Localization dynamics in weakly disordered systems

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The time dependence of the localization of a quantum particle in a disordered system is considered. It is assumed that the particle is placed into the system at the initial instant, and the character of its transition to a stationary localized state is tracked. In the one-dimensional case this problem can be solved exactly in all of time, starting with the atomic scale. The final dependence is found to be quite simple and reflects some new features of one-dimensional localization. The ensuing physical properties of the observable quantities are indicated. In the case of systems of large dimensionality, the spreading is discussed within the framework of perturbation theory and of the Mott description of the resonance states.

I. INTRODUCTION

A feature of a disordered electronic system is the onset of localized states.[1] The elucidation of the nature and character of these states has been the subject of a large number of studies. We wish to call attention here to another aspect of this phenomenon, namely, the dynamic features of the transition into a localized state, i.e., to the manner in which the electron becomes localized in time from an almost free state (see below). Clearly, such characteristics determine many important properties of the system, for example the transient injection current, the hopping kinetics,[2] and others.

The standard formulation of the problem is the following. Assume that an electron was placed on site n of a disordered lattice at an initial instant of time $t = 0$. The question is: what is the probability $W(t)$ that it will remain on the same site at an instant $t > 0$. Strictly speaking, the localization criterion is the behavior of $W(t)$ as $t \to \infty$ (Ref. 3). In the case of localized states $W(t \to \infty)$ tends to a finite limit W_0. The time by which $W(t)$ reaches values on the order of W_0 can be defined in the general case as the localization time T_{loc}. It was in just this formulation that the localization problem was investigated numerically for the one-dimensional state in Ref. 4, and T_{loc} was estimated at $T_{\mathrm{loc}} \approx 20\tau$, where τ is the Boltzmann time between collisions. Actually, the very character of the behavior of $W(t)$ is still a question for which an answer has not yet been found within the framework of analytic theories. We have found in the present study that $W(t)$ approaches W_0 in as a power-law function $(\tau/t)^3$.

We turn first to the one-dimensional case, since this problem can be solved exactly. Naturally, we use a continual version of the model with an infinitely broad band. Next, as indicated in Ref. 5, we must change to a description in terms of wave packets, assuming that the spatial dimension of the packet is $\Delta x \ll L_{\mathrm{loc}}$, where L_{loc} is the localization radius. The disorder will be taken into account mainly by the Berezinskiĭ method.[6] This approach led to a number of exact relations[7,8] (see also the review in Ref. 9). They touch upon mainly, however, the coordinate dependence of the first asymptotic expansion in the frequency $\omega \to 0$ of several correlators. Our task is, technically, to study the entire frequency dependence of the two-particle correlation function, subject to certain constraints on the coordinates. This principal and procedurally new result is contained in Eq. (17) [with allowance for (21), (22) and (23)–(25)]. It creates a unified rigorous

mathematical base for the treatment of the great variety of physical problems touched upon in the present paper.

2. FORMULATION OF THE PROBLEM

Let the state of the electron at the instant of time $t = 0$ be described by the function $\psi_i(x)$. Its evolution in the succeeding instants of time $t > 0$ is then specified by the function

$$\psi(y, t) = \sum_n \exp(i\varepsilon_n t) \psi_n(y) \int dx\, \psi_n^*(x) \psi_i(x), \qquad (1)$$

where ψ_n and ε_n are the eigenfunction and eigenvalues of the total Hamiltonian, with allowance for impurities. The corresponding amplitude of the transition to a state with $\psi_f(x)$ will be

$$A_{i \to f}(t) = \int dx\, \psi_i(x) \int dy\, \psi_f^*(y)\, (-iG_-(x, y; t)), \qquad (2)$$

where the advanced Green's function is defined in standard fashion:

$$G_-(x, y; t) = \int \frac{d\varepsilon}{2\pi} e^{i\varepsilon t} G_-(x, y; \varepsilon),$$

$$G_-(x, y; \varepsilon) = \sum_n \frac{\psi_n^*(x) \psi_n(y)}{\varepsilon - \varepsilon_n - i0}.$$

