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A GENERALIZATION OF THE HARTREE-FOCK METHOD FOR THE CASE OF A NON-IDEAL BOSE GAS

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A nonideal Bose gas at temperatures considerably below the critical temperature is described sufficiently completely by one-particle two-time temperature Green' s functions

$$\left\langle\left\langle a_q(t); D^+(t')\right\rangle\right\rangle = -i\theta(t-t')\left\langle[a_q(t), D^+(t')]\right\rangle,$$

$$\left\langle\left\langle a_{-q}^+(t); D^+(t')\right\rangle\right\rangle = -i\theta(t-t')\left\langle[a_{-q}^+(t), D^+(t')]\right\rangle, \tag{1}$$

where the notation of paper ([1]) is used; $a_q(t)$ and $a_{-q}^+(t)$ are annihilation and creation operators in the Heisenberg representation. The averaging is performed over the grand Gibbs ensemble. For $D = a_q$ one obtains the usual normal and anomalous Green' s functions.

The operator $a_q(t)$ satisfies the equation

$$i\,da_q(t)/dt = (q^2/2m - \mu)a_q(t) + A_q(t), \tag{2}$$

where μ is the chemical potential;

$$A_q = \frac{1}{V}\sum_{kp} v(k)a_p^+ a_{p+k}a_{-k+q} =$$

$$= \frac{N_0}{V}v(0) + \frac{N_0}{V}v(q)(a_q + a_{-q}^+) + \sqrt{\varepsilon}\,B_q + \varepsilon C_q; \tag{3}$$

$$B_q = \frac{\sqrt{N_0}}{V}\sum_k \{(v(q) + v(k))a_{+k}^+ + v(k)a_{-k}\}a_{-k+q}; \tag{4}$$

$$C_q = \frac{1}{V}\sum_{kp} v(k) a_p^+ a_{p+k} a_{-k+q}. \tag{5}$$

In expressions (4), (5) and below, the summation is over states in which the particles have momentum different from zero; $v(k) = \int \exp(ikx) v(x)\, dx$ is the Fourier component of the interaction potential $v(x)$; V is the volume of the system. In relation (3), in accordance with N. N. Bogolyubov' s theory of the nonideal Bose gas ([2]), the condensate has been separated out,

$$a_p = \delta_{p0}\sqrt{N_0} + (1 - \delta_{p0}) a_p, \tag{6}$$

where N_0 is the number of particles in the state with zero momentum, of the order of the total number of particles N.

The formal small parameter ε, set equal to unity in the final results, is introduced by the substitution (see ([3])) $v(p) \to \varepsilon v(p)$, $N_0 \to \varepsilon^{-1} N_0$. In the case of weak interaction with radius $d \gg v(0)m$, expansion in ε corresponds to the assumption of a high density of the system ($v(0)md^{-1}(d/a)^3 \sim 1$, $a/d \ll 1$, where $a = (V/N)^{1/3}$).

The expression for the chemical potential μ, as in paper ([3]), is obtained from the condition $\langle a_p \rangle = \delta_{p0}\sqrt{N_0}$, by averaging the equation of motion (2):

$$\mu = \frac{N_0}{V} v(0) + \frac{\varepsilon}{V}\sum_k \{(v(0) + v(k)) n_k + v(k) s_k\} +$$

$$+ \frac{\varepsilon^{3/2}}{\sqrt{N_0} V}\sum_{kp} v(k) \left\langle a_p^+ a_{p+k} a_{-k} \right\rangle, \tag{7}$$

where $n_k = \langle a_k^+ a_k \rangle$ and $s_k = \langle a_{-k} a_k \rangle$; the number of particles in the condensate N_0 is determined by the equation

$$N_0 = N - \sum_k n_k. \tag{8}$$

Starting from the equation of motion (2), we obtain equations for the Green functions (1). Passing to Fourier components,

$$\langle\langle A \mid B^+ \rangle\rangle_E = -\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{iEt} \langle\langle A(t); B^+(0) \rangle\rangle\, dt, \tag{9}$$

where $\operatorname{Im} E > 0$ for the retarded function, we shall have

$$E\langle\langle a_q \pm a^+_{-q} \mid D^+\rangle\rangle = \langle [a_q \pm a^+_{-q}, D]\rangle + (q^2/2m - \mu)\langle\langle a_q \mp a^+_{-q} \mid D^+\rangle\rangle + \langle\langle A_q \mp A^+_{-q} \mid D^+\rangle\rangle. \tag{10}$$

Applying the Hartree–Fock method, we must carry out in the right-hand side of (10) all possible pairings of operators, taking into account, as in the case of superconductivity [4], the anomalous averages $s_k = \langle a_{-k} a_k \rangle$.

