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Abstract

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PHYSICS

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AN EQUATION FOR “CLASSICAL” GREEN FUNCTIONS IN THE KINETIC APPROXIMATION

(Presented by Academician N. N. Bogolyubov on 25 III 1965)

In the present note a closed equation is obtained for the basic Green function (“lowest” order) for a classical statistical system of particles with short-range interaction, accurate to the cube of the formal expansion parameter characteristic of low-density systems, $n = N/V$ ⁽¹⁾. In previous works ^(2, 3) “classical” Green functions were introduced and a chain of equations for them was obtained, and also its simplest decoupling, corresponding to the approximation of a self-consistent field, was considered. The initial equations have the form

$$-iE\langle\langle A_{x_1}; A_y \rangle\rangle_E = \left[\frac{\mathbf{p}_1^2}{2m}; \langle\langle A_{x_1}; A_y \rangle\rangle_E \right] + 2 \int [\Phi(\mathbf{r}_1 - \mathbf{r}_2); \langle\langle A_{x_1 x_2}; A_y \rangle\rangle_E] dx_2 + \frac{n}{2\pi} [\delta(x_1 - y); F_1^{(0)}(x_1)], \quad (1)$$

$$-iE\langle\langle A_{x_1 x_2}; A_y \rangle\rangle_E = [H_2(x_1, x_2); \langle\langle A_{x_1 x_2}; A_y \rangle\rangle_E] + \quad (2)$$

$$+ 3 \sum_{1 \leq j < 2} \int [\Phi(\mathbf{r}_j - \mathbf{r}_3); \langle\langle A_{x_1 x_2 x_3}; A_y \rangle\rangle_E] dx_3 + \frac{n^2}{4\pi} \left[\sum_{1 \leq j < 2} \delta(x_j - y); F_2^{(0)}(x_1, x_2) \right],$$

where $x_1 \rightarrow (\mathbf{r}_1, \mathbf{p}_1)$, $y \rightarrow (\mathbf{r}', \mathbf{p}')$;

$$H_2(x_1, x_2) = \mathbf{p}_1^2/2m + \mathbf{p}_2^2/2m + \Phi(\mathbf{r}_1 - \mathbf{r}_2),$$

and the equilibrium distribution functions will be ⁽¹⁾

$$F_1^{(0)}(x_1) = C e^{-\mathbf{p}_1^2/2m\theta}, \quad C = (2\pi m\theta)^{-3/2}; \quad F_2^{(0)}(x_1, x_2) = C^2 e^{-H_2/\theta} + n \dots$$

We see that the quantity $\langle\langle A_{x_1}; A_y \rangle\rangle_E$ is proportional to n , while $\langle\langle A_{x_1 x_2}; A_y \rangle\rangle_E$ is proportional to n^2 . Therefore, in order to obtain a closed equation for the first Green function $\langle\langle A_{x_1}; A_y \rangle\rangle_E$, accurate to quantities of order of smallness n^3 , it is necessary to find an approximate expression for $\langle\langle A_{x_1 x_2}; A_y \rangle\rangle_E$, accurate to quantities of the same order. Let us note that with increasing distance $|\mathbf{r}_1 - \mathbf{r}_2|$ the correlation deviation ⁽³⁾

$$\langle\langle A_{x_1 x_2}; A_y \rangle\rangle_E - \frac{1}{2}n\{\langle\langle A_{x_1}; A_y \rangle\rangle_E F_1^{(0)}(\mathbf{p}_2) + \langle\langle A_{x_2}; A_y \rangle\rangle_E F_1^{(0)}(\mathbf{p}_1)\}$$

tends to zero. In particular, we shall consider the situation when the particles have some “radius of impenetrability,” for example, the case of elastic spheres, i.e. $\Phi(|\mathbf{r}|) = \infty$, $|\mathbf{r}| < r_0$ (r_0 is the diameter of a sphere). Then it is obvious that $\langle\langle A_{x_1 x_2}; A_y \rangle\rangle_E = 0$ for $|\mathbf{r}_1 - \mathbf{r}_2| < r_0$. Therefore it is convenient to consider the correlation deviation of the form

$$\langle\langle A_{x_1 x_2}; A_y \rangle\rangle_E - \frac{1}{2}n\{\langle\langle A_{x_1}; A_y \rangle\rangle_E F_1^{(0)}(\mathbf{p}_2) + \langle\langle A_{x_2}; A_y \rangle\rangle_E F_1^{(0)}(\mathbf{p}_1)\}e^{-\Phi(\mathbf{r}_1 - \mathbf{r}_2)/\theta},$$