We obtain the physically observable transition probability after averaging $|A(t)|^2$ over the random potential. It can be written in the form

$$W_{i \to f}(t) = \int \frac{d\omega}{2\pi} e^{i\omega t} W_{i \to f}(\omega), \qquad (3)$$

$$W_{i \to f}(\omega) = \int dx\, \psi_i(x) \int dy\, \psi_f^*(y) \int dx'\, \psi_i^*(x') \int dy'\, \psi_f(y')$$
$$\times \int \frac{d\varepsilon'}{2\pi} K(x, y; x', y'; \varepsilon' + \omega, \varepsilon'), \qquad (4)$$

$$K(x, y; x', y'; \varepsilon, \varepsilon') = \langle G_-(x, y; \varepsilon) G_+(x', y'; \varepsilon') \rangle,$$
$$G_+(x, y; \varepsilon) = (G_-(x, y; \varepsilon))^*, \qquad (5)$$

where the angle brackets denote the sought-for averaging. We can similarly express in simple fashion the electron-density distribution probability $\rho(y, t)$ at the instant of time t, if initially ($t = 0$) the state of the electron was described by the wave function $\psi_i(x)$. According to (1) and (5) we have

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$$\rho(y,t)=\langle|\psi(y,t)|^2\rangle=\int\frac{d\omega}{2\pi}e^{i\omega t}\rho(y,\omega),$$

$$\rho(y,\omega)=\int dx\,\psi_i(x)\int dx'\,\psi_i^*(x')$$

$$\times\int\frac{d\varepsilon'}{2\pi}K(x,y;x',y;\varepsilon'+\omega,\varepsilon'). \tag{6}$$

As to $\psi_{i,f}(x)$, we assume that they constitute a spatially bounded wave packet of size $\Delta x\ll L_{loc}$ with a carrier frequency $\varepsilon_F=mv_F^2/2$. According to the exact solution,[6-9] the localization radius is $L_{loc}=2\tau_2 v_F=2l_2$, where τ_2 and l_2 are the time and length of free path with respect to backward scattering. The energy width Δ_ε of the packet is found in turn to be such that

$$1/\varepsilon_F\ll1/\Delta\varepsilon\approx\Delta x/v_F\sim\Delta t\ll\tau_2,$$

where Δt is the time of the ballistic decay of the wave packet. It is convenient to represent $\psi(x)$ in the form

$$\psi(x)=\int\frac{dk}{2\pi}\varphi(k)e^{ikx}, \tag{7}$$

where $\varphi(k)$ is centered relative to $\pm k_F$ with a width of order $\Delta k\approx1/\Delta x$. By way of example, we consider a Gaussian packet of the type

$$\varphi(k)=N\left\{\exp\left[\frac{(k-k_F)^2}{2\alpha^2}\right]+\exp\left[-\frac{(k+k_F)^2}{2\alpha^2}\right]\right\},\quad N=\frac{\pi^{1/4}}{\alpha^{1/2}}, \tag{8}$$

where $k_F/\alpha\gg1$; then

$$\psi_0(x)=\frac{2N\alpha}{(2\pi)^{1/2}}\cos(k_Fx)\exp\left[-\frac{(\alpha x)^2}{2}\right]. \tag{9}$$

In the absence of disorder, the spreading of such a wave packet follows the law ($\psi_i(x)=\psi_f(x)=\psi_0(x)$)

$$W_0(t)=\exp\left[-\frac{1}{2}(t/\Delta t)^2\right],\quad\Delta t=\alpha/v_F. \tag{10}$$

This justifies the definition of Δt as the ballistic-decay time. Strictly speaking, Eq. (10) is valid so long as $t\leqslant\bar{t}=\Delta t(k_F/\alpha)$. At $t\geqslant\bar{t}$ the function W_0 falls off like $1/t$, but here $W_0(t)$ turns out to be already exponentially small, since $k_F/\alpha\gg1$. We shall consider hereafter also asymmetric wave packets of the type

$$\psi_+(x)=\pi^{-1/2}N\alpha\exp(ik_Fx)\exp[-(\alpha x)^2/2],\quad\psi_-(x)=\psi_f^*(x). \tag{11}$$

The presence of impurities makes possible transitions between two states with $\psi_+(x)$ and $\psi_-(x)$.

