Quantum master equation for a system of identical particles and the anisotropic distribution of the interacting electrons

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We consider an open quantum many-particle system in which there are dissipative processes. The evolution of this system is described by a kinetic equation for the density matrix. From the equation describing a random Markov process in this system, we obtain an equation for the single-particle statistical operator. This equation describes the evolution of a system of identical particles in a mean-field approximation. The equation for interacting particles in thermodynamic equilibrium was obtained. The distribution function of a system of interacting electrons in metals has multivalence in a certain region of wave vectors. Among many solutions one is isotropic. Other solutions have the anisotropy of the electron distribution over the wave vectors. The anisotropy arises as a result of repulsion and attraction between electrons.

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1. Introduction

The most general statistical description of any system in quantum mechanics is performed by using the statistical operator [1]. If the system state changes with time, then the statistical operator is a function of time:

\[ \hat{\rho} = \hat{\rho}(t). \] (1.1)

When the system takes a random Markov process, this function can be found from the kinetic equation of the form [2 – 14]

\[ i\hbar \dot{\hat{\rho}} = \left[ \hat{H}, \hat{\rho} \right] + \frac{1}{2} i\hbar \sum_{k,l} C_{kl} \left( \left[ \hat{a}_k \hat{\rho}, \hat{a}_l^+ \right] + \left[ \hat{a}_k, \hat{\rho} \hat{a}_l^+ \right] \right), \] (1.3)

This equation is called the Lindblad equation [6]. Here \( a_k \) is an operator, \( k = 1, 2, ... \) – the number of the operator, \( C_{kl} \) - constants.

Let us write the equation (1.3) for the quantum harmonic oscillator:

\[ i\hbar \dot{\hat{\rho}} = \left[ \hat{H}, \hat{\rho} \right] + \frac{1}{2} i\hbar A \left( \left[ \hat{a} \hat{\rho}, \hat{a}^+ \right] + \left[ \hat{\rho}, \hat{a} \hat{a}^+ \right] \right) + \frac{1}{2} i\hbar B \left( \left[ \hat{a}^+ \hat{\rho}, \hat{a} \right] + \left[ \hat{\rho}, \hat{a}^+ \hat{a} \right] \right), \] (1.4)
where

$$\hat{H} = \hbar \omega \left( \hat{a}^+ \hat{a} + \frac{1}{2} \right),$$

(1.5)

$A$ and $B$ are constants. The operator $\hat{a}$ has the form

$$\hat{a} = \frac{1}{\sqrt{2 \hbar \omega}} \left( \frac{i \hat{\rho}}{\sqrt{m}} + \sqrt{\kappa} \hat{x} \right).$$

(1.6)

Equation (1.4) surprisingly accurately describes the change of the state of the quantum harmonic oscillator with time, provided that

$$\frac{A}{B} = e^{\beta \hbar \omega},$$

(1.7)

where $\beta = 1/kT$ is the inverse temperature.

2. The hierarchy of statistical operators

Consider the system consisting of $N$ identical particles. The statistical operator $\hat{\rho}$ describing the state of this system can be written as follows:

$$\hat{\rho} = \hat{\rho}(1, 2, ..., N).$$

(2.1)

Here the numbers in parentheses denote the indices of the variables which are affected by this operator. The statistical operator like any other operator describing the state of the system of identical particles must be symmetric:

$$\hat{\rho}(..., i, ..., j, ...) = \hat{\rho}(..., j, ..., i, ...).$$

(2.2)

Let us assume the following normalization condition for the statistical operator:

$$\text{Tr}_{1...N} \hat{\rho}(1, ..., N) = N!.$$  

(2.3)

If the system state changes over time, the statistical operator is a function of time: $t$: $\hat{\rho} = \hat{\rho}(t)$. When we can be sure that the system takes a random Markov process, this function can be found from the equation

$$i \hbar \dot{\hat{\rho}} = [\hat{H}, \hat{\rho}] + i \hbar \hat{d} \hat{\rho}.$$  

(2.4)

