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On the theory of electrons localized in the field of defects

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We formulate a mathematical criterion for the localization of single-particle wave functions in a random field. The localization is characterized by the appearance of singular terms in the expressions for the correlation functions of various physical quantities as functions as the energy (independent of the dimensionality of the problem). We propose for one-dimensional problems a method which, in principle, allows one to evaluate directly correlators which contain products of several exact wave functions of electrons in a random field, pertaining to different energies and taken at different points.

The present paper does not pretend to give new physical results, but has as its aim the solution of some methodological problems. We discuss in section 1 the problem of particle localization in the random field of randomly distributed defects and we propose a mathematical formulation of a criterion for the localization of the wave functions of eigenstates. The applicability of the results of this section is not limited to the case of one-dimensional problems. The criterion formulated there refers equally well to two- and three-dimensional cases.

The second part of the paper refers solely to a one-dimensional conductor. It contains a general method which allows us—at least in principle—to write down and evaluate an arbitrary correlator of the product of any number of exact wave functions with different energies of an electron in the random field of static defects, taken at different points in space.

The necessity to evaluate such correlators arises in a whole set of problems, such as, for instance, the determination of the temperature dependence of the conductivity. It is well known that the localization of electrons in the field of defects is complete in the sense that all states with arbitrary energies are localized.[1] The static conductivity therefore vanishes at zero temperature. Mott and Twose[2] were the first to note this fact and later on this result was obtained exactly by one of the present authors.[3] At non-zero temperatures the conductivity behaves like that of a semiconductor. The finite magnitude of the conductivity is caused by jumps of the electrons along the localized states due to inelastic interaction processes between them and the thermal phonons or between themselves. This effect was considered in Ref. 4 for the electron-phonon inter-

action mechanism under well-defined, rather strong assumptions about the temperature and the frequencies of the phonons participating in the inelastic process, and the diagram method of Ref. 3 was used. Afterwards the same result was obtained in Ref. 5 where, in turn, a somewhat different method (an S-matrix method) was proposed for the corresponding calculations.

So far it is unclear how the electron-electron and the other interactions affect the localization of the electrons by the static defects. The difficulty is here first and foremost a mathematical one. To study the role of the interactions it is necessary to be able to evaluate to any order of perturbation theory the matrix elements between the exact wave functions of the states of the non-interacting particles. The existing methods[3,5] are too complicated to be used as a basis to carry out this program. To a certain extent these difficulties reflect, of course, the complexity of the problem. From our point of view, however, their main defect is that the starting point of Refs. 3 and 5 is the approximation of free electrons in the absence of impurities. As we see it, the basic point which is characteristic only for localized electrons—the presence in the matrix elements of singular, δ-functionlike terms in the energy—is, as a result of this, not explicitly visible and can appear in the answer only after lengthy calculations. Therefore, a simplification of the mathematical apparatus remains as before very desirable.

In the present paper we develop a method which is, from our point of view, most suitable for the mathematical description of a one-dimensional problem. The new method stems from Schmidt's method[6] of calculating the number of zeroes of an electron wave function which, as has already been shown in a number of papers,[7] is able to simplify the calculations considerably.

1. LOCALIZATION CRITERION IN THE GENERAL CASE

In this section we make a few simple remarks about different possibilities of formulating mathematically the localization of wave functions by static defects. We remind ourselves that the electrons are assumed to be non-interacting. This practically reduces the problem to a single-particle one.

We introduce the simplest retarded density correlator:

$$K(x) = \langle\langle \hat{\rho}(\mathbf{r}, t) - \bar{\rho}(\mathbf{r}), \hat{\rho}(0, 0) - \bar{\rho}(0) \rangle\rangle, \quad t > 0, \qquad (1)$$

where the symbol $\langle\langle \ldots \rangle\rangle$ implies averaging both over a thermodynamic ensemble for a given realization of the random potential and subsequently over different configurations of that potential. Here

$$\hat{\rho}(\mathbf{r}, t) = \sum_{\nu\nu',\sigma} \psi_\nu(x)\psi_{\nu'}(x) a^+_{\nu'\sigma} a_{\nu\sigma}$$

is the usual expression for the density operator in the second-quantization representation in terms of the wave functions $\psi_\nu(x)$ of the electron eigenstates with

energies ε_ν. (We take the functions in a finite volume to be real.) An elementary evaluation of Eq. (1) gives

$$K(x) = 2\left\langle \sum_{\nu\nu'} \exp\{-i(\varepsilon_{\nu'}-\varepsilon_\nu)t\} n_\nu(1-n_{\nu'})\psi_\nu(\mathbf{r})\psi_{\nu'}(\mathbf{r})\psi_\nu(0)\psi_{\nu'}(0) \right\rangle_v,$$

$$(1')$$

where $\langle \ldots \rangle_v$ corresponds to the averaging over the realizations of the random potential. We assume in what follows that the latter is characterized by uniform correlation functions which are invariant under the rotation and reflection group in the space of the appropriate dimensionality d. This expression can be written in the form

$$K(x) = 2\iint dE\, d\omega\, e^{-i\omega t} n_E(1-n_{E+\omega})$$
$$\times\left\langle \sum_{\nu\nu'} \delta(E-\varepsilon_\nu)\delta(E+\omega-\varepsilon_{\nu'})\psi_\nu(\mathbf{r})\psi_{\nu'}(\mathbf{r})\psi_\nu(0)\psi_{\nu'}(0) \right\rangle_v. \qquad (2)$$

Introducing the function

$$\langle\langle \rho_E(r)\rho_{E+\omega}(0) \rangle\rangle = \frac{1}{\nu(E)}\left\langle \sum_{\nu\nu'}\delta(E-\varepsilon_\nu)\delta(E+\omega-\varepsilon_{\nu'}) \right.$$
$$\times \psi_\nu(\mathbf{r})\psi_{\nu'}(\mathbf{r})\psi_\nu(0)\psi_{\nu'}(0) \Big\rangle_v \qquad (3)$$

$[\nu(E$ is the density of states for a single spin at an energy $E]$ we write the Fourier component of (2) with respect to time in the form

$$K(\mathbf{r}, \varepsilon) = 2i\iint \frac{\nu(E)n_E(1-n_{E+\omega})\langle\langle \rho_E(r)\rho_{E+\omega}(0) \rangle\rangle dE\, d\omega}{\varepsilon-\omega+i\delta}. \qquad (4)$$

The spectral density (3) has the following obvious properties:

$$\int_{\mathbf{r}} dr\langle\langle \rho_E(r)\rho_{E+\omega}(0) \rangle\rangle = \delta(\omega),$$
$$\int d\omega\langle\langle \rho_E(r)\rho_{E+\omega}(0) \rangle\rangle = \delta(r), \qquad (5)$$

which for the spatial Fourier components $\langle\langle \rho_E\rho_{E+\omega}(\mathbf{q}) \rangle\rangle$ means:

$$\langle\langle \rho_E\rho_{E+\omega}(q=0) \rangle\rangle = \delta(\omega), \quad \int d\omega\langle\langle \rho_E\rho_{E+\omega}(q) \rangle\rangle = 1. \qquad (5')$$

Moreover, one shows easily, by using the assumptions made about the correlation functions of the random potential that $\langle\langle \rho_E\rho_{E+\omega}(\mathbf{q}) \rangle\rangle \geqslant 0$.