which vanishes both for $|\mathbf{r}_1 - \mathbf{r}_2| < r_0$ and at large distances ($|\mathbf{r}_1 - \mathbf{r}_2| \gg r_0$). We represent this correlation deviation in the form

$$D(E; x_1, x_2, y) = \langle\langle A_{x_1 x_2}; A_y \rangle\rangle_E - \frac{1}{2}nC^2e^{-H_2/\theta} [G'_E(x_1, y) + G'_E(x_2, y)], \quad (3)$$

where

$$\langle\langle A_x; A_y \rangle\rangle_E = G'_E(x, y)F_1^{(0)}(\mathbf{p}),$$

and we shall set up an equation for it. To this end, from (2) we subtract the equation, composed in accordance with (1), for the quantity

$$\frac{1}{2}n\{\langle\langle A_{x_1}; A_y \rangle\rangle_E F_1^{(0)}(\mathbf{p}_2) + \langle\langle A_{x_2}; A_y \rangle\rangle_E F_1^{(0)}(\mathbf{p}_1)\}e^{-\Phi(\mathbf{r}_1 - \mathbf{r}_2)/\theta},$$

and, restricting ourselves to terms of order n^2 , after some algebraic transformations—

we obtain

$$\begin{aligned} -iED(E; x_1, x_2, y) &= [H_2; D(E; x_1, x_2, y)] + \\ &+ \frac{1}{2}nC^2e^{-H_2/\theta} [\Phi(\mathbf{r}_1 - \mathbf{r}_2); G'_E(x_1, y) + G'_E(x_2, y)] + R; \end{aligned} \quad (4)$$

where

$$R = \frac{n^2}{4\pi} \sum_{1 \leq j \leq 2} [\delta(x_j - y); F_2^{(0)}(x_1, x_2)] + \frac{n^2}{4\pi} e^{-\Phi(|\mathbf{r}_1 - \mathbf{r}_2|)/\theta} \sum_{1 \leq j \leq 2} [\delta(x_j - y); F_1^{(0)}(p_1)F_1^{(0)}(p_2)].$$

Let us now note that, to the accepted degree of accuracy, it is not difficult to obtain expressions for $D(E; x_1, x_2, y)$ and $G'_E(x, y)$ at $E = 0$. Indeed, using the definition of the Green functions, as well as relations (3),

$$\langle [A(t); B(0)] \rangle = \frac{1}{\theta} \frac{d}{dt} \langle A(t)B(0) \rangle;$$

$$\langle A_{x_1, \dots, x_s}(0) \rangle = \frac{n^s}{s!} F_s^{(0)}(x_1 \dots x_s)$$

and setting $A = A_x$, $B = A_y$, after simple transformations we obtain

$$\langle\langle A_{x_1}; A_y \rangle\rangle_{E=0} = \frac{1}{2\pi\theta} \{n^2 F_1^{(0)}(x_1)F_1^{(0)}(y) - n^2 F_2^{(0)}(x_1, y) - n F_1^{(0)}(x_1)\delta(x_1 - y)\},$$

$$\langle\langle A_{x_1 x_2}; A_y \rangle\rangle_{E=0} = \frac{1}{2\pi\theta} \left\{ \frac{n^3}{2} F_2^{(0)}(x_1, x_2)F_1^{(0)}(y) - \frac{n^3}{2} F_3^{(0)}(x_1, x_2, y) - \frac{n^2}{2} \sum_{1 \leq j \leq 2} [\delta(x_j - y); F_2^{(0)}(x_1, x_2)] \right\}, \quad (5)$$

where $F_3^{(0)}(x_1, x_2, y) = C^3 e^{-H_3/\theta} + \dots$

Thus all Green functions can be computed at $E = 0$. Formulas (5) were obtained from the assumption that the correlations vanish as $|t - \tau| \rightarrow \infty$. However, it is not difficult to verify these formulas directly by substituting them into equations (1) and (2) at $E = 0$, and to make sure that the equations are identically satisfied if one takes into account that $f_3^{(0)}$ satisfies the corresponding equilibrium chain of equations (1).