The problem consists thus of calculating the function $K(x;y;x',y';\varepsilon,\varepsilon')$ in the general case for arbitrary values of the coordinates and energies. We, however, confine ourselves to a region of coordinates that are close to one another with the difference between each pair of coordinates not larger than $\Delta x\ll l_2$, although the approach developed below uncovers a possibility of calculating K also in an arbitrary case.[10] It will be shown below that this dependence can be divided into a fast one of the type $\exp(ipx)$ and a slow one in the form $\exp(-x/l_2)$. Since $\Delta x\ll1$, the second dependence can be neglected. After integrating over the fast dependence with $\psi_{i,f}(x)$ in the form (7), we relate the internal energies (ε and ε') with the specified energies of the wave packets (k_i

and k_f). Naturally, they turn out to be close. The problem of finding the coordinate dependence of K becomes substantially simpler if no distinction is made in it between the energies ε and ε'. This is valid if $p-p'=\omega/v_F\ll1/\Delta x$, or for $t\gg\Delta x/v_F\approx\Delta t$.

4. CALCULATION OF FOUR-POINT CORRELATION FUNCTION

We turn to perturbation theory, choosing as the starting point the free Green's functions

$$G_-(x,y;\varepsilon)=\int\frac{dp}{2\pi}\frac{\exp[ip(x-y)]}{\varepsilon-E(p)-i0}=\frac{i}{v}\exp[-ip|x-y|],$$

$$G_+(x',y';\varepsilon')=-\frac{i}{v}\exp[ip'|x'-y'|],$$

where

$$p=(2m\varepsilon)^{1/2}-i0,\quad v=p/m,\quad p'=(2m\varepsilon')^{1/2}+i0,$$

and regarding the scattering by the impurities as a perturbation. The corresponding technique of summing the essential perturbation-theory-series diagrams obtained in this manner was proposed by Berezinskiĭ.[6] It is based on the idea of spatial ordering of the diagrams. Details of this technique can be found in the reviews.[7,8] According to this approach, in diagram notation, the sought-for object breaks up in the coordinate representation, by drawing sections through the outer vertices, into a product of individual blocks with fixed numbers of incoming and outgoing electron lines. The outermost blocks $R_m(z)$ produced in this manner obviously coincide with the left- and right-hand sides which were introduced already earlier by Berezinskiĭ (see Fig. 1a). Their distinguishing feature is that the number of pairs of single (G_-) and double (G_+) lines coincide. The corresponding equation for $R_m(z)$ is of the form

$$R_m(z)=\exp[-2i(p-p')mz]\bar{R}_m,\quad s\bar{R}_m=m(\bar{R}_{m+1}+\bar{R}_{m-1}-2\bar{R}_m), \tag{12}$$

where $s=2i\tau_2\omega$ and $\omega=v(p-p')-i0$. To consider the central part of the diagrams we must introduce new blocks, where the numbers of single and double lines are different. It is easy, however, to determine the explicit coordinate dependence of each such block.[11,13] Consider, for example, the block $T_m(z)$ shown in Fig. 1b, with $2m+1$ single and $2(m+1)$ double lines. An example of a diagram that contributes to T_m is shown in Fig. 2. Following the standard derivation,[6-8] we can find the following equation for T_m:
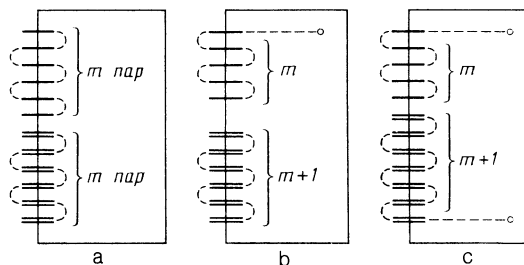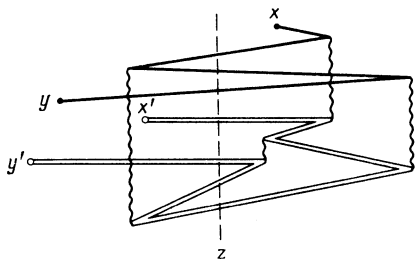

FIG. 1.