It is now convenient to compare Eq. (1') for $K(x)$ and the properties expressed by Eq. (5'). Starting from (1') we see that there are present in it, in general, constant terms with $\varepsilon_\nu = \varepsilon_{\nu'}$. However, if the states are delocalized, their wave functions are normalized to the volume V and the corresponding contribution to (1') is thus of the order $\sim 1/V$. The situation is different if the states are localized. In that case the correlator $K(x)$ acquires a constant (i.e., independent of the time difference) term:

$$2\left\langle \sum_\nu n_\nu(1-n_\nu)\psi_\nu^2(\mathbf{r})\psi_\nu^2(0) \right\rangle_v, \qquad (6)$$

which in terms of the spectral density is equivalent to a term of the form $A(\mathbf{q})\delta(\omega)$ in $\langle\langle \rho_E\rho_{E+\omega}(\mathbf{q}) \rangle\rangle$. The wave functions are normalized to the localization length (mean free path) and an estimate of the term (6) gives

$$\sim (1/l)^d \int dE\nu(E)n_E(1-n_E).$$

V. L. Berezinskiĭ and L. P. Gor'kov   1210

We put it that one of the possible criteria for localization may be formulated as follows. We introduce the single-particle spectral densities:

$$\rho_E(\mathbf{r}, \mathbf{r}') = \sum_\nu \delta(E - \varepsilon_\nu)\psi_\nu(\mathbf{r})\psi_\nu(\mathbf{r}').$$

In the average of the product of n quantities $\rho_{E_i}(\mathbf{r}, \mathbf{r}')$ pertaining to energies $E_1, \ldots, E_n$ and arbitrary points $(\mathbf{r}_i, \mathbf{r}'_i)$ there must be present δ-functionlike singularities corresponding to some of the energies E_i being equal. These energies correspond to localized states.[1]

Turning to Eqs. (5') we see that they, in turn, also express two possibilities. For the first of them, corresponding to the presence of localized states at an energy E, the δ-functionlike term is retained for finite $\mathbf{q}$ and for $q \neq 0$ we can write

$$\langle\!\langle \rho_E \rho_{E+\omega}(\mathbf{q})\rangle\!\rangle = A(\mathbf{q})\delta(\omega) + \rho_1(\mathbf{q}, \omega), \qquad (7)$$

and for small q

$$\langle\!\langle \rho_E \rho_{E+\omega}(\mathbf{q})\rangle\!\rangle = (1 - \alpha q^2)\delta(\omega) + q^2\rho_1(\omega), \qquad (7')$$

where according to (5')

$$\alpha = \int \rho_1(\omega)\, d\omega. \qquad (7'')$$

Delocalization would correspond to a spreading out of the δ-functionlike singularities in (5') at finite $\mathbf{q}$. The simplest variant corresponding to diffusive behavior means that the width $\Delta\omega$ of the singularity is quadratic in q: $\Delta\omega \propto q^2$. We have

$$\langle\!\langle \rho_E \rho_{E+\omega}(\mathbf{q})\rangle\!\rangle = \frac{1}{\pi}\frac{D_E q^2}{\omega^2 + (D_E q^2)^2}. \qquad (8)$$

It follows already from the possibility of such a statement of the problem that the diffusive spreading out of the singularity is just one particular case of the behavior of $\langle\!\langle \rho_E \rho_{E+\omega}(\mathbf{q})\rangle\!\rangle$ for small q and there can be many other possibilities for its dependence on ω and q which satisfy the normalization condition (5'), among which there is also a singular behavior for small ω and q. We deduce hence that delocalization does not necessarily imply a diffusive spreading out of the packet.

Comparing (7') and (6) [i.e., evaluating the Fourier component of (6), the term q^2] we get

$$\alpha = -\frac{1}{2d\nu(E)}\int r^2\, dr \left\langle \sum_\nu \delta(E - \varepsilon_\nu)\psi_\nu^2(\mathbf{r})\psi_\nu^2(0)\right\rangle_v \qquad (9)$$

(d is the dimensionality of the space). In other words, α can be expressed in terms of the mean square variance of the dipole moment.

Similar to the single-particle spectral density of the density-density correlator, we can introduce spectral densities for the current-current and current-density correlators. We can then use the equation of continuity to establish the following relations between these quantities:

$$\langle\!\langle j_E \rho_{E+\omega}(\mathbf{q})\rangle\!\rangle = \langle\!\langle \rho_E j_{E+\omega}(\mathbf{q})\rangle\!\rangle = \frac{\omega \mathbf{q}}{q^2}\langle\!\langle \rho_E \rho_{E+\omega}(\mathbf{q})\rangle\!\rangle,$$

$$\langle\!\langle j_{iE}j_{kE+\omega}(\mathbf{q})\rangle\!\rangle = \langle\!\langle j_E j_{E+\omega}^\perp(\mathbf{q})\rangle\!\rangle\left(\delta_{ik} - \frac{q_i q_k}{q^2}\right) + \langle\!\langle j_E j_{E+\omega}^\parallel(\mathbf{q})\rangle\!\rangle\frac{q_i q_k}{q^2}, \qquad (10)$$

$$\langle\!\langle j_E j_{E+\omega}^\parallel(\mathbf{q})\rangle\!\rangle = \frac{\omega^2}{q^2}\langle\!\langle \rho_E \rho_{E+\omega}(\mathbf{q})\rangle\!\rangle.$$

The response in the current of a many-particle system to an external vector potential $\mathbf{A}_\varepsilon(\mathbf{r})$ is given by the formula[8]

$$j_i(\mathbf{r}, \varepsilon) = -\frac{e^2\rho}{m}A_{i\varepsilon}(\mathbf{r}) + i\int d\mathbf{r}' \langle\!\langle [\hat{j}_i(x), \hat{j}_k(x')]\rangle\!\rangle_\varepsilon^{(R)} A_{k\varepsilon}(\mathbf{r}'),$$

where the integrand contains the retarded commutator of the current density operators. For the Fourier components with repsect to momenta we get[2]

$$j(\mathbf{q}, \varepsilon) = -2e^2 \iint \frac{\nu(E)\, dE\, d\omega[n_E - n_{E+\omega}]}{\varepsilon - \omega + i\delta}\frac{\omega^2}{q^2}\langle\!\langle \rho_E \rho_{E+\omega}(\mathbf{q})\rangle\!\rangle \mathbf{A}_\varepsilon(\mathbf{q}).$$

Using (8), letting $\mathbf{q} \to 0$ and substituting $\mathbf{A}_\varepsilon = \mathbf{E}/i\varepsilon$ we get in the diffusive case for the conductivity the well known expression:

$$\sigma = 2e^2\nu(E_F)D.$$

In the localized case we have according to (7')

$$\sigma(\varepsilon) = 2e^2\nu(E_F)\varepsilon^2\rho_1(\varepsilon),$$

where[2,3] in the one-dimensional case

$$\rho_1(\varepsilon) \propto \ln^2(\varepsilon\tau).$$

Without using Eqs. (10) we can directly write down the following expression for the conductivity in terms of the wave functions of the system:

$$\sigma_{ik}(\varepsilon) = \delta_{ik}\sigma(\varepsilon) = \frac{2\pi e^2}{m^2}\int \left\langle \sum_{\nu\nu'} \delta(E - \varepsilon_\nu)\delta(\varepsilon_\nu - \varepsilon_{\nu'} + \varepsilon)\right.$$

$$\left. \times (\psi_{\varepsilon_\nu}(\mathbf{r})\hat{p}_{i,r}\psi_{\varepsilon_{\nu'}}(\mathbf{r}))(\psi_{\varepsilon_\nu}(\mathbf{r}')\hat{p}_{k,r'}\psi_{\varepsilon_{\nu'}}(\mathbf{r}'))\right\rangle_v dr' \qquad (11)$$

(here $\hat{p}_{i,r} = -i\partial/\partial r_i$).

2. METHOD FOR EVALUATING AVERAGES OF WAVEFUNCTIONS IN THE ONE-DIMENSIONAL CASE

Equations (3), (6), (9), and (11) contain averages of the product of several electron wave functions with different or the same energies and at different points in space. It is possible to develop for the one-dimensional case a method for evaluating such averages which looks to us simpler and more general than the diagram method of one of the present authors[3] or the S-matrix method.[5] The present section is devoted to an exposition and discussion of that method.

One can in the one-dimensional case juxtapose the eigenvalue of the energy E_ν to the number of zeroes of its wave function $\psi_\nu(x)$ that satisfies the Schrödinger equation:

$$\{-(d^2/2m\, dx^2) + U(x)\}\psi_\nu(x) = E_\nu\psi_\nu(x).$$

This fact was used by Schmidt[6] as the basis for the evaluation of the single-particle density of states of a linear chain with a random distribution. The considerations given below are a further development of this approach. Schmidt's method[6] leading to the equations for a Markov process is valid for a potential $U(x)$ corresponding to a random set of short-range potentials and can be formulated both for a random Gaussian potential $U(x)$ (so-called white noise) and also

for a lattice in whose points defect atoms are randomly dispersed and have a potential range less than the size of the selected cell. In the Born approximation both procedures are absolutely equivalent, but below we prefer to emphasize the lattice formulation, bearing in mind possible generalizations. In conclusion we give a derivation also for a white-noise kind of potential.

