On the description of a two-dimensional Bose gas at low densities

On the description of a two-dimensional Bose gas at low densities

A A Ovchinnikov

Institute for Nuclear Research of the Russian Academy of Sciences, Moscow 117312, Russia

Abstract. We propose a new method to describe the interacting Bose gas at zero temperature. For the three-dimensional system the correction to the ground-state energy in density is reproduced. For a two-dimensional dilute Bose gas the ground-state energy in the leading order in the parameter $|\ln \rho \alpha^2|^{-1}$ where α is the scattering length is obtained.

1. Introduction

At the present time, two-dimensional (2D) models are attracting much attention in connection with the problems of high-T_c superconductivity and fractional quantum Hall effect. In this context the description of the 2D system of bosons may be important. For instance the system of planar fermions in the magnetic field is equivalent to the system of interacting bosons with the additional long-range Chern–Simons interaction. The problem of the hard-core bosons on a lattice at high densities is closely related to the description of different strongly correlated electronic systems. The conventional methods of describing the interacting Bose gas are inapplicable in both of the above-mentioned problems. In this context the new ways to treat the system in the two different physical limits where the perturbation theory is possible are of interest.

Various methods to describe the system of bosons with the pairwise interaction were introduced, and these in one way or another consisted in summing up an infinite subset of the terms in the perturbation series. An example of this procedure is the Bogoliubov [1] method which is correct in the high-density limit; this means that the range of the potential is much larger than the average particle spacing. In the opposite limit of the dilute Bose gas the perturbation theory [1] does not work; this is manifested in the divergence in the expression for the energy for the δ-function type of potential. Various modifications of this procedure using the pseudopotential or the diagrammatic expansion methods, for example, have been proposed [2]. However, the reason why the procedure in [1] can be applied when the two-body potential is not small and the wavefunction is not close to the unperturbed wavefunction is obscured. Generalization of this method to the 2D system is not straightforward owing to the behaviour of the modified scattering amplitude which approaches zero in the low-energy limit. In fact the methods in [2] can be considered as an application of the Bogoliubov approach to a system with the parameters chosen in such a way that this approximation is valid and at the same time the density ρ is small in the sense that $\alpha \rho^{1/d} \ll 1$ (α is of the order of the scattering length). Although this can be a basis for the solution of the 2D problem an estimate of the accuracy of the approximation [1] for a given potential is required.

The properties of a 2D dilute Bose gas at zero temperature were first studied in [3]. In the leading order in the expansion parameter the ladder diagrams at the non-zero value of chemical potential, related to the ground-state energy, can be calculated. However, in the framework of the diagrammatic method there exists a discrepancy in the estimate of the corrections to the ladder approximation, i.e. in the form of the expansion parameter at zero temperature [4]. The closely related method in [5] is based on the effective separation of the long and the short distances. Apart from the independent derivation of the expansion parameter, it is also desirable to develop a method which makes a connection between the diagrammatic low-density expansions and the strong-coupling Feynman–Bijl approach. Finally, for two dimensions in view of the success of the Laughlin wavefunction in the theory of the fractional quantum Hall effect the form of the wavefunction in coordinate space is of interest. The system at non-zero temperatures was considered in [5, 6].

In the present paper we suggest a new method to describe the system of bosons for the two limiting cases and we investigate the ground-state properties of the 2D Bose gas at zero temperature. Our method is closely related to the approach proposed by Lieb [7] which makes use of the distribution functions related to the ground-state wavefunction. We use the decomposition of the logarithm of the wavefunction into a series over the n-particle functions. We argue that at small densities the proposed expansion corresponds to the expansion of energy in the small parameter. Although in practice it is difficult to solve the corresponding system of equations beyond the leading-order approximation which in the framework of our approach corresponds to a wavefunction of the Jastrow form, convincing arguments in favour of the validity of this procedure in the leading order can be found. Of course the distribution functions can be calculated using a wavefunction of the Jastrow form. In this way the connection with the approach in [7] can be made.

The equation for the energy E_0 and the wavefunction $\Phi(x_1, \ldots, x_N)$ of the ground state for a system of N particles in the volume V interacting with the two-body potential $U(x)$ has the form

$$\left(-\sum_i \partial_i^2 + 2\sum_{i<j} U(x_{ij})\right)\Phi = E_0\Phi \qquad i, j = 1, \ldots, N \tag{1}$$

where $\partial_i = \partial/\partial x_i$, $x_{ij} = x_i - x_j$ and we denote by x_i the d-dimensional space vector of the ith particle throughout the paper. The ground-state wavefunction $\Phi(x_1, \ldots, x_N)$ is a symmetric and positive function of its arguments. According to [8] (see also [9]) one can look for the function Φ in the form