The Hamiltonian operator in this equation can be written as the sum

$$\hat{H}(1, ..., N) = \sum_{i=1}^{N} \hat{H}(i) + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1 \atop j \neq i}^{N} \hat{H}(i, j),$$

(2.5)

where $\hat{H}(i)$ is a single-particle Hamiltonian, i.e. the energy operator of a single particle without considering its interaction with other particles; $\hat{H}(i, j)$ is the operator of the interaction of two particles. A single-particle Hamiltonian may contain dissipative terms. A two-particle Hamiltonian should be symmetric:

$$\hat{H}(i, j) = \hat{H}(j, i).$$

(2.6)

Under this condition, the Hamiltonian (2.5) will also be symmetric.

Suppose that the action of the dissipative operator $\hat{d}$ on the statistical operator $\hat{\rho}$ leads to the expression

$$\hat{d} \hat{\rho} = \frac{1}{2} \left( [\hat{a} \hat{\rho}, \hat{a}^+] + [\hat{a}^+, \hat{\rho} \hat{a}] \right).$$

(2.7)

Here the indices $k$ and $l$ near the operator $\hat{a}$ are omitted.
Suppose that the dissipative processes occurring in the system are caused by the stochastic interaction of particles with a heat reservoir. Moreover, each particle interacts with it independently of other particles. In this case the many-particle operator \( \hat{a} \) in the expression (2.7) can be written as the sum

\[
\hat{a}(1, \ldots, N) = \sum_{i=1}^{N} \hat{a}(i),
\]

where the operator \( \hat{a}(i) \) characterizes the effect of the heat reservoir on one of the particles.

Substitution of the sum (2.8) in the formula (2.7) gives

\[
\hat{d} \hat{\rho} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left( [\hat{a}(i) \hat{\rho}, \hat{a}^+(j) \hat{h}\hat{h}] + [\hat{a}(i), \hat{\rho} \hat{a}^+(j)] \right).
\]

It is impossible to solve the equation (2.4) with such a complex right-hand side. Therefore the practical interest is carried by the single-particle kinetic equation for the statistical operator \( \hat{\rho}(1) \), which is defined by the relation

\[
\hat{\rho}(1) = \frac{1}{(N-1)!} \text{Tr}_{2,\ldots,N} \hat{\rho}(1, 2, \ldots, N).
\]

This definition and condition (2.3) implies the normalization condition

\[
\text{Tr}_1 \hat{\rho}(1) = N.
\]

We define the two-particle statistical operator \( \hat{\rho}(1, 2) \) as

\[
\hat{\rho}(1, 2) = \frac{1}{(N-2)!} \text{Tr}_{3,\ldots,N} \hat{\rho}(1, 2, \ldots, N).
\]

This operator satisfies the normalization condition

\[
\text{Tr}_{12} \hat{\rho}(1, 2) = N (N - 1).
\]

3. The quantum kinetic equation for single-particle density matrix

To obtain the equation for the single-particle operator \( \hat{\rho}(1) \), let us apply the operation of coagulation \( \text{Tr}_{2,\ldots,N} \) to both sides of the equation (2.4). As

\[
\text{Tr}_i \left[ \hat{H}(i), \hat{\rho}(1, \ldots, N) \right] \equiv 0
\]

by definition (2.10), we obtain

\[
\text{Tr}_{2,\ldots,N} \sum_{i=1}^{N} \left[ \hat{H}(i), \hat{\rho}(\ldots, i, \ldots) \right] = (N-1)! \left[ \hat{H}(1), \hat{\rho}(1) \right].
\]

