ON THE MOMENTUM DISTRIBUTION FUNCTION OF A FERMI-PARTICLE GAS IN THE HIGH-DENSITY LIMIT

I. O. KULIK

Physico-Technical Institute, Academy of Sciences, Ukrainian S.S.R.

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Field theoretical methods are used to study a fermion gas with Coulomb interactions at zero temperature. We renormalize the interaction lines and the free particle propagation lines so that we can take correlation and exchange effects of the interaction into account. We have evaluated in the high-density limit (Gell-Mann–Brueckner limit) the momentum distribution function of the particles at zero temperature. The applicability of the high-density approximation for describing the interaction between the electrons in a metal is discussed.

A timely problem of solid state theory is the study of the interaction between particles in systems with a large number of degrees of freedom. The use of quantum field-theoretical methods (see references 1 to 10 and others) based upon the introduction of Green's functions, i.e., particle propagation functions, has turned out to be very fruitful for solving this problem.

The present paper is devoted to a study of the effects of inter-particle interactions in a high-density electron gas. The first to pose a similar problem correctly were Gell-Mann and Brueckner[8] who evaluated the electron gas correlation energy as a power series in the reciprocal of the density. In the present paper we evaluate the momentum distribution function of the particles in the ground state (this turns out to be different from the Fermi distribution function) as a power series in the reciprocal of the electron gas density. We note that it turns out that there is an essential need to use a field-theoretical technique to evaluate the momentum distribution function of the particles, as the difference between the distribution function and the Fermi distribution function is itself a quantum effect.

We consider a system of interacting fermions with a Hamiltonian*

$$H = -\frac{\hbar}{2m}\sum_{\alpha}\int d\mathbf{x}\psi_{\alpha}^{+}(\mathbf{x})\,\Delta\psi_{\alpha}(\mathbf{x}) + \frac{1}{2}\sum_{\alpha,\,\beta}\int d\mathbf{x}d\mathbf{y}\,\psi_{\beta}^{+}(\mathbf{y})\,\psi_{\alpha}^{+}(\mathbf{x})\,v(|\mathbf{x}-\mathbf{y}|)\,\psi_{\alpha}(\mathbf{x})\,\psi_{\beta}(\mathbf{y}). \quad (1)$$

Here $\psi_{\alpha}(\mathbf{x})$ and $\psi_{\alpha}^{+}(\mathbf{x})$ are the field function operators in the Schrödinger representation ($\alpha = \pm 1/2$ is the spin index); $v(|\mathbf{x}|)$ is the Coulomb interaction potential:

$$v(\mathbf{x}) = \frac{1}{V}\sum_{\mathbf{q}\neq 0} v(q)\,e^{i\mathbf{q}\mathbf{x}}, \qquad v(q) = \frac{4\pi e^2}{q^2} \quad (2)$$

($\mathbf{q} \neq 0$ indicates that we consider a system of N electrons in a space filled with a compensating positive constant charge density). We note that although most equations in the following are valid for any $v(q)$ any actual calculations are performed for Coulomb forces.

To describe various properties of the interaction it is convenient to go over to a time-dependent form of the theory. We shall use the Matsubara field-theoretical technique[1,2] (at $T = 0$); to do this we introduce field functions $\psi_{\alpha}(\mathbf{x})$ in the "modified Heisenberg representation"

$$\psi_{\alpha}(x) = e^{Ht}\psi_{\alpha}(\mathbf{x})\,e^{-Ht}, \qquad x \equiv (\mathbf{x},\ t), \quad (3)$$

$$\partial\psi_{\alpha}/\partial t = [H,\ \psi_{\alpha}(x)]_{-} \quad (4)$$

[and similarly $\psi_{\alpha}^{+}(\mathbf{x})$].

The single-particle and two-particle electron Green's functions are defined by the usual equations

$$G_{\alpha\beta}(x;\ x') = \langle T(\psi_{\alpha}(x)\,\psi_{\beta}^{+}(x'))\rangle, \quad (5)$$

$$G_{\alpha\beta\gamma\delta}(x_1 x_2;\ x_1' x_2') = \langle T(\psi_{\alpha}(x_1)\,\psi_{\beta}(x_2)\,\psi_{\delta}^{+}(x_2')\,\psi_{\gamma}^{+}(x_1'))\rangle, \quad (6)$$

where $\langle \ldots \rangle$ indicates an average over the physical vacuum, i.e., over that state of the system of interacting particles with the lowest energy (ground state).

