

TWO-DIMENSIONAL BOSE GAS AT LOW DENSITY

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

At present time two-dimensional models attract much attention in connection with the problems of high- T_c superconductivity and fractional quantum Hall effect. In this context the description of the two-dimensional system of bosons may be important and 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 were introduced which in one way or another consisted in summing up an infinite subset of the terms in the perturbation series. The example of this procedure is the Bogoliubov's method ¹. In the limit of the dilute bose gas the perturbation theory ¹ does not work which manifests 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 obscured. The generalization of this 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 ² can be considered as an application of the Bogoliubov's approach to a system with the parameters chosen in such a way that both 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 a basis for the solution of 2D problem the estimate of the accuracy of the approximation ¹ for a given potential is required.

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 $\partial_i = \partial / \partial x_i$, $x_{ij} = x_i - x_j$ and 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 ⁴ (see also ⁵) one can seek

for Φ in the form $\Phi = \exp S$. We observe that the function $S = S(x_1, \dots, x_N)$ can be expanded in the following way

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

where $S_n(x_1, \dots, x_n)$ are symmetric functions depending on the relative particle spacing and 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 subsequently for $n = 2, 3, \dots$ and using the condition (3) one can show that the expansion (2) is an irreducible one 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 depending on the pair function $S_2(x) = S(x)$ only 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 the equations cannot be solved. For the dilute bose gas the perturbation theory can be used. One can argue that the expansion of the energy in the small parameter corresponds just to the expansion (2). Here we will demonstrate it in the lowest order which corresponds to the pairwise wave function. Suppose for a while that only the function $S(x)$ is not equal to zero. Integrating the equation (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 the periodic boundary conditions so that the integral over the total derivative is zero. Due to the condition (3) the contributions of S_3 to Eq.(5) and Eq.(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. It is the smallness of $S(x)$ at the distances $\sim \rho^{-1/d}$ ($d = 2, 3$) that allows one to neglect the S_3 function in the lowest order approximation. The equation (6) reproduces correctly

the correction in density 2 to the ground-state energy for 3D system and predicts the leading order term for 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 form of the solution of Eq.(6) that the variational energy is given by Eq.(5) with the accuracy up to the higher order terms in the expansion parameter.

If the second term in the left-hand side of the equation (6) can be neglected 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 to the expression $a = U_0 + \int_k k^2 S_k^2$ ($U_0 = \int dx U(x)$) we get

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

where the notation $\int_k = \int d^d k / (2\pi)^d$ is used. Eq.(7) is the Bogoliubov's expression for the energy. The corrections are determined by the function $S(x)$ which should be small in order 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 the equation (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 the equation (6) at $\rho = 0$:

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

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 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 $\phi_0(r) \rightarrow 1$ at $r \rightarrow \infty$. 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

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

Make use of the Fourier transformation in Eq.(6) and (8). In the region $r \gg \alpha$ we have $S_0(r) = -\alpha/r$. Hence the Fourier transform of the function $U - (\partial S_0)^2$ is independent of the momentum k at $k \ll 1/\alpha$. Up to the corrections in ρ the same is true for $S(x)$. At these k $S_{0k} = -\alpha/k^2$ 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 corrections to $\int dx e^{ikx}(U - (\partial S)^2) = \alpha$ does not change the result in the approximation considered. Evaluating the integral in Eq.(10) we obtain the well known result ² for 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 3D the solution of Eq.(6) is

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

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

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

which is valid with the accuracy up to the terms of order a^2 . At the distances much larger than the correlation length $S(r) \simeq -(a/\rho)^{1/2} / 2\pi r$. Using Eq.(12) one can justify the initial assumption about the behavior of σ_k . The other way 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 $k \ll 1/\alpha$. In the long distance region ($S(x) \ll 1$) we can neglect the terms of order $S^2(x)$ and the equation (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 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 using Eq.(12). $\delta\phi(r)$ is small ($\sim a$) at the distances $r \sim \rho^{-1/2}$. Comparing Eq.(12) with the function $\phi_0(r)$ we get the relation

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

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

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

Eq.(15) is our 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 necessary small at small distances our estimate of the right hand side of Eq.(13) as well as the equation (14) are valid by 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 of 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 that corresponds to the first term in Eq.(11).

The pair distribution function associated with the function Φ^3 can be calculated using the obtained wave function of the Jastrow form 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 (integral $\int dx S(x)$ diverges at large distances). The summation of "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 to the other wave functions of the Jastrow form used in the variational studies of the bose liquid ⁷ we obtain the correct behavior $F(k) \sim k$ at $k \rightarrow 0$ due to the behavior $S(r) \sim 1/r^{d-1}$ at the asymptotically large distances ⁶ (for a related discussion see ref.⁸).

Finally, the situation is different for one-dimensional problem. From the point of view of our method the low density limit coincide 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 which is in agreement with the exact solution of the problem for the δ -function potential ⁹. The same can be true for the lattice system. For instance for a system described by the Hamiltonian (for example, see ref.¹⁰)

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

at $U \rightarrow 0$ and the density of order of unity Eq.(7) is asymptotically exact in any dimensions.

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