We thus consider a lattice of points with cell size a, while in each site there is a probability p that there is a defect situated with a potential with a range which for the sake of simplicity we assume to be negligibly small compared to a. When $p \ll 1$ this arrangement corresponds, in particular, to a low impurity concentration $c = p/a$. The phase φ_E of the wave function is given by the relation

$$\operatorname{ctg} \varphi_E = \psi'/k\psi, \quad k = (2mE)^{\frac{1}{2}} \tag{12}$$

and satisfies the equation

$$\varphi_E' = k - (U(x)/k) \sin^2 \varphi_E. \tag{13}$$

In the figure we have depicted the lattice potential where in agreement with the assumptions about the character of the potential in the whole cell (j), except at the lattice sites, the motion is free:

$$\psi_i(x) = A_j(x) + B_j(x) = R_j \sin \varphi_j(x); \quad \frac{d}{dx} \varphi_j(x) = k. \tag{14}$$

The connection between the amplitudes of the traveling waves $\{A_j B_j\}$ and $\{A_{j+1} B_{j+1}\}$ is determined by the scattering by the potential located at the site $j+1$. For the sake of argument, we shall match together all quantities A_j, B_j, φ_j taken immediately to the right of the site j, as shown by the arrow in the figure.[7]

One checks easily that for such a choice of the quantities in the points j and $j+1$ the connection between the coefficients A_j and B_j is given by the matrix

$$\begin{Bmatrix} A_{j+1} \\ B_{j+1} \end{Bmatrix} = \frac{1}{\cos \gamma} \begin{Bmatrix} e^{-i(ka-\delta)}, & i \sin \gamma e^{-ika} \\ -i \sin \gamma e^{ika}, & e^{-i(ka-\delta)} \end{Bmatrix} \begin{Bmatrix} A_j \\ B_j \end{Bmatrix}, \tag{15}$$

in which γ and δ are characterized by the problem of the scattering by the defect atom (for the sake of simplicity the potential is taken to be symmetrical under $x \to -x$) where δ is the advance in phase of the previous wave and $\sin^2 \gamma$ the reflection coefficient.

We have

$$R_{j+1}^2 = (R_j^2/\cos^2 \gamma)[1 + \sin^2 \gamma - 2 \sin \gamma \sin(2\varphi_j + 2ak - \delta)],$$
$$R_j^2 = (R_{j+1}^2/\cos^2 \gamma)[1 + \sin^2 \gamma + 2 \sin \gamma \sin(2\varphi_{j+1} + \delta)] \tag{16}$$
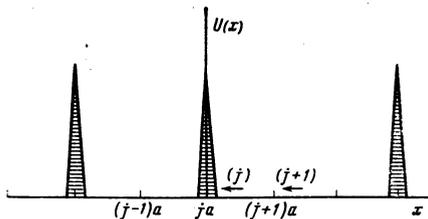

FIG. 1. Random potential $U(x)$ as potential of defects which are randomly positioned in lattice sites (lattice period a). The arrows indicate the positions where all quantities in the cell j and $j+1$ are matched.

and

$$\varphi_{j+1} = \varphi_j + ka - \delta + \frac{1}{2i} \ln \left\{ \frac{1 - i \sin \gamma \exp[-i(2\varphi_j + 2ka - \delta)]}{1 + i \sin \gamma \exp[i(2\varphi_j + 2ka - \delta)]} \right\}, \tag{17}$$

$$\varphi_j = \varphi_{j+1} - ka + \delta + \frac{1}{2i} \ln \left\{ \frac{1 + i \sin \gamma \exp[-i(2\varphi_{j+1} + \delta)]}{1 - i \sin \gamma \exp[i(2\varphi_{j+1} + \delta)]} \right\}. \tag{17'}$$

Equations (17) enable us to construct the phase φ_j as a monotonically increasing or decreasing function,[6] depending on whether we start the process from the left-hand or the right-hand end point. We shall mark the corresponding quantities with an index $>$ or $<$.

We still need equations for the derivatives $\zeta^> = \partial \varphi^> / \partial k$ and $\zeta^< = \partial \varphi^< / \partial k$. From (17) we get, for example,

$$\frac{\partial \varphi_{j+1}}{\partial k} = \left(\frac{\partial \varphi_j}{\partial k} + a \right) \frac{\cos^2 \gamma}{1 + \sin^2 \gamma - 2 \sin \gamma \sin(2\varphi_j + 2ka - \delta)}. \tag{18}$$

In correspondence with the definition of the phase[6] the quantity $\zeta^>$ is always positive.

We write

$$\alpha(j|n) = R_j/R_n \tag{19}$$

and introduce as a definition

$$\int_{-L}^{x_j} \alpha^2(x|x_i) dx = \sum_{0 < i < j} \alpha^2(i|j) a. \tag{20}$$

(The integral has here a symbolic meaning, but in what follows we shall often change to a continual description.) Using (16) and (18) one checks easily that

$$\zeta_j^> = \int_{-L}^{x_j} \alpha^2(x|x_i) dx, \tag{21}$$

as (20) satisfies Eq. (18) and the boundary condition $(\partial \varphi^>/\partial k)_{x=-L} = 0$. In turn, we have similarly

$$\zeta_j^< = -\int_{x_j}^{L} \alpha^2(x|x_i) dx = -\sum_{j < i < N} \alpha^2(i|j) a. \tag{21'}$$

In order not to encumber the paper with general formulae we choose first, to begin to demonstrate the idea of the method, the average of the electron Green function:

$$G_{i\omega_n}(x, x') = \sum_{\nu} \frac{\psi_\nu(x) \psi_\nu(x')}{i\omega_n - \varepsilon_\nu} \tag{22}$$

(here $\omega_n = (2n + 1)\pi T$; we denote the energy reckoned from the level of the chemical potential by ε_ν). We write (22) in the form

$$G_{i\omega_n}(x, x') = \int d\xi \sum_\nu \delta(\xi - \varepsilon_\nu) \frac{\psi_\nu(x) \psi_\nu(x')}{i\omega_n - \xi} \tag{22'}$$

and, we choose, for instance, $x < x'$ in the mean value of the spectral density.

$$\langle \rho_\xi(x, x') \rangle = \left\langle \sum_\nu \delta(\xi - \varepsilon_\nu) \psi_\nu(x) \psi_\nu(x') \right\rangle_U. \tag{23}$$

The eigenwave functions $\psi_\nu(x)$ in (22) are normalized to unity:

$$\int \psi_\nu^2(x) dx = 1. \tag{24}$$

If the case is quasi-classical, $kl \gg 1$, one can write that condition as

$$\frac{1}{2}\sum_{0<i<N} R_i^2 a = 1. \tag{24'}$$

Taking an arbitrary point j_0 we can rewrite (24') in terms of the quantity α from (19):

$$\frac{1}{2} R_{j_0}^2 \int_{-L}^{L} \alpha^2(x|j_0)\,dx = 1, \tag{25}$$

and the normalization constant $R_{j_0}^2$ is then according to (21) and (21') equal to

$$R_{j_0}^2 = 2 \Big/ \int \alpha^2(x|j_0)\,dx = \frac{2}{\xi^>(j_0) - \zeta^<(j_0)}. \tag{26}$$

The presence of a δ-function in (23) expresses the fact that the energy ξ is the eigenvalue for a given configuration of defects. The same fact can be represented by the condition that the solutions for the phase, satisfying the boundary condition $\varphi|_{\pm L} = \varphi_0$, from the left $\varphi_j^>$ and from the right $\varphi_j^<$, differ by an integer times π in any arbitrarily chosen point j_0 where we match the solution. Taking therefore the phase in the range[3] $(-\pi/2, \pi/2)$ we can write:

$$\delta(\xi - \varepsilon_\nu) = \delta(\varphi_{j_0}^> - \varphi_{j_0}^<)\,[\,(\partial\varphi^>/\partial\xi)_{j_0} \\ -(\partial\varphi^</\partial\xi)_{j_0}] = (1/v)\,\delta(\varphi_{j_0}^> - \varphi_{j_0}^<)\,(\zeta_{j_0}^> - \zeta_{j_0}^<). \tag{27}$$

As a result Eq. (23), takes at the points $x = j$, $x' = j'$ [inside the cell, (23) is determined by the free-motion Eq. (14)], when we use (26), the form

$$(2/v)\,\langle \delta(\varphi_{j_0}^> - \varphi_{j_0}^<)\,\sin\varphi_j \alpha_t(j|j_0)\,\sin\varphi_{j'}\alpha_t(j'|j_0)\rangle_v.$$

We write it in the form of an integral:

$$2\int_{-\pi/2}^{+\pi/2} \frac{d\varphi}{v}\langle\delta(\varphi_{j_0}^> - \varphi)\,\delta(\varphi - \varphi_{j_0}^<)\sin\varphi_j\alpha_t(j|j_0)\sin\varphi_{j'}\alpha_t(j'|j_0)\rangle_v.$$