One can obtain in the usual way an equation for G by starting from the equations of motion (4):

*Here and henceforth we measure energies and frequencies in the same units; they are connected through the equation $\varepsilon = \omega$. Similarly, we put $\mathbf{p} = \mathbf{k}$ ($\mathbf{p}$ – momentum; $\mathbf{k}$ – wave vector).

$$\left(\frac{\partial}{\partial t}-\frac{\hbar}{2m}\Delta\right)G_{\alpha\beta}(x;\ x')$$
$$-\sum_{\gamma}\int dyv(|\mathbf{x}-\mathbf{y}|)G_{\alpha\gamma\beta\gamma}(xy;\ x'y)=\delta^4(x-x')\delta_{\alpha\beta}. \tag{7}$$

When there are no periodic or external fields $G_{\alpha\beta}(x;\ x') = G(x-x')\delta_{\alpha\beta}$. To evaluate the Green's function explicitly we can use a formal expansion of Eq. (7) in a power series in v. In the zeroth approximation we get

$$G^{(0)}(x-x') = \begin{cases} -\frac{1}{V}\sum_{\mathbf{k}} n^{(0)}(k)\exp\{i\mathbf{k}(\mathbf{x}-\mathbf{x}')-\varepsilon_k^0(t-t')\}, & t<t' \\ \frac{1}{V}\sum_{\mathbf{k}}(1-n^{(0)}(k))\exp\{i\mathbf{k}(\mathbf{x}-\mathbf{x}')-\varepsilon_k^0(t-t')\}, & t>t' \end{cases} \tag{8}$$

where

$$n^{(0)}(k) = \begin{cases} 1, & k<k_F \\ 0, & k>k_F \end{cases}$$

is the Fermi distribution function at T = 0.

The contributions from the first and second approximations are given by the diagrams of Figs. 1 and 2. To obtain the corresponding contribution to G from a given diagram it is necessary to write

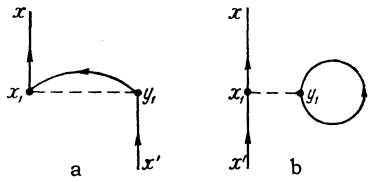

FIG. 1

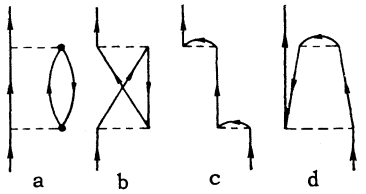

FIG. 2

for each full-drawn line $G^{(0)}(\mathbf{x}-\mathbf{x}')$ and for each dotted line $v(|\mathbf{x}-\mathbf{x}'|)$. The product obtained is then integrated over coordinate space at each vertex and over the time coordinates of the vertices with a different time coordinate* and multiplied by $(-1)^{n+l}2^l$, where n is the order of the diagram, i.e., the number of dotted interaction lines, and l the number of closed electron loops.† We note that diagrams of the type of Fig. 1b lead to a zero contribution as the momentum transferred along the dotted line is here zero while according to (2) $\mathbf{q} \neq 0$. We have omitted all such diagrams in Fig. 2.

As an example we shall write down the contribution from the diagram of Fig. 1a:

$$G_a^{(1)}(x-x') = -\int d^4x_1 dy_1 v(|\mathbf{x}_1-\mathbf{y}_1|)G^{(0)}(x-x_1)$$
$$\times G^{(0)}(x_1-y_1)G^{(0)}(y_1-x'). \tag{9}$$

We consider the Fourier-representation of the Green's functions. If we write

$$G(x-x') = V^{-1}\sum_{\mathbf{k}} G_k(t-t')\exp\{i\mathbf{k}(\mathbf{x}-\mathbf{x}')\},$$

we get from (5) (dropping for the sake of simplicity the spin indices):

$$G_k(t) = \begin{cases} \langle a_k e^{-Ht}a_k^+\rangle e^{E_0 t}, & t>0, \\ -\langle a_k^+ e^{Ht}a_k\rangle e^{-E_0 t}, & t<0. \end{cases} \tag{10}$$

We now follow Galitskii and Migdal[4] and write the operators a_k and a_k^+ in the energy representation, and (10) is then transformed to

$$G_k(t) = \begin{cases} \sum_s |(a_k)_{0s}|^2\exp\{-(E_s-E_0)t\}, & t>0 \\ -\sum_s |(a_k^+)_{0s}|^2\exp\{(E_s-E_0)t\}, & t<0 \end{cases} \tag{11}$$

(the sum over s is over all excited states of the system).

