)^2} = \varepsilon^2_{2l}(k_{2l}) + \varepsilon^2_{g}(2l),
\]

where \( \varepsilon^2_{g}(2l) \ll \varepsilon^2_{2l}(k_{2l}) \) should hold. Eq. (45) defines function \( \varepsilon^2_{g}(2l) \). Let us separate the term with \( p = l \) from the sum in (42). Then, subject to (45), we obtain the following infinite system of equations for the coefficients \( a_{2l} \):

\[
a_{2l}(E^2_B(k_{2l}) + \varepsilon^2_{g}(2l) + \varepsilon^2_{g}(2l) - \hbar^2\omega^2) + 4 \sum_{j=0,\pm 1,\pm 2,\ldots} \frac{\varepsilon^2_{2l}(k_{2j+1})}{2l - 2j - 1}
\]

\[
\times \sum_{p=1,2,\ldots} a_{2p} \left[ \frac{1}{2p - 2j - 1} + \frac{1}{2p + 2j + 1} \right] = 0, \quad l = 1, 2, \ldots, \infty,
\]

\[
\varepsilon^2_{g}(2l) = \frac{\varepsilon^2_{g}(2l)}{2l - 2j - 1}.
\]
with
\[\epsilon^2_b(2l) = \frac{4}{\pi^2} \sum_{j=0,\pm1,\pm2,...} \frac{\epsilon_2^2(k_{2j+1})}{4l^2 - (2j + 1)^2}.\] (47)

Similarly, Eq. (43) can be written as
\[a_{2l-1}(E_B^2(k_{2l-1}) + \epsilon_b^2(2l - 1) + \epsilon_g^2(2l - 1) - \hbar^2 \omega^2)\]
\[+ \frac{4}{\pi^2} \sum_{j=0,\pm1,\pm2,...} \frac{\epsilon_{2l-1}^2(k_{2j})}{2l - 2j - 1} \sum_{p=1,2,...} a_{2p-1} \left[ \frac{1}{2p - 1 - 2j} + \frac{1}{2p - 1 + 2j} \right] = 0,\]
where \(l = 1, 2, \ldots, \infty\) and
\[\epsilon_b^2(2l - 1) = \frac{4}{\pi^2} \sum_{j=0,\pm1,\pm2,...} \frac{\epsilon_{2l-1}^2(k_{2j})}{(2l - 1)^2 - 4j^2}.\] (49)
\[\epsilon_g^2(2l - 1) = \frac{4}{\pi^2} \sum_{j=0,\pm1,\pm2,...} \frac{\epsilon_{2l-1}^2(k_{2j})}{(2l - 2j - 1)^2} - \epsilon_{2l-1}^2(k_{2l-1}).\] (50)

It is convenient to introduce the coefficients \(f_l\):
\[f_l = \frac{\epsilon_b^2(l) + \epsilon_g^2(l)}{E_B^2(k_l)}; \quad l = 1, 2, \ldots, \infty.\] (51)

Consider the system of equations (46) for \(a_{2l}\)'s. This is an infinite system of linear homogeneous equations for the coefficients \(a_{2l}\). The system has a solution if its determinant is equal to zero. This condition yields the equation for \(\omega^2\), which has an infinite number of solutions \(\omega_{2j}^2 (j = 1, 2, \ldots, \infty)\). The sum in Eq. (46) contains only terms with alternating denominators. This favors the smallness of the sum, because
\[\sum_{j=0,\pm1,\pm2,...} \frac{1}{(2l - 2j - 1)(\pm2p - 2j - 1)} = 0\] (52)
for integers \(p, l, \text{ and } \pm p \neq l\). These properties allow us to construct a perturbation theory to solve equation (46).