$$\Phi(x_1, \ldots, x_N) = \exp[S(x_1, \ldots, x_N)].$$

We observe that the function $S(x_1, \ldots, x_N)$ can be expanded as follows:

$$S(x_1, \ldots, x_N) = \sum_{i<j} S_2(x_{ij}) + \sum_{i<k<l} S_3(x_i, x_k, x_l) + \cdots \tag{2}$$

where $S_n(x_1, \ldots, x_n)$ are the symmetric functions depending on the relative interparticle distances and subjected to the constraints

$$\int dx_n\, S_n(x_1, \ldots, x_n) = 0 \qquad n > 2. \tag{3}$$

Integrating equation (2) over the coordinates of $N - n$ particles subsequently for $n = 2, 3 \ldots$, and using the condition (3), one can show that the expansion (2) is irreducible, which means

that for a given function $S(x_1, \ldots, x_N)$ the set of functions S_n is unique. Substituting equation (2) into equation (1), we obtain the equation

$$E_0 = \sum_{i \neq j} F(x_{ij}) - \sum_{i \neq k \neq l} \partial S(x_{ik}) \, \partial S(x_{il}) + \cdots \tag{4}$$

$$F(x) = -\partial^2 S(x) - \partial S(x) \, \partial S(x) + U(x)$$

where the terms depending on the pair function $S_2(x) = S(x)$ only are indicated explicitly. Integrating equation (4) over the coordinates $n+1, \ldots, N$ and using equation (3) we obtain the n-particle equation for the functions S_n. In general the system of equations cannot be solved and assumptions about the higher-order functions S_n are required. For the dilute Bose gas the perturbation theory in the small parameter can be used. Although calculations in the high orders are too complicated, one can argue that the expansion of the energy in the small parameter corresponds simply to the expansion (2). Here we shall demonstrate this in the lowest order which corresponds to the pairwise wavefunction. It is plausible that this calculation is valid for higher-order terms. Suppose for a while that only the function $S(x)$ is not equal to zero. Integrating equation (4) over the coordinates $1, \ldots, N$, we obtain for the parameter a defined as

$$E_0 = N\rho a$$

$(\rho = N/V; \ E_0/V = a\rho^2)$ the equation

$$a = \frac{N-1}{N} \int dx \, F(x) \tag{5}$$

which is equivalent to $a = \int dx \, [U - (\partial S)^2]$ in the infinite-volume limit. Integrating equation (4) over the coordinates $3, \ldots, N$ and using equation (5), we obtain the equation

$$\partial^2 S(x) + \partial S \, \partial S(x) - U(x) - \rho \partial_1^2 \int dx_3 \, S(x_{13}) S(x_{23}) = -a/V \tag{6}$$

where the notation $x = x_{12}$ is used and terms of order $1/V$ are retained. The right-hand side is equal to zero in the limit $V \to \infty$. We assume periodic boundary conditions so that the integral over the total derivative is zero. Because of the condition (3) the contribution of S_3 to equation (5) is of the form $\rho \int dx_1 \, dx_2 \, [\partial_1 S(123)]^2$ and an example of its contribution to equation (6) is $\rho \int dx_3 \, \partial_3 S(123) \, \partial_3 S(13)$. One can use the solution of equation (6) to estimate the function S_3 with the help of the three-particle equation and to show that these integrals are suppressed. We shall show below that it is the smallness of $S(x)$ at distances of the order of $\rho^{-1/d}$ $(d = 2, 3)$ that allow one to neglect the function S_3 in the lowest-order approximation. Equation (6) reproduces the correction in density [2] to the ground-state energy for the three-dimensional (3D) system and predicts the leading order term for the 2D system.

Note also that equation (6) can be regarded as an equation for the trial variational wavefunction of the Jastrow form. In this case it follows from the form of the solution of equation (6) that the variational energy is given by equation (5) with accuracy up to higher-order terms in the expansion parameter.

If the second term on the left-hand side of equation (6) can be neglected, then the equation can be easily solved using Fourier transformation:

$$\rho k^2 S_k^2 - k^2 S_k - U_k = 0 \qquad S_k = \int dx \, \exp(ikx) S(x)$$

(where $U_k = \int dx \exp(ikx)U(x)$). Substituting the solution S_k of this equation into the expression for the energy given by

$$a = U_0 - \int dx \, [\partial S(x)]^2 = U_0 - \int_k k^2 S_k^2$$

($U_0 = \int dx \, U(x)$), we obtain

$$a = U_0 + \frac{1}{2\rho^2} \int_k [(k^4 + 4U_k \rho k^2)^{1/2} - k^2 - 2U_k \rho] \tag{7}$$

where the notation $\int_k = \int d^d k/(2\pi)^d$ is used. Equation (7) is the Bogoliubov expression for the energy. One can estimate the accuracy of equation (7) for a given two-body potential $U(x)$. The corrections are determined by the function $S(x)$ which should be small in order for the approximation (7) to be valid. Briefly, the potential should be relatively shallow compared with its width, and the spatial range should be much larger than the average particle spacing.

