

Two-dimensional Bose gas at low density

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

At present, two-dimensional models attract considerable attention in high- T_c superconductivity and fractional quantum Hall effect. In this context the description of the two-dimensional system of bosons might be important and the new ways of treating the system in the two different physical limits, where the perturbation theory is applicable, are of interest. Various methods to describe the system of bosons were introduced. These methods sum up in one way or another the infinite subset of terms in the perturbation series. An example of this procedure is the Bogolyubov's method.¹ In the limit of the dilute Bose gas the perturbation theory¹ does not work. This is evident in the divergence in the expression for the energy. Various modifications of this procedure using the pseudopotential or the diagrammatic expansion methods, for example, were proposed.² However, the reason why the procedure of Ref. 1 can be applied when the two-body potential is not small and the wave function is not close to the unperturbed one is not clear. The generalization of these methods to the 2D system is not straightforward due to the behavior of the modified scattering amplitude which approaches zero in the low energy limit. Actually the methods of Ref. 2 can be considered as an application of the Bogolyubov's approach to a system whose parameters are chosen in such a way that this approximation is valid and the density ρ is small in a sense $\alpha \rho^{1/d} \ll 1$ (α is the scattering length). Although this can be the basis for the solution of a 2D problem, the accuracy of the approximation¹ for a given potential is being estimated.

In the present letter we propose a new method to describe the system of bosons at low density. Our method is closely related to the approach used by Lieb.³

The equation for the energy E_0 and the wave function $\Phi(x_1, \dots, x_N)$ 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

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

where $\partial_i = \partial / \partial x_i$, $x_{ij} = x_i - x_j$ we denote by x_i the d -dimensional space vector of i th particle. The ground-state wave function $\Phi(x_1, \dots, x_N)$ is a symmetric and positive function of its arguments. According to Ref. 4 (see also Ref. 5), we can seek Φ in the form $\Phi = \exp S$. We see that the function $S = S(x_1, \dots, x_N)$ can be expanded as follows:

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

where $S_n(x_1, \dots, x_n)$ are symmetric functions which depend on the relative particle spacing and which are subjected to the constraints

$$\int dx_n S_n(x_1, \dots, x_n) = 0, \quad n > 2. \quad (3)$$

Integrating (2) over the coordinates of $N-n$ particles for $n=2,3,\dots$ and using the condition (3), we can show that expansion (2) is irreducible, which means that for a given function $S(x_1, \dots, x_N)$ the set of the functions S_n is unique. Substituting Eq. (2) into Eq. (1), we obtain

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

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

where the terms which depend only on the pair function $S_2(x) = S(x)$ are indicated explicitly. Integrating Eq. (4) over the coordinates $n+1, \dots, N$ and using Eq. (3), we obtain the n -particle equation for the functions S_n . In general, the system of equations cannot be solved. The perturbation theory can be used for the dilute Bose gas. One can argue that the expansion of the energy in the small parameter corresponds to the expansion (2). Here we will demonstrate it in the lowest order which corresponds to the pairwise wave function. Let us assume that only the function $S(x)$ is not equal to zero. Integrating Eq. (4) over the coordinates $1, \dots, N$, we obtain for the energy $E_0 = N\rho a$ ($\rho = N/V$, $E_0/V = a\rho^2$) the equation

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

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

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

where the notation $x = x_{12}$ is used and the terms of order $\sim 1/V$ are retained. We assume periodic boundary conditions, so that the integral over the total derivative is zero. Because of condition (3), the contributions of S_3 to Eqs. (5) and (6) are respectively $\rho \int dx_1 dx_2 [\partial_1 S(123)]^2$ and $2\rho \int dx_3 S(13) (\partial_1 \partial_3 - \partial_3^2) S(123)$. One can use the solution of Eq. (6) to estimate the function S_3 with the help of the three-particle equation. It can be solved in the leading-order approximation (which means that the terms $\sim S_2 S_3$ are omitted) in the momentum representation, and the integrals in the momentum space can be estimated. These integrals are suppressed by an extra power of the expansion parameter. The smallness of $S(x)$ at the distances $\sim \rho^{-1/d}$ ($d=2,3$) allows one to disregard the S_3 function in the lowest-order approximation. Equation (6) reproduces correctly the correction in density² to the ground-state energy for a 3D system and predicts the leading-order term for a 2D system.