Due to the identity

\[
\text{Tr}_{ij} \left[ \hat{H}(i, j), \hat{\rho}(1, \ldots, N) \right] \equiv 0,
\]

taking into account the property (2.6) and the definition (2.12) we have

\[
\text{Tr}_{2,\ldots,N} \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left[ \hat{H}(i, j), \hat{\rho}(1, \ldots, N) \right] =
\]

\[
= \text{Tr}_{2,\ldots,N} \left( \sum_{j=2}^{N} \left[ \hat{H}(1, j), \hat{\rho}(1, \ldots, N) \right] + \frac{1}{2} \sum_{i=2}^{N} \sum_{j=2}^{N} \left[ \hat{H}(i, j), \hat{\rho}(1, \ldots, N) \right] \right) =
\]
Similarly
\[ \operatorname{Tr}_{2...N} \hat{a} \hat{b} = \frac{1}{2} \operatorname{Tr}_{2...N} \left( [\hat{a}(1) \hat{b}, \hat{a}^+(1)] + [\hat{a}(1), \hat{b} \hat{a}^+(1)] + \sum_{i=2}^{N} \left( [\hat{a}(i) \hat{b}, \hat{a}^+(i)] + [\hat{a}(i), \hat{b} \hat{a}^+(i)] \right) \right) \]

\[ + \sum_{i=2}^{N} \sum_{j=2}^{N} \left( [\hat{a}(i) \hat{b}, \hat{a}^+(j)] + [\hat{a}(i), \hat{b} \hat{a}^+(j)] \right) \right) = \frac{1}{2} (N-1)! \left( [\hat{a}(1) \hat{b}(1), \hat{a}^+(1)] + [\hat{a}(1), \hat{b}(1) \hat{a}^+(1)] + \left[ \operatorname{Tr}_{2} \hat{a}(2) \hat{b}(2), \hat{a}^+(1) \right] + \left[ \hat{a}(1), \operatorname{Tr}_{2} \hat{b}(1, 2) \hat{a}^+(2) \right] \right), \]

as
\[ \operatorname{Tr}_1 [\hat{a}(i), \hat{b} \hat{a}^+(j)] = 0, \quad \operatorname{Tr}_j [\hat{a}(i) \hat{b}, \hat{a}^+(j)] = 0. \]

Bringing together these expressions, we obtain the equation
\[ i \hbar \hat{b}(1) = [\hat{H}(1), \hat{b}(1)] + \operatorname{Tr}_2 [\hat{H}(1, 2), \hat{b}(1, 2)] + \frac{1}{2} i \hbar \left( [\hat{a}(1) \hat{b}(1), \hat{a}^+(1)] + [\hat{a}(1), \hat{b}(1) \hat{a}^+(1)] + \left[ \operatorname{Tr}_2 \hat{a}(2) \hat{b}(2), \hat{a}^+(1) \right] + \left[ \hat{a}(1), \operatorname{Tr}_2 \hat{b}(1, 2) \hat{a}^+(2) \right] \right). \]

We denote the matrix elements \( \hat{b}(1), \hat{b}(1, 2), \hat{H}(1, 2) \) and \( \hat{a}(1) \) in an \( \alpha \)-representation as follows:
\[ \theta_{\alpha \alpha_1} = \theta_{11'}, \quad \theta_{\alpha_1 \alpha_2} = \theta_{12', 12'}, \quad H_{\alpha \alpha_1} = H_{11'}, \quad H_{\alpha_1 \alpha_2} = H_{12', 12'}, \quad a_{\alpha \alpha_1} = a_{11'}, \]
and write the equation (3.1) in matrix form as:
\[ i \hbar \theta_{11'} = \sum_{\alpha_2} \left( H_{12} \theta_{21'} - \theta_{12} H_{21'} \right) + \sum_{\alpha_2} \sum_{\alpha_3} \sum_{\alpha_4} \left( H_{12, 34} \theta_{34, 1'2} - \theta_{12, 34} H_{34, 1'2} \right) + \]
\[ + \frac{1}{2} i \hbar \sum_{\alpha_2} \sum_{\alpha_3} \left( 2 a_{12} \theta_{23} a_{31'}^+ - a_{12}^+ a_{23} \theta_{31'} - \theta_{12} a_{23}^+ a_{31'} \right) + \]
\[ + \frac{1}{2} i \hbar \sum_{\alpha_2} \sum_{\alpha_3} \left( \theta_{12, 34} \left( a_{42} a_{31'}^+ - a_{42}^+ a_{31'} \right) + \left( a_{12} a_{34}^+ - a_{12}^+ a_{34} \right) \theta_{42, 31'} \right). \]

