# AN APPROACH TO THE THEORY OF THE LOW-TEMPERATURE BOSE GAS

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A perturbation theory is developed for the calculation of the one-particle Green function of a Bose gas below the temperature of the phase transition associated with the appearance of a condensate. It is shown that the one-particle excitation spectrum has a phonon character.

THE properties of a Bose gas at zero temperature were first clarified from a microscopic point of view by Bogolyubov.[1] Starting from the physical notion of the existence of a macroscopically occupied level (condensate) he proposed the replacement of the creation and annihilation operators referring to this level by c-numbers proportional to the total number of particles in the system. Much later, a consistent perturbation-theory treatment based on this idea was developed by Belyaev[2] and also by Hugenholtz and Pines[3]. Recently Bogolyubov has put forward a new argument to support his method and its finite-temperature generalization, based on the plausible general principle of the extinction of correlations[4]. The Bogolyubov substitution evidently gives an exact result in the thermodynamic limit $N \to \infty$, $V \to \infty$, $N/V = \text{const}$; however, a number of authors[5] have cast doubt on the exactness of this approach.

In this paper we suggest an approach to the theory of the Bose gas which we believe to be more rigorous and at the same time simpler conceptually. The method allows us to consider the case of arbitrary temperature, so that in our formalism the phase transition associated with the vanishing of the condensate occurs in a natural way.

We briefly outline the logic of our approach. Like all the authors mentioned, we start from the fact that the existence of a condensate at low temperatures precludes the application of ordinary perturbation theory, in which the unperturbed Hamiltonian is that of noninteracting particles. This is expressed formally by the fact that if we decrease the temperature at fixed density nonphysical singularities appear in the Green function as calculated by ordinary perturbation theory. One way out of this difficulty is to develop a perturbation theory which starts out from a different unperturbed Hamiltonian; this operator must of course be exactly diagonalizable, which in practice means it must be quadratic in the annihilation and creation operators. The simplest way to obtain such a quadratic form (other then the Hamiltonian of noninteracting particles) is to carry out some canonical transformation. Our approach is based on doing just that; we perform a simple, specific canonical transformation. Its form is described in Sec. 1, where we also develop our graphical perturbation theory. In Sec. 2 we discuss the general consequences of the formalism developed; in particular we illustrate how the phase transition shows up as the point where the canonical transformation degenerates into the identity transformation and our perturbation theory goes over into the usual one.

## 1. GENERAL FORMALISM

We shall use a grand canonical ensemble and, accordingly, work with the generalized Hamiltonian (we set $\hbar = 1$, $m = 1/2$)

$$H' = H - \lambda N = \sum_{\mathbf{k}} (k^2 - \lambda) c_{\mathbf{k}}^+ c_{\mathbf{k}} + \frac{1}{4V} \times \sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4} (u_{\mathbf{k}_1-\mathbf{k}_3} + u_{\mathbf{k}_1-\mathbf{k}_4}) c_{\mathbf{k}_1}^+ c_{\mathbf{k}_2}^+ c_{\mathbf{k}_3} c_{\mathbf{k}_4}.$$

Here $V = L^3$ is the volume of the system, and the summation is taken over all points $\mathbf{k}$ of a lattice with cell volume $(2\pi/L)^3$. The potential $u_{\mathbf{k}}$ is assumed to be short-ranged and repulsive.

We shall be interested in the temperature Green function

$$G(\mathbf{k};\, \tau - \tau') = -\langle T c_{\mathbf{k}}(\tau) c_{\mathbf{k}}(\tau') \rangle,$$

where

$$c_{\mathbf{k}}(\tau) = \exp\{H'\tau\} c_{\mathbf{k}} \exp\{-H'\tau\}$$

and $\langle A \rangle$ denotes the average of the operator $A$ taken over a grand canonical ensemble:

$$\langle A \rangle = \mathrm{Sp}\,[\exp\{-\beta(H - \lambda N)\} A] \,/\, \mathrm{Sp}\,[\exp\{-\beta(H - \lambda N)\}].$$

Thus, $\langle A \rangle$ is a function of the parameters $\beta$ and $\lambda$.

