

GREEN FUNCTIONS AND THERMODYNAMIC FUNCTIONS OF A NON-IDEAL BOSE GAS

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The perturbation theory developed in a previous paper is used to calculate the Green function and thermodynamic functions of a low-density Bose gas.

IN this paper we derive an expression for the Green function and thermodynamic functions of a low-density Bose gas with the help of a method developed in a previous paper^[1] by L. D. Faddeev and the author (subsequently referred to as I). The formulae we obtain are valid for temperatures of the order of, but not too close to, the phase transition temperature. (The method is also applicable at lower temperatures, but in this case the formulae will be different from those obtained below).

1. FIRST APPROXIMATION FOR THE GREEN FUNCTION

We assume the following conditions satisfied:¹⁾

$$\theta \equiv \rho^{1/3} \max(t_0, a) \ll 1, \quad \rho^{2/3} \sim T, \quad (1.1)$$

Where $\rho = N/V$ is the density, t_0 the two-particle t-matrix for scattering at zero energy, a the range of the potential and θ a small dimensionless parameter.

In (1.1) the first condition is the usual one for the gas approximation; the second indicates the range of temperature in which we shall be interested. Connected with these conditions we have three characteristic momenta:

$$k_\alpha = \rho^{1/2} \max(t_0^{1/2}, a^{1/2}), \quad k_\beta = T^{1/2} \sim \rho^{1/3},$$

$$k_\gamma = \min(a^{-1}, t_0^{-1}), \quad (1.2)$$

with relative order of magnitude:

$$k_\alpha \sim \theta^{1/2} k_\gamma \ll k_\beta \sim \theta k_\gamma \ll k_\gamma. \quad (1.3)$$

It is natural to call k_α the correlation momentum (for $k \sim k_\alpha$ the energy spectrum is substantially different from that of an ideal gas), k_β the thermal momentum (k_β^{-1} is the thermal wavelength, which by virtue of the condition $T^{1/2} \sim \rho^{1/3}$ is comparable to the inter-particle spacing), and k_γ the

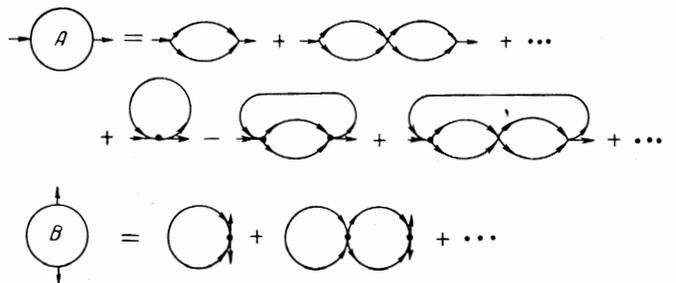
momentum characterizing the scattering in the interparticle potential.

Let us now consider the self-energy parts $A(p)$, $B(p)$ of the one-particle Green function (1.3). We notice that the contribution of a particular graph to A or B will be reduced if either of the following factors are included in it:

1) Anomalous elements (third-order vertices or the propagators G_{10} , G_{20} (see the Table in I)); these contain factors α or α^2 which tend to reduce the contribution of the graph (since α^2 , the condensate density, cannot exceed ρ).

2) Closed loops of normal propagators G_0 (those loops in which we can follow the direction of the arrows right around the loop); these reduce the contribution of the graph because the frequency summation introduces a factor $(e^{\beta\epsilon k} - 1)^{-1}$, which cuts off the momentum sum in the region $k \sim k_\beta$, while the cut-off due to the potential takes place at $k \sim k_\gamma \gg k_\beta$.