As a result, in equations (10) one should put

$$A_q \cong \left\{ \frac{N_0}{V}(v(0) + v(q)) + \frac{\varepsilon}{V}\sum_k (v(0) + v(k)) n_k \right\} a_q + \left\{ \frac{N_0}{V} v(q) + \frac{\varepsilon}{V}\sum_k v(k) s_{k-q} \right\} a^+_{-q}; \tag{11}$$

$$\mu \cong \frac{N_0}{V} v(0) + \frac{\varepsilon}{V}\sum_k \{(v(0) + v(k)) n_k + v(k) s_k\}. \tag{12}$$

The system of equations (10) becomes closed. However, in this case we obtain a gap in the spectrum of elementary excitations [5], which contradicts the known theorems on nonideal Bose systems [6,7]. The reason for this inconsistency lies in the fact that, in the case of the approximation (11), terms $\sim \sqrt{\varepsilon}$ in expression (3), which give a contribution of the same order as the terms in (11), are not taken into account.

In the approximation (11), the operator A_q is represented in the form of a linear combination

$$A_q \cong \alpha a_q + \beta a^+_{-q}, \tag{13}$$

where the coefficients α and β can be determined from the condition that the averaged commutators with the operators a_q and a^+_{-q} of the left- and right-hand sides of equality (13) coincide. Let us find the coefficients α and β from another principle. For this purpose, starting from (9), we introduce a scalar product of the operators A and B

$$(A, B) = -\langle\langle A \mid B^+\rangle\rangle_{E=0} = \int_{-\infty}^{\infty} \frac{e^{\omega/\theta} - 1}{\omega} J_{AB^+}(\omega)\, d\omega, \tag{14}$$

where $J_{AB^+}(\omega)$ is the spectral intensity [1], and θ is the temperature in energy units.

As is not difficult to verify, the scalar product (14) possesses all the necessary properties. We choose α and β in (13) from the condition that the scalar products of the right- and left-hand sides of the equality with the operators a_q and a^+_{-q} coincide. As a result we shall have

$$A_q + A^+_{-q} \cong \frac{(A_q + A^+_{-q},\, a_q + a^+_{-q})}{(a_q + a^+_{-q},\, a_q + a^+_{-q})}\,(a_q + a^+_{-q}), \tag{15}$$

where we have also used the fact that

$$(A_q + A^+_{-q},\, a_q - a^+_{-q}) \cong 0, \qquad (a_q + a^+_{-q},\, a_q - a^+_{-q}) \cong 0. \tag{16}$$

The approximate expression for the operator $A_q - A^+_{-q}$ is obtained from (15) by replacing the plus signs by minus signs. Thus, the approximation (15) used in the present work is a projection of the operator A_q onto the subspace with the operators $a_q + a^+_{-q}$ and $a_q - a^+_{-q}$, chosen as a basis. Substituting now the approximate expressions (15) into (10), we arrive at a closed system of equations for the functions (1). Solving this system for the Fourier components of the Green functions, we shall have the expressions

$$\langle\langle a_q + a^+_{-q} \mid D^+ \rangle\rangle = \frac{E\langle [a_q + a^+_{-q}, D^+]\rangle + V_q \langle [a_q - a^+_{-q}, D^+]\rangle}{E^2 - V_{qU} q}, \tag{17}$$

$$\langle\langle a_q - a^+_{-q} \mid D^+ \rangle\rangle = -\frac{E\left\langle [a_q - a^+_{-q}, D^+]\right\rangle + U_q \left\langle [a_q + a^+_{-q}, D^+]\right\rangle}{E^2 - V_{qU} q}, \tag{18}$$

