The Fermi – Dirac function and the anisotropic distribution of the interacting electrons

Boris V. Bondarev

Moscow Aviation Institute, Volokolamskoye Shosse 4, 125871 Moscow, Russia
E-mail: bondarev.b@mail.ru

The distribution function for a system of interacting electrons in metals is multivalent in a certain region of wave vectors. One solution among many is isotropic. For other solutions the distribution of electrons over the wave vectors is anisotropic. In the simplest case, the anisotropy arises as a result of the repulsion between electrons in states with the wave vectors $k$ and $-k$.

Key words: Anisotropy, distribution, interacting electrons.

1. Mean-field approximation

The equilibrium function $w_k$ of electron distribution over the wave vectors in the mean field approximation can be found from the equation [1 – 3]:

$$\ln \frac{1 - w_k}{w_k} = \beta (\bar{\varepsilon}_k - \mu),$$

(1)

where $w_k$ – the probability of the state described by the wave function $\psi_{kn}(r) \chi_{\sigma}(\xi)$ being occupied by one of the electrons from the equilibrium system with the wave vector $k$; $\beta = 1/kT$, $T$ – temperature,

$$\bar{\varepsilon}_k = \varepsilon_k + \sum_{k'} \varepsilon_{kk'} w_{k'},$$

(2)

– the average energy of an electron in one of the states with the wave vector $k$, $\varepsilon_k$ – the energy of electron without regard to its interaction with other electrons, $\varepsilon_{kk'}$ – the interaction energy of electrons with wave vectors $k$ and $k'$, $\mu$ – chemical potential.

If the electrons do not interact with each other, i.e. $\varepsilon_{kk'} = 0$, then from the equation (1) we find the function of Fermi – Dirac

$$w_k = \frac{1}{1 + e^{\beta (\varepsilon_k - \mu)}}.$$
2. Repulsion of electrons with wave vectors $k$ and $-k$

We assume the approximate formula for the interaction energy

$$\varepsilon_{kk'} = I \delta_{k+k'},$$  \hspace{1cm} (3)

where $I$ – a positive constant. According to this approximate formula only those electrons interact - the wave vectors of which are equal in absolute value and opposite in direction: $k' = -k$. In this case $I$ is the interaction energy of the electrons.

By the formula (2) the average energy of an electron will be equal to

$$\bar{\varepsilon}_k = \varepsilon_k + I w_{-k}. \hspace{1cm} (4)$$

According to this formula, the greater is the probability $w_{-k}$ of the state with the wave vector $-k$ being occupied, the larger is the energy of the electron with the wave vector $k$. Thus, the electron with the wave vector $-k$ as if displaces the electron from the state with the wave vector $k$.

Put the expression (4) in the equation (1). We obtain the equation (5)

$$\ln \frac{1 - w_k}{w_k} = \beta (\varepsilon_k + I w_{-k} - \mu).$$ \hspace{1cm} (5)

Change the vector $k$ to the vector $-k$ in the equation (5) and obtain the equation (6)

$$\ln \frac{1 - w_{-k}}{w_{-k}} = \beta (\varepsilon_k + I w_k - \mu).$$ \hspace{1cm} (6)

The equations (5) and (6) form a system with two unknowns $w_k$ and $w_{-k}$. It is easy to see that the probability $w_k$ is a complex function of the vector $k$, in which the electron kinetic energy $\varepsilon_k$ plays the role of intermediate variable:

$$w_k = w(\varepsilon_k).$$ \hspace{1cm} (7)

The system of the equations (5) and (6) has two types of solutions. The first are the isotropic distribution functions, which for all values of the wave vector satisfy the condition

$$w_{-k} = w_k.$$ \hspace{1cm} (8)

The isotropic distribution function is a solution of the equation
\[ \ln \frac{1 - w_k}{w_k} = \beta (\varepsilon_k + I w_k - \mu). \]  \hspace{1cm} (9)

There are also anisotropic distribution functions for which the condition (7) is not satisfied for some values of the wave vector:

\[ w_{-k} \neq w_k. \]

And such anisotropy of the electrons distribution over the Bloch states can take place even in the absence of external fields.

