On the use of standard temperature techniques in the theory of a degenerate Bose gas: Calculating the average in the approximation of a noninteracting Bose gas

B. V. Bobrov, S. A. Triger, and P. Schram*

Institute of High-Temperature Physics, Russian Academy of Sciences, 127412 Moscow, Russia

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This paper discusses whether the standard temperature diagram technique in perturbation theory can be used to describe a Bose gas below the Bose condensation temperature. It is shown that the average value of a product of several creation and annihilation operators for a noninteracting Bose gas can be expressed in terms of the average value of pairs of creation and annihilation operators at arbitrary temperatures without any limitation on the particle momentum. © *1995 American Institute of Physics.*

1. The basic description of the properties of superfluid helium involves the model of an interacting Bose gas with a short-range interaction potential, which includes the effect of Bose–Einstein condensation.[1] However, there are nontrivial problems associated with the use of this model. The first is that the ideal-gas assumption is a poor choice for an initial approximation; this is clear, e.g., from the fact that for temperatures $T<T_\Lambda$, where T_Λ is the Bose-condensation temperature, the pressure of an ideal Bose gas does not depend on the particle number density n.[1] This implies that inclusion of particle interactions is of fundamental importance in describing the properties of superfluid helium. In this situation, questions about the applicability of the standard form of the temperature diagram technique used in perturbation theory become extremely important. It is well known that generalization of the methods of standard diagram technique for the case of a Bose gas at temperatures $T<T_\Lambda$ is an extremely difficult problem.[2] The fact is that the basis for constructing the standard diagram technique is the circumstance that the average value of a product of several creation operators $\hat{a}_{\mathbf{p}}^{+}$ and annihilation operators $\hat{a}_{\mathbf{p}}$ (where $\hbar\mathbf{p}$ is the momentum of a particle; we will assume the particle spins are zero) for a system of noninteracting particles can be expressed in terms of average values of pairs of creation and annihilation operators. According to existing representations, this latter assertion is valid in the thermodynamic limit:

$$T\text{-lim:}\quad V\to\infty,\quad N\to\infty,\quad n=N/V=\text{const},\tag{1}$$

where N is the total number of particles in a system with volume V. This will only be true when we can neglect the contribution of average values of products that contain several creation and annihilation operators with the same momentum.[2] However, in the case of a Bose gas with $T<T_\Lambda$ the creation and annihilation operators for particles whose momentum equals zero is usually assumed to be proportional to the square root of the volume:

$$\hat{a}_0^{+}\sim\hat{a}_0\propto\sqrt{N}\propto\sqrt{V}.\tag{2}$$

This fact is used to justify the assertion that standard diagram techniques are inapplicable, and that special techniques are required. Since the publication of Ref. 3, this problem has been solved by assuming that the operators $\hat{a}_0^{+}$ and $\hat{a}_0$ can be treated as C-numbers.[4–6] However, the validity of this assertion cannot be rigorously proved.[7,8] Furthermore, in Ref. 9 an alternative canonical representation was proposed for the field operators without using the c-number representation of the operators $\hat{a}_0^{+}$ and $\hat{a}_0$. On the other hand, in Refs. 10 and 11 the results of applying standard diagram techniques were analyzed using the random phase approximation in order to describe a weakly nonideal Bose gas at temperatures $T<T_\Lambda$; based on this analysis, the authors explained features of the behavior of the dynamic structure factor of liquid helium. Meanwhile, a self-consistent equation of state for a Bose gas was obtained in Ref. 12 and in Ref. 13 the possibility of use of the standard diagram technique is possible. In light of these developments, the present work is aimed at a detailed investigation of the applicability of the temperature-diagram perturbation theory in its standard form. It will be shown here that the formal rules for computing average values remain in force even for $T<T_\Lambda$. In this case the average value of a product of several creation and annihilation operators for a noninteracting Bose gas is expressed in terms of average values of pairs of creation and annihilation operators without any limitation on the particle momentum or gas temperature.

