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Abstract

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MATHEMATICAL PHYSICS

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MODIFIED AND TRUE FORMULATIONS OF THE PROBLEM OF A NONIDEAL BOSE-EINSTEIN MANY-PARTICLE SYSTEM

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The modified formulation consists in the fact that, in the problem, the creation and annihilation operators a_0^+ and a_0 of particles with zero momentum are, from the very beginning, replaced in a completely definite way by the c-number $\sqrt{N_0}$, where N_0 is the number of particles in the condensate (see [1–3]).

The necessity of the modified formulation is connected with our desire to study the formal perturbation theory in the problem by the usual methods of quantum field theory*. These methods are not applicable, since, for example, for the case of temperature $\theta = 0$ the state of the ideal Bose condensate on which the perturbation theory is to be built is not a vacuum with respect to the operators a_0^+ and a_0. An analogous difficulty also occurs for the case of nonzero temperature $\theta \neq 0$.

Leaving aside here the discussion of the question of a complete and rigorous proof of the equivalence of both formulations [2,4,5], we shall set forth below a very simple argument which is sufficiently convincing**.

First of all let us explain why, in developing perturbation theory for a nonideal Bose–Einstein system, we cannot use the very convenient grand canonical ensemble with an unfixed total number of particles of the system, but are forced to resort to the canonical ensemble with a fixed total number of particles of the system.

Consider, at $\theta = 0$, an ideal system placed in a thermostat with chemical potential μ. Let us find the state in which our system will reside. For this it is necessary to consider the lowest eigenstate of the dynamical operator $\Omega = H - \mu N$, where H is the operator of the total energy, and N is the operator of the total number of particles.

The eigenstates of Ω are specified by sets of occupation numbers $\ldots n_p \ldots$, with each n_p able to take the values $0, 1, 2, \ldots$. The eigenvalues of Ω will be

Fig. 1. Diagram of states of a nonideal system in the grand canonical ensemble. μ –chemical potential, v –interaction parameter

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$$F_{\ldots n_p \ldots} = \sum_p (E(p) - \mu) n_p,$$

where $E(p) = p^2/2m$ is the kinetic energy of a single particle.

One must consider three cases: 1) $\mu < 0$; 2) $\mu > 0$; 3) $\mu = 0$. In the first case, $\mu < 0$, the minimizing set of occupation numbers will be the set $n_p = 0$ for all p. All particles of the Bose system go into the thermostat. In the second case, $\mu > 0$, the minimizing set will be the set $n_0 = \infty$, while the remaining $n_p = 0$. Particles from the thermostat will continually enter our Bose system. In the third case, $\mu = 0$, we are dealing with the true state of our system. However, the minimum value of Ω turns out to be infinitely degenerate. To this value belong all sets: n_0 arbitrary, the remaining $n_p = 0$. In fact, only at one value of the chemical potential μ can the ideal system be in equilibrium with the thermostat of the grand canonical ensemble.

* It is true that one may use the usual Wick theorem, expressing T-products in terms of N-products with pairings, and then "parametrize" not only the pairings but also nonzero averages of N-products.

** The results set forth in this note were obtained by the author at the end of 1959.

From the study of a nonideal Bose-Einstein system, carried out in the canonical ensemble, it follows that the diagram of possible equilibrium states of our system in the grand canonical ensemble has the form shown in Fig. 1. From consideration of Fig. 1 it is quite clear that we cannot adiabatically switch off the interaction in the grand canonical ensemble (μ fixed, v tends to zero), since in doing so we necessarily enter the forbidden region in the diagram of states.