The two-particle density matrix describing the fermion system state must be antisymmetric. This matrix can be approximately expressed by means of the single-particle density matrix as follows:
\[ \theta_{12, 1'2'} = \theta_{11'} \theta_{22'} - \theta_{12'} \theta_{21'}. \]

Substituting this expression into the equation (3.2), we obtain the equation for the single-particle density matrix
\[ i \hbar \theta_{11'} = \sum_{\alpha_2} \left( H_{12} \theta_{21'} - \theta_{12} H_{21'} \right) + \frac{1}{2} i \hbar \sum_{\alpha_2} \sum_{\alpha_3} \left( 2 a_{12} \theta_{23} a_{31'}^+ - a_{12}^+ a_{23} \theta_{31'} - \theta_{12} a_{23}^+ a_{31'} \right) + \]
\[ + \frac{1}{2} i \hbar \sum_{\alpha_2} \sum_{\alpha_3} \left( \theta_{12, 34} \left( a_{42} a_{31'}^+ - a_{42}^+ a_{31'} \right) + \left( a_{12} a_{34}^+ - a_{12}^+ a_{34} \right) \theta_{42, 31'} \right) + \]
where
\[ \overline{H}_{12} = H_{12} + 2 \sum_{\alpha_3} \sum_{\alpha_4} H_{13,24} \varrho_{43} \varrho_{43}. \] (3.5)

Let us write the equation (3.4) in operator form
\[ i \hbar \dot{\varrho} = [\overline{H}, \varrho] + \frac{1}{2} i \hbar \left( [\hat{a} \varrho, \hat{a}^+] + [\hat{a}^+ \varrho, \hat{a}] \right) + \frac{1}{2} i \hbar \left( [\text{Tr}_2(\hat{a}^+ \varrho) \hat{a} - \text{Tr}_2(\hat{a} \varrho) \hat{a}^+ + \varrho] + [\hat{a}^+ \varrho, \hat{a}^+] + [\hat{a}^+ \varrho, \hat{a}] \right), \] (3.6)
where \( \varrho = \varrho(1), \)
\[ \overline{H} = \overline{H}(1) + 2 \text{Tr}_2 \left[ \overline{H}(1, 2), \varrho(2) \right] \] (3.7)
is an averaged single-particle Hamiltonian. The equation (3.6) can be given more compact form if we use the notation
\[ \overline{H}' = \overline{H} + \frac{1}{2} i \hbar \left( \text{Tr}_2(\hat{a}^+ \varrho) \hat{a} - \text{Tr}_2(\hat{a} \varrho) \hat{a}^+ \right). \] (3.8)

In this case we have
\[ i \hbar \dot{\varrho} = [\overline{H}', \varrho] + \frac{1}{2} i \hbar \left( [\hat{a} \varrho, \hat{a}^+ (1 - \varrho)] + [(1 - \varrho) \hat{a}, \varrho \hat{a}^+] \right). \] (3.9)

In general the right sides of equations (3.8) and (3.9) may contain several terms describing dissipative effects which depend on different operators \( \hat{a}_k. \) Taking this into account we generalize the equation (3.8) and write it as follows:
\[ i \hbar \dot{\varrho} = [\overline{H}', \varrho] + \frac{1}{2} i \hbar \sum_{k,l} C_{kl} \left( [\hat{a}_k \varrho, \hat{a}_l^+ (1 - \varrho)] + [(1 - \varrho) \hat{a}_k, \varrho \hat{a}_l^+] \right), \] (3.10)
where
\[ \overline{H}' = \overline{H} + i \hbar \sum_{k,l} C_{kl} \left( \text{Tr}_2(\hat{a}_l^+ \varrho) \hat{a}_k - \text{Tr}_2(\hat{a}_k \varrho) \hat{a}_l^+ \right). \] (3.11)