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

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

$$\rho S_k^2 - k^2 S_k - U_k = 0, \quad S_k = \int dx e^{ikx} S(x).$$

Substituting the solution for the expression $a = U_0 = \int_k k^2 S_k^2 [U_0 = \int dx U(x)]$, we obtain

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

where the notation $\int_k = \int d^d k / (2\pi)^d$ is used. Equation (7) is the Bogolyubov's expression for the energy. 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 to its width and the spatial range should be much larger than the average particle spacing.

Let us solve Eq. (6) in the low density limit. The expansion parameters are respectively $|\ln \rho \alpha^2|^{-1}$ and $\alpha^{3/2} \rho^{1/2}$ in two and three dimensions.

1. Three-dimensional system. Define $S_0(x)$ as the solution of Eq. (6) at $\rho=0$:

$$\partial^2 S_0 + \partial S_0 \partial S_0 - U = -\alpha/V. \quad (8)$$

Using 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 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 must be supplemented by the boundary condition $\phi_0(r) \rightarrow 1$ as $r \rightarrow \infty$. At the distances much larger than the range of the potential the solution is $\phi_0(r) = 1 - \alpha/r$. For the energy we have

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

We will use the Fourier transformation in Eqs. (6) and (8). In the region $r \gg \alpha$ we have $S_0(r) = -\alpha/r$. Hence the Fourier transform of the function $U - (\partial S_0)^2$ does not depend on the momentum k at $k \ll 1/\alpha$. Up to the corrections in ρ this also holds for $S(x)$. At these k we have $S_{0k} = -\alpha k^2$, and S_k is the solution of the equation $\rho k^2 S_k^2 - k^2 S_k - \alpha = 0$. Substituting these functions into Eq. (9), we obtain

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

The integral in Eq. (10) converges at large k , so the correction to $\int dx e^{ikx}[U - (\partial S)^2] = \alpha$ does not change the result in the approximation we are considering. Evaluating the integral in Eq. (10), we obtain the well-known result² for the 3D system:

$$a = \alpha \left(1 + \frac{16}{15\pi^2} \alpha^{3/2} \rho^{1/2} \right). \quad (11)$$

2. Two-dimensional system. In 2D it is easy to determine the energy in the leading order in the small parameter, $a \sim |\ln \rho \alpha^2|^{-1}$. As in the 3D system, the solution of Eq. (6) is

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

where $\sigma_k = \int dx e^{ikx}[U(x) - \partial S \partial S(x)]$. At sufficiently small k we have $\sigma_k = a$, while at larger k , σ_k could depend on the momentum k . However, with sufficient accuracy we can set $\sigma_k = a$. We are interested in the behavior of $S(x)$ for $a \ll r \ll (a\rho)^{-1/2}$. In this region

$$S(x) = -a/4\pi + (a/2\pi) \ln[(a\rho)^{1/2} r], \quad (12)$$

which is valid with accuracy to the terms of order a^2 . At distances much larger than the correlation length, $S(r) \approx -(a/\rho)^{1/2}/2\pi r$. Using Eq. (12), we can justify the initial assumption about the behavior of σ_k . The other approach is to represent Eq. (6) in the form

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

where $\phi(x) = \exp S(x)$. The Fourier transform of the function $U(x)\phi(x)$ does not depend on the momentum at $k \ll 1/a$. In the long distance region [$S(x) \ll 1$] we can disregard the terms of order $S^2(x)$, and Eq. (13) has the solution of the same form as Eq. (12). The only difference is that the parameter a should be replaced by the value of the integral $\int dx U(x)\phi(x) = a[1 + O(a)]$.

