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Abstract

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ON A METHOD FOR COMPUTING QUANTUM DISTRIBUTION FUNCTIONS

(Presented by Academician N. N. Bogoliubov on 10 IV 1957)

Systematic methods for computing thermodynamically equilibrium quantum distribution functions must, naturally, make use of the well-developed techniques and concepts of quantum field theory, since in both cases we are dealing with the quantum theory of many particles. In ([5]), methods of field theory were applied to the problem of computing the free energy of interacting particles. In the present work we shall derive relations concerning distribution functions, in a form reminiscent of the results of the theory of propagation functions.

We shall restrict ourselves to the model of a one-component nonrelativistic Bose gas, although, of course, generalization to other cases is possible. We choose the Hamiltonian of the system in the form

$$H = \int \left[\psi^*(x')T_{x'x}\psi(x) + \frac{1}{2}\psi^*(x')\psi(x')\Phi(x'-x)\psi^*(x)\psi(x)\right] dx'\, dx \equiv$$

$$\equiv \psi^* T \psi + \frac{1}{2} n \Phi n. \tag{1}$$

On the right is given the abbreviated notation which we shall use below: $n(x) = \psi^*(x)\psi(x)$; $T = p^2/2m \equiv T_p$; $\Phi(x'-x) = \Phi(x-x')$ is the interaction potential; $\psi(x)$ is a second-quantized wave function in three-dimensional space, satisfying the commutation relations

$$[\psi, \psi] = 0, \qquad [\psi^*, \psi^*] = 0, \qquad [\psi, \psi^*] = 1$$

(i.e. $\psi(x)\psi^*(x') - \psi^*(x')\psi(x) = \delta(x-x')$).

The quantum distribution functions $f_r(x_1, x_1', \dots, x_r, x_r')$ are the functional derivatives at the point $v = 0$ of the generating functional

$$L[v] = \left\langle N \exp \int \psi^*(x') v_{x'x} \psi(x)\, dx'\, dx \right\rangle \equiv \left\langle N e^{\psi^* v \psi} \right\rangle, \tag{2}$$

where N is Wick' s symbol of normal product introduced by Wick.

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The functional (2) is the quantum generalization ([4]) of the classical generating functional ([2,3]). From x, x' in (2) one may pass to phase coordinates x, p by means of the Wigner transform. If, however, one sets $v_{xx'} = v_x \delta(x - x')$, then the consideration will be restricted to distribution functions only in the configuration space x.

Using the operator identity

$$\exp \psi^* u \psi = N \exp \psi^* (e^u - 1) \psi, \tag{3}$$

valid, for the above commutation relations, for ψ and ψ^*, one can transform (2) to the form

$$L[v] = \mathrm{Tr}\{R \exp[\psi^* \ln(v + 1)\psi]\}. \tag{4}$$

Here $\ln(v+1)$ should be understood as an operator that is an analytic function of the operator v. The state operator R in the case of thermodynamic equilibrium, corresponding to the temperature $kT = 1/\lambda$ and to a uniform mean spatial particle density n_0, has the form

$$R = \exp(\lambda \Psi - \lambda H + \mu \psi^* \psi). \tag{5}$$

According to the abbreviated notation we have adopted, here $\psi^* \psi = \int \psi^* \psi \, dx$ is the operator of the total number of particles; $\Psi = \int \varphi \, dx$ is the free energy (φ is its density); μ/λ has the meaning of the chemical potential. The quantities φ and μ are determined from the conditions

$$\mathrm{Tr}\, R = 1; \qquad \lambda \frac{\partial \varphi}{\partial \mu} = -n_0 \tag{6}$$

(the latter is equivalent to $\langle n \rangle = n_0$).

If the operator $e^{-\lambda H}$, using the ordering index s introduced by Feynman ([1]), is written in the form

$$\exp\left\{-\lambda \psi^* T \psi - \frac{\lambda}{2} n \Phi n\right\} = \exp\left\{-\int_0^\lambda \left[(\psi^* T \psi)_s + \frac{1}{2}(n \Phi n)_s\right] ds\right\}, \tag{7}$$

then in it one need not pay attention to the order in which the operators are written, since the order of their action is completely determined by the values of the index s.