To obtain the solution in the zero approximation, we set the sum in (46) to zero. Then the system of equations (46) is reduced to the equations
\[a_{2l}(E_B^2(k_{2l})[1 + f_{2l}] - \hbar^2 \omega^2) = 0, \quad l = 1, 2, \ldots, \infty\] (53)
and gives the solutions \(a_{2l_0} \neq 0, a_{2l \neq 2l_0} = 0\) and
\[\hbar^2 \omega^2(k_{2l_0}) = E_B^2(k_{2l_0})[1 + f_{2l_0}];\] (54)
here \(l_0, l = 1, 2, \ldots, \infty\). That is, in the zero approximation, expansions (31) and (32) consist only of a single \(2l_0\)-harmonic. In the higher approximations, we will include other harmonics.

In the first approximation, we take into account the sum in (46) and consider that \(a_{2l \neq 2l_0}\) are small but non-zero for all \(l, l_0\). Let \(\omega(2l_0)\) be the frequency, which is a solution of the
system of equations (46) and corresponds to the quasimomentum $k_{2l_0}^l$: $\omega(2l_0) \equiv \omega(k_{2l_0}^l)$. Then, in the set of coefficients $a_2, a_4, a_6, \ldots$, which are the solutions of Eq. (46) for the frequency $\omega(2l_0)$, the value of the harmonic $a_{2l_0}$ must be much larger (in modulus) than the values of all the other $a_{2l}$’s. Therefore, for the frequency $\omega(2l_0)$ we consider the harmonic $a_{2l_0}$ to be the principal and separate it from the sum in Eq. (46) by assuming that the contribution of the other harmonics $a_{2p \neq 2l_0}$ to the sum is small. From the system of equations (46), for $l \neq l_0$ we find

$$a_{2l \neq 2l_0}(2l_0) = a_{2l_0}(2l_0) \frac{A_{2l}(2l_0)\hbar^2 \omega^2(2l_0)}{E_B^2(k_{2l_0})[1 + f_{2l}] - \hbar^2 \omega^2(2l_0)}, \quad (55)$$

where $l = 1, 2, \ldots, \infty$ (except $l = l_0$), and the inequality $|a_{2l \neq 2l_0}(2l_0)| \ll |a_{2l_0}(2l_0)|$ must hold (otherwise the exact solution $\hbar^2 \omega^2(k_{2l_0})$ can be very different from the zero approximation (54)). If $|a_{2l \neq 2l_0}(2l_0)| \ll |a_{2l_0}(2l_0)|$, we can look for the quantity $A_{2l}(2l_0)$ using perturbation theory:

$$A_{2l}(2l_0) = A_{2l_0}^{(0)}(2l_0) + \delta A_{2l}(2l_0), \quad (56)$$

$$A_{2l}^{(0)}(2l_0) = -\frac{4}{\pi^2} \sum_{j=0, \pm 1, \ldots, \pm \infty} \frac{\epsilon_{2l}^2(k_{2j+1})}{2l - 2j - 1} \times \left[ \frac{1}{2l_0 - 2j - 1} + \frac{1}{2l_0 + 2j + 1} \right], \quad (57)$$

$$\delta A_{2l}(2l_0) = -\frac{4}{\pi^2} \sum_{j=0, \pm 1, \ldots, \pm \infty} \frac{\epsilon_{2l}^2(k_{2j+1})}{2l - 2j - 1} \times \sum_{p=1, 2, \ldots, \infty} \frac{A_{2p}(2l_0)}{E_B^2(k_{2p})[1 + f_{2p}] - \hbar^2 \omega^2(2l_0)} \left[ \frac{1}{2p - 2j - 1} + \frac{1}{2p + 2j + 1} \right] \approx -\frac{4}{\pi^2} \sum_{j=0, \pm 1, \ldots, \pm \infty} \frac{\epsilon_{2l}^2(k_{2j+1})}{2l - 2j - 1} \times \sum_{p=1, 2, \ldots, \infty} \frac{A_{2p}^{(0)}(2l_0)}{E_B^2(k_{2p})[1 + f_{2p}] - \hbar^2 \omega^2(2l_0)} \left[ \frac{1}{2p - 2j - 1} + \frac{1}{2p + 2j + 1} \right]. \quad (58)$$