Let us proceed with the solution of equation (6) in the low-density limit. The particle density is assumed to be small so that the dimensionless parameter $\alpha \rho^{1/d} \ll 1$. In this formula, α is the scattering length for the potential U and $\rho^{-1/d}$ is the average interparticle distance in d-dimensional space. The expansion parameters are $|\ln \rho \alpha^2|^{-1}$ and $\alpha^{3/2} \rho^{1/2}$ in two and three dimensions, respectively.

2. Three-dimensional system

Let us begin with the case of three spatial dimensions $d = 3$. Define $S_0(x)$ as the solution of equation (6) at $\rho = 0$:

$$\partial^2 S_0 + \partial S_0 \, \partial S_0 - U = -\alpha/V. \tag{8}$$

Here α is the unknown parameter and periodic boundary conditions are implied. In terms of the function $\phi_0(x) = \exp[S_0(x)]$ keeping the volume finite and taking into account the periodic boundary conditions, we find that

$$\alpha = \int dx \, [U(x) + S_0 \, \partial^2 S_0(x)] = \int dx \, U(x)\phi_0(x)$$

is proportional to the scattering length (which is equal to $4\pi\alpha$) for the potential $U(x)$. For the hard-sphere potential, α is the radius of the potential. In the infinite-volume limit the equation has the form $(-\partial^2 + U)\phi_0(x) = 0$ which is to be supplemented by the boundary condition $\phi_0(r) \to 1$ at $r \to \infty$ ($r = |x|$). At distances much larger than the range of the potential the solution is $\phi_0(r) = 1 - \alpha/r$. For the energy we have $a = \alpha + \int dx \, (S \partial^2 S - S_0 \partial^2 S_0)$ or, equivalently,

$$a = \alpha - \int_k (k^2 S_k^2 - k^2 S_{0k}^2). \tag{9}$$

Let us make use of the Fourier transformation in equations (6) and (8). In the region $r \gg \alpha$ where the condition $S_0(x) \ll 1$ is satisfied we have $S_0(r) = -\alpha/r$ and the main contribution

to the integral $\int dx \, (\partial S_0)^2$ comes from the integration over the region of small $r \sim \alpha$. Up to the corrections in ρ the same is true for the analogous integral for $S(x)$.

Therefore the Fourier transform of the function $U - (\partial S)^2$, and the same function for S_0, are independent of the momentum k at $k \ll 1/\alpha$. At these values of k, $S_{0k} = -\alpha/k^2$ and S_k is given by the solution of the equation $\rho k^2 S_k^2 - k^2 S_k - \alpha = 0$. Substituting these functions into equation (9), we obtain

$$a = \alpha + \frac{1}{2\rho^2} \int_k \left(\sqrt{k^4 + 4\alpha\rho k^2} - k^2 - 2\alpha\rho + \frac{2\alpha^2\rho^2}{k^2} \right). \tag{10}$$

The integral in this expression converges at large k and is saturated at the values $k \sim (a\rho)^{1/2} \ll 1/\alpha$ which justifies our assumption that $\int dx \, \exp(ikx)[U - (\partial S)^2] = \alpha$. The corrections to this formula do not change the result in the approximation considered. Evaluating the integral in equation (10), we obtain the well known result [2] for the expansion of the ground-state energy in powers of density in three dimensions:

$$a = \alpha[1 + (16/15\pi^2)\alpha^{3/2}\rho^{1/2}]. \tag{11}$$

3. Two-dimensional system

Let us proceed with the investigation of the 2D system. In two dimensions it is easy to find the solution of equation (6) and to determine the energy a as a function of the density ρ with accuracy up to terms of higher order in the small parameter $a \sim |\ln(\rho\alpha^2)|^{-1}$.