FIG. 2.

$$T_m(z) = \exp\left[-2i(p-p')(m+1)z\right]\widetilde{T}_m(z),$$

$$2i(p-p')(m+1)\widetilde{T}_m(z) - \frac{\partial}{\partial z}\widetilde{T}_m(z) = \frac{1}{2}\left(\frac{1}{l_1} + \frac{1}{l_2}\right)\widetilde{T}_m$$

$$+ \frac{(m+1)^2}{l_2}(\widetilde{T}_{m+1} - \widetilde{T}_m) - \frac{m(m+1)}{l_2}(\widetilde{T}_m - \widetilde{T}_{m-1}), \quad (13)$$

where we have separated the explicit (rapid) dependence of T_m on z. Clearly, the remaining dependence of T_m on z is due to the boundary condition, its scales are $1/l_i$, and $p - p' = \omega/v \approx 1/vt$, and can be neglected compared with the small parameter $\Delta x/l_i$ or $\Delta t/t$. In fact, the boundary condition for $\widetilde{T}_m(z)$ is

$$\widetilde{T}_m(z)|_{z=x} = \widetilde{R}_{m+1}(x).$$

In the region of small $z - x$ the function $\widetilde{T}_m(x)$ can then be represented in the form

$$\widetilde{T}_m(z) = \widetilde{T}_m(x) + (z-x)(\partial\widetilde{T}_m/\partial z)_{z=x}, \quad (14)$$

where $\widetilde{T}_m(x) = \widetilde{R}_{m+1}$, and according to (12) and (13) we have

$$\frac{\partial\widetilde{T}_m}{\partial z}\bigg|_{z=x} = -\frac{1}{2}\left(\frac{1}{l_1} + \frac{1}{l_2}\right)\widetilde{R}_{m+1} - \frac{(m+1)}{l_2}(\widetilde{R}_{m+1} - \widetilde{R}_m).$$

In the region of small $s \ll 1$ the last equation can be rewritten in the form

$$\frac{\partial\widetilde{T}_m}{\partial z} = -\frac{1}{2}\left(\frac{1}{l_1} + \frac{1}{l_2}\right)\widetilde{R}(\zeta) - \frac{1}{l_2}\zeta\frac{\partial\widetilde{R}}{\partial\zeta},$$

where $\zeta = ms$. Since $\zeta\partial\widetilde{R}/\partial\zeta \approx \widetilde{R}(\zeta)$ [see (19a)], the second term in (14) can be neglected compared with the first if $|z - x|/l_2 \ll 1$. In the region $s \gg 1$ we have for $\widetilde{R}_m(s)$ the high-frequency expansion $\widetilde{R}_m(s) \approx O(1/s^m)$, and according to (12) $(m + 1)\widetilde{R}_m \approx s\widetilde{R}_{m+1}$. Consequently, the condition for neglecting the second term compared with the first at $s \gg 1$ is the inequality $s|z - x|/l_2 \ll 1$. The estimates $s \approx \tau_2/t$ and $|z - x| \approx \Delta x$ allow us to rewrite this condition in the form $t \gg \Delta t$.

This approach can be used to analyze also other blocks that enter into the problem. In particular, for the block S_m (see Fig. 1c), which contains $2m + 1$ single and $2(m + 1) + 1$ double lines, we obtain the following equation:

$$S_m(z) = \exp\left[-2i(p-p')mz\right]\widetilde{S}_m(z),$$

$$2i(p-p')m\widetilde{S}_m - \frac{\partial}{\partial z}\widetilde{S}_m = -\left(\frac{2}{l_1} + \frac{1}{l_2}\right)\widetilde{S}_m$$

$$+ \frac{1}{l_2}(m+1)(m+2)(\widetilde{S}_{m+1} - \widetilde{S}_m) \quad (15)$$

$$- \frac{1}{l_2}m(m+1)(\widetilde{S}_m - \widetilde{S}_{m-1}).$$

It can be noted that in the limit as $s \to 0$, but with $\zeta = ms -$ const, Eq. (15) becomes equal, after a simple substitution, to the corresponding equation for the central part of $Z_m(z)$, introduced by Berezinskiĭ. As a result we have