Using the notation

\[ w_{-k} = w_1(\varepsilon_k), \quad w_k = w_2(\varepsilon_k), \]  \hspace{1cm} (10)

the equations (5) and (6) can be written as:

\[
\begin{align*}
\ln \frac{1 - w_1}{w_1} &= \frac{4}{\tau} (\epsilon + w_2), \\
\ln \frac{1 - w_2}{w_2} &= \frac{4}{\tau} (\epsilon + w_1),
\end{align*}
\]

(11) where

\[ \epsilon = \frac{\varepsilon - \mu}{I}, \quad \tau = \frac{4 kT}{I}. \]

In the equations (11) the unknowns are the functions

\[ w_1 = w_1(\varepsilon) \quad \text{and} \quad w_2 = w_2(\varepsilon). \]

When the electrons distribution over the wave vectors is isotropic, we should put in the equations (11) \( w_1 = w_2 = w_0 \). It is convenient to rewrite the obtained equation as:

\[ \epsilon = \frac{\tau}{4} \ln \frac{1 - w_0}{w_0} - w_0. \]  \hspace{1cm} (12)

The equation (12) determines the dependence \( w_0 = w_0(\epsilon) \), the graphs of which for different values of temperature are shown in Fig.1 as monotonically decreasing curves.

When the electrons distribution over the wave vectors is anisotropic, in the equations (11) the probabilities \( w_1 \) and \( w_2 \) should be considered as different functions of energy \( \epsilon \): \( w_1 = w_1(\varepsilon) \), \( w_2 = w_2(\varepsilon) \). In order to establish these relationships, we introduce new variables \( d \) and \( s \) by means of relations
\[ w_2 - w_1 = d, \quad w_1 + w_2 = 1 + s. \]  

Without loss of the generality we can take the difference \(d\) between two values of the distribution functions \(w_1\) and \(w_2\) as the non-negative value: \(d \geq 0\), the greatest value of \(d\) being equal to one: \(d \in [0, 1]\). The parameter \(s\) can take values from \(-1\) to 1: \(s \in [-1, 1]\). We solve the equation (13) with respect to the probabilities \(w_1\) and \(w_2\):

\[ w_1 = \frac{1}{2} (1 + s - d), \quad w_2 = \frac{1}{2} (1 + s + d). \]  

With the help of (14) we transform the system of the equations (11). To do this at first we subtract one equation from the other and then add the equations. As a result, we obtain the following system of the equations:

\[
\begin{aligned}
\frac{(1 + d)^2 - s^2}{(1 - d)^2 - s^2} &= e^{4d/\tau}, \\
\epsilon &= \frac{\tau}{8} \ln \frac{(1 - s)^2 - d^2}{(1 + s)^2 - d^2} - \frac{1}{2} (1 + s).
\end{aligned}
\]  

The first equation in this system can be easily solved with respect to \(s\):

\[ s(d) = \pm \sqrt{\frac{(1 - d)^2 e^{4d/\tau} - (1 + d)^2}{e^{4d/\tau} - 1}}. \]

By virtue of relations (14) the probabilities of \(w_1\) and \(w_2\) can also be viewed as the functions of the parameter \(d\): \(w_1 = w_1(d), \ w_2 = w_2(d)\). The second equation of (15) allows us to express the energy \(\epsilon\) of an electron through the parameter \(d\). With the help of the dependencies obtained it is easy to construct the graphs of the functions \(w_1 = w_1(\epsilon)\) and \(w_2 = w_2(\epsilon)\) for the different values of the temperature. Such graphs are shown in the Fig. 2.

The character of the electrons distribution in Bloch states depends on the relationship between the metal temperature \(T\) and the critical temperature \(T_c\):

\[ T_c = \frac{I}{4k}. \]  

At the temperatures \(T \geq T_c\) the distribution function \(w = w(\epsilon)\) is single-valued and satisfies the condition (8) for all values of the electron energies \(\epsilon\).
At $T < T_c$ there is a range of the energy values $(\epsilon_1, \epsilon_2)$ at each point of which the function $w = w(\epsilon)$ can take any of three values: $w_1(\epsilon) < w_0(\epsilon) < w_2(\epsilon)$. Outside this interval, the distribution function $w = w(\epsilon)$ takes only one value $w_0(\epsilon)$. The function $w_k = w_0(\epsilon_k)$ is a solution of the equation (12) and describes an isotropic electron distribution over the wave vectors.

At $T < T_c$ in a narrow layer $S(\epsilon_1, \epsilon_2)$ below the Fermi surface $\epsilon_k = \mu$ the anisotropic electrons distribution over the wave vectors is possible. This distribution is described by functions

$$w_k = w_2(\epsilon_k), \quad w_{-k} = w_1(\epsilon_k)$$

at $\epsilon \in (\epsilon_1, \epsilon_2)$.