2. Let us consider a system of interacting Bose particles with zero spin, characterized by an interparticle interaction potential

$$\nu(\mathbf{r})=\nu_0\delta(\mathbf{r}),\quad \nu_0>0\tag{3}$$

at temperature $T=0$. The thermodynamic properties of such a system are fully characterized by the single dimensionless parameter

$$\lambda=\frac{\nu_0 m n^{1/3}}{4\pi\hbar^2},\tag{4}$$

where m is the particle mass. Then the average energy E (or the energy of the ground state), being a sum of the average kinetic energy K and potential energy U of the system, can be written in the form

$$\begin{gathered}E=K+U=Nn\nu_0\varepsilon(\lambda),\\ K=Nn\nu_0\varphi(\lambda),\quad U=Nn\nu_0\gamma(\lambda),\end{gathered}\tag{5}$$

where, by definition,

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$$K=\sum_{\mathbf{p}} \frac{\hbar^2 p^2}{2m} f_{\mathbf{p}} \geq 0, \quad \varphi(\lambda) \geq 0, \tag{6}$$

and $f_{\mathbf{p}}$ is the single-particle momentum distribution function. At the same time, according to (3), (5) the pressure P in this system equals

$$P=-\left(\frac{\partial E}{\partial V}\right)_N = n^2 \nu_0 \left(\varepsilon(\lambda)+\frac{\lambda}{3}\, \varepsilon'(\lambda) \right), \tag{7}$$

taking into account the virial theorem for a system with the interparticle interaction potential (3), we have

$$PV=\frac{2}{3} K+U \tag{8}$$

or

$$P=n^2 \nu_0 \left[\varepsilon(\lambda)-\frac{1}{3}\, \varphi(\lambda) \right]. \tag{9}$$

Comparing (7) and (9), and taking (5) into account, we obtain the equation

$$\lambda \varepsilon'(\lambda)=-\varphi(\lambda) \leq 0. \tag{10}$$

Consequently, for any value of the parameter λ we have

$$\begin{gathered} \varepsilon(\lambda)=\varepsilon_0-\int_0^\lambda \frac{dx}{x}\, \varphi(x), \\ \varepsilon_0=\lim_{\lambda\to 0} \varepsilon(\lambda), \quad \lim_{\lambda \to 0} \varphi(\lambda)=0. \end{gathered} \tag{11}$$

In this way we find that for arbitrary λ [see (6)]

$$\begin{gathered} \varepsilon(\lambda) \leq \varepsilon_0, \\ \mu=n\nu_0 \varepsilon(\lambda)+n^{-1}P=n\nu_0 \left[2\varepsilon(\lambda)-\frac{1}{3}\, \varphi(\lambda) \right] \\ \leq 2n\nu_0\varepsilon_0, \end{gathered} \tag{12}$$

where μ is the chemical potential, and the difference between $\varepsilon(\lambda)$ and ε_0 is entirely determined by the single-particle distribution function $f_{\mathbf{p}}$ [see (6)]; the "condensate" particles (with $\hbar\mathbf{p}=0$) make no contribution to this difference.

3. Let us discuss the distribution function of an ideal Bose gas. The basic problem to be addressed is the existence of the Bose–Einstein condensation effect at temperatures

$$T<T_\Lambda^0, \quad T_\Lambda^0=\frac{\hbar^2}{2m}\left[\frac{4\pi^2 n}{\Gamma(3/2)\zeta(3/2)} \right]^{2/3}, \tag{13}$$

where T_Λ^0 is the temperature for Bose–Einstein condensation of an ideal Bose gas, $\Gamma(x)$ is the gamma function, and $\zeta(x)$ is the Riemann function. The approach that is closest to first principles in this case is that proposed in Ref. 14, which is based on the assumption that the transition to the thermodynamic limit (1) can be made in the expressions that result from the averaging. Then the single-particle distribution function is

$$f_{\mathbf{p}}^0=\langle \hat{a}_{\mathbf{p}}^+ \hat{a}_{\mathbf{p}} \rangle^0. \tag{14}$$