Let, for instance, $j_0 = j$. We can then rewrite this average also differently:

$$\langle\rho_t(x,x')\rangle = \frac{2}{v}\iint_{-\pi/2}^{+\pi/2} d\varphi d\varphi'\langle\delta(\varphi_j^> - \varphi)\sin\varphi \\ \times\delta(\varphi - \varphi^<(j|j',\varphi'))\alpha_t(j'|j)\sin\varphi'\delta(\varphi' - \varphi_{j'}^<)\rangle_v. \tag{28}$$

In other words, since this is a Markov process, we can perform the averaging in (28) over all defect configurations separately over the sections $-\infty = -L < j < j' < L = +\infty$. Accordingly we introduce the following quantities:

$$w_t(\varphi) \equiv w_t^>(\varphi) = \langle\delta(\varphi_{t,j}^> - \varphi)\rangle \tag{29}$$

the stationary phase distribution function, found going from the left. The analogous quantity obtained by going from the right is

$$w_t^<(\varphi) = \langle\delta(\varphi - \varphi_{t,j}^<)\rangle. \tag{29'}$$

The function for the transition from the point j' to the point j (from right to left) has the form

$$w_{jj',t}^{<(t)}(\varphi,\varphi') = \langle\alpha_t(j'|j)\delta(\varphi - \varphi_t^<(j|j',\varphi'))\rangle, \tag{30}$$

where the notation $\varphi^<(j|j',\varphi')$ indicates the result of solving the equation for the phase (from the right to the left) at the point j under the condition that the phase at the point j' equalled φ'. Thus

$$\langle\rho_t(x,x')\rangle = \frac{2}{v}\iint_{-\pi/2}^{+\pi/2} d\varphi d\varphi' w_t^>(\varphi)\sin\varphi\, w_{jj',t}^{<(t)}(\varphi,\varphi')\sin\varphi'\, w_t^<(\varphi'), \tag{31}$$

where one can use Schmidt's method[6] to obtain easily the equations for any of the probability functions which occur here, connecting through the transformations (16), (17) the neighboring points j and $j+1$. We thus have, according to Schmidt,[6] for the stationary probability distribution function $w(\varphi)$ the equation

$$w_t^>(\varphi_{j+1}) = (1-p)\,w_t^>(\varphi_{j+1} - ka) \\ + p w_t^>(\varphi_j(\varphi_{j+1}))\,(d\varphi_j(\varphi_{j+1})/d\varphi_{j+1}), \tag{32}$$

which expresses the fact that the site $j+1$ is unoccupied with a probability $1 - p$ and occupied by a defect with a probability p. Schmidt's Eq. (32) is the basic one for deriving all further formulae.

We also note that for the symmetrical defect chosen by us Eq. (17) admits the substitution $\varphi^> \to -\varphi^<$. Since (17) defines a function $\varphi^>$ which increases monotonically from left to right, and (17') a function $\varphi^<$ which decreases monotonically from right to left, the stationary phase probability distribution functions satisfy the condition

$$w_t^<(\varphi) = w_t^>(-\varphi) \equiv w_t(-\varphi). \tag{33}$$

The generalization of the representation (31) to the case of correlators of products of a large number of $\rho_\xi(x, x')$ and the proof that the result of the averaging is independent of the choice of the point j_0 where we match the solutions are given by us in the Appendix.

So far in our considerations we had no need to resort to any simplifying assumptions regarding the potential, bar the assumption that it has a short range. However, we make here the following remark. Backward scattering of the electrons is important for the localization. At the same time the molecules in the experimentally studied organic conductors are rather large. The random potential then turns out to be relatively smooth which diminishes the amplitude for the backward scattering of an electron. (It is, of course, possible that for a number of substances a model in which the impurities split the chain into almost isolated sections is more suitable, but this case requires special considerations.) Starting here, therefore, and everywhere in what follows we use the Born approximation $\gamma \ll 1$.

The localization length

$$l = 2a/p\gamma^2 = 2/c\gamma^2 \tag{34}$$

will be assumed to be large compared to "atomic" distances (while $ak \sim 1$) and also large compared to the average distance between defects

$$l \gg \bar{x} = a/p. \tag{35}$$

Using the fact that γ is small we simplify Eqs. (16), (17):

$$R_{j+1}^2 = R_j^2[1 + 2\gamma^2 - 2\gamma\sin(2\varphi_j + 2ak - \delta)], \tag{36}$$

$$R_j^2 = R_{j+1}^2[1 + 2\gamma^2 + 2\gamma\sin(2\varphi_{j+1} + \delta)], \tag{36'}$$

V. L. Berezinskii and L. P. Gor'kov   1213

$$\varphi_{j+1}=\varphi_j+ka-\delta-\gamma\cos\,(2\varphi_j+2ka-\delta), \qquad (37)$$

$$\varphi_j=\varphi_{j+1}-ka+\delta+\gamma\cos\,(2\varphi_{j+1}+\delta). \qquad (37')$$

We have dropped in (36), (37) terms of the form $\gamma^2\sin m\varphi$. From a formal point of view they are according to (34) of the necessary (second) order of magnitude in γ but in all equations below they would occur with a fast-oscillating factor $\sin m\varphi$ which drops out unless we make special assumptions about the magnitude of ka (to be more precise, require that k and $2\pi/a$ are commensurable). Indeed, in the vicinity of an arbitrarily positioned Fermi level all probabilities depend solely on differences in the energies and in the phases corresponding to them and do not contain in the main approximation a dependence on the phases φ_ξ themselves.

As an example we write down the equation which is satisfied by the stationary distribution function of several phases, $w(\varphi_{\xi_0},\varphi_{\xi_1},\dots,\varphi_{\xi_i})$. We derive this equation by analogy with (32) and using Eq. (37). As in (32) the Jacobian—a product of factors

$$d\varphi_j/d\varphi_{j+1}=1-2\gamma\sin\,(2\varphi_{j+1}+\delta)$$

occurs on the right-hand side. Retaining everywhere only terms of order γ^2 (the terms which are linear in γ contain fast-oscillating factors depending on one of the phases) and rewriting $w(\varphi_{\xi_0},\dots,\varphi_{\xi_i})\equiv w(\theta_1,\dots,\theta_i)$, where $\theta_i=\varphi_{\xi_i}-\varphi_{\xi_0}$ we get as a result of elementary calculations

$$-\sum_i \nu_i\frac{\partial w}{\partial\theta_i}+\sum_i\frac{\partial^2}{\partial\theta_i^2}[(1-\cos 2\theta_i)w]$$
$$+\sum_{i>k}\frac{\partial^2}{\partial\theta_i\partial\theta_k}[(1+\cos 2(\theta_i-\theta_k)-\cos 2\theta_i-\cos 2\theta_k)w]=0, \qquad (38)$$

where, in turn, $\nu_i=(k_i-k_0)l$ and l is defined through (34).

We did not manage to find the general solution of (38). The limit $\nu_i\gg 1$ denotes the statistical independence and corresponds to a vanishing of the dependence on the angle θ_i of the function $w(\theta_1,\dots,\theta_i)$. Equation (38) has asymptotic solutions for all $\nu_i\gg 1$.

Let us discuss in detail the case of two phases: $w(\varphi_1,\varphi_2)\equiv w(\theta)$. For the sake of argument let $\nu>0$. In that case

$$-\nu\frac{\partial}{\partial\theta}w(\theta)+2\frac{\partial^2}{\partial\theta^2}(\sin^2\theta w(\theta))=0. \qquad (39)$$

The first integral of Eq. (39) is

$$-\nu w(\theta)+2\frac{\partial}{\partial\theta}(\sin^2\theta w(\theta))=-\frac{\nu}{\pi^2} \qquad (39')$$

(the probability distribution function of the two phases is normalized to unity). Equation (39) has a singularity at $\theta=0$.