Fig. 1. Diagram of the states of a nonideal system in the grand canonical ensemble.
μ –chemical potential, v –interaction parameter

In the canonical ensemble we shall use the formula given by the adiabatic theorem:

$$\Delta E = -\frac{\hbar}{i} \lim_{\alpha \to +0} \alpha g \frac{\partial}{\partial g} \ln \langle S_\alpha(0, -\infty \mid g) \rangle_{g=1}, \tag{1}$$

where ΔE is the shift of the ground-state energy due to the interaction,

$$S_\alpha(0,-\infty \mid g) = 1 + \sum_{n=1}^{+\infty} g^n \left(-\frac{i}{\hbar}\right)^n \int_{-\infty}^{0} dt_1 \int_{-\infty}^{t_1} dt_2 \ldots \int_{-\infty}^{t_{n-1}} dt_n \times$$

$$\times \langle H_{int}(t_1) \ldots H_{int}(t_n)\rangle e^{\alpha(t_1+\ldots+t_n)}, \tag{2}$$

where, in turn,

$$H_{int}(t) = e^{\frac{i}{\hbar}H_0 t} H_{int} e^{-\frac{i}{\hbar}H_0 t}.$$

The averaging $\langle \ldots \rangle$ is to be performed over the Bose condensate of the ideal system, in which all N particles of the system are in the state with zero momentum $p = 0$.

In (1), (2) we cannot use the field technique of pairings for zero momentum $p = 0$, although for momenta $p \neq 0$ we can do this. First we must calculate the averages

$$S_n = \left(-\frac{i}{\hbar}\right)^n \int_{-\infty}^{0} dt_1 \int_{-\infty}^{t_1} dt_2 \ldots \int_{-\infty}^{t_{n-1}} dt_n \langle H_{int}(t_1) \ldots H_{int}(t_n)\rangle e^{\alpha(t_1+\ldots+t_n)}, \tag{3}$$

and then from them, according to (1), (2), one must form the expression for the correction of the n-th order

$$\Delta E_n = \lim_{\varepsilon \to 0} \varepsilon n \sum_{m_1=0} \sum_{m_2=0} \ldots \sum_{m_n=0} \Delta(m_1 + 2m_2 + \ldots + nm_n - n) \times \tag{4}$$

$$\times (-1)^{m_1+m_2+\ldots+m_n} \frac{(m_1+m_2+\ldots+m_n-1)!}{m_1! m_2! \ldots m_n!} S_1^{m_1} S_2^{m_2} \ldots S_n^{m_n}, \qquad \varepsilon = \frac{\hbar}{i}\alpha.$$

The contribution S_n is constructed by enumerating the contributions from all possible n-th order diagrams arranged in different ways with respect to the time axis (diagrams with denominators).

The rules for constructing the contribution from each diagram are as follows. Vertices are quartic and incomplete quartic; solid particle lines run only in the direction of the time axis.

1) To an interaction line there corresponds the factor

$$-\frac{1}{V} v(q),$$

where q is the momentum transferred at the vertex.

Fig. 2. One of 4 possible diagrams for S_4

Figure 2: Fig. 2. One of 4 possible diagrams for S_4

2) To the cut between the $k-1$-st and k-th vertices of the diagram there corresponds the factor (the vertices are numbered opposite to the direction of the time axis)

$$\frac{1}{\mathcal{E}+(n-k+1)\varepsilon},$$

where $\mathcal{E}$ is the sum of the energies $E(p)$ of the diagram lines intersected by this cut.

3) To the entire diagram assign the factor $\frac{1}{g}\frac{1}{n\varepsilon}$, where g is the number of elements in the group of topological automorphisms that transform the diagram into itself.

4) To the missing ends of solid lines in incomplete four-vertices assign the operators a_0^+, a_0 (a_0^+ leaves the vertex, a_0 enters it), and place before the diagrams, as a factor, the average of the product of the operators a_0^+, a_0 corresponding to all incomplete vertices of the diagram.

The operators in the product should be arranged in accordance with the arrangement of the diagram' s vertices relative to the time axis.

It is very important to keep ε in the denominators $1/\mathcal{E}$ with the correct coefficients $n-k+1$.

For lack of space we do not give here the results obtained for all diagrams up to and including fourth order. We shall dwell only on the most important specific diagrams of fourth and sixth order.

Fig. 2. One of 4 possible diagrams for S_4

The corresponding diagrams for S_4 and S_6 are illustrated in Figs. 2 and 3. The diagrams S_4 are two-connected, the diagrams S_6 three-connected. They consist of one and the same diagram S_2, repeated several times. All possible arrangements of these connected parts of the diagrams for S_4 and S_6 relative to one another must be enumerated.