The canonical transformation mentioned in the Introduction has the form

$$c_{\mathbf{k}} = a_{\mathbf{k}} + \delta_{\mathbf{k}0}\alpha V^{1/2}, \qquad c_{\mathbf{k}}^{+} = a_{\mathbf{k}}^{+} + \delta_{\mathbf{k}0}\alpha V^{1/2}. \tag{1}$$

Here $\delta_{\mathbf{kk}'}$ is the Kronecker $\delta$-function, and $\alpha$ is a real number which for the present we regard as arbitrary. In terms of the new variables the operator $H'$ has the following form:

$$H' = C_0 + \gamma(a_0 + a_0^{+}) + \sum_{\mathbf{k}} f_{\mathbf{k}} a_{\mathbf{k}}^{+} a_{\mathbf{k}} + {}^1/_2 \sum_{\mathbf{k}} h_{\mathbf{k}} (a_{\mathbf{k}} a_{-\mathbf{k}} + a_{\mathbf{k}}^{+} a_{-\mathbf{k}}^{+})$$

$$+ \frac{\alpha}{2V^{1/2}} \sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3} (u_{\mathbf{k}_1} + u_{\mathbf{k}_2})(a_{\mathbf{k}_1}^{+} a_{\mathbf{k}_2}^{+} a_{\mathbf{k}_3} + a_{\mathbf{k}_3}^{+} a_{\mathbf{k}_2} a_{\mathbf{k}_1})$$

$$+ \frac{1}{4V} \sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4} (u_{\mathbf{k}_1-\mathbf{k}_3} + u_{\mathbf{k}_1-\mathbf{k}_4}) a_{\mathbf{k}_1}^{+} a_{\mathbf{k}_2}^{+} a_{\mathbf{k}_3} a_{\mathbf{k}_4};$$

$$C_0 = V(-\lambda\alpha^2 + {}^1/_2 u_0 \alpha^4), \qquad \gamma = V^{1/2}\alpha(-\lambda + u_0\alpha^2),$$

$$f_{\mathbf{k}} = k^2 - \lambda + (u_{\mathbf{k}} + u_0)\alpha^2, \qquad h_{\mathbf{k}} = u_{\mathbf{k}}\alpha^2.$$

We now consider the Green function

$$\tilde{G}(\mathbf{k}; \tau - \tau') = -\langle T a_{\mathbf{k}}(\tau) a_{\mathbf{k}}^{+}(\tau') \rangle,$$

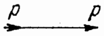
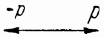
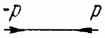
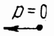
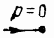
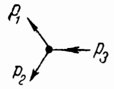
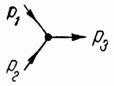
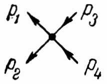
where $a_{\mathbf{k}}(\tau)$ is defined analogously to $c_{\mathbf{k}}(\tau)$; we shall develop for this quantity a perturbation theory which takes as unperturbed Hamiltonian the set of all terms in $H'$ which are quadratic in the operators $a_{\mathbf{k}}$, $a_{\mathbf{k}}^{+}$. As usual, it is most convenient to work with the Fourier components of the Green function, defined by

$$\tilde{G}(\mathbf{k}, \omega_n) = \frac{1}{2} \int_{-\beta}^{\beta} \tilde{G}(\mathbf{k}, \tau) e^{i\omega_n \tau} d\tau, \qquad \omega_n = 2\pi n/\beta.$$

From now on we denote the set of variables $\mathbf{k}$, $\omega_n$ by the single letter $p$.

The perturbation series can be represented in terms of diagrams composed of the elements listed in the table, where we also give the expressions corresponding to them (we have used the notation $\epsilon_{\mathbf{k}}^2 = f_{\mathbf{k}}^2 - h_{\mathbf{k}}^2$). As a consequence of the fact that the unperturbed Hamiltonian is not diagonal, we have to deal with three types of line; there are also vertices of five different types, corresponding to the structure of the perturbation operator.

The Green function $\tilde{G}(p)$ is composed of all diagrams with one incoming and one outgoing line which do not contain any completely unlinked parts (that is, parts unlinked even to one of the external lines). We get the expression corresponding to any such diagram by writing down the product of the expressions for each element composing it, taking into account the conservation of momentum and frequency at each vertex, summing over each independent momentum and frequency and multiplying the result by $R^{-1}(-\beta)^{v+1-l}$, where $v$ is the number of vertices, $l$ the number of lines, and R the order of the symmetry group of the diagram.