In the first sum in (11) $E_S = E_S(N-1)$, in the second sum $E_S = E_S(N+1)$. We have $E_S(N-1) - E_0(N) = \epsilon_S - \mu + O(N^{-1})$; $E_S(N+1) - E_0(N) = \epsilon_S + \mu + O(N^{-1})$, where $\mu = \partial E_0/\partial N$ is the chemical potential and $\epsilon_S = E_S(N) - E_0(N)$ the excitation energy ($\epsilon_S > 0$). Hence,

$$G_k(t) = \begin{cases} e^{-\mu t}\sum_s |(a_k)_{0s}|^2 e^{-\varepsilon_s t}, & t>0 \\ -e^{-\mu t}\sum_s |(a_k^+)_{0s}|^2 e^{\varepsilon_s t}, & t<0. \end{cases} \tag{12}$$

$G_k(t)\,e^{\mu t}$ is thus a regular function as $t \to \pm\infty$ and can thus be expanded in a Fourier integral. We change thus to the expansion

$$G_k(t) = \frac{1}{2\pi i}\int_C G_k(\varepsilon)e^{-\varepsilon t}d\varepsilon, \tag{13}$$

where the integration contour C is a vertical straight line in the complex plane of the variable ϵ which cuts the real axis in the point $\epsilon = \mu$ (Fig. 3).

One can obtain from (12) Lehmann's expansion[11]

$$G_k(\varepsilon) = \int_{-\infty}^{\infty}\frac{\rho(k,E)}{E+\mu-\varepsilon}dE, \tag{14}$$

where $\rho(k, E)$ is a real positive function. $G_k(\epsilon)$

*The times corresponding to the end points of dotted lines are the same as we assume the interaction v to be instantaneous.

†Similar rules for assignments are, for instance, also used in reference 3 for the usual time-dependent Green's functions.

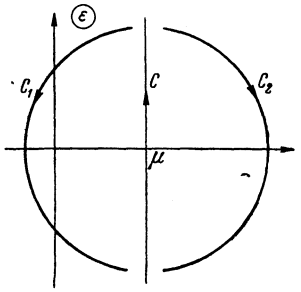

FIG. 3

is a regular function in the upper and lower half-plane of the complex variable ϵ but may have singularities (poles) on the real axis.*

It can be seen from Eq. (10) that once the single-particle Green's function G is known, one can evaluate the momentum distribution function of the particles:

$$n(k) = \langle a_k^+ a_k \rangle \tag{15}$$

using the relation

$$n(k) = -\lim_{t \to -0} G_k(t). \tag{16}$$

n(k) is equal to the quantum-mechanical average of the number of particles in a state with a well defined momentum k. When there is no interaction $n(k) = n^{(0)}(k)$ [see Eq. (8)] which corresponds to a filled Fermi-sphere (Fermi-filling). The effect of the interaction leads to a transition of electrons from the Fermi sphere and occupation of states with $k > k_F$; as a result there occur holes ($k < k_F$) and particles ($k > k_F$).

Migdal and Galitskii[4,7] considered the distribution function (15) and established some general properties of this function. In particular, they showed that the discontinuity in n(k) at $k = k_F$ remains whatever the interaction between the particles. This fact is confirmed in the present paper by a direct calculation of the momentum distribution function of the particles n(k) as a power series in the reciprocal of the density of the electron gas.