The contribution to ΔE of the indicated diagrams, in accordance with (4), should be calculated by the formulas (in (4) we retain only those terms that lead to contributions to ΔE of the same type as the contributions from the diagrams under consideration in S_4 and S_6):

$$\Delta E_4 = \lim_{\varepsilon\to 0}\varepsilon\left(-4S_4+2S_2^2\right), \tag{5}$$

Fig. 3. One of 15 possible diagrams for S_6

Figure 3: Fig. 3. One of 15 possible diagrams for S_6

$$\Delta E_6 = \lim_{\varepsilon \to 0} \varepsilon \left(-6S_6 + 6S_4 S_2 - 2S_2^3\right). \tag{6}$$

After carrying out the necessary calculations we obtain

$$\Delta E_4 = \sum_{p,p'} \frac{v^2(p)}{2V^2} \frac{v^2(p')}{2V^2} \frac{1}{4E^2(p)} \frac{1}{2E(p')} \left(4N^3 + \cdots\right), \tag{7}$$

$$\begin{aligned} \Delta E_6 = & -\sum_{p,p',p''} \frac{v^2(p)}{2V^2} \frac{v^2(p')}{2V^2} \frac{v^2(p'')}{2V^2} \frac{1}{8E^3(p)} \frac{1}{2E(p')} \frac{1}{2E(p'')} \left(16N^4 + \cdots\right) \\ & -\sum_{p,p',p''} \frac{v^2(p)}{2V^2} \frac{v^2(p')}{2V^2} \frac{v^2(p'')}{2V^2} \frac{1}{4E^2(p)} \frac{1}{4E^2(p')} \frac{1}{2E(p'')} \left(20N^4 + \cdots\right). \end{aligned} \tag{8}$$

Now let us turn to the modified formulation. We can likewise use formulas (1), (2), (3). Only now, instead of a_0, a_0^+, there will stand the c-number $\sqrt{N_0}$, and, in addition, instead of $E(p)$ there will stand $E(p) - \mu$, where μ is the chemical potential. Wick' s pairing technique is applicable without reservation. In particular, one may restrict oneself to considering only connected diagrams. Of course, the diagrams are now constructed for the thermodynamic potential $F = E - \mu N$.

Fig. 3. One of 15 possible diagrams for S_6

The rules for constructing the contributions from diagrams for $\Delta F(\mu, N_0)$ are completely analogous to the rules given above for constructing contributions from diagrams for ΔE. Only: 1) it is necessary to discard disconnected diagrams; 2) replace the factors N, $N-1$, etc. by N_0; 3) instead of $E(p)$ put $E(p) - \mu$.

Let us give the expression needed for $\Delta F_2(\mu, N_0)$:

$$\Delta F_2(\mu, N_0) = -\frac{N^2}{2V^2} \sum_p v^2(p) \frac{1}{2(E(p) - \mu)}. \tag{9}$$

The two parameters of the modified formulation, μ and N_0, should be eliminated by means of the conditions

$$\frac{\partial F(\mu, N_0)}{\partial N_0} = 0, \qquad \frac{\partial F(\mu, N_0)}{\partial \mu} = -N, \tag{10}$$

where the derivatives have the meaning of ordinary partial derivatives of functions of two independent variables.

From (10) we obtain, to within terms of second order,

$$\mu = \frac{N}{V} v(0) - \frac{N^2}{2V^2} \sum_p v^2(p) \frac{1}{E(p)} + \cdots, \tag{11}$$

$$N_0 = N - \frac{N^2}{4V^2} \sum_p v^2(p) \frac{1}{E^2(p)} + \cdots. \tag{12}$$

Let us note that in the modified formulation $\Delta E = \Delta F + \mu(N - N_0)$. Selecting the corresponding terms in this expression, it is easy to verify that, to within accuracy, they have the form (7) and (8). Thus the equivalence of the true and modified formulations is established, at least for zero temperature, for the quantity of the ground-state energy shift.

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Note: Figure translations are in progress. See original paper for figures.