| Diagram element | Notation | Contribution |
|---|---|---|
|  | $G_0(p)$ | $(i\omega_n + f_{\kappa})/[(i\omega_n)^2 - \varepsilon_{\kappa}^2]$ |
|  | $G_{10}(p)$ | $-h_{\kappa}/[(i\omega_n)^2 - \varepsilon_{\kappa}^2]$ |
|  | $G_{20}(p)$ | $-h_{\kappa}/[(i\omega_n)^2 - \varepsilon_{\kappa}^2]$ |
|  | $V_{10}$ | $\gamma$ |
|  | $V_{01}$ | $\gamma$ |
|  | $V_{21}(p_1, p_2)$ | $V^{-1/2}\alpha(u_{\kappa_1} + u_{\kappa_2})$ |
|  | $V_{12}(p_1, p_2)$ | $V^{-1/2}\alpha(u_{\kappa_1} + u_{\kappa_2})$ |
|  | $V_{22}(p_1, p_2, p_3, p_4)$ | $V^{-1}(u_{\kappa_1-\kappa_3} + u_{\kappa_1-\kappa_4})$ |

Among the diagrams composed of the elements listed are some which contain parts without external lines, linked to the rest of the diagram by a single line; the latter must have frequency $\omega_n = 0$ and momentum $k = 0$. We shall call such parts zero-momentum insertions; some examples of such insertions are given in Fig. 1.

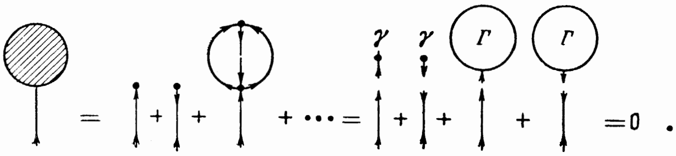


FIG. 1

We now take advantage of the arbitrariness of the constant $\alpha$ and demand that the sum of all zero-momentum insertions vanish (the diagrammatic expression for this sum is given in Fig. 1). This condition is equivalent to the requirements

$$\langle a_0(\tau) \rangle = \langle a_0 \rangle = 0, \qquad \langle a_0^{+}(\tau) \rangle = \langle a_0^{+} \rangle = 0,$$

so that when it is fulfilled $\alpha V^{1/2}$ is to be interpreted as the expectation value of the operators $c_0$ and $c_0^{+}$:

$$\langle c_0 \rangle = \langle c_0^{+} \rangle = \alpha V^{1/2}$$

and the connection between $G(p)$ and $\tilde{G}(p)$ has a particularly simple form:

$$G(p) = -\beta\delta_{p0}\alpha^2 V + \tilde{G}(p). \tag{2}$$

The precise formulation of the condition is discussed in the next section; here we merely point out that if it is fulfilled, it is sufficient when calculating any Green function to consider only diagrams without zero-momentum insertions.

To conclude this section we write down the expression for $\tilde{G}(p)$ in terms of the irreducible self-energy parts (cf. Fig. 2):

$$\tilde{G}(p) = \frac{i\omega_n + f_{\mathbf{k}} + A(-p)}{(i\omega_n + f_{\mathbf{k}} + A(-p))(i\omega_n - f_{\mathbf{k}} - A(p)) + (h_{\mathbf{k}} + B(p))^2}. \tag{3}$$

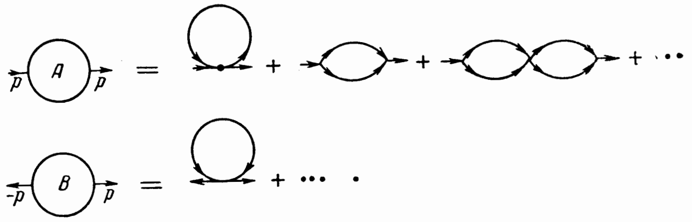


FIG. 2

## 2. DISCUSSION OF THE FORMALISM

1. We now discuss the precise formulation of the condition leading to the choice of the parameter $\alpha$. If we denote by $\Gamma$ the sum of the contributions of all diagrams with a single ingoing or outgoing arrow, we can write our condition in the form of an algebraic relation:

$$(G_0(0) + G_{10}(0))(\gamma + \Gamma) = 0.$$

The first factor in this expression is non-zero; for the second we have, as shown in the Appendix:

$$\gamma + \Gamma = \alpha V^{1/2}(f_0 + A_0 - h_0 - B_0), \tag{4}$$

so that we arrive at the equation

$$\alpha(f_0 + A_0 - h_0 - B_0) = 0. \tag{5}$$

This equation has the trivial solution $\alpha = 0$; it may also have a nontrivial solution if the second factor is zero. Detailed perturbation-theory calculations show that at sufficiently low temperatures the nontrivial solution does indeed exist; thus we must choose for the Green function the expression corresponding to this nontrivial solution. As the temperature is raised the nontrivial solution disappears, and then we must use for the Green function the expression obtained by ordinary perturbation theory.