As in the 3D case the solution of equation (6) can be represented in the form

$$S_k = -(1/2\rho) \left(\sqrt{1 + 4\sigma_k\rho/k^2} - 1 \right)$$

where S_k is the Fourier transform of the function $S(x)$ and the function σ_k is defined by

$$\sigma_k = \int dx \, \exp(ikx)[U(x) - \partial S \partial S(x)].$$

At sufficiently small k we have $\sigma_k = a$ while, at larger k, σ_k could depend on the momentum k. However, it can be shown that in fact with the accuracy of order $O(a^2)$ one can take $\sigma_k \simeq a$ for all $k \ll \alpha^{-1}$. We are interested in the behaviour of the function $S(x)$ in the region $\alpha \ll r \ll (a\rho)^{-1/2}$. As in three dimensions $(a\rho)^{-1/2}$ is the characteristic length, a kind of correlation length in the problem. In this region, $S(x)$ can be calculated as

$$S(x) = -\frac{1}{2\rho} \int_k \exp(ikx) \left[\left(1 + \frac{4a\rho}{k^2} \right)^{1/2} - 1 \right]. \tag{12}$$

Evaluating this expression we find that

$$S(x) = -a/4\pi + (a/2\pi) \ln[(a\rho)^{1/2}r] \tag{13}$$

which is valid in the indicated region with accuracy up to the terms of order a^2. One can see from equation (12) that the function $S(x)$ decreases quickly at distances much larger than the correlation length $(a\rho)^{-1/2}$:

$$S(x) \simeq -(1/2\pi)(a/\rho)^{1/2}(1/r) \qquad r \gg (a\rho)^{-1/2}.$$

Now, using equation (13), one can estimate the function σ_k:

$$|\sigma_k - a| < (a^2/2\pi)\ln(k/\sqrt{a\rho}) + O(a^2).$$

This relation justifies the initial assumption about the behaviour of σ_k. The other way to obtain the solution (13) is to represent equation (6) in the form

$$[\partial^2 - U(x)]\phi(x) = \rho\phi(x)\partial_1^2 \int dx_3\, S(x_{13})S(x_{23}) - (a/V)\phi(x) \qquad (14)$$

where $\phi(x) = \exp[S(x)]$. The Fourier transform of the function $U(x)\phi(x)$ does not depend on the momentum at $k \ll 1/\alpha$. In the large-distance region where $S(x) \ll 1$ we can expand the function $\phi(x) \simeq 1 + S(x)$ and neglect terms of order $S^2(x)$. Then equation (14) has a solution of the same form as equation (13). The only difference is that the parameter a is replaced by the value of the integral $\int dx\, U(x)\phi(x)$. To calculate this, one has to integrate both sides of equation (14) over the space vector in the finite volume V:

$$\int dx\, U(x)\phi(x) = a + \rho \int dx\, (1 - \phi(x))\chi(x)$$

$$\chi(x_{12}) = \partial_1^2 \int dx_3\, S(x_{13})S(x_{23}). \qquad (15)$$

In general the limit $V \to \infty$ of an integral of some function over the volume does not coincide with the integral of the limiting function, because in the finite volume the function may have an asymptote which is a constant divided by V. This is indeed the case for the function $\chi(x)$ since the integral $\int dx\, \chi(x)$ is equal to zero in the finite volume. However, one can substitute the product of the limiting functions $[1 - \phi(x)]\chi(x)$ into equation (15) since both functions approach zero at $r \to \infty$. Alternatively, one can use equation (6) directly in the infinite-volume limit. The function $\chi(r)$ can be evaluated using equation (12):

$$\chi(r) \simeq aS(r) \qquad (\alpha \ll r \ll (a\rho)^{-1/2})$$
$$\chi(r) \simeq (1/2\pi)(a^{1/2}/\rho^{3/2})(1/r^3) \qquad (r \gg (a\rho)^{-1/2}).$$

The integral on the right-hand side of equation (15) is determined by the long-distance region ($S(x) \ll 1$) and can be estimated as $O(a^2)$. Thus the solution of equation (6) as a function of the parameter a is found.

On the other hand at sufficiently small r the function $\phi(x)$ can be found approximately as the solution of the equation $[-\partial^2 + U(x)]\phi(x) = 0$ because the right-hand side of equation (14) is of the order of ρ. The solution is $\phi_0(r) = C\ln(r/\alpha)$ where C is an arbitrary constant and α is the scattering length for the potential $U(r)$ (the region $r \gg \alpha$ is implied). In two dimensions the scattering length is defined by the behaviour of the scattering amplitude at low energies which (for our equation) is given by

$$\bar{f}(k) = \pi/[\ln(\tfrac{1}{2}k\alpha) + \gamma - \tfrac{1}{2}i\pi] + O(k\alpha)$$

where $|\bar{f}(k)| = (2\pi k)^{1/2}|f(k)|$ is the modified scattering amplitude, k is the momentum and $\gamma = 0.5772$ is the Euler constant. For the 2D hard-sphere potential the scattering length α is equal to the radius of the potential. The correction $\delta\phi(r) \sim a\rho r^2$ to the solution of the homogeneous equation can be easily estimated using equation (13). The correction is