As usual, the angle brackets imply averaging over the grand canonical ensemble; the label 0 implies the ideal-gas approximation for which the average is determined by the Bose–Einstein distribution

$$f_{\mathbf{p}}^0=\left\{ \exp\left[\left(\frac{\hbar^2 p^2}{2m}-\mu_V \right) \frac{1}{T} \right]-1 \right\}^{-1} \tag{15}$$

but only for a system whose chemical potential μ_V is negative for large but finite volumes V, i.e.,

$$\mu_V<0. \tag{16}$$

In this case the condition for normalizability

$$N=\sum_{\mathbf{p}} f_{\mathbf{p}}^0 \tag{17}$$

can be written in the form

$$n=\int \frac{d^3p}{(2\pi)^3} \left\{ \exp\left[\left(\frac{\hbar^2 p^2}{2m}-\mu \right) \frac{1}{T} \right]-1 \right\}^{-1} \tag{18}$$

but only when the chemical potential μ is a negative quantity, i.e.,

$$\mu=T-\lim \mu_V<0. \tag{19}$$

However, according to (18), condition (19) is violated for $T=T_\Lambda^0$. Consequently, in order to treat temperatures $T<T_\Lambda^0$ we must include the fact that in a large but finite volume V the chemical potential μ_V can be written in the form

$$\mu_V=\mu-\frac{\alpha}{V}+\ldots \tag{20}$$

Then condition (16) becomes

$$\begin{gathered} \mu<0, \\ \mu=0, \quad \alpha>0, \end{gathered} \tag{21}$$

while Eq. (17) for $T<T_\Lambda^0$ is

$$N=N_0+V\int \frac{d^3p}{(2\pi)^3} \left\{ \exp\left(\frac{\hbar^2 p^2}{2mT} \right)-1 \right\}^{-1}. \tag{22}$$

Thus, for $T<T_\Lambda^0$,

$$\mu=0, \quad \alpha=\frac{TV}{N_0}, \quad N_0=N\left[1-\left(\frac{T}{T_\Lambda^0} \right)^{3/2} \right], \tag{23}$$

and consequently

$$f_{\mathbf{p}}^0=\left\{ \exp\left[\left(\frac{\hbar^2 p^2}{2m}+\frac{\alpha}{V} \right) \frac{1}{T} \right]-1 \right\}^{-1}, \tag{24}$$

or in the thermodynamic limit

$$f_{\mathbf{p}}^0=N_0\delta_{\mathbf{p},0}+\left\{ \exp\left(\frac{\hbar^2 p^2}{2mT} \right)-1 \right\}^{-1} (1-\delta_{\mathbf{p},0}). \tag{25}$$

According to this discussion, $f_{\mathbf{p}}^0$ is determined by Eqs. (15), (19)–(21) at arbitrary temperatures. We can assume that the analogous situation holds when we investigate an ideal Bose gas and correlation functions of higher order.

As an example of this, let us consider the pair correlation function $n_2^0(\mathbf{r}_1,\mathbf{r}_2)$, defined in terms of the field operators $\hat{\psi}^+$ and $\hat{\psi}$ in the following way:

$$n_2^0(\mathbf{r}_1,\mathbf{r}_2)=\langle\hat\psi^+(\mathbf{r}_1)\hat\psi^+(\mathbf{r}_2)\hat\psi(\mathbf{r}_2)\hat\psi(\mathbf{r}_1)\rangle^0$$

$$=V^{-2}\sum_{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_3\mathbf{p}_4}\langle\hat a^+_{\mathbf{p}_1}\hat a^+_{\mathbf{p}_2}\hat a_{\mathbf{p}_3}\hat a_{\mathbf{p}_4}\rangle^0$$

$$\times\exp(-i\mathbf{p}_1\mathbf{r}_1-i\mathbf{p}_2\mathbf{r}_2+i\mathbf{p}_3\mathbf{r}_2+i\mathbf{p}_4\mathbf{r}_1). \quad (26)$$