We write the equations (3.10) and (3.11) in matrix form:
\[ i \hbar \dot{\varrho}_{11'} = \sum_{\alpha_2} \left( \overline{\Pi}_{12} \varrho_{21'} - \varrho_{12} \overline{\Pi}'_{12} \right) + \sum_{\alpha_2} \left( \frac{1}{2} i \hbar \sum_{\alpha_3} \left( 2 \Gamma_{12,31'} \varrho_{23} - \Gamma_{23,12} \varrho_{31'} - \Gamma_{31'},23 \varrho_{12} \right) + \frac{1}{2} i \hbar \sum_{\alpha_3} \sum_{\alpha_4} \left( \varrho_{12} \varrho_{34} \left( \Gamma_{43,21'} - \Gamma_{21',43} - \Gamma_{23,41'} + \Gamma_{41',23} \right) + \left( \Gamma_{12,34} - \Gamma_{34,31} - \Gamma_{43,31} - \Gamma_{31',32} + \Gamma_{32,14} \right) \varrho_{43} \varrho_{21'} \right), \] (3.12)
where
\[ \overline{\Pi}_{12}' = H_{12} + \sum_{\alpha_3} \sum_{\alpha_4} \left( \frac{1}{2} i \hbar \left( \Gamma_{12,43} - \Gamma_{43,12} \right) \varrho_{43} \right). \] (3.13)
\[ \Gamma_{12,31'} = 2 \sum_{k,l} C_{kl} a_{12,k} a_{31',l}^+. \] (3.14)

4. The principle of detailed balance

Suppose that at some point in time the density matrix becomes diagonal:
\[ \varrho_{11'} = W_1 \delta_{11'}, \] (4.1)
where $W_1 = W_{\alpha_1}$ is the probability of the state $\alpha_1$ being filled by a particle. The substitution of matrix (4.1) into (3.12) leads to the equation

$$
\dot{W}_1 = \sum_{\alpha_2} \left( P_{12} (1 - W_1) W_2 - P_{21} (1 - W_2) W_1 \right),
$$

(4.2)

where

$$
P_{12} = \Gamma_{12,21}
$$

(4.3)

is the probability of the transition of a particle from state $\alpha_2$ to state $\alpha_1$ during a time unit. The transition probability $P_{12}$ can always be represented as

$$
P_{12} = P_{12}^{(0)} e^{-\frac{1}{2} \beta (\bar{\varepsilon} - \bar{\varepsilon})},
$$

(4.4)

where

$$
P_{12}^{(0)} = P_{21}^{(0)},
$$

$\bar{\varepsilon}_i$ – the average energy of a particle in the state $\alpha_i$, which is an eigenvalue of operator (3.13):

$$
\bar{\varepsilon}_1 = \varepsilon_1 + 2 \sum_{\alpha_2} H_{12,12} W_2,
$$

(4.5)

where $\varepsilon_1 = H_{11}$.

When a fermion system comes to the state of thermodynamic equilibrium, the particle distribution over the states must be subjected to the principle of detailed balance. We show that this distribution follows from the equation (4.2). Since the probability $W_1$ no longer depends on time, the right side of this equation is equal to zero. Moreover, according to the principle of detailed balance each term should be equal to zero. Thus the principle of detailed balance in this case is expressed by

$$
P_{12} (1 - W_1) W_2 = P_{21} (1 - W_2) W_1.
$$

(4.6)

We substitute the expression (4.4) into this equation. After simple transformations we obtain the equality

$$
\frac{1 - W_1}{W_1} e^{-\beta \bar{\varepsilon}_1} = \frac{1 - W_2}{W_2} e^{-\beta \bar{\varepsilon}_2},
$$

in which the left side depends on $\alpha_1$, and the right one - on $\alpha_2$. This is only possible if both sides are equal to the same constant value. Denote this value $e^{-\beta \mu}$, where $\mu$ is the chemical potential. We get the equation

$$
\frac{1 - W}{W} = e^{-\beta (\bar{\varepsilon} - \mu)}.
$$

(4.7)

Using the equality (4.5) we could show that this equation has an anisotropic solution [15].