Thus the principal series of diagrams for $A(p)$ and $B(p)$ is composed of the following (see the figure):



a) All diagrams with two third-order vertices but no other anomalous elements and no loops of the type described in (2) above; these diagrams contribute to $A(p)$;

b) all diagrams with one anomalous propagator but no other anomalous elements or loops; these contribute to $B(p)$;

¹⁾We use a system of units in which $\hbar = k = 2m = 1$, where \hbar is Planck's constant, k Boltzmann's constant and m the mass of the particles.

c) all diagrams with one loop but no anomalous elements; these contribute to $A(p)$.

The contributions of the graphs described cannot be greater in order of magnitude than $k_\alpha^2 \sim \theta^3 k_\gamma^2$. It can be shown that the most important of the graphs we have neglected contribute to order $t_0 k_\alpha T \sim k_\gamma^2 \theta^{1/2}$. Thus we need sum only the principal series, the error so introduced being of order $k_\gamma^2 \theta^{1/2} / k_\gamma^2 \theta^3 = \theta^{1/2}$. The result of this summation (after neglecting terms of the same or higher order than those already dropped) can be expressed in terms of the two-particle t -matrix defined by the equation

$$t(\mathbf{k}_1, \mathbf{k}_2; z) = u(\mathbf{k}_1 - \mathbf{k}_2) - (V)^{-1} \sum_{\mathbf{k}_3} u(\mathbf{k}_1 - \mathbf{k}_3) (2k_3^2 - z) t(\mathbf{k}_3, \mathbf{k}_2; z), \quad (1.4)$$

and has the form

$$f_{\mathbf{k}} + A(p) = k^2 - \lambda + [\alpha^2 + (4\pi)^{-3/2} \zeta(3/2) T^{3/2}] [t(\mathbf{k}/2, \mathbf{k}/2; i\omega_n - k^2/2) + t(\mathbf{k}/2, -\mathbf{k}/2; i\omega_n - k^2/2)],$$

$$h_{\mathbf{k}} + B(p) = \alpha^2 t(\mathbf{k}, 0; 0) \quad (1.5)$$

where $\zeta(s)$ is the Riemann ζ function. Substituting (1.5) in (1.5) we obtain the nontrivial solution for α^2 :

$$\alpha^2 = \lambda / t_0 - 2(4\pi)^{-3/2} \zeta(3/2) T^{3/2} \equiv \Lambda / t_0, \quad (1.6)$$

This is valid for $\Lambda > 0$, since for a repulsive potential $t_0 \equiv t(0, 0, 0) > 0$.

If $\Lambda < 0$, Eq. (1.5) has only the trivial solution $\alpha = 0$; in this case $h_{\mathbf{k}} + B(p) \equiv 0$, while for the quantity $f_{\mathbf{k}} + A(p)$ we have

$$f_{\mathbf{k}} + A(p) = k^2 - \lambda + (4\pi)^{-3/2} \zeta(3/2) T^{3/2} [t(\mathbf{k}/2, \mathbf{k}/2; i\omega_n - k^2/2) + t(\mathbf{k}/2, -\mathbf{k}/2; i\omega_n - k^2/2)]. \quad (1.7)$$

The equation $\Lambda = 0$ defines the first approximation to the phase transition curve in the (λ, T) plane. The Green functions and the quasi-particle energy spectrum defined by its poles are given for small momenta ($k \ll k_\gamma$) by the formulae:

$$\begin{aligned} \tilde{G}(\mathbf{k}, \omega_n) &= (i\omega_n + k^2 + \Lambda) / ((i\omega_n)^2 - k^4 - 2\Lambda k^2), \\ E(\mathbf{k}) &= (k^4 + 2\Lambda k^2)^{1/2}, \quad \Lambda > 0; \\ \tilde{G}(\mathbf{k}, \omega_n) &= (i\omega_n - k^2 + |\Lambda|)^{-1}, \\ E(\mathbf{k}) &= k^2 + |\Lambda|, \quad \Lambda < 0. \end{aligned} \quad (1.8)$$

Near the transition point, where Λ is small, the dropped terms of order $t_0 k_\alpha T$ may have an important effect. Hence the expressions for the

Green functions, and the thermodynamic formulae derived from them, are correct only so long as $|\Lambda| > t_0 k_\alpha T$.