On the other hand, at the sufficiently small r the function $\phi(x)$ can be found approximately as the solution of the equation $[-\partial^2 + U(x)]\phi(x) = 0$ [see Eq. (13)]. 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 $U(r)$ ($r \gg \alpha$). In two dimensions it is defined by the behavior of the scattering amplitude at low energy

$$\bar{f}(k) = \frac{\pi}{\ln k\alpha/2 + \gamma - i\pi/2} + O(k\alpha),$$

where $|\bar{f}(k)| = (2\pi k)^{1/2} |f(k)|$ is the modified scattering amplitude, k is the momentum, and γ is the Euler constant. For the 2D hard-sphere potential, 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 estimated from Eq. (12). The quantity $\delta\phi(r)$ is small ($\sim a$) at the distances $r \sim \rho^{-1/2}$. Comparing Eq. (12) with the function $\phi_0(r)$, we obtain the relation

$$C \ln(r/\alpha) = 1 - a/4\pi + (a/2\pi) \ln[(a\rho)^{-1/2}r], \quad (14)$$

which should be valid in the region $\alpha \ll r \ll (a\rho)^{-1/2}$ within logarithmic accuracy. Thus, in the leading order in the small parameter we have $|\ln \rho\alpha^2|^{-1}$, $C = a/2\pi$ and the energy is

$$a = \frac{4\pi}{|\ln \rho\alpha^2|} + O\left(\frac{1}{|\ln \rho\alpha^2|^2}\right). \quad (15)$$

Equation (15) is the final result for the two-dimensional system. 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 the other words, although the function S_3 is not necessarily small at small distances, our estimate of the right hand side of Eqs. (13) and Eq. (14) is valid within an order of magnitude.

The result (15) has a simple physical interpretation. The energy of the two particles located in the two-dimensional volume V is $\sim \bar{f}/V$, where the amplitude \bar{f} should be normalized at the momentum on the order of the correlation length which characterizes the screening of the pair wave function due to the other particles. Multiplying the result by the number of pairs, we obtain the result (15) in three dimensions, which corresponds to the first term in Eq. (11).

The pair distribution function, which is associated with the function Φ (Ref. 3), can be calculated using the Jastrow-type wave function with the help of the cluster expansion.⁶ Formally, the problem is similar to the calculation for the classical liquid, although the expansion in density for the corresponding partition function is not valid [the integral $\int dx S(x)$ diverges at large distances]. The summation of the "chain" diagrams should be performed. The same approximation can be used to calculate the Feynman structure factor $F(k)$ which determines the energy of the low-lying excitations:

$$F(k) = \frac{1}{1 - 2\rho S_k}.$$

In contrast with the other wave functions of the Jastrow type, which are used in the variational studies of the Bose liquid,⁷ we obtain the correct behavior $F(k) \sim k$ in the limit $k \rightarrow 0$, because of the behavior $S(r) \sim 1/r^{d-1}$ at asymptotically large distances⁶ (for a related discussion see Ref. 8).

Finally, the situation is different for the one-dimensional problem. From the point of view of our method, the low density limit coincides with the weak coupling limit. In this case the expression (7) is correct, regardless of the shape of the potential, while for the strong coupling the perturbation theory is inapplicable, in agreement with the exact solution of the problem for the δ -function potential.⁹ This is also true for the lattice system. For example, a system described by the Hamiltonian (see, e.g., Ref. 10),

$$H = -t \sum_{\langle ij \rangle} (b_i^+ b_j + \text{h.c.}) + U \sum_i n_i(n_i - 1), \quad n_i = b_i^+ b_i,$$

in the limit $U \rightarrow 0$ and with a density on the order of unity [Eq. (7)], is asymptotically exact in any dimension.

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