of the order of unity at distances of the order of the correlation length $(a\rho)^{-1/2}$; however, it is small $(\delta\phi(r) \sim a)$ at distances $r \sim \rho^{-1/2}$. At $r \sim \rho^{-1/2}$, equation (13) is still valid. Comparing the solution given by equation (13) with the function $\phi_0(r)$ we obtain the relation

$$C \ln(r/\alpha) = 1 - a/4\pi + (a/2\pi) \ln[(a\rho)^{1/2}r] \tag{16}$$

which should be valid in the region $\alpha \ll r \ll (a\rho)^{-1/2}$ with logarithmic accuracy. In particular, for $r \sim \rho^{-1/2}$, it is valid with accuracy up to the terms of the order of a. Thus in the leading order in the small parameter $|\ln(\rho\alpha^2)|^{-1}$, $C = a/2\pi$ and the energy is

$$a = 4\pi/|\ln(\rho\alpha^2)| + O[1/|\ln(\rho\alpha^2)|^2] \tag{17}$$

in agreement with the result in [3]. Equation (17) is our final result for the 2D system. Let us comment on the accuracy of this expression. It was shown that the leading-order corrections to equation (16) are of the order of a at $r \simeq \rho^{-1/2}$ since terms of the order of $[S(x)]^2$ are suppressed as $(a \ln a)^2$. The equation for a has the form

$$(a/4\pi)|\ln(a\rho\alpha^2)| = 1 + O(a).$$

Although from this equation the first two terms in the expansion of energy can be found, i.e.

$$a = 4\pi\{1/|\ln(\rho\alpha^2)| - \ln|\ln(\rho\alpha^2)|/[\ln(\rho\alpha^2)]^2\} \tag{18}$$

our method and the method in [3] do not allow one to determine terms of the order of $a^2 \sim 1/[\ln(\rho\alpha^2)]^2$. With logarithmic accuracy the second term (which is of the order of $a^2 \ln a$) in equation (18) is of the order of the omitted terms and the expansion (18) makes sense only in the extreme dilute limit $\ln|\ln(\rho\alpha^2)| \gg 1$. Below we consider the corrections due to the three-particle component of the wavefunction and show that the correct expansion parameter is a. We disagree with the statement in [4] that the terms corresponding to the three-particle collisions are suppressed as a power of $\rho\alpha^2$. The second term in equation (18) is in agreement with the corresponding term in the formula in [4].

Naively, from the three-particle equation the function S_3 can be estimated to within an order of magnitude as $S(1, 2, 3) \sim S(13)S(23) +$ permutations. Then the contribution of S_3 to equation (6) at distances of the order of $\rho^{-1/2}$ which is determined by the integral $\rho \int dx_3 \, S(13)(\partial_1\partial_3 - \partial_3^2)S(123)$ (see equation (3)) is suppressed owing to the smallness of the function $S(x)$ at these distances. In fact the three-particle equation can be solved in the leading order in the expansion parameter (which means that terms of the order of S_2S_3 in this equation should be neglected) in the momentum representation and the corresponding integral in the momentum space can be estimated (see the appendix).

At the same time, at short distances where the two particles interact strongly, the pair function is not expected to be very different from the solution of the two-body problem whether or not the function S_3 is taken into account. In other words, although the function S_3 is not necessarily small at short distances, our estimate of the right-hand side of equation (14) as well as equation (16) are valid to within an order of magnitude. Note that the 'momentum' corresponding to the two-particle equation is of the order of the correlation length which characterizes the screening of the pair wavefunction due to the other particles. Hence the result (17) has a simple physical interpretation. Namely the energy of the two particles interacting with the potential U located in the two-dimensional volume V is of the order of $\bar{f}/V$ where the modified scattering amplitude $\bar{f}$ should be normalized at $k \sim \rho^{1/2}$.

Multiplying the result by the number of pairs we obtain the result (17). In three dimensions this corresponds to the first term in equation (11).

At non-zero temperatures the behaviour of a 2D dilute Bose gas is completely different from the behaviour of the system in three dimensions. In particular, in contrast with the 3D system, the expansion parameter at zero temperature is different from the diluteness parameter found from the condition that the critical temperature T_c is close to the prediction obtained using the Bogoliubov form of the spectrum ($\ln|\ln(\rho\alpha^2)| \gg 1$) [6]. The determination of T_c beyond this extreme dilute limit remains an open question.