Taking into account the definition of the creation and annihilation operators in occupation-number space,[14] we can easily verify that

$$\langle\hat a^+_{\mathbf{p}_1}\hat a^+_{\mathbf{p}_2}\hat a_{\mathbf{p}_3}\hat a_{\mathbf{p}_4}\rangle^0=f^0_{\mathbf{p}_1}f^0_{\mathbf{p}_2}(\delta_{\mathbf{p}_1,\mathbf{p}_4}\delta_{\mathbf{p}_2,\mathbf{p}_3}+\delta_{\mathbf{p}_1,\mathbf{p}_3}\delta_{\mathbf{p}_2,\mathbf{p}_4})$$

$$\times(1-\delta_{\mathbf{p}_1,\mathbf{p}_2})$$

$$+\langle\hat a^+_{\mathbf{p}_1}\hat a^+_{\mathbf{p}_1}\hat a_{\mathbf{p}_1}\hat a_{\mathbf{p}_1}\rangle^0\delta_{\mathbf{p}_1,\mathbf{p}_2}\delta_{\mathbf{p}_1,\mathbf{p}_3}\delta_{\mathbf{p}_1,\mathbf{p}_4}. \quad (27)$$

Furthermore, taking into account that, according to (15)

$$\langle\hat a^+_{\mathbf{p}}\hat a^+_{\mathbf{p}}\hat a_{\mathbf{p}}\hat a_{\mathbf{p}}\rangle^0=\frac{\sum\limits_{k=0}^{\infty}k(k-1)\exp[(\hbar^2p^2/2m-\mu_V)k/T]}{\sum\limits_{l=0}^{\infty}\exp[(\hbar^2p^2/2m-\mu_V)l/T]}$$

$$=2(f^0_{\mathbf{p}})^2, \quad (28)$$

we find

$$\langle\hat a^+_{\mathbf{p}_1}\hat a^+_{\mathbf{p}_2}\hat a_{\mathbf{p}_3}\hat a_{\mathbf{p}_4}\rangle^0=f^0_{\mathbf{p}_1}f^0_{\mathbf{p}_2}(\delta_{\mathbf{p}_1,\mathbf{p}_4}\delta_{\mathbf{p}_2,\mathbf{p}_3}+\delta_{\mathbf{p}_1,\mathbf{p}_3}\delta_{\mathbf{p}_2,\mathbf{p}_4}). \quad (29)$$

Substituting (29) into (26) and using (17), we obtain

$$n_2^0(\mathbf{r})=n_2^0(\mathbf{r}_1-\mathbf{r}_2)=V^{-2}\sum_{\mathbf{p}_1\mathbf{p}_2}f^0_{\mathbf{p}_1}f^0_{\mathbf{p}_2}\{1+\exp[i(\mathbf{p}_2$$

$$-\mathbf{p}_1)\mathbf{r}]\}=n^2+\left|V^{-1}\sum_{\mathbf{p}}f^0_{\mathbf{p}}\exp(i\mathbf{p}\mathbf{r})\right|^2 \quad (30)$$

for arbitrary temperatures.

Note that, according to (15), (25), it is possible to make the change in (30) from summation over momentum to integration in the course of carrying out the thermodynamic limit only when $T>T^0_\Lambda$. In this case,

$$\lim_{r\to\infty}n_2^0(r)=n^2, \quad (31)$$

which expresses the well-known principle of weakening of correlations.[15] At the same time, for $T<T^0_\Lambda$, according to (25)

$$\lim_{r\to\infty}n_2^0(r)=n^2+n_0^2, \quad n_0=N_0/V. \quad (32)$$

Thus, for an ideal Bose gas at temperatures $T<T^0_\Lambda$ the principle of correlation decay for the pair correlation functions is violated. Note that the analogous assertion for the single particle correlation function is well known:[15]

$$n_1^0(\mathbf{r}_1-\mathbf{r}_2)=\langle\hat\psi^+(\mathbf{r}_1)\hat\psi(\mathbf{r}_2)\rangle^0. \quad (33)$$

