THE CONNECTION BETWEEN THE STATISTICAL VARIATIONAL PRINCIPLE AND THE METHOD OF PARTIAL SUMMATION OF DIAGRAMS OF THERMODYNAMIC PERTURBATION THEORY IN A MODIFIED FORMULATION OF THE PROBLEM OF A

NONIDEAL BOSE-EINSTEIN SYSTEM

1960

SovietRxiv

Abstract

Full Text

MATHEMATICAL PHYSICS

V. V. TOLMACHEV

THE CONNECTION BETWEEN THE STATISTICAL VARIATIONAL PRINCIPLE AND THE METHOD OF PARTIAL SUMMATION OF DIAGRAMS OF THERMODYNAMIC PERTURBATION THEORY IN A MODIFIED FORMULATION OF THE PROBLEM OF A NONIDEAL BOSE-EINSTEIN SYSTEM

(Presented by Academician N. N. Bogolyubov, 10 June 1960)

The modified formulation of the problem of a nonideal Bose-Einstein system differs from the true one in that, in the latter, the operators a_0^+ and a_0 for the creation and annihilation of particles with zero momentum are replaced in a quite definite way by the C-number $\sqrt{N_0}$ ([1–3]).

In the modified formulation, the Hamiltonian operator and the operator of the total number of particles in the representation of second quantization have the form

$$\begin{aligned}\mathcal{H} = &\sum_p E(p) a_p^+ a_p + \frac{N_0^2}{2V} v(0) + \frac{N_0}{V} v(0) \sum_p a_p^+ a_p \\ &+ \frac{N_0}{2V} \sum_p v(p) a_p^+ a_{-p}^+ + \frac{N_0}{2V} \sum_p v(p) a_p a_{-p} + \frac{N_0}{V} \sum_p v(p) a_p^+ a_p \\ &+ \frac{\sqrt{N_0}}{V} \sum_{p,p_1,p_2} v(p_1) \Delta(p - p_1 - p_2) a_p^+ a_{p_2} a_{p_1} \\ &+ \frac{\sqrt{N_0}}{V} \sum_{p,p_1',p_2'} v(p_1') \Delta(p - p_1' - p_2') a_{p_1'}^+ a_{p_2'}^+ a_p \\ &+ \frac{1}{2V} \sum_{p_1,p_2,p_1',p_2'} v(p_1 - p_1') \Delta(p_1 + p_2 - p_1' - p_2') a_{p_1'}^+ a_{p_2'}^+ a_{p_2} a_{p_1},\end{aligned} \tag{1}$$

$$\mathcal{N} = N_0 + \sum_p a_p^+ a_p, \tag{2}$$

where N_0 is the number of particles in the condensate; V is the volume in which the system is contained; $E(p) = p^2/2m$ is the kinetic energy of an individual particle; $v(p)$ is the pair-interaction potential in the momentum representation, $v(p) > 0$; $\Delta(p)$ is the Kronecker Δ-symbol; the operators a_p^+ and a_p for the creation and annihilation of particles with momentum p are bosonic, i.e., they satisfy the Bose commutation relations $a_p a_{p'}^+ - a_{p'}^+ a_p = \Delta(p-p')$. The operators $\mathscr{H}$ and $\mathscr{N}$ do not commute with each other.

The quantity N_0 is chosen from the following considerations. Let us construct the grand sum of states for (1) and (2) and take the corresponding thermodynamic potential F. For it,

$$-\beta F = \ln \operatorname{Sp} e^{-\beta\Omega}, \qquad \Omega = \mathscr{H} - \mu\mathscr{N}, \tag{3}$$

where $\beta = 1/\theta$; $\theta = kT$; k is Boltzmann' s constant; T is the absolute temperature; μ is the chemical potential. In accordance with (3), the thermodynamic potential F may be regarded as a function of the independent variables N_0 and μ. We determine the quantity N_0 from the condition

$$\partial F(N_0, \mu)/\partial N_0 = 0, \tag{4}$$

which is necessary for the preservation of the thermodynamic relations in the modified formulation.

Finally, we can also eliminate the chemical potential μ from the modified formulation with the aid of the condition

$$\partial F(N_0, \mu)/\partial \mu = -N, \tag{5}$$

introducing the mean total number of particles of the system N.