2. THE THERMODYNAMIC POTENTIAL $\Omega = -pV$

To obtain the thermodynamic functions we start from the formula

$$E - \frac{\lambda}{2} N = -\frac{T}{2} \sum_{\mathbf{k}, \omega_n} e^{i\omega_n \epsilon} [(i\omega_n + k^2) \tilde{G}(\mathbf{k}, \omega_n) - 1] \equiv Vf(\lambda, T), \quad (2.1)$$

where $\epsilon \rightarrow +0$, and N, E are the mean values respectively of the number of particles and the energy. (Notice that the replacement of G by \tilde{G} is of no importance in view of the factor $i\omega_n + k^2$.) Using standard thermodynamic relations for the quantity $E - (\lambda/2)N$, we can rewrite (2.1) as an equation for the pressure $p = -\Omega/V$:

$$p - T \frac{\partial p}{\partial T} - \frac{\lambda}{2} \frac{\partial p}{\partial \lambda} = -f(\lambda, T). \quad (2.2)$$

The solution of (2.2) has the form:

$$p = \lambda^2 / 2t_0 + 2\lambda^2 \int_0^\lambda f(\mu, \mu^2 T / \lambda^2) \mu^{-3} d\mu \quad (2.3)$$

as will now be demonstrated.

The values of $f(\lambda, T)$ used in the integral in (2.3) fall on the curve $\lambda^2/T = \text{const.}$; the lower end of this curve corresponds to low temperatures and densities. The right-hand side of (2.3) obeys Eq. (2.2), and the quantity obtained by dividing it by λ^2 and letting $\lambda \rightarrow 0$ with $\lambda^2/T = \text{const.}$ has the limit $(2t_0)^{-1}$. The left-hand side has the same properties, since it is easy to prove that when λ and T tend to zero in this fashion p has its asymptotic form for $T = 0$ and low density, viz. $\lambda^2/2t_0$.

Thus, formula (2.3) is proved. It is exact, and has the advantage over the usual method of deriving $p = -\Omega/V$ (namely integration over the coupling constant) that the integration is over ensemble parameters which can be varied experimentally. If the curve intersects the phase transition curve, we must remember that $f(\lambda, T)$ is given by different formulae on opposite sides of the intersection. At the transition point all terms of the perturbation series for $\tilde{G}(p)$ either vanish or go over smoothly into the corresponding terms of ordinary perturbation theory. Obviously therefore the Green function itself, and hence $f(\lambda, T)$ are continuous at the transition point. The pressure is expressed, by (2.3), as an integral of a continuous function and hence is itself continuous

along with its first derivatives. Discontinuities or infinities can occur only in the second derivatives, so that we have a second-order transition.

To calculate $f(\lambda, T)$ in explicit form we note that the principal contribution to the sum over momenta comes from the region $k \sim k_\beta$, where to a first approximation we can treat the corrections $A(p)$ and $B(p)$ as constant. Using this fact, we obtain the following formula for the condensed state:

$$\begin{aligned} f_c(\lambda, T) &= \\ & - T(2V)^{-1} \sum_{\mathbf{k}, n} e^{i\omega_n \varepsilon} \left[\frac{(i\omega_n + k^2)(i\omega_n + k^2 + \Lambda)}{(i\omega_n)^2 - k^4 - 2\Lambda k^2} - 1 \right] \\ & = \frac{3}{2}(4\pi)^{-3/2} \zeta(5/2) T^{5/2} - (4\pi)^{-3/2} \zeta(3/2) \Lambda T^{3/2} + O(T\Lambda^{3/2}) \end{aligned} \quad (2.4)$$

and for the normal state:

$$\begin{aligned} f_n(\lambda, T) &= \\ & - T(2V)^{-1} \sum_{\mathbf{k}, n} e^{i\omega_n \varepsilon} [(i\omega_n + k^2)/(i\omega_n - k^2 + \Lambda) - 1] \\ & = \frac{3}{2}(4\pi)^{-3/2} \zeta(5/2) T^{5/2} + (4\pi)^{-3/2} \zeta(3/2) \Lambda T^{3/2} \\ & + O(T|\Lambda|^{3/2}), \end{aligned} \quad (2.5)$$