Let us transform in (7) the term due to the interaction. To this end we introduce $\xi_s(x)$, a Gaussian random function of x and s, having the correlation function

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$$M\xi_{s_1}(x_1)\xi_{s_2}(x_2) = \Phi(x_1 - x_2)\delta(s_1 - s_2) \tag{8}$$

and zero mean value $M\xi_s(x) = 0$. Here M denotes statistical averaging over the ensemble of realizations of the introduced random function. By the known rules for writing the characteristic function of a Gaussian random process, we find

$$\exp\left\{-\frac{1}{2}\int_0^\lambda ds \iint n_s(x')\Phi(x'-x)n_s(x)\,dx'\,dx\right\} = M\exp\left\{i\int_0^\lambda ds \int \xi_s(x)n_s(x)\,dx\right\}. \tag{9}$$

Taking into account (4), (5), (7), (9), we have

$$L[v] = e^{\lambda\Psi}M\ \mathrm{Tr}\exp\left\{(\psi^*\ln(1+v)\psi)_0 + \mu\psi^*\psi - \int_0^\lambda (\psi^*T\psi)_s\,ds + i\int_0^\lambda (\psi^*\xi_s\psi)_s\,ds\right\}. \tag{10}$$

Thus, by means of a continual Fourier transformation, the problem is reduced to the consideration of noninteracting particles in a fluctuating external field. The symbol M makes it possible not to write explicitly the continual integration implied by it, with weight $\mathrm{const}\cdot\exp\left\{-\int \xi_s\Phi^{-1}\xi_s\,\frac{ds}{2}\right\}$.

Evaluation of the trace over ψ^*, ψ leads to the result

$$L[v] = e^{\lambda\Psi}M\exp\{-\mathrm{Tr}\ln|1-K-vK|\}, \tag{11}$$

where

$$K = \exp\left[\mu - \int_0^\lambda T_s\,ds + i\int_0^\lambda \xi_s\,ds\right],$$

and Tr refers to the operators v, T, ξ_s.

Expanding the functional (11) in powers of v, we obtain

$$\lambda\Psi = -\ln f^{(0)}; \qquad f_1(x,x') = \frac{f^{(1)}_{xx'}}{f^{(0)}}; \qquad f_2(x,x';y,y') = \frac{f^{(2)}_{xx'yy'} + f^{(2)}_{xy'yx'}}{f^{(0)}}; \ldots \tag{12}$$

$$f^{(r)}_{xx'_1\ldots x_r x'_r} = M\exp\{-\mathrm{Tr}\ln|1-K|\}\left(\frac{K}{1-K}\right)_{x_1x'_1}\cdots\left(\frac{K}{1-K}\right)_{x_rx'_r}. \tag{13}$$

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In the absence of interaction, K becomes $K_0 = e^{\mu-\lambda T}$, and $f^{(r)}$ becomes the corresponding functions of an ideal gas, which we shall denote by $f^{0(r)}$. Let us consider the interaction-induced deviation of $f^{(r)}$ from the ideal values. We introduce the following functions $F^{(r)}$, describing this deviation:

$$f^{(0)} = f^{0(0)} F^{(0)}; \qquad \frac{f^{(1)}}{f^{(0)}} = \frac{f^{0(1)}}{f^{0(0)}} + \frac{F^{(1)}}{F^{(0)}};$$

$$\frac{f^{(2)}_{xx'yy'}}{f^{(0)}} = \frac{f^{0(2)}_{xx'yy'}}{f^{0(0)}} + \frac{f^{0(1)}_{xx'}}{f^{0(0)}} \frac{F^{(1)}_{yy'}}{F^{(0)}} + \frac{F^{(1)}_{xx'}}{F^{(0)}} \frac{f^{0(1)}_{yy'}}{f^{0(0)}} + \frac{F^{(2)}_{xx'yy'}}{F^{(0)}}; \ldots \tag{14}$$

As follows from (11), (12), the functions thus defined can be represented by the sum

$$\mathrm{Tr}\,[F^{(r)} v_1 \ldots v_r] = M \sum_{j=0}^{\infty} \sum_{m_1,\ldots,m_{j+r}=1}^{\infty} \frac{1}{m_1 \ldots m_j} \mathrm{Tr}[(kB)^{m_1}] \ldots$$

$$\ldots \mathrm{Tr}[(kB)^{m_j}]\, \mathrm{Tr}[v_1 B (kB)^{m_{j+1}}] \ldots \mathrm{Tr}[v_{rB} (kB)^{m_{j+r}}], \tag{15}$$

where $k = K - K_0$; $B = (1 - K_0)^{-1}$; $r = 0, 1, 2, \ldots$.