When $T<T^0_\Lambda$, this function does not go to zero in the limit $|\mathbf{r}_1-\mathbf{r}_2|\to\infty$, like a normal system, but rather has a finite limit [see (25)]:

$$\lim_{r\to\infty}n_1^0(r)=n_0. \quad (34)$$

However, although the limiting relation (34) corresponds to C-number behavior of the operators $\hat a_0^+$ and $\hat a_0$, Eq. (32) contradicts it, a fact that is not difficult to verify directly. We therefore can argue that (12) and (32) invalidate the argument that it is possible to treat the operators $\hat a_0^+$ and $\hat a_0$ as C-numbers. This is also clear from "physical" considerations. In fact, according to (12) and (34) we should be able to assert that

$$\hat a_0^+\sim\hat a_0\propto\sqrt{N_0}. \quad (35)$$

However, the average number of particles in the Bose condensate N_0 is a function of temperature [see (23)]. Hence the operators $\hat a_0^+$ and $\hat a_0$ should be not simply C-numbers, which is possible in principle, but rather should depend explicitly on temperature, which can only be a consequence of the averaging procedure.

4. Let us turn to the question of whether temperature diagram techniques can be used in the standard form to describe a Bose gas at temperatures $T<T_\Lambda$. As we already noted in the introduction, the basic problem is to prove that for a noninteracting Bose gas the average value of a product of several creation and annihilation operators can be written in terms of the average values of pairs of creation and annihilation operators. We now call attention to a remarkable fact contained in Eq. (29): the average value of four creation and annihilation operators is in reality a product of two average values of pairs of creation and annihilation operators [see (14)], without any limitation on the particle momentum. This allows us to treat the ideal Bose gas in a unified fashion for arbitrary temperatures in terms of a single-particle distribution function representation in the form (15), (19)–(24).

Thus, if we can prove the validity of the analogous assertion for an arbitrary number of creation and annihilation operators, then this is sufficient (see Ref. 2) to justify formal use of the temperature diagram technique of perturbation theory to describe a Bose gas for arbitrary temperatures. By the word "formal" we mean implementation of the diagram technique in discussing systems within a large but finite volume V (see above) and then taking the thermodynamic limit in the final expressions for the quantities to be calculated.

In order to simplify the discussion, let us introduce an additional notation for the average value of $2N$ creation and annihilation operators with arbitrary labels for the case of an ideal Bose gas:

$$\langle\hat a^+_{\mathbf{p}_1}\hat a^+_{\mathbf{p}_2}\dots\hat a^+_{\mathbf{p}_N}\hat a_{\mathbf{q}_1}\hat a_{\mathbf{q}_2}\dots\hat a_{\mathbf{q}_N}\rangle^0\equiv\langle1,\dots,N|1,\dots,N\rangle^0, \quad (36)$$

in particular, according to (14),

$$\langle\alpha|a\rangle^0=f^0_{\mathbf{p}_\alpha}\delta_{\mathbf{p}_\alpha,\mathbf{q}_a}. \quad (37)$$

Furthermore, we will introduce a notation for products of pairs of creation and annihilation operators with differing indices:

$$\{\langle\alpha|a\rangle^0\langle\beta|b\rangle^0\ldots\langle\gamma|c\rangle^0\}\equiv\langle\alpha|a\rangle^0\langle\beta|b\rangle^0\ldots\langle\gamma|c\rangle^0\times(1-\delta_{\alpha,\beta})\ldots(1-\delta_{\alpha,\gamma})\times(1-\delta_{\beta,\gamma}), \tag{38}$$

for the average value of $2N$ creation and annihilation operators with the same indices:

$$[\langle 1,\ldots,N|1,\ldots,N\rangle^0]=\langle 1,\ldots,N|1,\ldots,N\rangle^0\delta_{1,2}\delta_{1,3}\ldots\delta_{1,N}, \tag{39}$$

for products of pairs with indices that do not coincide, and for average values of products of creation and annihilation operators with labels that do coincide:

$$\{\langle\alpha|a\rangle^0\ldots[\langle\beta,\ldots|b,\ldots\rangle^0]\}=\{\langle\alpha|a\rangle^0\ldots\}[\langle\beta,\ldots|b,\ldots\rangle^0]\times(1-\delta_{\alpha,\beta})\ldots . \tag{40}$$