We turn to the calculation of n(k). We get in first approximation from (9) (see Fig. 1a)

$$G_k^{(1)}(t) = e^{-\mu t} \Sigma_k^{(1)} \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\nu t}}{(\varepsilon_k^0 - \mu - i\nu)^2} d\nu, \tag{17}$$

$$\Sigma_k^{(1)} = \frac{1}{V} \sum_q v(q)\, n^{(0)}(k+q). \tag{18}$$

Using (16) we get from this for the distribution function

$$n^{(1)}(k) = -\Sigma_k^{(1)} \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\nu}{(\varepsilon_k^0 - \mu - i\nu)^2} = \Sigma_k^{(1)} \delta(\varepsilon_k^0 - \mu). \tag{19}$$

The diagram of Fig. 1a leads thus everywhere except at $k = k_F$ to a zero value of n(k), while at $k = k_F$, n(k) turns out to be infinite. The same is true, as one can easily check, for the diagrams of Fig. 2c, d, Fig. 4 a – e, and so on.

However, if we sum all such diagrams (i.e., if we "renormalize") the infinities disappear. We renormalize the free particle propagation lines, by taking the sum of the infinite class of diagrams of the kind of Fig. 1a, Fig. 2c,d, Fig. 4 a–e, and so on. We shall call all such diagrams exchange diagrams.* We denote the corresponding renormalized propagation function by $S(x - x')$. In Fig. 5 we give the graphic equation for S where the thin line corresponds to $G^{(0)}$ and the thick line to S. One verifies easily that an expansion of S for small v leads to the exchange diagrams for S which were enumerated in the foregoing.

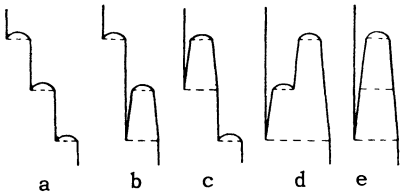

FIG. 4

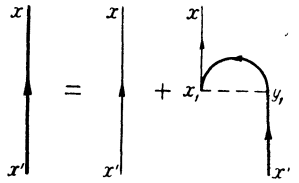

FIG. 5

The equation for S can also be obtained from (7) if we put

$$G_{\alpha\beta}(x; x') = S(x - x')\, \delta_{\alpha\beta},$$

$$G_{\alpha\beta\gamma\delta}(x_1 x_2; x_1' x_2') = S(x_1 - x_1')\, S(x_2 - x_2')\, \delta_{\alpha\gamma}\delta_{\beta\delta} - S(x_1 - x_2')\, S(x_2 - x_1')\, \delta_{\alpha\delta}\delta_{\beta\gamma}. \tag{20}$$

It has the form

*We note that the poles of the Fourier component of the time-dependent causal Green's function $G_k^c(\varepsilon)$ (in the usual Heisenberg representation) lie either above or below the real axis, which corresponds to the presence of damping of the corresponding quasi-particles. Similar problems have been considered by a number of authors.[3,5,6] In the present paper we aim mainly at studying the momentum distribution function of the particles for which the technique used here is relatively more convenient.

*We call exchange diagrams those diagrams which are obtained by iterations from diagrams of lower order by successively adding to one of the propagation lines the simplest diagram of Fig. 1a.

$$\left(\frac{\partial}{\partial t} - \frac{\hbar}{2m}\Delta\right) S(x-x') + \int dy\, v(|x-y|)\, S(x-y)\, S(y-x') = \delta^4(x-x'). \quad (21)$$

Using the Fourier representation we write (21) in the form

$$(\varepsilon_k^0 - \varepsilon) S_k(\varepsilon) + \frac{1}{V}\sum_q v(q) \frac{1}{2\pi i} \int_{C+C_1} S_{k+q}(\varepsilon')\, d\varepsilon'\, S_k(\varepsilon) = 1 \quad (22)$$

(see Fig. 3 for the integration contour).

One can easily verify that the solution of this non-linear integral equation has the simple form

$$S_k(\varepsilon) = \frac{1}{\varepsilon_k^0 - \varepsilon - \Sigma_k^{(1)}} = \frac{1}{\varepsilon_k - \varepsilon}, \quad (23)$$

where the quantity $\Sigma_k^{(1)}$ is according to (18) equal to

$$\Sigma_k^{(1)} = \frac{e^2}{\pi\hbar} k_F \left\{1 + \frac{k_F^2 - k^2}{2kk_F} \ln\left|\frac{k_F + k}{k_F - k}\right|\right\}. \quad (24)$$