We can write these as one equation:

$$\begin{aligned} f(\lambda, T) &= \frac{3}{2}(4\pi)^{-3/2} \zeta(5/2) T^{5/2} \\ & - (4\pi)^{-3/2} \zeta(3/2) |\Lambda| T^{3/2} + O(T|\Lambda|^{3/2}). \end{aligned} \quad (2.6)$$

Hence, from (2.3), the pressure is:

$$\begin{aligned} p_c &= (4\pi)^{-3/2} \zeta(5/2) T^{5/2} + \lambda^2 / 2t_0 - (4\pi)^{-3/2} \zeta(3/2) \lambda T^{3/2} \\ & + (4\pi)^{-3} \zeta^2(3/2) t_0 T^3 + O(T\Lambda^{3/2}), \\ p_n &= (4\pi)^{-3/2} \zeta(5/2) T^{5/2} + (4\pi)^{-3/2} \zeta(3/2) \lambda T^{3/2} \\ & - (4\pi)^{-3} \zeta^2(3/2) t_0 T^3 + O(T|\Lambda|^{3/2}). \end{aligned} \quad (2.7)$$

Here the first term is the important one, while all the rest are of the same order, namely of order $t_0 T^{1/2} \sim \theta \ll 1$ relative to the principal one.

We can actually improve the accuracy of the formulae (2.7) by finding the density with high precision and thence recalculating the pressure from the relation $\rho = (\partial p / \partial \lambda)_T$. The density of uncondensed particles is given by the formula

$$\rho_1 = N_1/V = -TV^{-1} \sum_{\mathbf{k}, n} e^{i\omega_n \varepsilon} \mathcal{G}(\mathbf{k}, \omega_n). \quad (2.8)$$

In the normal state the density follows directly from this expression:

$$\rho_n = (4\pi)^{-3/2} \zeta(3/2) T^{3/2} - (4\pi)^{-1} T |\Lambda|^{1/2}, \quad (2.9)$$

where the first term is the value obtained from p_n in (2.7) by differentiation with respect to λ . The remaining term therefore gives a correction to the

pressure:

$$\Delta p_n = (6\pi)^{-1} T |\Lambda|^{3/2}. \quad (2.10)$$

In the condensed state (2.8) gives:

$$\rho_{1c} = (4\pi)^{-3/2} \zeta(3/2) T^{3/2} - (8\pi)^{-1} T (2\Lambda)^{1/2}. \quad (2.11)$$

By considering the equation $\gamma + \Gamma = 0$ in I in detail we can also obtain a very accurate value for α^2 . Here we give only the result:

$$\begin{aligned} \alpha^2 = \rho_0 = \lambda / t_0 &- 2(4\pi)^{-3/2} \zeta(3/2) T^{3/2} \\ & + (3/8\pi) T (2\Lambda)^{1/2}, \end{aligned} \quad (2.12)$$

$$\begin{aligned} \rho_c = \rho_0 + \rho_{1c} = \lambda / t_0 &- (4\pi)^{-3/2} \zeta(3/2) T^{3/2} \\ & + (4\pi)^{-1} T (2\Lambda)^{1/2}, \end{aligned} \quad (2.13)$$

$$\Delta p_c = (12\pi)^{-1} T (2\Lambda)^{1/2}. \quad (2.14)$$

For a Bose system of hard spheres, (2.7) agrees with the results of Lee and Yang,^[2] derived by a pseudopotential method. To make the comparison, we have to put $t_0 = 8\pi a$ and eliminate the chemical potential λ so as to express the answer in terms of the density.