4. The distribution functions

Another approach to the description of the dilute Bose gas based on the equations for the distribution functions related to the function Φ was proposed in [7]. We shall show below that the assumptions made in [7] can be justified in the framework of our approach. Let us briefly describe this method. The n-particle distribution function is defined by

$$g_n(x_1, \ldots, x_n) = Z^{-1} V^n \int dx_{n+1} \ldots dx_N \, \Phi(x_1, \ldots, x_N)$$

$$Z = \int dx_1 \ldots dx_N \, \Phi(x_1, \ldots, x_N). \tag{19}$$

The energy is related to the pair distribution function $g_2(x_{12}) = g(x)$ by means of

$$a = \frac{N-1}{N} \int dx \, U(x) g(x). \tag{20}$$

Using equation (1) we obtain the equation for $g(x)$:

$$[-\partial^2 + U(x)]g(x) = \tfrac{1}{2} E_0 g(x) - \rho \int dx_3 \, g_3(1, 2, 3) U(x_{23})$$

$$- \frac{1}{2} \frac{(N-2)(N-3)}{V^2} \int dx_3 \, dx_4 \, g_4(1, 2, 3, 4) U(x_{34}). \tag{21}$$

The first and the third terms on the right-hand side are of the order of N while the left-hand side is of the order of unity. In the leading order, cancellation of these terms occurs and corrections of the order of $1/N$ are important. The approximation for the distribution functions g_3 and g_4 used in [7] to evaluate the right-hand side of equation (21) is the superposition approximation:

$$g_n(x_1, \ldots, x_n) = \prod_{i<j}^{n} \tilde{g}(x_{ij}). \tag{22}$$

From physical considerations it is clear that in the limit $V \to \infty$ the function $\tilde{g}(x) \to g(x)$ while for a finite volume it can be found using the set of the equations

$$\int dx_n \, g_n(x_1, \ldots, x_n) = V g_{n-1}(x_1, \ldots, x_{n-1}).$$

For instance, for the four-particle function g_4, substituting the *ansatz* (22) into the formula $\int dx_3\, dx_4\, g_4(1, 2, 3, 4) = V^2 g(x_{12})$ we find that the corresponding pair function is

$$\tilde{g}^{(4)}(x) = g(x)\left(1 - \frac{2}{V} \int dx_3\, f(x_{13})f(x_{23})\right)$$

where the function $f(x) = 1 - g(x)$ can be taken in the infinite-volume limit. These corrections are not important in the second term of the right-hand side of equation (21). Substituting the expressions for the functions g_3 and g_4 into equation (21) and taking the limit $V \to \infty$, we obtain an equation for the pair distribution function $g(x)$. Assuming that the function $f(x)$ is small and retaining terms of the leading order in $f(x)$, we find that

$$[-\partial^2 + U(x)]g(x) = 2a\rho f(x) - a\rho^2 \int dx_3\, f(x_{13})f(x_{23}). \qquad (23)$$

This equation is valid for those r where the function $f(x)$ is small ($f(x) \ll 1$).

Equation (23) can be solved in the same way as equation (6). For instance the solution of equation (23) for the 2D problem in the region where $f(x) \ll 1$ is

$$g(x) = 1 + a/4\pi + (a/2\pi)\ln[(a\rho)^{1/2}r]$$

for $r \ll (a\rho)^{-1/2}$. Repeating the arguments leading to equation (16), we obtain the result (17).

In three dimensions the solution of equation (23) at distances $r \ll (a\rho)^{-1/2}$ is

$$g(x) = [1 + (16/15\pi^2)a^{3/2}\rho^{1/2}] - a/r.$$

Comparing this function with the solution of the homogeneous equation $\phi_0(r) = C(1 - \alpha/r)$ which is valid with accuracy of the order of $\alpha^{3/2}\rho^{1/2}$ at $r < \rho^{-1/3}$ we obtain the result (11).

Let us comment on the relation of our approach to that of [7]. The function $g(x)$ can be calculated using the obtained wavefunction of the Jastrow form. Formally the problem is similar to the calculation of the distribution functions of the classical liquid. Although the expansion in density for the corresponding partition function is not valid (integral $\int dx\, S(x)$ diverges at large distances) the formulae in [7] resulting in equation (23) can be obtained to the lowest order in the expansion parameter. One can establish direct correspondence between equations (6) and (23). The function $g(x)$ at long distances can be calculated by means of the cluster expansion (see, e.g., [10, 11]). The connected diagrams with the lines corresponding to the function $\phi(x) - 1$ between points 1 and 2 are considered. At small momenta the Fourier transform of the function $\phi(x) - 1$ may be replaced by S_k. In the integrals corresponding to diagrams of the cluster expansion, long distances where the function $S(x)$ is small are important. Therefore, only diagrams that do not contain the two different paths connecting points 1 and 2 are required. These diagrams can be referred to as 'chain' diagrams. Adding one more line to each of these diagrams leads to an extra suppression. Since $S(r) \to 0$ at $r \to \infty$, it is clear that the sum of the 'chain' diagrams gives the exact result for the asymptote of the distribution function. The 'chain' diagrams can be summed in the momentum representation. We obtain the following relation:

$$f_k = -S_k/(1 - \rho S_k). \qquad (24)$$

Substituting the solutions of equations (6) and (23) into equation (24) we find that this relation is valid with the accuracy required for the estimates (11) and (17).