This method is true if for all $l_0$ and $l$ (except $l = l_0$),

$$|\delta A_{2l}(2l_0)| \ll |A_{2l_0}^{(0)}(2l_0)|. \quad (59)$$

Next, we consider Eq. (46) with $l = l_0$ and substitute $a_{2l \neq 2l_0}$ (55) into (46). In this case, $a_{2l_0}$ is canceled in Eq. (46), and we obtain the following equation for the frequency:

$$\hbar^2 \omega^2(2l_0) = E_B^2(k_{2l_0})[1 + f_{2l_0}] - \hbar^2 \omega^2(2l_0) \delta A_{2l_0}(2l_0). \quad (60)$$

Although equation (58) was obtained for $\delta A_{2l}(2l_0)$ when $l \neq l_0$, we may formally set $l = l_0$ in (58). Such a $\delta A_{2l_0}(2l_0)$ is denoted in (60) as $\delta A_{2l_0}(2l_0)$. Let us also denote

$$-\hbar^2 \omega^2(2l_0) \delta A_{2l_0}(2l_0) = q_{2l_0} E_B^2(k_{2l_0}), \quad (61)$$
Fig. 1: [Color online] Values of $f_{2l}/g$ for various $l$ for the 1D system of $N = 1000$ $^4$He atoms with interatomic potential (64) and $a = 2\,\text{Å}$, $a/\bar{R} = 0.5$. The symbols code the different values of $u_0 = \frac{U_0}{k_B}$: $u_0 = 0.1$ (circles), $u_0 = 1$ (diamonds), $u_0 = 10$ (crosses), and $u_0 = 100$ (triangles). The scale factor $g$ is different for different curves: $g = 0.1u_0N^2/\bar{R}^2$ for $u_0 = 0.1$; 1; 10 and $g = 1$ for $u_0 = 100$. Note that we have changed the value of $|f_{2l}/g|$ for $l = 1596$ (the bottom triangle): the figure shows $f_{2l}/g = -2$, but the real value is $f_{2l}/g = -6.35$.

then (60) takes the form

$$\hbar^2\omega^2(2l_0) = E_B^2(k_{2l_0})[1 + f_{2l_0} + q_{2l_0}].$$

From Eqs. (61) and (62) we get the equation

$$q_{2l_0} = -\delta A_{2l_0}(2l_0)[1 + f_{2l_0} + q_{2l_0}]$$

for the new parameter $q_{2l_0}$. In this case, $\delta A_{2l_0}(2l_0)$ is given by (58) and depends on $q_{2l_0}$.

It is difficult to analyze the obtained equations analytically, but the numerical analysis is rather simple. We used the “semi-transparent sphere” potential

$$U(|x_1 - x_2|) = \begin{cases} U_0 > 0, & |x_1 - x_2| \leq a \\ 0, & a < |x_1 - x_2| \leq L \end{cases}$$