The general form of the solution is:

$$w(\theta)=-\frac{\nu}{2\pi^2\sin^2\theta}\exp\left(-\frac{\nu}{2}\operatorname{ctg}\theta\right)\int^\theta\exp\left(\frac{\nu}{2}\operatorname{ctg}\theta'\right)d\theta'.$$

For the final definition of it we must require the finiteness (integrability) of $w(\theta)$ for $\theta=0$ and impose the

periodicity condition $w(\theta+\pi)=w(\theta)$. [In other words, when $\theta<0$ $w(\theta)\equiv w(\theta+\pi)$.] One checks easily that such a solution is

$$w(\theta)=\frac{\nu}{2\pi^2\sin^2\theta}\exp\left(-\frac{\nu}{2}\operatorname{ctg}\theta\right)\int_0^{\pi-0}\exp\left(\frac{\nu}{2}\operatorname{ctg}\theta'\right)d\theta'. \qquad (40)$$

The asymptotic properties of the solution for $\nu\ll 1$ follow at once from (40). In particular, one checks easily that for small $\theta\sim\nu$ we can expand (40) as follows

$$w(\theta)=\frac{1}{\nu}w_0\left(\frac{\theta}{\nu}\right)+w_1\left(\frac{\theta}{\nu}\right)+\dots. \qquad (41)$$

The main term $(1/\nu)w(\theta/\nu)$ is then non-vanishing only when $\theta>0$:

$$\frac{1}{\nu}w_0\left(\frac{\theta}{\nu}\right)=\frac{\nu}{2\pi\theta^2}\exp\left(-\frac{\nu}{2\theta}\right), \qquad (42)$$

and thus when $\theta<0$ the first-order term is important:

$$w_1\left(\frac{\theta}{\nu}\right)=\frac{\nu^2}{2\pi^2\theta^2}\exp\left(\frac{\nu}{2|\theta|}\right)\int_{-\infty}^{-\nu/|\theta|}\frac{dx}{x^2}e^{x/2}, \qquad (43)$$

with an asymptotic behavior when $|\theta|/\nu\gg 1$

$$w_1(\theta/\nu)\approx-\nu/2\pi^2\theta \qquad (43')$$

In applications one must often evaluate rather complicated correlators of wave functions which occur in different matrix elements. When writing down and solving the appropriate equations it turns out to be more convenient to look not for transition probabilities of the kind $w_{jj'}(\varphi,\varphi')$ in Eq. (31) (see A.6) themselves, but to use a somewhat different method which we now explain, evaluating again by the proposed method the frequency dependence of the conductivity due to static defects.[3]

Substituting the expressions for the wave functions (14) into (11) and retaining under the integral sign of the correlator only slowly varying factors at the points x and x' we get

$$(\pi e^2 v^2/2)\int dx'\left\langle\sum_{vv'}\delta(\xi-\varepsilon_v)\delta(\varepsilon_{v'}-\varepsilon_v-\omega)\right.$$
$$\left.\times\sin\theta(x)R_t(x)R_{t'}(x)\sin\theta(x')R_t(x')R_{t'}(x')\right\rangle,$$

where $\xi'=\xi+\omega$, $\theta(x)=\varphi_{\xi'}(x)-\varphi_\xi(x)$. As the average depends only on $|x-x'|$ let $x<x'$ and take the matching point in x'. We rewrite the conductivity in the form

$$\sigma(\omega)=4\pi^2 e^2\int_0^\infty dR\int_{-\pi/2}^{\pi/2}d\theta g(R,\theta)w(-\theta)\sin\theta \qquad (44)$$

(the extra π is due to the integral over φ). The function $g(R,\theta)$ is thus

$$g(R,\theta)=\langle\sin\theta(x)\alpha_t(x|x')\alpha_{t+\omega}(x|x')\delta(\theta-\theta'(x'))$$
$$\times\delta(\varphi-\varphi_t'(x'))\rangle_v, \qquad (45)$$

and we can write down an equation for it without introducing a transition probability, but connecting instead of that directly its values in the points x_j and x_{j+1} similarly to (32):

$$g(R+a,\theta_{j+1})=(1-p)g\left(R,\theta_{j+1}-\frac{\omega a}{v}\right)+pg(R,\theta_j(\theta_{j+1}))$$
$$\times\left(\frac{R_{t,j}}{R_{t,j+1}}\right)\left(\frac{R_{t',j}}{R_{t',j+1}}\right)\frac{d\theta_j}{d\theta_{j+1}}\frac{d\varphi_{t,j}}{d\varphi_{t,j+1}}.$$

V. L. Berezinskiĭ and L. P. Gor'kov   1214

Expanding this relation we find the equation ($\nu = l\omega/v = \omega\tau$)

$$l\frac{\partial g}{\partial R} = -\nu\frac{\partial g}{\partial\theta} + (1-\cos 2\theta)\frac{\partial^2 g}{\partial\theta^2} + 2\sin 2\theta\frac{\partial g}{\partial\theta} - (1-\cos 2\theta)g. \quad (46)$$

We take its Laplace transform

$$g_\lambda(\theta) = \int_0^\infty dR\, g(R,\theta)e^{-\lambda R}.$$

We have

$$-l\sin\theta\, w(\theta) + \lambda l g_\lambda(\theta) = -\nu g_\lambda'(\theta)$$
$$+ (1-\cos 2\theta)g_\lambda''(\theta) + 2\sin 2\theta\, g_\lambda'(\theta) - (1-\cos 2\theta)g_\lambda(\theta). \quad (46')$$

We have used the boundary condition $g(R=0,\theta) \equiv w(\theta)\sin\theta$ which is obvious from (45). We have not solved Eq. (46') in its general form. However, for small ν small angles are important:

$$-\theta l w(\theta) = -\nu g_\lambda' + 2\theta^2 g_\lambda'' + 4\theta g_\lambda' - \lambda l g_\lambda. \quad (46'')$$

The solution of (46") can be expressed in terms of Bessel functions.

To evaluate the conductivity (44) one requires only $g_{\lambda=0}(\theta)$. We see that the main contribution to (44) comes from the region $\nu \ll |\theta| \ll 1$. To find the solution we proceed as follows. On the one hand, in the small angle region we easily solve Eq. (46") ($\lambda = 0$):

$$g(\theta) = \frac{l}{\nu}\left\{\int_0^\theta \theta' w(\theta')\left[1 - \exp\frac{\nu}{2}\left(\frac{1}{\theta'} - \frac{1}{\theta}\right)\right]d\theta' + \alpha\exp\left(-\frac{\nu}{2\theta}\right) + \varkappa\right\},$$
$$\theta > 0, \quad (47)$$

$$g(\theta) = \frac{l}{\nu}\left\{\int_0^{|\theta|} x w(-x)\left[1 - \exp\frac{\nu}{2}\left(\frac{1}{|\theta|} - \frac{1}{x}\right)\right]dx + \varkappa\right\}, \quad \theta < 0.$$

(We have taken solutions finite at $\theta = 0$; α and $\varkappa$ are integration constants.)

For large angles we can neglect the term with ν. As a result (46') becomes

$$-\frac{l\nu}{4\pi^2}\frac{\pi-\theta}{\sin^2\theta} = \frac{\partial^2}{\partial\theta^2}(g\sin\theta)$$

and can be integrated:

$$g\sin\theta = \frac{l\nu}{4\pi^2}\left\{(\pi-\theta)\ln\sin\theta + 2\int_0^\theta \ln\sin\theta' d\theta' + c_1\theta + c_2\right\}.$$

One must match the expansion of this expression in the region $\theta \ll 1$ and $\pi - \theta \ll \pi$ with the asymptotic solution (47) in the region $1 \gg |\theta| \gg \nu$ using the fact that $g(\theta) = -g(\pi+\theta)$ when $\theta < 0$. This procedure enables us to determine the constants c_1, c_2, α, and $\varkappa$. We write down the main terms of the function $g(\theta)$ in the region $\nu \ll |\theta| \ll 1$:

$$g(\theta) = \frac{l\nu}{4\pi^2}\left\{\begin{array}{ll}(\pi/\theta)\ln(\theta/\nu); & \theta > 0 \\ \ln|\theta| + \ln\nu; & \theta < 0\end{array}\right.$$

Using them in (44) we find[3]

$$\sigma(\omega) = (l\nu^2/\pi)\ln^2\nu.$$

The answer is the same as the equations in Refs. 3, 5 if we substitute for the localization length (34) $l = 2l_-$ (see Ref. 7) where l_- is the kinetic mean free path for backward scattering.