$$S_m(z) = \exp\left[-|z|(2/l_1 + 1/l_2)\right]Z(\zeta, z). \quad (16)$$

The main conclusion that can be drawn from the foregoing analysis of the blocks T_m and S_m is that no dangerous dependence, say of the form $\exp(ipmz)$, appears in blocks in which the numbers of double and single lines are not equal. As to the dependence of type $\exp[i(p - p')mz]$, it is cancelled out in the usual manner[6-8] when the blocks are joined together in the derivation of the complete expression for the correlator K. Thus, even by proceeding directly to calculate the function K and following the foregoing analysis of the blocks it contains we can establish the complete form of the coordinate dependence of K at all possible arrangements of the coordinates. As already stated, the difference between p and p' can be disregarded. After separating the rapid dependence, all the coordinates in the remaining part of K can be regarded as equal, and this part becomes simply equal to the autocorrelator. This is valid again for the parameter $\Delta x/l_2$. We ultimately obtain for K the expression

$$K(x, y; x', y'; \varepsilon, \varepsilon') = v^{-2}\exp\left[-ip(|x-y| - |x'-y'|)\right]$$
$$+ 4v^{-2}\cos\left[p(x-y)\right]\cos\left[p(x'-y')\right]A(\omega)$$
$$+ 2v^{-2}\cos\left[p(x+y-x'-y')\right]B(\omega), \quad (17)$$

$$A(\omega) = \sum_{m=0}^{\infty}\widetilde{R}_{m+1}\widetilde{R}_{m+1}, \quad B(\omega) = \sum_{m=0}^{\infty}\widetilde{R}_m\widetilde{R}_{m+1}. \quad (18)$$

The following interpretation of (17) and (18) can be proposed. In a region where the coordinates x, y, x', y' differ by less than l_2, there is no impurity scattering. The preceding analysis was in fact devoted to a proof of this statement. In this case the numbers of pairs of lines in the right-hand and left-hand sides are equal or differ by unity, and the coordinate dependence stems only from the outer vertices. The term with A in (17) corresponds to the case when the electron lines in each pair of outer vertices, x, y or x', y', are oppositely directed, and the term with B corresponds to the variant in which the electron lines are connected to all the outer vertices from one side. The first term in (17) corresponds to free propagation of the electron.

Equation (12) is a functional form of the confluent hypergeometric equation,[13] and its solution, which satisfies the condition $R_0(s) = 1$ and decreases as $m \to \infty$ is of the form

$$\widetilde{R}_m(s) = s\Gamma(m+1)\Psi(m+1, 2; s), \quad (19)$$

where Γ is the gamma function and Ψ a confluent hypergeometric function. The validity of the relation can be verified by substituting (19) in (12) and using the known relations for functions associated with Ψ (Ref. 13). In the limit as $s \to 0$ and $m \to \infty$, but with $\zeta = ms -$ const, Eq. (19) takes the form of the known solution[6,7]

$$\widetilde{R}_m(s) = 2\zeta^{1/2}K_1(2\zeta^{1/2}), \quad (19a)$$

where $K_1(\zeta)$ is a modified Bessel function. To calculate A and B it is convenient to use in (18) an integral representation for $R_m(s)$, in the form

$$\tilde{R}_m(s) = \int_0^\infty e^{-y} \left(1 + \frac{s}{y}\right)^{-m} dy. \tag{20}$$

This form of the solution (12) was first indicated in Ref. 6. As a result,

$$A(\omega) = \frac{1}{3s} - \frac{1}{6} \int_0^\infty \frac{u^2 \, du}{s+u} e^{-u}, \tag{21}$$

$$B(\omega) = \frac{1}{3s} + \frac{1}{3} \int_0^\infty \frac{u^2 \, du}{s+u} e^{-u}. \tag{22}$$

The functions A and B represent at $x \gg 1$ the first perturbation-theory orders:

$$A = 1/s^2 + O(1/s^3), \quad B = 1/s + O(1/s^2).$$

At low frequencies we have, besides the pole singularity corresponding to localization, also a logarithmic singularity, and it is this which determines the localization rate. A and B take a rather simple form in the temporal representation:

$$A(t) = \frac{1}{2\tau_2} \left[\frac{1}{3} - \frac{1}{3} \left(\frac{2\tau_2}{t+2\tau_2}\right)^3 \right], \tag{23}$$

$$B(t) = \frac{1}{2\tau_2} \left[\frac{1}{3} + \frac{2}{3} \left(\frac{2\tau_2}{t+2\tau_2}\right)^3 \right]. \tag{24}$$