The same approximation can be used to calculate the Feynman structure factor $F(k)$ which determines the energy of the low-lying excitations (phonons). In this case the distribution function related to the square of the wavefunction Φ (defined as in equation (19)) should be calculated. The structure factor $F(k)$ can be expressed through the Fourier transform of the pair distribution function as

$$F(k) = \rho + \rho^2 \int dx \, \exp(ikx)[G(x) - 1]$$

$$G(x_{12}) = V^2 \int dx_3 \ldots dx_N \, |\Phi(x_1, x_2, \ldots, x_N)|^2$$

where the normalization of the wavefunction $\langle \Phi | \Phi \rangle = 1$ is implied. Calculating the sum of the 'chain' diagrams we find that

$$F(k) = \rho[1/(1 - 2\rho S_k)].$$

In contrast with the other wavefunctions of the Jastrow form used in the variational studies of the Bose liquid [10] we obtain the correct behaviour $F(k) \sim k$ at $k \to 0$ owing to the behaviour $S(r) \sim 1/r^{d-1}$ at asymptotically large distances [11] (for a related discussion see [12]). The phonon energy

$$\omega(k) = \rho k^2 / F(k) = \sqrt{k^4 + 4a\rho k^2}$$

is in agreement with the predictions of other approaches [1, 2]. The formula for the spectrum is valid at $k \ll (a\rho)^{1/2}$. In order to determine the dispersion in the region $k \sim \rho^{1/2}$, where one would expect the existence of the roton minimum, apart from the calculation of $G(r)$ at $r \sim \rho^{-1/2}$, corrections to the Feynman variational formula for $\omega(k)$ are required. We hope to discuss this problem elsewhere. The momentum distribution n_k can be readily calculated. In terms of the wavefunction it has the form

$$n_k = N \int dx \, \exp(ikx) \int dx_2 \ldots dx_N \, \Phi(x, x_2, \ldots, x_N) \Phi(0, x_2, \ldots, x_N)$$

($\int_k n_k = \rho$; the normalization $\langle \Phi | \Phi \rangle = 1$ is implied). The only difference in comparison with the previous calculations is that the two lines of the 'chain' diagram connecting points 1 and 2 with the other points correspond to the function $\exp[S(x)]$ while the rest of the lines are related to the function $\exp[2S(x)]$. The result is as follows:

$$n_k = \rho^2 S_k^2 / (1 - 2\rho S_k) = \tfrac{1}{2}[(k^2 + 2a\rho)/\sqrt{k^4 + 4a\rho k^2} - 1]$$

which coincides with the known expression [1,2]. In two dimensions the expression (17) should be substituted for a. In two dimensions the condensate fraction is $N_0 = N[1 - (1/4\pi)a]$.

Finally, the situation is different for the one-dimensional problem. From the viewpoint of our method the low-density limit coincides with the weak-coupling limit. In this case, equation (7) is correct in the weak-interaction limit regardless of the shape of the potential while, for strong coupling, the perturbation theory is inapplicable which is in agreement with the exact solution of the problem for the δ- function potential [13]. The same can be true for the lattice system. For instance for a system described by the Hamiltonian (see, e.g., [14])

$$H = -t \sum_{\langle ij \rangle} (b_i^+ b_j + \text{HC}) + U \sum_i n_i(n_i - 1) \qquad n_i = b_i^+ b_i$$

at $U \to 0$ and a density of the order of unity, equation (7) is asymptotically exact in any dimensions.

5. Conclusion

In conclusion, we presented a method to describe the interacting Bose gas at zero temperature. The expansion in the irreducible functions for a logarithm of the ground-state wavefunction was used. For low densities the equation for a Jastrow wavefunction was solved. It was argued that the contribution of the three-particle component of the wavefunction to the equation is suppressed. For a 3D system the leading-order correction for the ground-state energy in the particle density was reproduced. For the 2D dilute Bose gas the ground-state energy in the leading order in the parameter $|\ln(\rho\alpha^2)|^{-1}$ where α is the 2D scattering length was obtained.