One sees from Eq. (20) that the renormalization which we have performed corresponds to taking the exchange effects exactly into account in all orders. It is clear from (23), as $\Sigma_k^{(1)}$ is independent of ϵ, that when the exchange effects are taken into account exactly the Fermi-filling is conserved, i.e., the distribution function n(k) evaluated by using (23) has the shape of a Fermi step-function; the limiting momentum k_F is connected with the chemical potential μ by the relation*

$$\varepsilon_{k_F} = \mu, \qquad \mu = \hbar k_F^2/2m - \frac{e^2}{\pi\hbar} k_F, \qquad k_F = (3\pi^2 n)^{1/3}. \quad (25)$$

It will be shown in the following that taking the non-exchange part of the interaction into account leads to a change in the rectangular form of the distribution function.

We must introduce for the following the energy operator M(x − x′) which is defined through the relation (see, for instance, reference 3)

$$G(x-x') = G^{(0)}(x-x') + \int d^4x_1\, d^4x_2\, G^{(0)}(x-x_1)\, M(x_1-x_2)\, G^{(0)}(x_2-x'). \quad (26)$$

That G is of this form is clear from the structure of the graphs for the single-particle Green's function which start or end with a free electron line $G^{(0)}$ (see Figs. 1, 2, 4).

If we write down the Fourier expansion of the energy operator

$$M(x-x') = \frac{1}{V}\sum_k e^{ik(x-x')} \frac{1}{2\pi i} \int_C d\varepsilon\, e^{-\varepsilon(t-t')} M_k(\varepsilon), \quad (27)$$

we get from (26)

$$G_k(\varepsilon) = G_k^{(0)}(\varepsilon) + G_k^{(0)}(\varepsilon)\, M_k(\varepsilon)\, G_k^{(0)}(\varepsilon), \quad (28)$$

where $G_k^{(0)}(\epsilon) = (\epsilon_k^{(0)} - \epsilon)^{-1}$.

We can now express the distribution function n(k) in terms of M, using (16), and we get

$$n(k) = n^{(0)}(k) - \frac{1}{2\pi i}\int_C \frac{M_k(\varepsilon)}{(\varepsilon_k^0 - \varepsilon)^2} d\varepsilon = n^{(0)}(k) + \nu(k). \quad (29)$$

The integral in Eq. (29) can be evaluated by means of the residue theorem; to do this we first split $M_k(\epsilon)$:

$$M_k(\varepsilon) = M_k^+(\varepsilon) + M_k^-(\varepsilon), \quad (30)$$

where $M_k^+(\epsilon)$ is that part of $M_k(\epsilon)$ which is regular (without poles) in the right hand half-plane Re $\epsilon > \mu$ (Fig. 3) and $M_k^-(\epsilon)$ is regular in the left-hand half-plane Re $\epsilon < \mu$ [if $M_k(\epsilon)$ contains a part which is regular for all ϵ, i.e., a constant, it must be contained in $M_k^-(\epsilon)$]. After this splitting up we get from Eq. (29)

$$\nu(k) = -\frac{1}{2\pi i}\int_{C+C_1} \frac{M_k^-(\varepsilon)}{(\varepsilon_k^0 - \varepsilon)^2} d\varepsilon - \frac{1}{2\pi i}\int_{C+C_2} \frac{M_k^+(\varepsilon)}{(\varepsilon_k^0 - \varepsilon)^2} d\varepsilon, \quad (31)$$

where C_1 and C_2 are the semi-circles of infinite radius which lie respectively in the left- and the right-hand half-planes (Fig. 3). Applying the residue theorem to (31) we get

$$\nu(k) = \begin{cases} \nu^+(k), & k > k_F \\ \nu^-(k), & k < k_F, \end{cases} \quad (32)$$

$$\nu^{\pm}(k) = \pm\left(\frac{d}{d\varepsilon} M_k^{\pm}(\varepsilon)\right)_{\varepsilon=\varepsilon_k^0}. \quad (33)$$