At $T = 0$ the isotropic distribution function has the form

$$w_k = \begin{cases} 
1 & \text{at } \epsilon_k \leq \mu - I, \\
-\frac{1}{I}(\epsilon_k - \mu) & \text{at } \mu - I < \epsilon_k < \mu, \\
0 & \text{at } \epsilon_k \geq \mu,
\end{cases} \quad (17)$$

and the anisotropic distribution is such that

$$w_k = 1 \text{ at } \epsilon_k \leq \mu - I,$$

$$w_k = 1, \quad w_{-k} = 0 \text{ or } w_k = 0, \quad w_{-k} = 1 \text{ at } \mu - I < \epsilon_k < \mu, \quad (18)$$

$$w_k = 0 \text{ at } \epsilon_k \geq \mu.$$

The formulae (18) show that below the Fermi surface there is a layer $S$, defined by the inequalities

$$\mu - I < \epsilon_k < \mu, \quad (19)$$

in which the distribution of the electrons over the wave vectors is anisotropic, i.e. of two states with wave vectors $k$ and $-k$ in this layer one is vacant and the other is necessarily occupied.

It can be shown that the electrons in an anisotropic distribution have a lower energy than in the isotropic. Therefore, in a layer of the electrons the anisotropic distribution is occupied and the isotropic one is empty.

Calculation show that anisotropic solutions have lower energy than the isotropic. Accordingly the real solutions are shown in Fig. 3 – 5.
3. Anisotropy parameter

The difference \( d = w_2 - w_1 \) between the two values of the anisotropic distribution function takes its maximum value \( d_{\text{max}} \) at \( \epsilon = 0.5 \). At the same time \( w_0 = 0.5 \) and \( s = 0 \). The dependence \( d_{\text{max}} \) on the temperature can be found from the first equation of the system (15), putting in it \( s = 0 \):

\[
\frac{2d_{\text{max}}}{\tau} = \ln \frac{1 + d_{\text{max}}}{1 - d_{\text{max}}}. \tag{20}
\]

The graph of this function is shown in the Fig. 6.

4. The average energy of one electron

The dependence of the average energy \( \overline{\varepsilon}_k \) of one electron on its kinetic energy \( \varepsilon_k \) is given by (4). As it can be seen from this formula, the energy of the electron with wave vector \( k \) depends on whether a state with wave vector \( -k \) is vacant or occupied. The average energy of an electron \( \overline{\varepsilon} \) can be represented as a function of its kinetic energy \( \varepsilon \) as follows:

\[
\overline{\varepsilon}(\varepsilon) = \varepsilon + I w_1(\varepsilon). \tag{21}
\]

The graphs of this function for different values of the temperature are shown in the Fig. 7.

5. Conclusions

In this work we show the existence of the anisotropy in the distribution of the interacting electrons over the wave vectors. In the simplest case, such anisotropy arises as a result of the repulsion between electrons in the states with the wave vectors \( k \) and \( -k \).

It can be shown that the anisotropy arises also in the other dependencies of the interaction energy \( \varepsilon_{kk'} \) of the electrons.

The following paper should be devoted to the physical phenomena that are the consequences of the anisotropy of the distribution functions.

References

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Fig. 1.

Fig. 2.
Fig. 3.

Fig. 4.
Fig. 5.

Fig. 6.
Fig. 7.
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Fig. 1. The isotropic distribution function of the conduction electrons over the energy at the different values of the temperature $\tau$: 1 – $\tau = 0$; 2 – $\tau = 0.25$; 3 – $\tau = 0.8$.

Fig. 2. The anisotropic distribution function of the conduction electrons over the energy at the different values of the temperature $\tau$: 1 – $\tau = 0$; 2 – $\tau = 0.25$; 3 – $\tau = 0.8$; 4 – $\tau = 0.95$.

Fig. 3. The anisotropic distribution function of the conduction electrons over the energy at the different values of the temperature $\tau = 0$ with the lowest energy.

Fig. 4. The anisotropic distribution function of the conduction electrons over the energy at the different values of the temperature $\tau = 0.25$ with the lowest energy.

Fig. 5. The anisotropic distribution function of the conduction electrons over the energy at the different values of the temperature $\tau = 0.8$ with the lowest energy.

Fig. 6. The anisotropy parameter of the electron distribution $d_{\text{max}}$ as a function of the temperature $\tau$.

Fig. 7. The dependence of the average electron energy $\overline{\varepsilon}$ on its kinetic energy $\varepsilon$ for the temperature $\tau$: 1 – $\tau = 0$; 2 – $\tau = 0.5$; 3 – $\tau = 0.8$. 

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