Finally, Eq. (6) allows us to point out those changes caused by a case important for localized states, when

there are more than two wave functions with the same energy in the averaged quantity:

$$F(x-x') = \langle\sum_t \delta(\xi-\varepsilon_\nu)\psi_t^2(x)\psi_t^2(x')\rangle_\nu. \quad (48)$$

Let the point of joining be x' and let $x' > x$. In agreement with (26) and (27) we have for (48)

$$F(x-x') = (1/v)\langle\delta(\varphi^>(x')$$
$$-\varphi^<(x'))\alpha_t^2(x|x')[\zeta^>(x') - \zeta^<(x')]^{-1}\rangle_\nu. \quad (48')$$

We can proceed here in two ways. Firstly, we can introduce a probability distribution function for the phases and their derivatives simultaneously. For instance, the stationary function corresponding to the interval $(-\infty, x)$ is

$$w_t(\varphi, \zeta) = \langle\delta(\varphi-\varphi_t^>(x))\delta(\zeta_t^>(x)-\zeta)\rangle. \quad (49)$$

We can obtain an equation for it independently, but we can also use Eq. (38) together with the definition

$$\zeta_t = \lim_{k\to 0}(\varphi_{t+\tau k} - \varphi_t)/k.$$

For (49) we have

$$-l\frac{\partial}{\partial\zeta}w_t(\varphi,\zeta) + 2\frac{\partial^2}{\partial\zeta^2}[\zeta^2 w_t(\varphi,\zeta)] = 0. \quad (50)$$

It is, however, convenient to use in (48') the representation

$$R^2(x') = [\zeta^>(x') - \zeta^<(x')]^{-1} = \int_0^\infty ds\,\exp(-s[\zeta^>(x') - \zeta^<(x')]). \quad (51)$$

There occur then under the integral sign in (48') two factors each of which can be averaged independently

$$F(x-x') = \frac{1}{v}\int_0^\infty ds\int_{-\pi/2}^{\pi/2}d\varphi\bar{g}(R,s,\varphi)w_t(-\varphi,s). \quad (52)$$

One obtains the equation for the function $w_\xi(\varphi, s) \equiv w(s)$ by taking the Laplace transform of (50)

$$-lsw(s) + 2s^2(\partial^2 w(s)/\partial s^2) = 0, \quad (53)$$

and the equation determining $\bar{g}(R, s, \varphi) \equiv \bar{g}(R, s)$ is derived, like (46), by using (18) in the Born approximation

$$\zeta_{j+1} = (\zeta_j + a)\{1 + \frac{1}{2}\gamma^2 + 2\gamma\sin(2\varphi_j + 2ka - \delta)\}. \quad (54)$$

After simple calculations we find

$$l(\partial\bar{g}/\partial R) = -ls\bar{g} + 2s^2(\partial^2 g/\partial s^2) + 4s(\partial\bar{g}/\partial s). \quad (55)$$

The boundary condition for (55) is $\bar{g}(R=0,s) = w(s)$. The solutions of both (53) and (55) can be expressed in terms of Bessel functions, but we shall not obtain these formulae here (see Refs. 3, 4).

In concluding this section we give a brief derivation of the main equations for the case when the potential $U(x)$ represents Gaussian white noise with δ-function pair correlations.

For the energy range $E = E_0 + \varepsilon$, where $\varepsilon = v(k - k_0) \ll E_0$ it is convenient to introduce $\psi = \psi^+ + \psi^-$:

$$\psi^\pm(x) = a_\pm\exp(\pm ik_0 x),$$

where we can neglect the ε-dependence of v. The ap-

V. L. Berezinskii and L. P. Gor'kov   1215

proximate Schrödinger equation has the form

$$v(da_\pm/dx)=\pm i\varepsilon a_\pm \mp i[a_\pm + a_\mp \exp(\mp 2ik_0 x)]U(x).$$

We introduce the amplitude $a(x)$ and the phase $\varphi(x)$, for instance, by the relation

$$a_\pm(x)=a(x)\exp(\pm i\varphi(x)).$$

One then gets easily equations for the new quantities:

$$v(da/dx)=-U(x)\sin(2k_0 x+2\varphi)a, \tag{56}$$

$$v(d\varphi/dx)=\varepsilon-[1+\cos(2k_0 x+2\varphi)]U(x). \tag{57}$$

Assuming $a(x)$ and $\varphi(x)$ to be slowly changing functions it is convenient to write:

$$v\frac{da}{dx}=-\frac{a}{2i}[U_+(x)e^{2i\varphi}-U_-(x)e^{-2i\varphi}],$$

$$v\frac{d\varphi}{dx}=\varepsilon-U_0(x)-\frac{1}{2}U_+(x)e^{2i\varphi}-\frac{1}{2}U_-(x)e^{-2i\varphi},$$

where we have introduced the notation

$$U_0(x)\equiv U(x),\quad U_\pm(x)\equiv U(x)\exp(\pm 2ik_0 x). \tag{58}$$

As before, we denote the solutions of the equations for the phase with the boundary condition $\varphi(x_0)=\varphi_0$ for $x>x_0$ and $x<x_0$ by $\varphi_\varepsilon^>(x|x_0,\varphi_0)$ and $\varphi_\varepsilon^<(x|x_0,\varphi_0)$, respectively. We introduce again the factor

$$\alpha_\varepsilon(x|x')=\frac{a(x)}{a(x')}=\exp\left\{-\frac{1}{v}\int_{x'}^{x}U(\xi)\sin(2k_0\xi+2\varphi(\xi))\,d\xi\right\},$$

which describes the change in the amplitude when we go from x' to x. We have exactly:

$$\alpha_\varepsilon(x|x'')\alpha_\varepsilon(x''|x')=\alpha_\varepsilon(x|x'),$$

$$\frac{vd}{dx}\alpha_\varepsilon(x|x')=-\frac{1}{2i}[U_+(x)e^{2i\varphi(x)}-U_-(x)e^{-2i\varphi(x)}]\alpha_\varepsilon(x|x'),$$

$$\frac{vd}{dx'}\alpha_\varepsilon(x|x')=\frac{\alpha_\varepsilon(x|x')}{2i}[U_+(x')e^{2i\varphi(x')}-U_-(x')e^{-2i\varphi(x')}].$$

To derive (26) we vary Eq. (57):

$$v(d\delta\varphi/dx)=\delta\varepsilon+2U(x)\sin(2k_0 x+2\varphi)\delta\varphi.$$

Comparing this with the equation for $\alpha_\varepsilon(x|x')$ we find for the two forms of the variation ($\delta\varepsilon$ and $\delta\varphi_0$):

$$(\partial/\partial k)\varphi_\varepsilon(x|x_0,\varphi_0)=\int_{x_0}^{x}\alpha_\varepsilon^2(x'|x)\,dx,$$

$$(\partial/\partial\varphi_0)\varphi_\varepsilon(x|x_0,\varphi_0)=\alpha_\varepsilon^{-2}(x|x_0).$$

In order to obtain the analog of Eqs. (32) we must write down the Fokker–Planck equations for the interval

$$l\gg\Delta x\gg k_0^{-1}$$

assuming that the correlation radius for the average $\langle U(x)U(x')\rangle$ is small compared to the mean free path l. In the approximation $k_0 l\gg 1$ the following moments of (58) are nonvanishing:

$$1/l=(\Delta x v^2)^{-1}\iint_{\Delta x>\xi'>\xi>0}\langle U_+(x+\xi')U_-(x+\xi)\rangle\,d\xi\,d\xi'$$

$$=v^{-2}\int_0^\infty\langle U(\xi)U(0)\rangle\exp(2ik_0\xi)\,d\xi,$$

$$1/l^*=(\Delta x v^2)^{-1}\iint_{\Delta x>\xi'>\xi>0}\langle U_-(x+\xi')U_+(x+\xi)\rangle\,d\xi\,d\xi' \tag{59}$$

$$=v^{-2}\int_0^\infty\langle U(\xi)U(0)\rangle\exp(-2ik_0\xi)\,d\xi,$$

$$1/l_0=(\Delta x v^2)^{-1}\iint_{\Delta x>\xi'>\xi>0}\langle U_0(x+\xi')U_0(x+\xi)\rangle\,d\xi\,d\xi'=v^{-2}\int_0^\infty\langle U(\xi)U(0)\rangle\,d\xi.$$

If we assume that $U(x)=U(-x)$ (in the sense that both have the same probability distribution) then $1/l$ is real and $l=l^*$.