To eliminate R , subtract from equation (4) the same equation, but at $E = 0$. According to expressions (5) and formula (3), the quantity $D(E = 0; x_1, x_2, y)$ is proportional to n^3 . Therefore, to the accepted accuracy we obtain

$$-iE\Delta_E = [H_2; \Delta_E] + f(E; x_1, x_2, y),$$

$$\Delta_E = D(E; x_1, x_2, y); \quad G_E(x, y) = G'_E(x, y) - G'_{E=0}(x, y), \quad (6)$$

$$f(E; x_1, x_2, y) = \frac{1}{2} n C^2 e^{-H_2/\theta} [\Phi(\mathbf{r}_1 - \mathbf{r}_2); G_E(x_1, y) + G_E(x_2, y)].$$

Let us note that $f(E; x_1, x_2, y)$ is an analytic function of E in the upper and lower complex half-planes, and infinity is not a singular point. By its definition, Δ_E must also possess this property. It can be shown that the solution of equation (6), the only one and regular in the upper (plus sign) or lower (minus sign) complex half-plane of E , will be

$$\Delta_E = \int_0^{\pm\infty} e^{i\alpha E} S_{-\alpha}^{(2)} f(E; x_1, x_2, y) d\alpha.$$

Here $S_{-\alpha}^{(2)}$ is the operation of replacing the arguments x_1, x_2 by $x_1(\alpha), x_2(\alpha)$, determined by the solution of the “two-body” problem with Hamiltonian H_2 and initial conditions $x_1(0) = x_1; x_2(0) = x_2$.

Now, substituting the expression for $\langle\langle A_{x_1 x_2}; A_y \rangle\rangle_E$, in accordance with the adopted notation, into equation (1), we obtain a closed equation for the Fourier-image of the first Green function in the form

$$\begin{aligned} i \left(\frac{\mathbf{p}_1 \vec{v}}{m} - E \right) G_{\overline{E\vec{v}}}(\mathbf{p}_1, \mathbf{p}') F_1^{(0)}(\mathbf{p}_1) &= i E G_{0\vec{v}}(\mathbf{p}_1, \mathbf{p}') F_1^{(0)}(\mathbf{p}_1) + \\ &+ n C^2 e^{-i\vec{v}\mathbf{r}_1} \int [\Phi(\mathbf{r}_1 - \mathbf{r}_2); e^{-H_2/\theta} (G_{\overline{E\vec{v}}}(\mathbf{p}_1, \mathbf{p}') e^{i\vec{v}\mathbf{r}_1} + \\ &+ \int_0^{\pm\infty} S_{-\alpha}^{(2)} e^{iE\alpha} [\Phi(\mathbf{r}_1 - \mathbf{r}_2); G_{\overline{E\vec{v}}}(\mathbf{p}_1, \mathbf{p}') e^{i\vec{v}\mathbf{r}_1}] d\alpha] dx_2 + \\ &+ n C^2 e^{-i\vec{v}\mathbf{r}_1} \int [\Phi(\mathbf{r}_1 - \mathbf{r}_2); e^{-H_2/\theta} (G_{\overline{E\vec{v}}}(\mathbf{p}_2, \mathbf{p}') e^{i\vec{v}\mathbf{r}_2} + \\ &+ \int_0^{\pm\infty} S_{-\alpha}^{(2)} e^{iE\alpha} [\Phi(\mathbf{r}_1 - \mathbf{r}_2); G_{\overline{E\vec{v}}}(\mathbf{p}_2, \mathbf{p}') e^{-i\vec{v}\mathbf{r}_2}] d\alpha] dx_2, \end{aligned} \quad (7)$$

where

$$G_E(x, y) = \int G_{\overline{E\vec{v}}}(\mathbf{p}, \mathbf{p}') e^{i\vec{v}(\mathbf{r}-\mathbf{r}')} d\vec{v},$$

$$G_{0\vec{v}}(\mathbf{p}, \mathbf{p}') = \frac{1}{(2\pi)^4 \theta} \left\{ n^2 F_1^{(0)}(\mathbf{p}') \int (1 - e^{-\Phi(r)/\theta}) e^{-i\vec{v}\mathbf{r}} d\mathbf{r} - n \delta(\mathbf{p} - \mathbf{p}') \right\}.$$