where

$$V_q = \frac{q^2}{2m} - \mu + \frac{N}{V}\nu(0) + \frac{\sqrt{\varepsilon}\,(B_q - B^+_{-q}, a_q - a^+_{-q}) + \varepsilon\,(C_q - C^+_{-q}, a_q - a^+_{-q})}{(a_q - a^+_{-q}, a_q - a^+_{-q})}, \tag{19}$$

$$U_q = \frac{q^2}{2m} - \mu + \frac{N_0}{V}\nu(0) + 2\,\frac{N_0}{V}\nu(q) + \frac{\sqrt{\varepsilon}\,(B_q + B^+_{-q}, a_q + a^+_{-q}) + \varepsilon\,(C_q + C^+_{-q}, a_q + a^+_{-q})}{(a_q + a^+_{-q}, a_q + a^+_{-q})}. \tag{20}$$

The spectrum of elementary excitations is determined by the relation

$$E_q = \pm\sqrt{V_{qU} q}. \tag{21}$$

In the zeroth approximation in ε we arrive at the results of Ref. [2]

$$\left(\mu \simeq \frac{N_0}{V}\nu(0), \quad V_q \simeq \frac{q^2}{2m}, \quad U_q = \frac{q^2}{2m} + 2\,\frac{N_0}{V}\nu(q)\right).$$

In this case, putting $D = a_q \pm a^+_{-q}$, we shall have

$$(a_q + a_{-q}^+, a_q + a_{-q}^+) \simeq 2\left(\frac{q^2}{2m} + 2\,\frac{N_0}{V}\nu(0)\right)^{-1}, \qquad (a_q - a_{-q}^+, a_q - a_{-q}^+) \simeq \frac{4m}{q^2}. \tag{22}$$

In the first approximation in ε, in expressions (19) and (20) the scalar products $(C_q \pm C_{-q}^+, a_q \pm a_{-q}^+)$ must be calculated in the zeroth approximation. The result reduces to all possible pairings of the operators entering C_q (see (11)) and, thus, coincides with the result obtained in the Hartree-Fock approximation. The scalar products $(B_q \pm B_{-q}^+, a_q \pm a_{-q}^+)$ we shall calculate in the first nonvanishing approximation. For this we use the approximate equation

$$i\frac{d}{dt}\left\langle\!\left\langle B_q + B_{-q}^+; a_q^+ - a_{-q}\right\rangle\!\right\rangle = -\left\langle\!\left\langle B_q + B_{-q}^+; i\frac{d}{dt'}(a_q^+ - a_{-q})\right\rangle\!\right\rangle \simeq$$

$$\simeq \left(\frac{q^2}{2m} + 2\,\frac{N_0}{V}\nu(q)\right)\left\langle\!\left\langle B_q + B_{-q}^+; a_q^+ + a_{-q}\right\rangle\!\right\rangle + \sqrt{\varepsilon}\,\left\langle\!\left\langle B_q + B_{-q}^+; B_q^+ + B_{-q}\right\rangle\!\right\rangle. \tag{23}$$

Passing to the Fourier components (9), putting $E = 0$ and using (22), from (23) we obtain

$$(B_q + B_{-q}^+, a_q + a_{-q}^+) \simeq -\sqrt{\varepsilon}\left(\frac{q^2}{2m} + 2\,\frac{N_0}{V}\nu(q)\right)^{-1}(B_q + B_{-q}^+, B_q + B_{-q}^+) \simeq$$

$$\simeq -\frac{\sqrt{\varepsilon}}{2}(B_q + B_{-q}^+, B_q + B_{-q}^+)(a_q + a_{-q}^+, a_q + a_{-q}^+). \tag{24}$$

Similarly we find

$$(B_q - B_{-q}^+, a_q - a_{-q}^+) \simeq -\frac{\sqrt{\varepsilon}}{2}(B_q - B_{-q}^+, B_q - B_{-q}^+)(a_q - a_{-q}^+, a_q - a_{-q}^+). \tag{25}$$