From the equation (4.7) we find that the equilibrium distribution of noninteracting particles over states is described by the Fermi-Dirac function

$$
W = \frac{1}{1 + e^{\beta (\varepsilon - \mu)}}.
$$

(4.8)

5. The electrons in a metal

Consider electrons in metal. Equation (4.7) is transformed to

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

(5.1)

Here, the function $w_k$ describes the electron distribution over wave vectors $k$,

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

(5.2)
is the average energy of an electron, $\varepsilon_k$ is the energy of an electron without taking into account its interaction with other electrons, $\varepsilon_{kk'}$ is the interaction energy of electrons with wave vectors $k$ and $k'$. Assume the following approximate formula for the interaction energy

$$
\varepsilon_{kk'} = I \delta_{k+k'} - J \delta_{k-k'}, \tag{5.3}
$$

where $I$ is the repulsion energy of electrons with vectors $k$ and $-k'$, $J$ is the attraction energy of the electrons with vectors $k$ and $k'$. The substitution of (5.3) into (5.2) gives

$$
\varepsilon_k = \varepsilon_k + I w_{-k} - J w_k, \tag{5.4}
$$

and the equation (5.1) becomes

$$
\ln \frac{1-w_k}{w_k} = \beta \left( \varepsilon_k + I w_{-k} - J w_k - \mu \right). \tag{5.5}
$$

Replace in this equation the vector $k$ by the vector $-k$:

$$
\ln \frac{1-w_{-k}}{w_{-k}} = \beta \left( \varepsilon_k + I w_k - J w_{-k} - \mu \right), \tag{5.6}
$$

where

$$
\varepsilon_{-k} = \varepsilon_k.
$$

The equations (5.5) and (5.6) form a system with two unknowns $w_k$ and $w_{-k}$.

This system has the solutions of two types. One of them describes the isotropic distribution of electrons over wave vectors and the other describes the anisotropic distribution. If $w_{-k} = w_k$, then each of the equations (5.5) and (5.6) turns into the equation

$$
\ln \frac{1-w_k}{w_k} = \beta \left( \varepsilon_k + (I - J) w_k - \mu \right). \tag{5.7}
$$

In the equations (5.5) and (5.6) the unknown functions $w_k$ and $w_{-k}$ are complex functions, in which the role of an intermediate variable is played by the kinetic energy $\varepsilon_k$ of an electron: $w_{-k} = w_1(\varepsilon_k)$ and $w_k = w_2(\varepsilon_k)$. The functions $w_1 = w_1(\varepsilon)$ and $w_2 = w_2(\varepsilon)$ are the solutions of the equations

$$
\ln \frac{1-w_1}{w_1} = \frac{2}{\tau} \left( 2 \varepsilon + (1 - f) w_2 - (1 + f) w_1 \right), \tag{5.8}
$$

$$
\ln \frac{1-w_2}{w_2} = \frac{2}{\tau} \left( 2 \varepsilon + (1 - f) w_1 - (1 + f) w_2 \right), \tag{5.9}
$$

where

$$
\epsilon = \frac{\varepsilon - \mu}{J + I}, \quad \tau = \frac{4 \theta}{J + I},
$$

the ratio of the energy $I$ and $J$ is determined by the parameter

$$
f = \frac{J - I}{J + I}.
$$

Without loss of generality, we may accept the condition

$$
w_1(\epsilon) \leq w_2(\epsilon). \tag{5.10}
$$

Let us introduce new variables $d$ and $s$ by means of relations

$$
w_2 - w_1 = d, \quad w_1 + w_2 = 1 + s. \tag{5.11}
$$
Due to (5.10) the quantity \( d \) is non-negative: \( d \geq 0 \). The maximal value of \( d \) is equal to one: \( d \in [0, 1] \).

The quantity \( s \) takes on values from \(-1 \) to \( 1 \): \( s \in [-1, 1] \). Let us solve equations (5.11) with respect to \( w_1 \) and \( w_2 \):

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

(5.12)

We transform equations (5.8) and (5.9) using (5.12) to a form convenient for their numerical solution.