for the domain $x_1, x_2 \in [0, L]$ and solved the system of equations (46) for $l = 1, 2, \ldots, l_{\text{max}}$ ($l_{\text{max}} \approx 10N\bar{R}/a$) and several values of $a/\bar{R}$ and $u_0 = \frac{U_0}{k_B}$ using perturbation theory (55)–(63). The summations in (45), (47), (57), and (58) were performed over $p = 1, 2, \ldots, l_{\text{max}}$ and $j = 0, \pm 1, \ldots, \pm l_{\text{max}}$, increasing $l_{\text{max}}$ by a factor of 10 changed the results negligibly. For $^4$He atoms ($a \approx 2\,\text{Å}, m \approx 6.65 \cdot 10^{-24}\text{g}$) the numerical analysis shows that the numbers $f_{2l}$ (51) are very small ($|f_{2l}| \lesssim 1/N$, see Fig. 1) when $u_0a/\bar{R} \lesssim 10$. In this case, the largest among $|f_{2l}|$'s is equal to $|f_{2l}| \approx 0.1u_0 a^p N^{-p}$ with $p \approx 1$–2. The inequalities $|a_{2l \neq 2l_0}(2l_0)| \ll |a_{2l_0}(2l_0)|$ and (59) are satisfied provided that $u_0a/\bar{R} \lesssim 1$. The values of $a_{2l_0}(2l_0)/a_{2l_0}(2l_0)$ and $\delta A_{2l_0}(2l_0)/A_{2l_0}^{(0)}(2l_0)$ for the different sets of parameters are shown in Figs. 2 and 3. When $u_0a/\bar{R} \gg 1$, several values
Fig. 2: [Color online] The set of quantities $a_{2l}(2l_0)/a_{2l_0}(2l_0)$ for wave packet $\tilde{n}(x)$ (Eqs. (31), (32)) for the 30th frequency ($l_0 = 30$). The $a_{2l}$ are obtained by the formula (55), where $A_{2l}(2l_0) = A_{2l}^{(0)}(2l_0)$ and $A^{(0)}_{2l}(2l_0)$ is given by (57). Shown are the curves for $u_0 = 0.1$ (circles), 1 (diamonds), 10 (crosses), and 100 (triangles). We consider $N = 1000$ $^4$He atoms with the interatomic potential (64) for $a = 2$ Å, $a/\bar{R} = 0.5$ and $q_{2l_0} = 0$. The values of $a_{2l}(2l_0)$ are multiplied by a factor $10^h$, which is equal to $10^5$ for $u_0 = 0.1; 1; 10$. For $u_0 = 100$ we assume $10^h = 10^5$ when $l \leq 750$ and $10^h = 10$ when $l > 750$. The discontinuity in the curve $\triangle\triangle\triangle$ at $l = 750$ is fictitious and is only caused by the change in the coefficient $10^h$.

$a_{2l}(2l_0)/a_{2l_0}(2l_0)$ and all $\delta A_{2l}(2l_0)/A^{(0)}_{2l}(2l_0)$ are of the order of unity (in modulus); therefore, our perturbation theory does not work. We verified this for $N = 100, 1000, 10000$ and many values of $l_0$.

In the numerical analysis, we used $\hbar^2 \omega^2$ (62) with $q$ as a free parameter. We varied $q$ from -100 to 100 and compared it with the theoretical $q$ which is given by the left-hand side of (63). The solution for $q$ is that $q$ for which the theoretical $q$ is equal to the free $q$. We obtained $|q| \lesssim 0.01/N$ for $u_0 a/\bar{R} \lesssim 1$, $N = 100, 1000$ and $l_0 = 1, 2, \ldots, l^{max}$ with $l^{max} \approx 10N\bar{R}/a$. Note that (63) is an algebraic equation of infinite degree with respect to $q_{2l_0}$. Therefore, there must be an infinite number of roots $q_{2l_0}$. All roots, except $q_{2l_0} = 0$ are probably complex.

Thus, the numerical analysis shows that $|f_{2l}| \lesssim 1/N$ and $|q(2l_0)| \lesssim 0.01/N$ for all $l$ and $l_0$ provided that $u_0 a/\bar{R} \lesssim 1$. In this case, Eq. (62) takes the form

$$\hbar^2 \omega^2(k) = E_B^2(k),$$

which is equivalent to the famous Bogoliubov formula (11).

An analysis of the system of equations (48) for odd harmonics also leads to the Bogoliubov dispersion law. In this case, the formulae and figures are similar; therefore, we skip them.

As mentioned in the Introduction, one of the difficulties in the case of zero BCs is determining the quasimomentum of the quasiparticle. The above analysis allows one to find quasimomentum. Because $|a_{2l}(2l_0)/a_{2l_0}(2l_0)| \ll 1$ for all $l, l_0 = 1, 2, \ldots, l^{max}$ (for $l \neq l_0$),
Fig. 3: [Color online] Values of $\delta A_{2l}(2l_0)/[A_{2l}^{(0)}(2l_0)u_0]$ for various $l$’s for the system of $N = 1000$ $^4$He atoms with interatomic potential (64): $l_0 = 30, q_{2l_0} = 0, a = 2 \text{ Å},$ and $a/R = 0.5$. Shown are the curves for $u_0 = 0.1$ (circles), 1 (diamonds), 10 (crosses), and 100 (triangles). The values of $A_{2l}^{(0)}(2l_0)$ and $\delta A_{2l}(2l_0)$ are obtained by the formulae (57), (58).