One can show that the ground state energy E_0 is a sum of the energy of the non-interacting particles with a distribution function n(k) plus an extra term connected with interparticle correlations:

$$E_0 = 2\sum_k \varepsilon_k^0 n(k) + \sum_K \zeta(k), \quad (34)$$

where by analogy with (33) $\zeta^{\pm}(k) = \pm M_k^{\pm}(\epsilon_k^0)$. To evaluate the distribution function it is now necessary to start from renormalized diagrams in which $G^{(0)}$ is replaced by S. The contributions to G in the lowest approximation are the diagrams of Figs. 2a, b (we retain for the renormalized free particle propagation function S in the diagrams the previous notation of a full-drawn line). One can, however, easily verify that the diagram of Fig. 2a leads to an infinite contribution; this is connected with the divergence of integrals for small momentum transfers q. These divergences can be removed by renormalizing the interaction lines (see

*We note that Eq. (23) is not a trivial consequence of the introduction of the principal part of the energy operator Σ (see reference 4). A similar equation would occur if we summed only the diagrams of Fig. 1a, Fig. 2c, Fig. 4a, and so on. The difference lies in the meaning of the quantities μ and k_F.

also references 5, 6, 9, 10, and others). To do this it is necessary to sum the class of the most strongly divergent diagrams which are given in Fig. 6. Here the same momentum **q** is transferred along each of the interaction lines. These diagrams correspond to virtual creation and annihilation processes of electron-hole pairs ($k > k_F$ and $k < k_F$), as each upward line in the diagram corresponds to a factor $1-n^{(0)}(k)$ in the k-representation while a downward line correspond to a factor $n^{(0)}(k)$. Gell-Mann and Brueckner[8] were the first to perform such a summation for an electron gas (in a different technique).

To sum the diagrams given in Fig. 6 we introduce an effective interaction potential $V(x-x')$ which we define by the graphic equation of Fig. 7

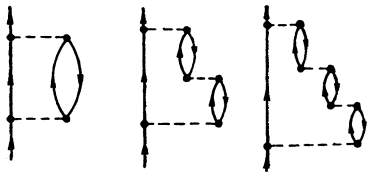

FIG. 6

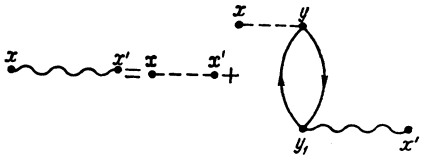

FIG. 7

(the wavy line corresponds to V). We have thus

$$V(x-x') = v(\mathbf{x}-\mathbf{x}')\,\delta(t-t') + \int dy\,dy_1\, v(\mathbf{x}-\mathbf{y})\, F(y-y_1)\, V(y_1-x'), \quad (35)$$

$$F(x-x') = 2S(x-x')\,S(x'-x). \quad (36)$$

For the Fourier component of the function $F(x-x')$ we get*

$$F_q(t) = -\frac{2}{V}\sum_{\mathbf{k}} n^{(0)}(k)\,(1-n^{(0)}(k+q)) \times \exp\{-(\varepsilon^0_{k+q}-\varepsilon^0_k)\,t\}. \quad (37)$$

The function F determined by Eq. (37) is the same as the electron-hole pair propagation function introduced by Gell-Mann and Brueckner.[8]†

*We can replace S here by the renormalized function $G^{(0)}$ obtained from Eq. (8).

†F is that part of the polarization operator which takes the virtual pair creation processes into account. Similarly, V is in the present approximation the propagation function of the Bose branch of the excitations in the system of interacting fermions (i. e., the plasmon propagation function).

If we write

$$F_q(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F_q(\omega)\, e^{i\omega t}\, d\omega,$$

we get from (37)*

$$F_q(\omega) = -(mk_F/\pi^2\hbar)\, R_q(u), \qquad u = \omega/q;$$

$$R_q(u) = \frac{1}{2}\left\{1 - u\left(\operatorname{arctg}\frac{2+q}{2u} - \operatorname{arctg}\frac{2-q}{2u}\right) + \frac{1}{2q}\left(1+u^2-\frac{q^2}{4}\right)\ln\frac{4u^2+(2+q)^2}{4u^2+(2-q)^2}\right\} \quad (38)$$

(in the last equation we have gone over to dimensionless variables q/k_F, ϵ/ϵ_F, u/u_F, where $u_F = \hbar k_F/m$ is the velocity at the Fermi surface).