To do this we first subtract one equation from another, then we add these equations. As a result, we obtain the following system:

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

(5.13)

These equations allow us to represent the energy \( \epsilon \) and the probabilities \( w_1 \) and \( w_2 \) as functions of the parameter \( d \). Using these functions it is not difficult to construct the graphs of the functions \( w_1 = w_1(\epsilon) \) and \( w_2 = w_2(\epsilon) \) for different values of temperature. These graphs are shown in Fig. 1 for the case when the interaction energy of electrons \( I \) and \( J \) is such that \( J = 3I \). At the same time \( f = 1/2 \).

The solution of equation (5.7) is also a function of electron kinetic energy \( \varepsilon_k \): \( w_k = w_0(\varepsilon_k) \). The function \( w_0 = w_0(\varepsilon) \) can be found from the equation

\[
\ln \frac{1-w_0}{w_0} = \frac{4}{\tau} (\epsilon - f w_0),
\]

(5.14)

which is a corollary of equation (5.7). The solution \( w_{TT0} = w_0(\varepsilon) \) of equation (5.14) is among the solutions of equations (5.8) and (5.9). Indeed, if we put in these equations \( w_1 = w_2 \), then each of them takes the form (5.14).

Fig. 1 shows the graphs of all three functions \( w_0 = w_0(\varepsilon) \), \( w_1 = w_1(\varepsilon) \) and \( w_2 = w_2(\varepsilon) \). From this figure it is clear that at sufficiently low temperatures the distribution function for some values of the energy \( \epsilon \) can take not one but several values. The multivaluedness of functions \( w = w(\varepsilon) \) suggests that at the same temperature there can be different equilibrium macrostates of a system of conduction electrons in metal. These macrostates differ from each other by the distributions of electrons in Bloch states. In fact, only the macrostate of electrons, in which their energy is minimal, is realized, provided that this state is stable and cannot be destroyed by any external effects.

The graphs in Fig. 1 give an idea of the changes in the distribution of electrons in states that occur when the metal temperature changes. When the temperature \( \tau \geq 1 \), only the isotropic distribution of electrons over wave vectors described by the function \( w_k = w_k(\varepsilon_k) \) is possible. The graph of the function \( w_0 = w_0(\varepsilon) \) for all values of the temperature passes through the point \( \Omega \) with coordinates \( \varepsilon = \mu + \frac{1}{2} (J-I) \) and \( w = \frac{1}{2} \). As the temperature decreases, the slope of the curve at this point increases. When the temperature is sufficiently low, the curve of \( w_0 = w_0(\varepsilon) \) bends so that it becomes similar to the letter \( Z \).

For \( \tau = 1 \) on the curve \( w_0 = w_0(\varepsilon) \) at the point \( \Omega \) a closed curve \( Z \) originates. Its size increases as the temperature decreases. The shape of the curve also changes. The value \( \tau = 1 \) corresponds to the critical temperature

\[
T_c = \frac{I + J}{4 k_B}.
\]

(5.15)

At \( \tau \in (\tau', 1) \), where \( \tau' \) is some critical value, the vertical line intersects the curve \( Z \) no more than in two points (the curve \( Z \) in Fig. 1c). At \( \tau < \tau' \) the curve \( Z \) bends so that the vertical line intersects it four times in some places (Fig. 1b). In the limit, \( \tau \to 0 \), the curve \( Z \) transforms into a polygon \( AB_1C_1OC_2B_2A \), that looks like the letter \( Z \). This polygon is shown in Fig. 1a. The curve \( w_0 = w_0(\varepsilon) \) divides the curve \( Z \) into two parts. The lower part corresponds to \( w_1 = w_1(\varepsilon) \) and the upper - to \( w_2 = w_2(\varepsilon) \).

Let us give more detailed consideration to the distribution of electrons over states at \( T = 0 \). In the
limit, $\tau \to 0$, the solution of (5.14) takes on the form

$$w_0(\varepsilon) = \begin{cases} 
1 & \text{if } \varepsilon \leq \mu + J - I, \\
\frac{\varepsilon - \mu}{J - I} & \text{if } \mu \leq \varepsilon \leq \mu + J - I, \\
0 & \text{if } \varepsilon \geq \mu.
\end{cases}$$ \hspace{1cm} (5.16)$$

The graph of this function is shown in Fig. 1a as the dotted broken line $B_2AOC_1$.