To derive the Fokker–Planck equations we must accurately write down expressions for the increases up to terms of second order in $U(x)$. For the increase in the phase $\Delta\varphi(\xi)=\varphi(\Delta x+\xi)-\varphi(\xi)(\Delta\varphi=\Delta_0\varphi+\Delta_1\varphi+\Delta_2\varphi)$ we have

$$\Delta_0\varphi=(k-k_0)\Delta x,$$

$$\Delta_1\varphi(\xi)=-\frac{1}{v}\int_0^\xi d\xi'\left[U_0(x+\xi')+\frac{1}{2}U_+(x+\xi')\exp[2i\varphi(\xi')]\right.$$
$$\left.+\frac{1}{2}U_-(x+\xi')\exp[-2i\varphi(\xi')]\right],$$

$$\Delta_2\varphi(\Delta x)=-\frac{i}{v}\int_0^{\Delta x}d\xi'[U_+(x+\xi')e^{2i\varphi(x)}-U_-(x+\xi')e^{-2i\varphi(x)}]\Delta_1\varphi(\xi').$$

Using (59) we get

$$\left\langle\frac{\Delta_0\varphi}{\Delta x}\right\rangle=k-k_0,\quad\left\langle\frac{\Delta_2\varphi}{\Delta x}\right\rangle=\frac{2}{l''}=i\left(\frac{1}{l}-\frac{1}{l^*}\right),$$

$$\frac{1}{\Delta x}\langle\Delta\varphi_\varepsilon\Delta\varphi_{\varepsilon'}\rangle=\frac{2}{l_0}+\left(\frac{1}{l}+\frac{1}{l^*}\right)\cos(2\varphi_\varepsilon-2\varphi_{\varepsilon'}).$$

In the general case we must add to these formulae

$$\left\langle\frac{\Delta\alpha_\varepsilon}{\Delta x'}\right\rangle=-\frac{1}{4}\left(\frac{1}{l}+\frac{1}{l^*}\right)\alpha_\varepsilon,$$

$$\left\langle\frac{\Delta\alpha_\varepsilon\Delta\alpha_{\varepsilon'}}{\Delta x}\right\rangle=-\frac{1}{2}\left(\frac{1}{l}+\frac{1}{l^*}\right)\cos 2(\varphi_\varepsilon-\varphi_{\varepsilon'})\alpha_\varepsilon\alpha_{\varepsilon'},$$

$$\left\langle\frac{\Delta\alpha_\varepsilon\Delta\varphi_{\varepsilon'}}{\Delta x}\right\rangle=\frac{1}{2}\left(\frac{1}{l}+\frac{1}{l^*}\right)\sin 2(\varphi_\varepsilon-\varphi_{\varepsilon'})\alpha_\varepsilon.$$

We take an average function $F(\ldots,\varphi_{\varepsilon_i}(x),\ldots)$ and define

$$\langle F(\ldots,\varphi_{\varepsilon_i}(x),\ldots)\rangle=\int\prod_i d\varphi_{\varepsilon_i}w(\ldots,\varphi_{\varepsilon_i},\ldots;x)F(\ldots,\varphi_{\varepsilon_i},\ldots), \tag{60}$$

i.e., we introduce a phase probability distribution function $w(\ldots,\varphi_{\varepsilon_i},\ldots;x)$. Considering the change of that average over the interval Δx we get by means of the formulae given above

$$\frac{\partial}{\partial x}\langle F\rangle=\sum_i\left\langle\frac{\partial F}{\partial\varphi_{\varepsilon_i}}\frac{\Delta\varphi_{\varepsilon_i}}{\Delta x}\right\rangle+\frac{1}{2}\sum_{i,k}\left\langle\frac{\partial^2 F}{\partial\varphi_{\varepsilon_i}\partial\varphi_{\varepsilon_k}}\frac{\Delta\varphi_{\varepsilon_i}\Delta\varphi_{\varepsilon_k}}{\Delta x}\right\rangle$$

$$=\sum_i\left[(k_i-k_0)-\frac{2}{l''}\right]\left\langle\frac{\partial F}{\partial\varphi_{\varepsilon_i}}\right\rangle$$

$$+\frac{1}{2}\sum_{i,k}\left\langle\left[\frac{2}{l_0}+\left(\frac{1}{l}+\frac{1}{l^*}\right)\cos 2(\varphi_{\varepsilon_i}-\varphi_{\varepsilon_k})\right]\frac{\partial^2 F}{\partial\varphi_{\varepsilon_i}\partial\varphi_{\varepsilon_k}}\right\rangle$$

and substituting Eq. (60) into the definitions of the averages and integrating by parts we find immediately an equation for the distribution function $w(\ldots,\varphi_{\varepsilon_i},\ldots;x)$:

$$\frac{\partial w}{\partial x}=-\sum_i\left(k-k_0-\frac{2}{l''}\right)\frac{\partial w}{\partial\varphi_{\varepsilon_i}}$$

$$+\frac{1}{2}\sum_{i,k}\frac{\partial^2}{\partial\varphi_{\varepsilon_i}\partial\varphi_{\varepsilon_k}}\left(\left[\frac{2}{l_0}+\left(\frac{1}{l}+\frac{1}{l^*}\right)\cos 2(\varphi_{\varepsilon_i}-\varphi_{\varepsilon_k})\right]w\right).$$

To obtain equations for more general transition functions, in particular, ones which contain factors $\alpha_\varepsilon(y|x)$ we can use the same method, substituting instead of an arbitrary function $F(\ldots,\varphi_{\varepsilon_i}(x),\ldots)$ into (60)

$$F\to\prod_i\alpha_{\varepsilon_i}\bar F(\ldots,\varphi_{\varepsilon_i},\ldots),$$

where $\bar F$ is a new arbitrary function.

APPENDIX

Let there be an average of a product of several $\rho_{\xi_i}(x_i, x_j)$ which appears when we average a product of several Green functions:

$$\prod(\xi_1, \ldots, \xi_n | x_1, \ldots, x_{2n}) = \left\langle \prod_{l=1}^{n} \rho_{\xi_l}(x_i, x_j) \right\rangle_v , \qquad (A.1)$$

where the coordinates of the wave functions may be placed in order of increasing values: $x_1 < x_2 < \cdots < x_{2n}$. We assume that all ξ_i are different. This product then has the form

$$\prod(\xi_1, \ldots, \xi_n | x_1, \ldots, x_{2n})$$
$$= v^{-n} \left\langle \prod_l \delta(\varphi_{\xi_i}{}^>(j_0) - \varphi_{\xi_i}{}^<(j_0)) \alpha_{\xi_i}(x | j_0) \sin \varphi_{\xi_i}(x_i) \right\rangle_v . \qquad (A.2)$$

We have chosen the joining point $x_0 \equiv j_0$ arbitrarily so that

$$-L = -\infty < x_1 < x_2 \ldots, < x_m < x_0 < x_{m+1} < \ldots, < x_{2n} < L = \infty. \qquad (A.3)$$

In (A.2) $\alpha(x_i | j_0)$ can be written as

$$\alpha(x_i | j_0) = \alpha(x_i | x_{i+1}) \alpha(x_{i+1} | x_{i+2}) \ldots \alpha(x_m | j_0) \qquad (A.4)$$

in agreement with the sequence (A.3), if $x_i < j_0$ and

$$\alpha(x_i | j_0) = \alpha(x_i | x_{i-1}) \alpha(x_{i-1} | x_{i-2}) \ldots \alpha(x_{m+1} | j_0), \qquad (A.4')$$

if $x_i > j_0$.

We introduce the stationary probability distributions $w^>$ and $w^<$:

$$w^>(\varphi_1, \ldots, \varphi_n) = \left\langle \prod_{l=1}^{n} \delta(\varphi_{\xi_i}{}^> - \varphi_l) \right\rangle_v ,$$
$$w^<(\varphi_1, \ldots, \varphi_n) = \left\langle \prod_{l=1}^{n} \delta(\varphi_l - \varphi_{\xi_i}{}^<) \right\rangle_v \qquad (A.5)$$

and the generalized transition functions going from i to $i+1$:

$$w_{i,i+1}^{>(s)}(\varphi_1{}^i, \ldots, \varphi_n{}^i | \varphi_1{}^{i+1}, \ldots, \varphi_n{}^{i+1})$$
$$= \left\langle \prod_{l=1}^{n} \delta(\varphi_l{}^{i+1} - \varphi_{\xi_i}{}^>(x_{i+1} | \varphi_l{}^i, x_i)) \prod \alpha_{\xi_p}^{s_p}(x_{i+1} | x_i) \right\rangle , \qquad (A.6)$$

and similarly for the functions

$$w_{i,i+1}^{<(s)}(\varphi_1{}^i, \ldots, \varphi_n{}^i | \varphi_1{}^{i+1}, \ldots, \varphi_n{}^{i+1}),$$