Taking as μ expression (7), in the first approximation in ε we shall have

$$V_q = \frac{q^2}{2m^*} - 2\,\frac{\varepsilon}{V}\sum_k \nu(k+q)s_k - \frac{\varepsilon}{2}(B_q - B_{-q}^+, B_q - B_{-q}^+), \tag{26}$$

$$U_q = \frac{q^2}{2m^*} + 2\,\frac{N_0}{V}\nu(q) - \frac{\varepsilon}{2}(B_q + B_{-q}^+, B_q + B_{-q}^+), \tag{27}$$

where the quantity m^* is determined by the relation

$$\frac{q^2}{2m^*} = \frac{q^2}{2m} - \frac{\varepsilon}{V}\sum_k (\nu(k) - \nu(k+q))(n_k + s_k). \tag{28}$$

It remains for us to estimate the scalar products entering the right-hand sides of (26) and (27). According to (4), we have

$$\begin{aligned}(B_q - B^+_{-q}, B_q - B^+_{-q}) = \frac{N_0}{V^2}\sum_{kk'}((v(k) - v(k+q))a^+_k a_{k+q} + \\ + v(k)a_{-k}a_{k+q} - v(k+q)a^+_k a^+_{-k-q}, \\ (v(k') - v(k'+q))a^+_{k'}a_{k'+q} + v(k')a_{-k'}a_{k'+q} \\ - v(k'+q)a^+_{k'}a^+_{-k'-q}).\end{aligned} \tag{29}$$

Let us express all scalar products in the right-hand sides of (29) through $(a^+_k a_{k+q}, a^+_k, a_{k'+q})$. For this purpose we shall use the relations obtained from the corresponding equations for the Green functions in the zeroth approximation at $E = 0$

$$\frac{N_0}{V}(v(k)a_{-k}a_{k+q} - v(k+q)a^+_k a^+_{-k-q}, D) = \\ = -\langle[a^+_k a_{k+q}, D^+]\rangle + (\xi_{k+q} - \xi_k)(a^+_k a_{k+q}, D),$$

$$\begin{aligned}(\xi_{k+q} + \xi_k)(a_{-k}a_{k+q} + a^+_k a^+_{-k-q}, D) = \langle[a_{-k}a_{k+q} - a^+_k a^+_{-k-q}, D^+]\rangle \\ - \frac{N_0}{V}(v(k) + v(k+q))(a^+_k a_{k+q} + a_{-k}a^+_{-k-q}, D),\end{aligned} \tag{30}$$

where

$$\xi_k = \frac{k^2}{2m} + \frac{N_0}{V}v(k).$$

Using (30) and the equations conjugate to them, as a result of simple calculations we arrive at the expression

$$(B_q - B_{-q}^+, B_q - B_{-q}^+) = -\frac{2}{V}\sum_k (v(k) + v(k+q))s_k$$
$$- \frac{2}{V}\sum_k (v(k) - v(k+q))n_k - \frac{q^2}{m}\frac{1}{N_0}\sum_k n_k +$$
$$+ \frac{1}{N_0}\sum_{kk'}\left(\frac{q^2}{2m} + \frac{k\cdot q}{m}\right)\left(\frac{q^2}{2m} + \frac{k'\cdot q}{m}\right)(a_k^+ a_{k+q}, a_{k'}^+ a_{k'+q}). \tag{31}$$

The scalar product $(a_k^+ a_{k+q}, a_{k'}^+ a_{k'+q})$ can be calculated in the random-phase approximation. The quantity $(B_q + B_{-q}^+, B_q + B_{-q}^+)$ is calculated analogously. It is easy to see that the second term in expression (26), as $q \to 0$, cancels the first term in (31). Thus, for $q \to 0$, $U_q \sim q^2$, and there is no gap in the spectrum of elementary excitations (21). The quantity V_q, therefore, has the form $V_q = q^2/2m^{**}$. The expression for U_q may be represented in the form

$$U_q = q^2/2m^{**} + 2(N_0/V)v^*(q).$$

As a result, from (21) we obtain the usual expression for the spectrum of elementary excitations [2] with renormalized mass and potential $v^*(q)$.

For $D = a_q$ we obtain expressions for the one-particle Green functions. Starting from them, in the usual way [1], expressions for n_k and s_k can be constructed.

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