In the limit, $\tau \to 0$, the equations (5.8) and (5.9) give the following dependence of the probability $w$ on the electron kinetic energy $\varepsilon$, which describes the anisotropic distribution of electrons over wave vectors:

$$w(\varepsilon) = \begin{cases} 1 & \text{if } \varepsilon \leq \mu - I, \\
w_i(\varepsilon) & \text{if } \mu - I \leq \varepsilon \leq \mu + J, \\
0 & \text{if } \varepsilon \geq \mu + J,
\end{cases}$$ \hspace{1cm} (5.17)

where $i = 1$ or 2. The values of the functions $w_1 = w_1(\varepsilon)$ and $w_2 = w_2(\varepsilon)$ form pairs, such that

$$w_1(\varepsilon) = 0 \quad \text{and} \quad w_2(\varepsilon) = 1$$ \hspace{1cm} (5.18)

at $\mu - I \leq \varepsilon \leq \mu + J$, or

$$w_1(\varepsilon) = \frac{1}{J}(\varepsilon - \mu + I) \quad \text{and} \quad w_2(\varepsilon) = 1$$ \hspace{1cm} (5.19)

at $\mu - I \leq \varepsilon \leq \mu + J - I$, or

$$w_1(\varepsilon) = 0 \quad \text{and} \quad w_2(\varepsilon) = \frac{1}{J}(\varepsilon - \mu)$$ \hspace{1cm} (5.20)

at $0 \leq \varepsilon \leq \mu + J$. The broken line $AB_1C_1O$ in Fig. 1a corresponds to $w_1 = w_1(\varepsilon)$, and the line $AB_2C_2O$ to $w_2 = w_2(\varepsilon)$.

6. Conclusions

The quantum Markov equation for $N$-particle density matrix describes the evolution of a strictly open system with allowance for the dissipative operator. From this equation, we obtained the approximate kinetic equation for a single-particle density matrix. This equation describes the evolution of a system of identical particles. We obtained the integral equation for the function of distribution of particles in states where a many-particle system is in thermodynamic equilibrium. We showed that for equilibrium systems of interacting particles the distribution over wave vectors is anisotropic.
References

[1] J. von Neumann, Mathematical Foundations of Quantum Mechanics (Nauka, Moscow, 1964).
[2] Y.R.Shen, Phys. Rev. 155 (1967) 921.
[3] M.Grover, R.Silbey, Chem. Phys. 52 (1970) 2099, 54 (1971) 4843.
[4] A.Kossakowski, Rep. Math. Phys. 3 (1972) 247.
[5] V.Gorini, A.Kossakowski and E.C.G.Sudarshan, J. Math. Phys. 17 (1976) 821.
[6] G.Lindblad, Commun. Math. Phys. 48 (1976) 119.
[7] V.Gorini, A.Frigerio, N.Verri, A.Kossakowski and E.C.G.Sudarshan, Rep. Math. Phys. 13 (1978) 149.
[8] K.Blum, Density Matrix Theory and Application (Plenum, New York, London, 1981).
[9] R.L.Stratonovich, Nonlinear Nonequilibrium Thermodynamics (Nauka, Moscow, 1985).
[10] R.Alicki, K.Lendy, Quantum Dynamical Semigroups and Applications. Lecture Notes in Physics. vol. 286 (Springer-Verlag, Berlin, 1987).
[11] J.L.Neto, Ann. Phys. (NY) 173 (1987) 443.
[12] B.V.Bondarev, Physica A 176 (1991) 366.
[13] B.V.Bondarev, Physica A 183 (1992) 159.
[14] B.V.Bondarev, Teoret. Mat. Fis. 100 (1994) 33.
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Fig. 1. The distribution function of conductivity electrons in energies for the case when $J=3l$, and at different temperatures $\tau$: a) $\tau = 0$; b) $\tau = 0.5$; c) $1 - \tau = 0.75$; 2 - $\tau = 0.95$. 