One can easily solve Eq. (35) if one goes over to the Fourier representation. The result is

$$V_q(\omega) = v(q)/[1 - v(q)\,F_q(\omega)], \quad (39)$$

or in dimensionless variables

$$V_q(u) = 4\pi/[q^2 + \alpha r_s R_q(u)], \quad (40)$$

$\alpha = (4/\pi)(4/9\pi)^{1/3} = 0.663$. Here r_S is the usual parameter occurring in the theory of a free electron gas (see, for instance, reference 12) which is defined as $r_S = r_0/a_0$, where $4\pi r_0^3/3 = V/N = 1/n$; $a_0 = \hbar^2/me^2$ is the Bohr radius; $r_S \sim e^2$. At $T = 0$ the quantity r_S turns out to be in the case of the electron gas the only dimensionless parameter in the theory, and the approximation $r_S \to 0$ (i.e., $n \to \infty$) the only reasonable physical approximation in which there is a small parameter.

As the function $R_q(u)$ does not tend to zero as $q \to 0$, but according to (38) is equal to

$$R_0(u) = 1 - u\,\operatorname{arctg} u^{-1}, \quad (41)$$

the result of the summation is to replace the Coulomb potential $v(q) = 4\pi/q^2$ which leads to a divergence as $q \to 0$ by the screened potential $V_q(u) \approx 4\pi/(q^2 + \alpha r_S R_0(u))$ which no longer diverges for small momenta.

We now shall compute $n(k)$ directly. It is necessary in the first non-vanishing approximation in V to sum the diagrams of Fig. 6. We have in that approximation (the summation is over **q**)

$$M_k^+(\varepsilon) = \frac{1}{V}\sum_{|\mathbf{k}+\mathbf{q}|<k_F} v(q)\,\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\,\frac{F_q(\omega)\,V_q(\omega)}{-\varepsilon+\varepsilon^0_{k+q}+i\omega},$$

$$M_k^-(\varepsilon) = -\frac{1}{V}\sum_{|\mathbf{k}+\mathbf{q}|>k_F} v(q)\,\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\,\frac{F_q(\omega)\,V_q(\omega)}{\varepsilon-\varepsilon^0_{k+q}+i\omega}, \quad (42)$$

whence we get, using Eq. (33) (the summation is over **q**)

*arctg = $\tan^{-1}$.

$$\nu^+(k) = \frac{1}{V}\sum_{|\mathbf{k}+\mathbf{q}|<k_F} v^2(q)\frac{1}{2\pi} \times \int_{-\infty}^{\infty} \frac{F_q(\omega)}{(\varepsilon_k^0 - \varepsilon_{k+q}^0 + i\omega)^2}\,d\omega, \quad k > k_F,$$

$$\nu^-(k) = -\frac{1}{V}\sum_{|\mathbf{k}+\mathbf{q}|<k_F} v^2(q)\frac{1}{2\pi} \times \int_{-\infty}^{\infty} \frac{F_q(\omega)}{(\varepsilon_{k+q}^0 - \varepsilon_k^0 + i\omega)^2}\,d\omega, \quad k < k_F. \tag{43}$$

It is clear, first of all, that the relation

$$\sum_{k<k_F} \nu^-(k) + \sum_{k>k_F} \nu^+(k) = 0,$$

which expresses the conservation of particle number, is satisfied. This relation is also valid in the higher approximations.

Changing in Eq. (43) to dimensionless variables, we get

$$\nu^+(k) = \beta r_s^2 \int_{-\infty}^{\infty} du \int \frac{dq}{q} \int_{|\mathbf{k}+\mathbf{q}|<1} \frac{dx}{(-kx + q/2 + iu)^2} \times \frac{R_q(u)}{q^2 + \alpha r_s R_q(u)}, \quad k > 1,$$

$$\nu^-(k) = -\beta r_s^2 \int_{-\infty}^{\infty} du \int \frac{dq}{q} \int_{|\mathbf{k}+\mathbf{q}|>1} \frac{dx}{(-kx + q/2 + iu)^2} \times \frac{R_q(u)}{q^2 + \alpha r_s R_q(u)}, \quad k < 1, \tag{44}$$

where

$$\beta = (2/\pi^3)(4/9\pi)^{2/3} = 0.0175, \qquad x = \cos(\mathbf{k}, \mathbf{q}).$$

