# STATISTICAL EQUATION FOR A PARTICLE OF A CRYSTAL IN THE REGION OF A NODE

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## Abstract

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# STATISTICAL EQUATION FOR A PARTICLE OF A CRYSTAL IN THE REGION OF A NODE

*(Presented by Academician N. N. Bogolyubov, 18 I 1968)*

The one-particle distribution function $\rho_1(q_1)$ (which determines the probability density that, upon observing a system of $N$ particles in a volume $V$, some particle will be found at the point $q_1$) and the binary distribution function $\rho_2(q_1, q_2)$ (which gives the probability density of finding one particle of the system at the point $q_1$, and a second particle at the point $q_2$) are connected with each other by the equation ($^1$)

$$\theta \frac{\partial \rho_1(q)}{\partial q^\alpha} + \int_V \frac{\partial \Phi(|q-q'|)}{\partial q^\alpha} \rho_2(q, q')\, dq' = 0, \tag{1}$$

where $\theta = kT$ ($T$ is the absolute temperature); $\Phi(|q-q'|)$ is the potential of pair interaction between particles, and $\alpha = 1, 2, 3$.

In ($^2$), in accordance with experiment ($^3$) and in contrast to ($^4$), it was established that the regions of motion of particles in a crystal about the corresponding nodes do not overlap up to the melting temperature, and that the linear dimensions $b$ of these regions are small in comparison with the distance $a$ between nearest neighbors ($b = 0.1a$).

This result justifies the assumption of multiplicativity of the binary distribution function of crystal particles:

$$\rho_2(q, q') = \rho_1(q)\rho_1(q'), \tag{2}$$

since

$$|q - q'| \geq b \tag{3}$$

and each particle simultaneously interacts with an entire ensemble of equal nearest neighbors and with particles on other coordinate spheres.

The solution of the statistical many-body problem in the approximation of multiplicativity of the binary distribution function is called the self-consistent-field approximation. Substituting (2) into (1), we obtain a closed nonlinear equation for the one-particle distribution function in this approximation,

$$\theta \ln \lambda \rho_1(q) + \int_V \Phi(|q-q'|)\rho_1(q')\,dq' = 0, \tag{4}$$

which is called the self-consistent-field equation ($\lambda$ is a normalization constant).

Equation (4), without taking condition (3) into account, is not applicable to a crystal. In liquids and gases no such condition exists. Consequently, equation (4) is likewise not applicable to them.

The inapplicability of the self-consistent method to liquids and gases makes it illegitimate to construct a theory of crystallization and of the crystal by starting from a consideration of a liquid in the self-consistent-field approximation and using the periodic solution of equation (4) that branches off for certain parameters of the liquid.

In works ($^{5,6}$) equation (4) was applied to liquids and gases, and also to crystals without taking into account, and contrary to, condition (3). As was shown in ($^{7}$), such an application of this equation in the theory of solids leads to absurd results. The defect of equation (4), if (2) is taken without the restriction (3), consists in the fact that it leads to the inclusion of the particles' self-energy. In addition, it also has the drawback that it does not allow one to determine the period of the crystal, since as $\theta \to 0$ it is satisfied for an arbitrary period ($^{6}$). Determining the period of the crystal with the aid of (4), as is done in ($^{5,6}$), is not correct ($^{7,8}$). The period of the crystal in the self-consistent-field approximation, like condition (3), can be determined only by invoking thermodynamics ($^{2}$). Let us define the equation for the one-particle distribution function $\rho_1(q)$ in a crystal in the self-consistent-field approximation, taking into account (3), which, consequently, will be free of the defect of equation (4).

According to ($^{2}$), the function $\rho_1(q)$ in a crystal has the form

$$\rho_1(q) = \sum_{i=0}^{N-1} \rho(q-a_i), \tag{5}$$

where the $\delta$-like function $\rho(q-a_i)$ has a sharp maximum at the site $a_i$ of the crystal lattice and is nonzero only in a neighborhood $b$ of this site. It determines the probability density of finding a given particle at the point $q$ near the site $a_i$, and is called the species distribution function of the particle near the $i$-th site. We shall find the equation for this distribution function.

Substituting (5) into (4) and taking (3) into account, we obtain

$$\theta \ln \lambda \sum_i \rho(q-a_i) + \sum_j (1-\delta_{ij}) \int_V \Phi(|q-q'|)\rho(q'-a_j)\,dq' = 0, \qquad (6)$$

where $\delta_{ij}$ is the Kronecker symbol.

Equation (6) for a crystal is free of the organic defect of equation (4).

In equation (6) $q$ is arbitrary. For $q$ in the region of some site, for example the initial one, for which $i=0$ and $a_0=0$, in the sum of the first term of equation (6) only one term remains, $\rho(q-a_0)=\rho(q)$, while in the sum of the second term all terms except $j=0$ remain. Making in equation (6) also the substitution $q'-a_j=q_1$, for the function $\rho(q)$ we obtain the equation

$$\theta \ln \lambda \rho(q) + \int_V K(|q-q_1|)\rho(q_1)\,dq_1 = 0, \qquad (7)$$

where

$$K(|q-q_1|) = \sum_{j=1}^{N-1} \Phi(|q-q_1-a_j|) = \sum_{k=1}^{M} z_k \Phi(|q-q_1-v_k a|) \qquad (8)$$

(the summation is carried out over coordination spheres; see (2)).

Equation (7), like equation (6), is free of the defect of equation (4) and determines the distribution function of a particle in the region of a site of the crystal lattice; its solution makes it possible to obtain all the equilibrium properties of the crystal, since it gives the possibility of finding its free energy*. Indeed, following (9), the solution of equation (7) can be found by the method of iteration. In the harmonic approximation we obtain

$$\rho(q) = C \exp\left\{-\frac{1}{\theta}\left[u_0 + \frac{1}{2}\sum_{\alpha,\beta} F_{\alpha,\beta} q^\alpha q^\beta\right]\right\}, \qquad (9)$$

*

On the basis of the results of works (2,9), equation (7) is derived in (10) by another method–starting from the Liouville equation while using a number of additional assumptions.

where $C$ is determined from the normalization condition $\int \rho(a)\,dq = 1$, $u_0$ is the energy of a particle at a site of the crystal lattice, $F_{\alpha\beta} = (\partial^2 u_0/\partial q^\alpha \partial q^\beta)_{a_0}$.

Using (9), we find the configurational part of the free energy of the crystal, which is equal to

$$F = -\frac{3}{2}N\theta \ln(2\pi\theta) + \frac{N\theta}{2}\ln(f_1 \cdot f_2 \cdot f_3) + U^0, \tag{10}$$

where $f_\alpha$ are the elements of the matrix $\|F_{\alpha\beta}\|$, reduced to the principal axes, $U^0 = \frac{1}{2}Nu_0$.

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