harmonic $a_{2l_0}$ strongly dominates the wave packet $\tilde{n}(x)$ (31). Therefore, $k_{2l_0} = \pi 2l_0/L$ is the quasimomentum of the quasiparticle. Similarly, one can obtain that for an odd harmonic, the quasimomentum is $k_{2l_0-1} = \pi (2l_0 - 1)/L$. Thus, we have a general formula for the quasiparticle quasimomentum, $k_{l_0} = \pi l_0/L$ ($l_0 = 1, 2, \ldots, \infty$), which agrees with the results of papers [7–9, 41].

3 Discussion

The question arises: Have we found all solutions for the frequencies? The answer is yes. Indeed, system (46) can be solved for a finite number of $l$: $l = 1, 2, \ldots, l_{\text{max}}$. By equating the corresponding determinant to zero, we obtain an algebraic equation of degree $l$ for $\omega^2$. Hence, the $l_{\text{max}}$ solutions must exist. But we found exactly $l_{\text{max}}$ values of $\omega^2(2l_0)$, which correspond to $l_0 = 1, 2, \ldots, l_{\text{max}}$ and quasimomenta $k_2, k_4, \ldots, k_{2l_{\text{max}}}$. So there are no other solutions. Similarly for system (48). We can look at this from the other side. Condition (54) virtually numbers the frequencies $\omega^2$; therefore, the equality $E_{Bi}^2(k_{2p})[1 + f_{2p}] = \hbar^2 \omega^2(2l_0)$ is only possible if $p = l_0$. This prohibits zero denominators $E_{Bi}^2(k_{2p})[1 + f_{2p}] - \hbar^2 \omega^2(2l_0)$ in (58) and hence large values of $|\delta A_{2l_0}(2l_0)|$ in (63) at $u_0 a/R \lesssim 1$. Therefore, the singular denominators in (63) do not lead to additional solutions for $q_{2l_0}$’s. Similarly for $q_{2l_0+1}$’s.

Note that the exact solution for the ground-state energy $E_0$ of a 1D system of point bosons $(U(|x_j - x_l|) = 2\delta(x_j - x_l))$ is close to Bogoliubov’s $E_0$ only for $N \gtrsim 1000$ [22, 42]. Consequently, since Gross’ approximation $\tilde{\Psi}(r, t) = \Psi(r, t)$ [18] is in fact the zero approximation
of Bogoliubov’s approach [1], Gross’ equation (2) can be applied to systems with \( N \gtrsim 1000 \). The criterion for the applicability of Bogoliubov’s model in the 1D case for zero BCs and the point potential \( U(|x_j - x_l|) = 2c\delta(x_j - x_l) \) is \( 2/\pi \ln N \sqrt{\gamma} \ll 1 \) (at \( T = 0 \)) [8] where \( \gamma = \frac{2mc}{\hbar^2 n} \).

This criterion can be written as:

\[
\gamma \ll b = \left( \frac{2\pi}{\ln N \sqrt{\gamma}} \right)^2. \tag{66}
\]

For \(^4\)He atoms we have \( a \approx 2 \AA \) and \( \hbar^2/(2ma^2) \approx 1.5k_B \) K, so the condition (66) is equivalent to \( u_0 \ll 1.5ba/\bar{R} \), since \( n = 1/\bar{R} \) and \( c = \nu(0)/2 = u_0a \) for the potential (64). For the system to be uniform far from the walls, the inequality \( N \sqrt{\gamma} \gg 1 \) should be satisfied [8,22]. Therefore, we have \( b \sim 1 \) for a not too large \( N \), and \( b \to 0 \) for \( N \to \infty \). The usability condition \( u_0a/\bar{R} \ll 1 \) of the perturbation theory constructed above is equivalent to the condition \( u_0 \ll \bar{R}/a \). For real-world systems, \( \bar{R}/a \geq 1 \). According to these estimates, the condition \( u_0 \ll 1.5ba/\bar{R} \) required for Bogoliubov’s approach to work, sets a narrower range of variability of \( u_0 \) as compared to the range \( u_0 \ll \bar{R}/a \), in which our perturbation theory holds. Thus, our method works over the entire range of parameters for which Bogoliubov’s approach holds.