Let us now turn to the statistical variational principle. We first perform the Bogoliubov canonical transformation of the Bose operators a_p^+ and a_p to new Bose operators b_p^+ and b_p: $a_p = u_p b_p + v_p b_{-p}^+$, where u_p, v_p satisfy the conditions $u_p^2 - v_p^2 = 1$, $u_p = u_{-p}$, $v_p = v_{-p}$. Next we represent the operator Ω in the form of the sum $\Omega = \Omega_0 + \Omega_{\text{int}}$, $\Omega_0 = \sum_p \varepsilon(p) b_p^+ b_p$. The parameters u_p, v_p, and $\varepsilon(p)$ of such a decomposition are chosen in the best way according to the statistical variational principle (see (4)),

$$F \leq \min\{F_0 + \langle \Omega_{\text{int}} \rangle\}, \tag{6}$$

where $-\beta F_0 = \ln \operatorname{Sp} e^{-\beta\Omega_0}$, $\langle ... \rangle = \operatorname{Sp} e^{-\beta\Omega_0} ... / \operatorname{Sp} e^{-\beta\Omega_0}$.

As a result we obtain the following system of equations (in the case $\theta = 0$ it coincides with that obtained, for example, in [5]):

$$\begin{gathered}\varepsilon(p) = A(p)(u_p^2 + v_p^2) + B(p)2u_pv_p,\\ B(p)(u_p^2 + v_p^2) + A(p)2u_pv_p = 0,\\ A(p) = E(p) - \mu + \frac{N_0}{V}v(0) + \frac{N_0}{V}v(p) + \\ + \frac{1}{V}\sum_{p'}(v(0) + v(p-p'))(n_{p'}u_{p'}^2 + (1+n_{p'})v_{p'}^2),\\ B(p) = \frac{N_0}{V}v(p) + \frac{1}{V}\sum_{p'}v(p-p')(1+2n_{p'})u_{p'}v_{p'},\end{gathered} \tag{7}$$

where $n_p = 1/(e^{\beta\varepsilon(p)} - 1)$. We could also have obtained the system (7) from the requirements $\langle b_p\Omega_{\text{int}}b_p^+\rangle_{\text{conn}} = 0$, $\langle b_pb_{-p}\Omega_{\text{int}}\rangle = 0$, where the subscript "conn" on the average means that, in expanding the average, we must not contract b_p with b_p^+.

Substituting into the conditions (4), (5) the variational estimate for F, given by $\min\{F_0 + \langle\Omega_{\text{int}}\rangle\}$, we obtain

$$\mu = \frac{N_0}{V}v(0) + \frac{1}{2V}\sum_{p'}(v(0) + v(p'))(n_{p'}u_{p'}^2 + (1+n_{p'})v_{p'}^2) + $$

$$+ \frac{1}{2V}\sum_{p'}v(p')(1+2n_{p'})2u_{p'}v_{p'} + \dots, \tag{8}$$

$$N = N_0 + \frac{1}{2V}\sum_{p'}(n_{p'}u_{p'}^2 + (1+n_{p'})v_{p'}^2) + \dots \tag{9}$$

We shall now establish the connection between the formulated statistical variational principle and the method of partial summation of diagrams of the formal perturbation theory for the modified formulation. We shall show which diagrams are summed by the variational principle. We shall develop the diagrams for the one-particle temperature Green' s function

$$G(p;\tau-\tau') = \langle T(a_p(\tau)a_p^+(\tau'))\rangle, \tag{10}$$

where $a_p(\tau) = e^{\tau\Omega}a_pe^{-\tau\Omega}$, $a_p^+(\tau) = e^{\tau\Omega}a_p^+e^{-\tau\Omega}$, $\langle\dots\rangle = \operatorname{Sp} e^{-\beta\Omega}\dots / \operatorname{Sp} e^{-\beta\Omega}$.

Passing to the interaction representation, in the manner standard for field theory we arrive at the following rules for constructing the diagrams contributing to (10). The only new feature will be the use, instead of the field-theoretic Wick theorem, of the temperature theorem on contractions [6,7]

In addition to complete four-legged vertices, the diagrams may contain incomplete triple and double vertices, in which one or two particle lines are missing.

One must imagine the set of diagrams with two external lines and without vacuum loops.

Fig. 1. Elimination of pair vertices. a—pair vertices; b—pair propagators corresponding to summation excluding pair vertices; c—Dyson equations

Fig. 1. Elimination of pair vertices. *a*—pair vertices; *b*—pair propagators corresponding to summation excluding pair vertices; *c*—Dyson equations.