2. It follows from expression (2) for the Green function $G(p)$ that $\alpha^2$ can be interpreted as the density of zero-momentum particles, i.e., the density of the condensate. It then follows from the above considerations that at sufficiently low temperatures the condensate does indeed exist. The temperature at which the nontrivial solution of Eq. (5) disappears is the temperature of the phase transition associated with the vanishing of the condensate; at this temperature our perturbation theory goes over into the usual one.

We note that the condition that there should exist a nontrivial solution to Eq. (5) is also the condition for the one-particle excitation spectrum to have a phonon character. In fact, it follows from (3) that if the second factor in (5) vanishes, then the denominator of the Green function $\tilde{G}(p)$ also vanishes, so that the point $\mathbf{k} = 0$, $\omega_n = 0$ is a pole of the Green function. Above the transition temperature the spectrum no longer has a phonon character.

3. To illustrate the general assertions made above we shall write out explicitly the result of summing a particular infinite series of diagrams for the self-energy parts: we carry out the ladder sum over all four-line vertices in the diagrams shown in Fig. 2. The result has the form:

$$f_{\mathbf{k}} + A_0 = k^2 - \lambda + 2\alpha^2 t_0 + 2t_0(4\pi\beta)^{-3/2}\zeta(3/2),$$
$$h_{\mathbf{k}} + B_0 = \alpha^2 t_0,$$

where $\zeta(s)$ is the Riemann $\zeta$-function, $t_0 = 8\pi f$ and f is the zero-energy scattering amplitude. The nontrivial solution of (5) has the form

$$\rho_0 = \alpha^2 = \lambda / t_0 - 2(4\pi\beta)^{-3/2}\zeta(3/2) \equiv \Lambda / t_0$$

and exists only for positive $\Lambda$.

The Green functions $\tilde{G}(p)$ and $\tilde{G}_n(p)$ corresponding respectively to the nontrivial and trivial solutions are given for small $\mathbf{k}$ and $\omega_n$ by the expressions

$$\tilde{G}(p) = \frac{i\omega_n + k^2 + \Lambda}{(i\omega_n)^2 - k^4 - 2\Lambda k^2}, \quad \tilde{G}_n(p) = [i\omega_n - k^2 + \Lambda]^{-1}.$$

We must choose the first expression for $\Lambda$ positive, the second for $\Lambda$ negative. For $\Lambda = 0$ the expressions for $\tilde{G}(p)$ and $\tilde{G}_n(p)$ coincide: the curve $\Lambda = 0$ gives the phase transition line in the $(\lambda, \beta)$ plane. Thus, these results confirm our assertion that we must choose the nontrivial solution if it exists.

The formulae given here are evidently exact in the low-density limit. We shall discuss them in more detail, and use them to derive the thermodynamic formulae in a separate paper.

4. Our choice of the constant $\alpha$ in the canonical transformation is not the only possible one. Calculation with an arbitrary $\alpha \neq 0$ leads to exactly the same expression for the Green function $G(p)$, if we use the fact that

$$G(p) = \tilde{G}(p) - \beta V\alpha^2\delta_{p0} - 2\beta V^{1/2}\alpha\langle a_0\rangle\delta_{p0}.$$

However, our choice of $\alpha$ simplifies the structure of the diagrams.

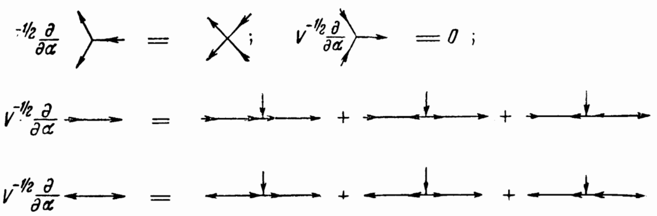


FIG. 3

We can actually use canonical transformations more general than (1), e.g.,

$$c_{\mathbf{k}} = \xi_{\mathbf{k}} a_{\mathbf{k}} + \eta_{\mathbf{k}} a_{-\mathbf{k}}^{+} + \delta_{\mathbf{k}0}\alpha V^{1/2},$$

$$c_{\mathbf{k}}^{+} = \xi_{\mathbf{k}} a_{\mathbf{k}}^{+} + \eta_{\mathbf{k}} a_{-\mathbf{k}} + \delta_{\mathbf{k}0}\alpha V^{1/2},$$