which determine the set of quantities α and phases in the point $x_i < x_{i+1}$ if the set of phases is given in the point x_{i+1}. The $\varphi_{\xi_i}^>(x_{i+1} | \varphi^i, x_i)$ and $\varphi_{\xi_i}^<(x_i | \varphi_i^{i+1}, x_{i+1})$ which occur in these definitions are, respectively, the solutions of Eqs. (17) and (17') in the points $x_{i+1}(x_i)$ under the condition that in the point $x_i(x_{i+1})$ the phase equals $\varphi_i^i(\varphi_i^{i+1})$ for an energy ξ_i. In the vector $s = \{s_1, \ldots, s_n\}$ each component s_i indicates the power of the factor $\alpha_{\xi_i}(x_{i+1} | x_i)$ in the product $\Pi \, \alpha_{\xi_p}^{s_p}(x_i | x_{i+1})$. The vector s is determined by the coordinate distribution in (A.3) and by the writing down of the factors $\alpha_{\xi_i}(x_i | j_0)$ in the ordered form (A.4) or (A.4'). The

separate component s_i can thus have the values 0, 1, and 2. The rules for the construction of the average are simple. It is clear that the intervals $(-\infty, x_1)$ and (x_{2n}, ∞) are associated, respectively, with the stationary probability distributions $w^>(\varphi_1, \ldots, \varphi_n)$ and $w^<(\varphi_1, \ldots, \varphi_n)$. Each interval (x_i, x_{i+1}) in (A.3) is associated with a transition function of the form (A.6), $w^{>(s)}$, if $x_i \leq j_0$ and $w^{<(s)}$, if $x_i \geq j_0$. Finally, each of the ψ-functions in (A.1) gives not only $\alpha_{\xi_i}(x_i | j_0)$, but, according to (14), also a factor $\sin \varphi_{\xi_i}(x_i)$. The expression obtained must be integrated over all phases occurring in it in the points x_i and j_0. The meaning and advantage of such a representation of (A.1) lies in the fact that it is divided into a product of factors, each of which can, in agreement with the assumption about the Markovian nature of the random process, be averaged independently in the intervals (A.3). The functions (A.5) and (A.6) satisfy, of course, equations with partial derivatives.

In actual problems one does normally not use the expressions for the transition probabilities as it is easier to write down recurrence relations relating the point j_0 to one of the coordinates occurring in (A.1).

For a proof that nothing depends on the choice of the point j_0 we note that as long as the point j_0 lies in one of the intervals (A.3), (A.4), the independence of the results with respect to its position is determined exclusively by the properties of the probability distribution:

$$w_{x_m, x_{m+1}}^{>(s)}(\varphi_1{}^m, \ldots, \varphi_n{}^m | \varphi_1{}^{m+1}, \ldots, \varphi_n{}^{m+1}) = \int w_{x_m, x_0}^{>(s)}(\varphi_1{}^m, \ldots, \varphi_n{}^m | \varphi_1', \ldots, \varphi_n')$$
$$\times w_{x_0, x_{m+1}}^{>(s)}(\varphi_1', \ldots, \varphi_n' | \varphi_1{}^{m+1}, \ldots, \varphi_n{}^{m+1}) \prod_{c=1}^{n} d\varphi_l' .$$

If the point j_0 changes an interval of (A.3) we must use for a proof of the independence the relations

$$w_{x, x'}^{>(s)}(\varphi_1, \ldots, \varphi_n | \varphi_1', \ldots, \varphi_n') = w_{x, x'}^{<(s-2)}(\varphi_1, \ldots, \varphi_n | \varphi_1', \ldots, \varphi_n'). \qquad (A.7)$$

The verification of the latter statement consists in the observation that δ-functions such as $\delta(\varphi' - \varphi^>(x' | x, \varphi))$ express the fact that $\varphi = \varphi^<(x | x', \varphi')$ and therefore

$$\delta(\varphi' - \varphi^>(x' | x, \varphi)) = \delta(\varphi - \varphi^<(x | x', \varphi')) [\partial \varphi^>(x' | x, \varphi) / \partial \varphi]^{-1}.$$

Differentiating (17) and using the boundary condition we find easily

$$\partial \varphi_t(i' | i, \varphi) / \partial \varphi = \alpha_t^{-2}(i' | i),$$

which proves (A.7).

We show in conclusion that the results are independent of the choice of the intervals $(0, \pi)$ or $(0, 2\pi)$. The possibility to change from one interval to the other is connected with the fact that when $k_F l \gg 1$ all stochastic equations are invariant with respect to the transformation $\varphi_{\xi_i} \to \varphi_{\xi_i} \pm \pi$ for each variable φ_{ξ_i} independently. We show how one can use that fact through the example of averaging a two-point expression of the kind

$$\sum_v f_1(\varphi_j) f_2(\varphi_{j'}) \delta(\xi - \xi_v),$$

i.e., we shall consider Eq. (28), dropping the unimportant factor $\alpha(j|j')$. The total expression for this average is

$$A_{jj'} = \frac{2}{v}\int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \langle [\delta(\varphi_j^> - \varphi) + \delta(\varphi_j^> - \varphi - \pi)] f_1(\varphi)$$
$$\cdot \delta(\varphi - \varphi^< (j|j', \varphi')) f_2(\varphi') \delta(\varphi' - \varphi_{j'}^<) \rangle_v.$$

Here $\langle \delta(\varphi_{j(j')}^> - \varphi) \rangle$ and $\langle \delta(\varphi - \varphi^<(j|j', \varphi')) \rangle$ are, respectively, the probability distribution function and the transition probability referring to the interval $(0, 2\pi)$. We have

$$A_{jj'} = \frac{2}{v}\int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \langle \delta(\varphi_j^> - \varphi) [f_1(\varphi)\delta(\varphi - \varphi^<(j|j', \varphi'))$$
$$+ f_1(\varphi + \pi)\delta(\varphi + \pi - \varphi^<(j|j', \varphi'))] f_2(\varphi') \delta(\varphi' - \varphi_{j'}^<) \rangle_v$$

$$= \frac{2}{v}\int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \langle \delta(\varphi_j^> - \varphi) [f_1(\varphi)\delta(\varphi - \varphi^<(j|j', \varphi')) f_2(\varphi') \delta(\varphi' - \varphi_{j'}^<)$$
$$+ f_1(\varphi + \pi)\delta(\varphi - \varphi^<(j|j', \varphi')) f_2(\varphi' + \pi)\delta(\varphi' + \pi - \varphi_{j'}^<)] \rangle_v.$$

As was explained above

$$\langle \delta(\varphi_{j(j')}^> - \varphi) \rangle = \langle \delta(\varphi_{j(j')}^> - \varphi - \pi) \rangle = \tfrac{1}{2} w^>(\varphi),$$

where $w^>(\varphi)$ is the probability distribution (29) referring to the interval $(0, \pi)$. If the functions f_1 and f_2 are both even or odd with respect to the substitution $\varphi \to \varphi \pm \pi$ we get again Eq. (31).

When there are several energies we can perform the indicated transformations independently for each variable φ_{ε_i}.

[1] Hence it follows that in the averaged single-particle Green functions there is no information about localization or delocalization.

[2] Writing it down in terms of the spectral density means that among all integrations the integration over E must be performed last. In accordance with §37 of Ref. 8 we must then drop the term with $e^2\bar{\rho}A/m$.

[3] See the Appendix about the choice of interval.

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Kinetic phenomena in semiquantum liquids

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The temperature dependence of the viscosity and of the thermal conductivity of liquids is obtained in the semiquantum region, i.e., below the Debye temperature but above the quantum degeneracy temperature. The viscosity is inversely proportional and the thermal conductivity is proportional to the temperature.

From the point of view of the symmetry of particle arrangement, liquids do not differ from gases and are on the average homogeneous and isotropic systems that have no long-range order. In contrast to gases, however, they have a clearly pronounced short-wave order, a substantial manifestation of which is the presence of the vibrational particle motion characteristic of solids. Melting of a solid is accompanied by a relatively small change of the density and therefore affects relatively little the properties of short range order and of the vibrational motion. In liquids, however, there is a translational particle motion much more pronounced than in solids. This motion, however, which in fact is what destroys the long-range order, has nothing in common with the free translational motion of particles in gases. It is the result of individual acts of jumping from one equilibrium position, about the

particle had executed oscillatory motion, to a neighboring vacant equilibrium position. It is of course more accurate to speak of acts of the simultaneous rearrangement of the configuration of the equilibrium positions of a group of particles. Since any such rearrangement entails the surmounting of a potential barrier, the characteristic frequency $1/\tau$ (τ is the lifetime in the given equilibrium position) of the translational motion decreases very rapidly (exponentially) when the interaction increases. In a strong-interaction system, such as a liquid, this frequency is much lower than the characteristic frequency Ω of the vibrational motion of the particle about the equilibrium positions.

The described picture is the basis of the theory developed by Frenkel[1] for kinetic phenomena in ordinary