Acknowledgments

Appendix

Here we estimate the contribution of the three-particle function $S_3(x_1, x_2, x_3)$ to equation (6). The three-particle equation is obtained after integration of the basic equation (1) over the coordinates $4, \ldots, N$. It is necessary to take into account equations (5) and (6) for the terms that depend on only one of the variables x_{12}, x_{13}, x_{23}. In the coordinate space the equation is

$$\tfrac{1}{2}(\partial_1^2 + \partial_2^2 + \partial_3^2)S_3(1,2,3) + \partial_1 S(12)\, \partial_1 S(13) + \partial_2 S(21)\, \partial_2 S(23) + \partial_3 S(31)\, \partial_3 S(32) + \ldots$$
$$= (1/V\rho)[F(12) + F(13) + F(23)] \tag{A1}$$

where the ellipsis (...) stands for the terms of the order of $S_2 S_3$ and S_3^2. These terms are not important for the solution of equation (A1) in the leading order. The right-hand side is equal to zero in the infinite-volume limit. In the momentum representation the function $S(k_1, k_2, k_3)$ is defined as

$$\int dx_1\, dx_2\, dx_3 \exp(ik_1 x_1 + ik_2 x_2 + ik_3 x_3)S(1,2,3) = (2\pi)^d \delta^d(k_1 + k_2 + k_3)S(k_1, k_2, k_3).$$

The solution of equation (A1) is

$$S(k_1, k_2, k_3) = -[2/(k_1^2 + k_2^2 + k_3^2)](k_1 k_2 S_{k_1} S_{k_2} + k_1 k_3 S_{k_1} S_{k_3} + k_2 k_3 S_{k_2} S_{k_3}). \tag{A2}$$

The contribution of the function S_3 to the left-hand side of equation (6) has the following form:

$$2\rho \int dx_3\, S(13)(\partial_1 \partial_3 - \partial_3^2)S_3(1,2,3) \tag{A3}$$

which is a function of the variable $x_{12} = x$. Substituting the solution (A2) into the integral in momentum space corresponding to the Fourier transform of the function (A3) we obtain the following expression:

$$2\rho \int_p \frac{2p^2 - kp}{p^2 + k^2 - kp} S_p[k(k-p)S_k S_{k-p} + p(p-k)S_p S_{k-p} + kp S_k S_p] \quad (A4)$$

where k is the external momentum. It is possible to estimate the integral in equation (A4) at different values of the momentum k with the help of equation (12). For example at $k = 0$ we have

$$4\rho \int_p p^2 S_p^3.$$

This integral is easily estimated as $O(a^2)$ and $O[a(a^{3/2}\rho^{1/2})]$ in 2D and 3D space, respectively. On analysis of equation (A4) it is easy to show that these estimates are valid at arbitrary k. Therefore the considered contribution does not change the result in the approximation required for the derivation of equations (11) and (17).

References

[1] Bogoliubov N N 1947 *J. Phys. (Moscow)* **11** 23
[2] Lee T D and Yang C N 1957 *Phys. Rev.* **105** 1119
     Lee T D, Huang K and Yang C N 1957 *Phys. Rev.* **106** 1135
     Beliaev S T 1958 *Zh. Eksp. Teor. Phys.* **33** 289
     Brueckner K A and Sawada K 1957 *Phys. Rev.* **106** 1117
[3] Schick M 1971 *Phys. Rev.* A **3** 1067
[4] Hines D F, Frankel N E and Mitchell D J 1978 *Phys. Lett.* **68A** 12
[5] Popov V N 1972 *Teor. Mat. Fiz.* **11** 354 (Engl. Transl. 1972 *Theor. Math. Phys.* **11** 565)
[6] Fisher D S and Hohenberg P C 1988 *Phys. Rev.* B **37** 4936
[7] Lieb E H 1963 *Phys. Rev.* **130** 2518
[8] Bijl A 1940 *Physica* **7** 869
     Jastrow R 1955 *Phys. Rev.* **98** 1479
[9] Bogoliubov N N and Zubarev D N 1955 *Zh. Eksp. Teor. Phys.* **28** 129
[10] McMillan W L 1965 *Phys. Rev.* **138** A442
     Aviles J B 1958 *Ann. Phys., NY* **5** 251
     Hiroike K 1962 *Prog. Theor. Phys.* **27** 342
     Reatto L 1969 *Phys. Rev.* **183** 334
     Francis W P, Chester G V and Reatto L 1970 *Phys. Rev.* A **1** 86
[11] Reatto L and Chester G V 1967 *Phys. Rev.* **155** 88
[12] Kane C L, Kivelson S, Lee D H and Zhang S C 1991 *Phys. Rev.* B **43** 3255
[13] Lieb E H and Liniger W 1963 *Phys. Rev.* **130** 1605
[14] Rokhsar D S and Kotliar B G 1991 *Phys. Rev.* B **44** 10328