where $\xi_{\mathbf{k}}$ and $\eta_{\mathbf{k}}$ are real functions subject to the condition $\xi_{\mathbf{k}}^2 - \eta_{\mathbf{k}}^2 = 1$. One possible way of fixing $\xi_{\mathbf{k}}$ and $\eta_{\mathbf{k}}$ is to demand that the transformed Hamiltonian contain no nondiagonal quadratic terms of the type $a_{\mathbf{k}}a_{-\mathbf{k}}$ and $a_{\mathbf{k}}^{+}a_{-\mathbf{k}}^{+}$; the most natural approach is based on the condition that averages of the type $\langle a_{\mathbf{k}}a_{-\mathbf{k}}\rangle$ and $\langle a_{\mathbf{k}}^{+}a_{-\mathbf{k}}^{+}\rangle$ should vanish. In diagrammatic terms, this condition consists in the vanishing of the contribution to B(p) from those diagrams in which the outgoing lines enter the same four-line vertex. If in enforcing this condition we restrict ourselves to first-order diagrams, we arrive at a variant of the theory proposed by Tolmachev[6].

## APPENDIX

We shall prove (4) with the help of a variant of an auxiliary construction frequently encountered in the literature. Consider a canonical transformation slightly more general than (1), viz.:

$$c_{\mathbf{k}} = a_{\mathbf{k}} + \delta_{\mathbf{k}0}\alpha V^{1/2}, \qquad c_{\mathbf{k}}^{+} = a_{\mathbf{k}}^{+} + \delta_{\mathbf{k}0}\bar{\alpha} V^{1/2},$$

where $\alpha$ is now a complex number and $\bar{\alpha}$ its complex conjugate. The only ways in which the transformed Hamiltonian and the corresponding vertices and lines differ from their form for real $\alpha$ are: in the diagonal quantities $C_0$, $G_0(p)$ and $f_k$ the quantity $\alpha^2$ is replaced by $|\alpha|^2$; the nondiagonal quantities $G_{10}(p)$, $V_{10}$, and $V_{21}$ contain $\alpha$, while $G_{20}$, $V_{01}$ and $V_{12}$ are obtained by complex conjugation.

We note that differentiation with respect to $\alpha V^{1/2}$ (or $\bar{\alpha}V^{1/2}$) of any diagram element apart from vertices of the type $V_{01}$, $V_{10}$ leads to the affixing to the element of an incoming or outgoing arrow with p = 0 (cf. the examples in Fig. 3). In view of our complementary condition the diagrams do not contain $V_{01}$ or $V_{10}$. Hence, differentiation of an arbitrary diagram with respect to $\alpha V^{1/2}$ (or $\bar{\alpha}V^{1/2}$) leads to the affixing to it of an incoming or outgoing arrow in all possible ways.

Consider the thermodynamic potential $\Omega$. Contributions to it arise from the constant $C_0$, the thermodynamic potential $\Omega_0$ corresponding to the quadratic terms in H′, and the sum of all linked vacuum diagrams. Let us associate with the second term a diagram composed of a single closed loop without vertices. Then by direct comparison of the diagrams for the left and right sides we can verify the validity of the relations

$$\gamma + \Gamma = \frac{\partial(\Omega/V^{1/2})}{\partial\alpha}\bigg|_{\alpha=\alpha}, \qquad f_0 + A_0 = \frac{\partial^2(\Omega/V)}{\partial\alpha\partial\bar{\alpha}}\bigg|_{\alpha=\bar{\alpha}},$$

$$h_0 + B_0 = \frac{\partial^2(\Omega/V)}{\partial\alpha^2}\bigg|_{\alpha=\bar{\alpha}}.$$

It is easy to verify that $\Omega$ depends on $\alpha$ and $\bar{\alpha}$ only through the product $\alpha\bar{\alpha} = z$. Hence the above relation can be rewritten

$$\gamma + \Gamma = \alpha\frac{\partial(\Omega/V^{1/2})}{\partial z}, \qquad f_0 + A_0 = \frac{\partial(\Omega/V)}{\partial z} + z\frac{\partial^2(\Omega/V)}{\partial z^2},$$

$$h_0 + B_0 = z\frac{\partial^2(\Omega/V)}{\partial z^2}$$

whence (4) follows immediately.

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[4] N. N. Bogolyubov, Quasi-averages in Problems of Statistical Physics, Dubna preprint D-781 (1961).

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