Let us transform equation (7). Using property (1)

$$S_{-\alpha}^{(2)} [\Phi(\mathbf{r}_1 - \mathbf{r}_2) + T_1 + T_2; G_{\overline{E}v}(\mathbf{p}_1, \mathbf{p}') e^{i\overline{v}\mathbf{r}_1}] = \frac{\partial S_{-\alpha}^{(2)}}{\partial \alpha} G_{\overline{E}v}(\mathbf{p}_1, \mathbf{p}') e^{i\overline{v}\mathbf{r}_1},$$

it is not difficult to show that

$$\begin{aligned} & \int dx_2 [\Phi(\mathbf{r}_1 - \mathbf{r}_2); e^{-H_2/\theta} (G_{\overline{E}v}(\mathbf{p}_1, \mathbf{p}') e^{i\overline{v}\mathbf{r}_1} + \\ & + \int_0^{\pm\infty} S_{-\alpha}^{(2)} e^{iE\alpha} [\Phi(\mathbf{r}_1 - \mathbf{r}_2); G_{\overline{E}v}(\mathbf{p}_1, \mathbf{p}') e^{i\overline{v}\mathbf{r}_1}] d\alpha)] = \\ = & \int dx_2 \left[\Phi(\mathbf{r}_1 - \mathbf{r}_2); e^{-H_2/\theta} \left(i \int_0^{\pm\infty} S_{-\alpha}^{(2)} e^{iE\alpha} \left(\frac{\mathbf{p}_1 \vec{v}}{m} - E \right) G_{\overline{E}v}(\mathbf{p}_1, \mathbf{p}') e^{i\overline{v}\mathbf{r}_1} d\alpha \right) \right]. \end{aligned}$$

Introduce the operator of uniform rectilinear motion $S_{\alpha}^{(1)}$. It replaces $\mathbf{r}_1(0)$ by $\mathbf{r}_1(0) + (\mathbf{p}_1(0)/m)\alpha$ and does not change the momentum $\mathbf{p}_1(0)$. Denote further by $\Sigma = \lim_{\alpha \rightarrow \infty} S_{-\alpha}^{(2)} S_{\alpha}^{(1)}$. This operator, acting on $\mathbf{r}_1, \mathbf{r}_2; \mathbf{p}_1, \mathbf{p}_2$, transforms them respectively into $\mathbf{Q}_1, \mathbf{Q}_2; \mathbf{P}_1, \mathbf{P}_2$, which depend only on the differences $(\mathbf{p}_2 - \mathbf{p}_1)$, $(\mathbf{r}_1 - \mathbf{r}_2)$ and do not depend on α .

Introduce for the variable \mathbf{r}_2 a cylindrical coordinate system. As the cylindrical axis ξ take the straight line passing through the point \mathbf{r}_1 and parallel to the vector $(\mathbf{p}_2 - \mathbf{p}_1)$. Denote the polar radius and polar angle respectively by a, φ . Then, after simple transformations, using the fact that (1)

$$H_2 = \frac{1}{2m}(\mathbf{p}_1^2 + \mathbf{p}_2^2) + \Phi(\mathbf{r}_1 - \mathbf{r}_2) = \frac{1}{2m}\{\mathbf{P}_1^2 + \mathbf{P}_2^2\},$$

equation (7) can be represented in the form

$$\begin{aligned} & iG_{\overline{E}v}(\mathbf{p}_1, \mathbf{p}') F_1^{(0)}(\mathbf{p}_1) \left\{ \frac{\mathbf{p}_1 \vec{v}}{m} - E \right\} = iEG_{\overline{0}v}(\mathbf{p}_1, \mathbf{p}') F_1^{(0)}(\mathbf{p}_1) + \\ & + e^{i\overline{v}\mathbf{r}_1} n \int_0^{2\pi} d\varphi \int_0^{\infty} da a \int_{(\mathbf{p}_2)} d\mathbf{p}_2 \int_{-\infty}^{+\infty} d\xi \left| \frac{\mathbf{p}_2 - \mathbf{p}_1}{m} \right| \times \\ & \times \frac{\partial}{\partial \xi} \left\{ e^{-(\mathbf{P}_1^2 + \mathbf{P}_2^2)/2m\theta} [G_{\overline{E}v}(\mathbf{P}_1, \mathbf{p}') e^{i\overline{v}(\mathbf{K}_1 + \mathbf{r}_1)} + G_{\overline{E}v}(\mathbf{P}_2, \mathbf{p}') e^{i\overline{v}(\mathbf{K}_2 + \mathbf{r}_2)}] \right. \\ & \left. - i\overline{v} e^{-(\mathbf{P}_1^2 + \mathbf{P}_2^2)/2m\theta} \left[G_{\overline{E}v}(\mathbf{P}_1, \mathbf{p}') e^{i\overline{v}(\mathbf{K}_1 + \mathbf{r}_1)} \frac{\mathbf{J}_1}{m} + \frac{\mathbf{J}_2}{m} e^{i\overline{v}(\mathbf{K}_2 + \mathbf{r}_2)} G_{\overline{E}v}(\mathbf{P}_2, \mathbf{p}') \right] \right\} + \end{aligned}$$