3. VARIOUS THERMODYNAMIC FUNCTIONS

1. The fundamental function p and its first derivatives—the number of particles and entropy per unit volume—are, as we have seen, continuous at the transition point; hence the energy per unit volume E/V , which is equal to $-p + T \partial p / \partial T + \lambda \partial p / \partial \lambda$, is also continuous.

2. To investigate the behavior of the density ρ with temperature at constant pressure we consider $(\partial \rho / \partial T)_p$

$$\begin{aligned} (\partial \rho_c / \partial T)_p &= -\frac{5}{2} (4\pi)^{-3/2} \zeta(5/2) t_0^{-1} T^{5/2} \rho^{-1} \\ & \times [1 + (4\pi)^{-1} t_0 T (2\Lambda)^{-1/2}] < 0, \\ (\partial \rho_n / \partial T)_p &= -\frac{5}{16\pi} \zeta\left(\frac{5}{2}\right) \zeta^{-1}\left(\frac{3}{2}\right) T |\Lambda|^{-1/2} < 0. \end{aligned} \quad (3.1)$$

The density decreases with increasing temperature. If we extrapolate Eqs. (3.1) to the neighborhood of the transition point, we find that the curve $\rho(T)$ has a kink at this point, with a vertical tangent. This qualitative result apparently remains true even though the actual behavior of the functions in the neighborhood of the transition point may not be well described by (3.1).

3. The specific heat at constant pressure $C_p = T[\partial(S/m\rho)/\partial T]_p$ increases as the transition point is approached, as we see from the formulae

$$\begin{aligned} (C_p)_c &= \frac{25}{2} (4\pi)^{-3} \zeta^2(5/2) t_0^{-1} T^4 \rho^{-3} [1 + (4\pi)^{-1} t_0 T (2\Lambda)^{-1/2}], \\ (C_p)_n &= \frac{25}{4} (4\pi)^{1/2} \zeta^2(5/2) \zeta^{-3}(3/2) T^{1/2} |\Lambda|^{-1/2}, \end{aligned} \quad (3.2)$$

The curve $C_p(T)$ is asymmetric with respect to the transition temperature T_0 , the specific heat being larger at the point $T_0 - \Delta T$ than at $T_0 + \Delta T$.

4. For the speed of sound in the normal state, $u = [(\partial p / \partial(m\rho))_{S/\rho}]^{1/2}$, we find

$$u_n = [^{10/3}\zeta^{(5/2)}\zeta^{-1(3/2)}T]^{1/2}. \quad (3.3)$$

In the condensed state waves of two different types can be propagated; their velocities are given by the standard equation^[3]

$$u^4 - u^2 \left(\frac{TS^2\rho_s}{C_V\rho_n} + \left(\frac{\partial p}{\partial\rho} \right)_S \right) + \left(\frac{\partial p}{\partial\rho} \right)_T \frac{TS^2\rho_s}{C_V\rho_n} = 0,$$

where S and C_V refer to unit mass, $\rho = M/V$ is the total mass density and ρ_s/ρ_n is the ratio of the superfluid and normal densities. In our case $\rho_s = m\alpha^2$, $\rho_n = m(\rho - \alpha^2)$ (on the right-hand side here $\rho = N/V$); the other quantities appearing in the equation may easily be calculated. The result is

$$u_1 = (^{10/3}\zeta^{(5/2)}\zeta^{-1(3/2)}T)^{1/2}, \quad u_2 = (2\Lambda)^{1/2}. \quad (3.4)$$

We see that the velocity of first sound u_1 is given by the same expression before and after the transition, while the velocity of second sound u_2 coincides with the "microscopic" velocity obtained from the energy spectrum (1.8). In our case the ratio u_2/u_1 is small (of order $\theta^{1/2}$).

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