Obviously,

$$\{\langle\alpha|a\rangle^0\}=[\langle\alpha|a\rangle^0]=\langle\alpha|a\rangle^0. \tag{41}$$

According to the definition of creation and annihilation operators in occupation-number space, for a noninteracting gas each average over a product of $2N$ creation and annihilation operators (36) can be written in the form of all possible products (38) of averages of pairs, and products (39) of smaller numbers of operators with indices that coincide in the form

$$\langle 1,\ldots,N|1,\ldots,N\rangle^0=\sum_{m=0}^{N}\left\{\underbrace{\langle\alpha|a\rangle^0\ldots\langle\beta|b\rangle^0}_{m}\left[\langle\underbrace{\gamma,\ldots,\delta}_{N-m}|\underbrace{c,\ldots,d}_{N-m}\rangle^0\right]\right\}, \tag{42}$$

while in each of the "terms" the labels α, β,... and a, b,... can take on any of the possible values: $1,\ldots,N$, but cannot be repeated [see (27)].

If we take (28) into account, it is not difficult to prove by induction that

$$\langle\underbrace{\hat{a}^+_{\mathbf{p}}\ldots\hat{a}^+_{\mathbf{p}}}_{N}\underbrace{\hat{a}_{\mathbf{p}}\ldots\hat{a}_{\mathbf{p}}}_{N}\rangle^0=N!(f^0_{\mathbf{p}})^N. \tag{43}$$

Then, keeping in mind that $N!$ possible pairs of creation and annihilation operators result from averaging a product of $2N$ creation and annihilation operators, we have according to (37), (43) that

$$[\langle 1,\ldots,N|1,\ldots,N\rangle^0]=\left[\underbrace{\langle\alpha|a\rangle^0\ldots\langle\beta|b\rangle^0}_{N}\right]\equiv\underbrace{\langle\alpha|a\rangle^0\ldots\langle\beta|b\rangle^0\delta_{\alpha,\beta}\ldots}_{N}, \tag{44}$$

where each of the labels runs from 1 to N, but does not repeat. Consequently,

$$\langle 1,\ldots,N|1,\ldots,N\rangle^0=\sum_{m=0}^{N}\left\{\underbrace{\langle\alpha|a\rangle^0\ldots\langle(\beta|b\rangle^0}_{m}\left[\underbrace{\langle\gamma|c\rangle^0\ldots\langle\delta|d\rangle^0}_{N-m}\right]\right\}, \tag{45}$$

i.e., the average of the product is represented in the form of products of averaged pairs of creation and annihilation operators with all possible combinations of coinciding and noncoinciding indices. But this implies that

$$\langle 1,\ldots,N|1,\ldots,N\rangle^0=\underbrace{\langle\alpha|a\rangle^0\langle\beta|b\rangle^0\ldots\langle\gamma|c\rangle^0}_{N}, \tag{46}$$

where the indices can take on any values from 1 to N and do not repeat, which we were required to prove. Furthermore, it is clear from this discussion that there are no limitations on the particle momenta.

Equation (46) corresponds to Wick's theorem in the limits of the temperature diagram technique,[2] since the chronological ordering procedure when Green's function is being determined does not influence the calculation of the average value.

Thus, the formal rules of standard temperature diagram technique remain in force for temperatures $T<T_\lambda$ as well; however, for treatments that start with a large but finite volume V, this is true only in the final expressions, i.e., after passing to the thermodynamic limit (1). In fact, this limitation reduces to preserving the summation over momenta for systematic treatment of particles in the Bose–Einstein condensate [see (25)].

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*Technical University, Eindhoven, Netherlands.

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