$$\begin{aligned}
 & + e^{-i\bar{v}\bar{r}_1 n} \int d\mathbf{r}_2 \int d\mathbf{p}_2 \left[\Phi(\mathbf{r}_1 - \mathbf{r}_2); e^{-(\mathbf{p}_1^2 + \mathbf{p}_2^2)/\theta} \int_0^{\pm\infty} (S_\alpha^{(2)} S_\alpha^{(1)} - \Sigma) \right. \\
 & \quad \times \left\{ i \left(E - \frac{\mathbf{p}_2 \bar{v}}{m} \right) e^{i(E - \mathbf{p}_2 \bar{v}/m)\alpha} G_{E\bar{v}}(\mathbf{p}_2, \mathbf{p}') e^{i\bar{v}\mathbf{r}_2} + \right. \\
 & \quad \left. \left. + i \left(E - \frac{\mathbf{p}_1 \bar{v}}{m} \right) e^{i(E - \mathbf{p}_1 \bar{v}/m)\alpha} G_{E\bar{v}}(\mathbf{p}_1, \mathbf{p}') e^{-i\bar{v}\mathbf{r}_1} \right\} d\alpha \right].
 \end{aligned}$$

Here $\mathbf{K}_1 = \mathbf{Q}_1 - \mathbf{r}_1$, $\mathbf{K}_2 = \mathbf{Q}_2 - \mathbf{r}_2$; $\mathbf{J}_1 = \mathbf{P}_1 - \mathbf{p}_1$; $\mathbf{J}_2 = \mathbf{P}_2 - \mathbf{p}_2$.

Let us transform the equation obtained for a system of elastic spheres. We shall first consider the situation in which $\Phi(\mathbf{r}_1 - \mathbf{r}_2) = 0$, $|\mathbf{r}_1 - \mathbf{r}_2| > r_0 + \delta$; $\Phi(\mathbf{r}_1 - \mathbf{r}_2) = U$, $|\mathbf{r}_1 - \mathbf{r}_2| < r_0$, and then pass to the limit as $\delta \rightarrow 0$, $U \rightarrow \infty$. By directly taking into account the dynamics of a binary collision, we can reduce this equation to a somewhat simpler form:

$$\begin{aligned}
 & G_{E\bar{v}}(\mathbf{p}_1, \mathbf{p}') F_1^{(0)}(\mathbf{p}_1) \{ \mathbf{p}_1 \bar{v}/m - E \} = EG_{0v}(\mathbf{p}_1, \mathbf{p}') F_1^{(0)}(\mathbf{p}_1) + \\
 & + inr_0^2 \int_{(v_2)} d\mathbf{p}_2 \int_{(\mathbf{g}\cdot\mathbf{j})>0} d\mathbf{j} \left(\frac{\mathbf{p}_2 - \mathbf{p}_1}{m} \cdot \mathbf{j} \right) F_1^{(0)}(\mathbf{p}_1) F_1^{(0)}(\mathbf{p}_2) \{ G_{E\bar{v}}(\mathbf{p}_1, \mathbf{p}') + \\
 & + G_{E\bar{v}}^*(\mathbf{p}_2, \mathbf{p}') e^{ir_0(\bar{v}\cdot\mathbf{j})} - G_{E\bar{v}}(\mathbf{p}_1, \mathbf{p}') - G_{E\bar{v}}(\mathbf{p}_2, \mathbf{p}') e^{-ir_0[\bar{v}\cdot\mathbf{j}]} \}, \quad (8)
 \end{aligned}$$

where \mathbf{p}_1^* , \mathbf{p}_2^* (which are functions of $\mathbf{p}_1, \mathbf{p}_2, \alpha, \varphi$) and $\mathbf{p}_1, \mathbf{p}_2$ are the momenta of the particles before and after the collision; \mathbf{j} is a unit vector along the line joining the centers of the two colliding spheres, directed from the center of molecule I. The minus sign corresponds to the case $\text{Im } E > 0$, the plus sign to the case $\text{Im } E < 0$.

The equation obtained is the analogue of the classical Boltzmann equation (with account of the finite sizes of the particles) in the Green-function method. This can be verified if one applies to the Boltzmann equation in Bogoliubov's form¹ the method developed in³.

The investigation of equation (8) will be the subject of our next paper.

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

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