Each term of this sum is put in correspondence with a diagram having j closed loops and r open lines. On each line there are m_α vertices k. To a segment of a line connecting two vertices or going from a vertex to the edge of the diagram there corresponds the operator B, which in the momentum representation has the form $(1 - e^{\mu-\lambda T})^{-1} = f_0(p) + 1$. Before averaging M, to a vertex lying between segments with momenta p and p' there corresponds the operator

$$k_{p'p} = ie^{\mu} \int_0^{\lambda} ds\, \exp\{(s-\lambda)T_{p'} - sT_p\}\, \xi_{sp'p} +$$

$$+ i^2 e^{2\mu} \int_0^{\lambda} ds \int_0^{s} dt \int \exp\{(s-\lambda)T_{p'} + (t-s)T_q - tT_p\}\, \xi_{sp'q} \xi_{tqp}\, dq + \ldots \tag{16}$$

The moments of a Gaussian random function, as is known, are expressed through the correlation function. This means that under the averaging M all operators ξ are joined pairwise in all possible ways; on the graph such a joining of vertices is denoted by dotted interaction lines. Equation (8) in the momentum representation has the form

$$M \xi_{sp'p} \xi_{tk'k} = \delta(p' + k' - p - k)\, \nu(p' - p)\, \delta(s - t);$$

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Fig. 1

Figure 1: Fig. 1

$$\left(\nu(x) = (2\pi)^{-3} \int e^{ixz} \Phi(z)\, dz\right). \tag{17}$$

Therefore, to each interaction line there corresponds $\nu(x)$, and it may be interpreted as the exchange of an interaction quantum, with momentum conservation taking place.

The number of interaction lines in the diagram determines the order of the given term in powers of the square of the interaction constant, or, in other words, the degree in respect to

of the interaction potential Φ. Calculation of the terms corresponding to diagrams of a given order makes it possible to find the exact terms of the expansion of the distribution functions in powers of Φ.

The first correction, due to the interaction, is linear in υ and is described by diagrams having only one interaction line. In Fig. 1 the diagrams a, b, and c are all possible diagrams describing the first correction to $F^{(0)}$, defined by the sum (15) ($r = 0$). The graphs b and c may be excluded from consideration by a renormalization of the chemical potential. The term b is proportional to $\int \upsilon(\chi) d\chi = \Phi(0)$ and describes the self-action of a particle. The term c, proportional to $\upsilon(0)$, describes the mean repulsive action of the whole gas as a whole. The nonzero quantities $\Phi(0)$ and $\upsilon(0)$ can be excluded from $\Phi(x)$, replacing them by an additional uniform external potential $\Phi(0) + \int \Phi n_0 dx$, and the latter can be included in the chemical potential by the replacement $\mu/\lambda - \Phi(0) - \int \Phi n_0 dx \to \mu/\lambda$. Therefore, in calculating the first correction one must take into account only diagram a for $F^{(0)}$ and only c and d for the functions $F^{(1)}$ and $F^{(2)}$, respectively.

Fig. 1

Upon substituting expression (16) into the corresponding terms (15), in the present approximation it is sufficient to retain only the first term of this expression. After averaging, taking (17) into account, we shall have

$$F^{(1)}_{p'p} = -\delta(p' - p)\lambda f_0(p)[f_0(p) + 1] \int f_0(p + \chi)\upsilon(\chi) d\chi; \tag{18}$$

$$\begin{aligned} F^{(2)}_{p'pk'k} = & -\delta(p' + k' - p - k)\upsilon(p' - p) f_0(p') f_0(k') f_0(p) f_0(k) \times \\ & \times \frac{e^{\lambda T_{p'} + \lambda T_{k'}} - e^{\lambda T_p + \lambda T_k}}{T_{p'} + T_{k'} - T_p - T_k}\, e^{-2\mu}. \end{aligned} \tag{19}$$

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The function standing in (18) as the multiplier of $\delta(p' - p)$ is the correction to the unperturbed momentum distribution $f_0(p)$.

In the diagrams considered by us, several interaction lines may emerge from a single vertex. In this they differ from the diagrams of the work [(5)], being the result of a splitting of the latter. Thus, the graph of the work [(5)] having the form a (Fig. 1) is nothing other than the sum of our diagrams a and b.

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

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