The rules for composing contributions from diagrams are as follows (cf. ([2,3])):

1) For each line (internal and external) with momentum p, leaving a vertex at which τ' stands and ending at a vertex at which τ stands, write the factor

$$G_0(p;\tau-\tau') = e^{-\varepsilon_0(p)(\tau-\tau')}\{(1+n_p^{(0)})\theta(\tau-\tau') + n_p^{(0)}\theta(\tau'-\tau)\},$$

where

$$n_p^{(0)} = \frac{1}{e^{\beta\varepsilon_0(p)}-1}; \qquad \theta(\tau)=1 \text{ for } \tau>0, \qquad \theta(\tau)=0 \text{ for } \tau<0;$$

$$\varepsilon_0(p) = E(p) - \mu + \frac{N_0}{V}v(0) + \frac{N_0}{V}v(p).$$

To an internal line with momentum p, beginning and ending at one and the same vertex, assign the factor $G_0(p;-0) = n_p$.

2) For a complete vertex introduce the factor

$$-\frac{1}{V}\,v(p_1-p_1')\,\Delta(p_1+p_2-p_1'-p_2'),$$

where p_1 and p_2 refer to the lines entering the vertex, and p_1' and p_2' refer to the corresponding outgoing lines. If the vertex is incomplete, then in this factor the momenta corresponding to the lines absent from the vertex are to be replaced by zeros. In addition, multiply the indicated expression by $\sqrt{N_0}$ for each line absent from the incomplete vertex.

3) Perform summation over all momenta p standing on internal lines, and integration from 0 to β over all τ standing at internal vertices.

4) A factor $1/n!$, where n is the order of the diagram.

We shall eliminate from the diagrams the pair vertices shown in Fig. 1a, by summing the contributions from parts of diagrams consisting exclusively of the indicated pair vertices. The notation for these contributions, described by new propagators, is given in Fig. 1b. Among these propagators only two are independent. Figure 1c gives a graphical representation of the Dyson equations expressing the summation being performed.

As the next step we shall eliminate the first-order self-energy parts proper, i.e. eliminate the vertices shown in Fig. 2a, bearing in mind the possibility of infinitely many insertions of these vertices into one another. The notation for the new propagators is given in Fig. 2b. Among them, again, only two are independent. Fig. 2b is completely analogous to Fig. 1b. In Fig. 2c a graphical representation of the corresponding Dyson equations is given. The indicated equations have, as solutions, functions of the following structure:

$$G^{--}(p;\tau) = \begin{cases} u_p v_p n_p e^{\varepsilon(p)\tau} + u_p v_p (1+n_p) e^{-\varepsilon(p)\tau}, & \tau > 0, \\ u_p v_p (1+n_p) e^{\varepsilon(p)\tau} + u_p v_p n_p e^{-\varepsilon(p)\tau}, & \tau < 0, \end{cases} \tag{11}$$

$$G^{-+}(p;\tau) = \begin{cases} v_p^2 n_p e^{\varepsilon(p)\tau} + u_p^2 (1+n_p) e^{-\varepsilon(p)\tau}, & \tau > 0, \\ u_p^2 (1+n_p) e^{\varepsilon(p)\tau} + v_p^2 n_p e^{-\varepsilon(p)\tau}, & \tau < 0, \end{cases} \tag{12}$$

$$G^{++}(p;\tau) = G^{--}(p;\tau), \qquad G^{+-}(p;\tau) = G^{-+}(p;-\tau);$$

u_p, v_p, and $\varepsilon(p)$ are determined from equations (7).

Fig. 2. Elimination of first-order self-energy parts.
a –eliminated vertices; *b* –propagators corresponding to summation; *c* –Dyson equations.

Thus we have shown the equivalence of the statistical variational principle and the summation of a special class of temperature diagrams.

An analogous result holds in the problem of a nonideal Fermi–Dirac system.

Physicochemical Institute
named after L. Ya. Karpov

Received
7 VI 1960

CITED LITERATURE

1. N. N. Bogolyubov, *J. of Phys.*, **9**, 23 (1947); *Vestn. MGU*, No. 7, 43 (1947).

2. S. T. Belyaev, *ZhETF*, **34**, 415, 433 (1958).

3. N. M. Hugenholtz, D. Pines, *Phys. Rev.*, **116**, 489 (1959).

4. N. N. Bogolyubov, see in the dissertation of I. A. Kvasnikov, V. A. Steklov Mathematical Institute, Academy of Sciences of the USSR, 1958.

5. M. Girardeau, R. Arnowitt, *Phys. Rev.*, **113**, 755 (1959); M. Girardeau, *Phys. Rev.*, **115**, 1090 (1959).

6. T. Matsubara, *Progr. Theor. Phys.*, **14**, 35 (1955).

7. D. J. Thouless, *Phys. Rev.*, **107**, 1162 (1957); C. Bloch, C. de Dominicis, *Nuclear Phys.*, **7**, 459 (1958).

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