On the other hand, a direct comparison of solutions of the Gross-Pitaevskii equation (5) with exact Bethe-ansatz solutions shows that Gross’ equation describes well the Bose system with the interatomic potential \( U(|x_j - x_l|) = 2c\delta(x_j - x_l) \) and \( \gamma \lesssim 0.1, N \gg 1 \) [22]. The condition \( \gamma \lesssim 0.1 \) can be written for the potential (64) as \( 2mu_0K \cdot K = \lesssim 0.1\hbar^2 n \), inasmuch as \( \gamma = \frac{2mc}{\hbar^2 n} \) and \( c = \nu(0)/2 = u_0K \cdot K \). For \(^4\)He atoms (see above) this condition gives \( u_0a/\bar{R} \lesssim 0.15(a/\bar{R})^2 \). Since for real systems \( a/\bar{R} < 1 \), the condition \( u_0a/\bar{R} \lesssim 0.15(a/\bar{R})^2 \) sets a much stronger restriction than the applicability condition \( u_0a/\bar{R} \lesssim 1 \) of the perturbation theory. In other words, our perturbation theory works over the entire parameter range in which Gross’ equation holds.

Interestingly, Bogoliubov’s solutions [1,2] for \( E_0 \) and \( E(k) \) are valid for a much wider range of parameters than the scope (60) of Bogoliubov’s method: for a 1D system of point bosons, the exact solutions for the ground-state energy \( E_0 \) [22,42,43] and the dispersion law \( E(k) \) [41,7,43] are close to Bogoliubov’s solutions at \( \gamma \lesssim 1, N \gg 1 \) (even for \( N \to \infty \), which is inconsistent with condition (66)). The cause of this is still unclear.

The form of the asymptotic law \( E(k \to 0) \) for the Bose gas is also of interest. In works [1,2,3,45,46] the asymptotic law \( E(k \to 0) = |c_1|k + |c_3|k^3 + \ldots \) was found. The formula (65) agrees with this law. In paper [47] the relation \( E(k) = |c_1|k \) was obtained. However, Eqs. (3.3) and (3.6) of this paper clearly lead to the formula \( E(k \to 0) = |c_1|k + |c_3|k^3 + \ldots \). Another result, \( E(k \to 0) = |c_1|k + |c_2|k^2 + \ldots \), was obtained in [48,49]. We do not comment on these results because we did not investigate this issue. Note only that in papers [41,48,49] a point-like potential was considered, and the solutions \( E(k) \) were additionally obtained for the so-called hole-like excitations, which were not found in the models [1,2,5,46,47].
However, this does not mean that the models [1, 2, 5, 46, 47] and our approach do not catch the hole-like excitations. According to the analysis in [44, 50], when the coupling is weak, the hole-like excitation is a collection of identical interacting phonons. In the present case, because the phonons are Bogoliubov’s quasiparticles, only Bogoliubov’s quasiparticles are elementary excitations.

4 Conclusion

We have found the dispersion law of a one-dimensional weakly interacting zero-temperature Bose gas under zero boundary conditions by solving Gross’ equation using special perturbation theory. Such a method is mainly analytical (numerical analysis is only used to prove the smallness of certain quantities and to determine the range of applicability of the method). Note that all frequencies $\omega$ can be found numerically from the systems of equations (46) and (48) by setting the determinants of the two corresponding matrices to zero. This approach is mostly numerical and is beyond the scope of this study.

Our analysis shows that the dispersion law of a Bose gas with zero BCs coincides with the dispersion law of the same periodic system. A similar result was previously obtained by other methods [7–9, 41]. According to results in [51], the ground-state energy of a Fermi system is the same for periodic and twisted BCs.

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