One can immediately easily evaluate the magnitude of the discontinuity $\Delta = \nu^+(1) - \nu^-(1)$ from (44):

$$\Delta = -\beta r_s^2 \int_{-\infty}^{\infty} du \int_0^{\infty} q\,dq \int_{-1}^{1} \frac{dx}{u + i(x + q/2)} \frac{R_q'(u)}{(q^2 + \alpha r_s R_q(u))^2}. \tag{45}$$

Integrating over x and replacing $R_q(u)$ by $R_0(u)$ we get the main term of the expansion of Δ as $r_s \to 0$ in the form

$$\Delta \approx 2Ar_s,$$

where the numerical constant A is equal to

$$A = -\frac{\beta}{\alpha}\int_0^{\infty} \frac{R_0'(u)}{R_0(u)} \operatorname{arctg}\frac{1}{u}\,du = -\frac{\beta}{\alpha}\int_0^{\infty} \frac{\ln R_0(u)}{1+u^2}\,du \qquad (A > 0). \tag{46}$$

One can also obtain from (44) the asymptotic behavior of $\nu^{\pm}(k)$ near k = 1. It is of the form

$$\nu^{\pm}(k) \approx \pm Ar_s g(|k-1|/\sqrt{\alpha r_s}), \qquad |k-1| \ll 1, \tag{47}$$

where the function $g(\xi)$ is equal to

$$g(\xi) = \frac{f(\xi)}{f(0)},$$

$$f(\xi) = -\int_0^{\infty} \frac{R_0'(u)}{R_0(u) - \xi^2/u^2} \times \left\{\operatorname{arctg}\frac{1}{u} - \frac{\xi}{uR_0^{1/2}(u)} \operatorname{arctg}\frac{R_0^{1/2}(u)}{\xi}\right\} du. \tag{48}$$

One can find the asymptotic behavior of $g(\xi)$ as $\xi \ll 1$:

$$g(\xi) \approx 1 + \gamma\xi\ln\xi, \qquad \gamma = (\beta/\alpha A)(\pi/2)^2(1 + 4\sqrt{3}/\pi) \tag{49}$$

(in practice, this asymptotic behavior is, however, insufficient as one needs to know $g(\xi)$ as $\xi \sim 1$).

It is clear from (47) that the particle distribution function $\nu^+(k)$ and the hole distribution function $\nu^-(k)$ near the Fermi surface will be symmetrical (Fig. 8). The magnitude of the discontinuity of the total distribution function $n(k) = n^{(0)}(k) + \nu(k)$ at k = 1 is equal to $Z = 1 - \Delta \approx 1 - 2Ar_s$ ($r_s \to 0$).

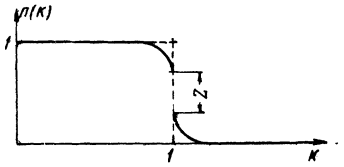

FIG. 8

In conclusion we determine the total number of particles outside the Fermi sphere (which is also equal to the number of holes inside the Fermi sphere) $N' = 2\Sigma\nu^+(k)$, $k > k_F$; this can be done conveniently by starting directly from (44). The main term in the expansion as $r_s \to 0$ is of the form

$$\bar{n} = N'/N \approx Br_s^{3/2}, \tag{50}$$

$$B = -\frac{3\pi\beta}{4\sqrt{\alpha}}\int_0^{\infty} \ln\left(1 + \frac{1}{u^2}\right)\frac{R_0'(u)}{\sqrt{R_0(u)}}\,u\,du. \tag{51}$$

A numerical integration of Eqs. (46) and (51) leads to the following values of the constants A, B, and γ:

$$A = 0.089, \qquad B = 0.051, \qquad \gamma = 1.61.$$

The dimensionless quantity $\epsilon = Br_s^{3/2}$ characterizes the degree of deviation from the perfect degenerate Fermi gas. r_s changes for different metals between the limits $r_s = 1.8$ to 5.6, whence $\epsilon = 0.12$ to 0.67. One may thus expect that for metals with the highest electron density the approximation considered here is sufficiently good (there remains,

of course, the additional circumstance that we replaced the metal lattice by a uniform positive background).

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230