It is of interest to compare the present results with those of simple diffusion. The latter can be investigated also by using the present approach. In this case Eqs. (17) and (18) remain in force, and on the equation for R_m changes[14]:

$$s\tilde{R}_m = \tilde{R}_{m+1} + \tilde{R}_{m-1} - 2\tilde{R}_m,$$

from which follows

$$\tilde{R}_m = \exp(-\lambda m),$$

where $s = \sinh^2(\lambda/2)$, and

$$A_D(s) = \tfrac{1}{2} \{(2+s)[s(s+4)]^{-1/2} - 1\}, \quad B_D(s) = [s(s+4)]^{-1/2}.$$

Consequently, the behavior of these two processes in the region $t \ll \tau_2 (s \gg 1)$ turns out thus to be similar, since it is governed in both cases by the first perturbation-theory terms and turns out to be substantially different at times that are long compared with τ_2. Here [cf. Eq. (24)]

$$B_D(t) = \frac{1}{2\tau_2} \left(\frac{\tau_2}{2\pi t}\right)^{1/2} \left[1 + O\left(\frac{\tau_2}{t}\right)\right] \tag{25}$$

and $A_D(t)$ are described by decreasing relations typical of one-dimensional diffusion.

4. RATE AND PECULIARITIES OF ONE-DIMENSIONAL RELAXATION

As seen from (17), the frequency and coordinate dependences of the function K were separated. It is clear from physical considerations that the frequency dependence reflects the properties of the energy spectrum of the system. In fact, the density-of-states correlator introduced in Ref. 15

$$F_\omega(z) = \left\langle \sum_{m,n} \delta(\varepsilon_F - \varepsilon_m) \delta(\varepsilon_F + \omega - \varepsilon_n) \psi_m^2(x) \psi_n^2(x') \right\rangle, \tag{26}$$

where $z = x - x'$, can be expressed in terms of K in the form

$$F_\omega(z) = \frac{1}{4\pi^2} \left[\frac{2}{v_F^2} + K(x, x; x', x'; \varepsilon_F, \varepsilon_F + \omega) + K(x', x'; x, x; \varepsilon_F + \omega, \varepsilon_F) \right]. \tag{27}$$

Substituting here the expression for K from (17), we get

$$F_\omega(z) = [N(0)]^2 \left\{ \left(1 - \frac{2}{3} \sin^2 k_F z\right) \right.$$
$$\times \left[1 + \frac{\pi}{2\tau_2} \delta(\omega)\right] + \frac{2}{3} C(\omega) \sin^2 k_F z \left. \right. ,$$

$$C(\omega) = (2\omega\tau_2)^2 \int_0^\infty \frac{\cos(2\omega\tau_2 y)}{y+1} dy, \tag{28}$$

where $N(0) = 1/\pi v_F$ is the one-electron density of states. The appearance of a term with $\delta\omega$ in (28) indicates that we are dealing with localized states.[16] The function $C(\omega)$ admits of both high-and low-frequency expansions:

$$C(\omega) = \begin{cases} 1 - 6/(2\omega\tau_2)^2, & 2\omega\tau_2 \gg 1, \\ (2\omega\tau_2)^2 \ln(1/2\omega\tau_2), & 2\omega\tau_2 \ll 1. \end{cases}$$

With this expression for $C(\omega)$, Eq. (28) yields, after averaging within the limits of the atomic scale, the first term obtained in Ref. 15 for the asymptotic expansion of $F_\omega(z)$.

On the other hand, the coordinate dependence of the function K reflects the structural singularities of the wave function of the localized state. According to (6), the electron-density distribution function at the instant of time t takes, for an initial state described by (9), the form

$$\rho(x, t) = \frac{1}{2l_2} \left[\frac{2}{3} + \frac{1}{3} \left(\frac{2\tau_2}{t+2\tau_2}\right)^3 \right]$$
$$+ \frac{\cos(2k_F x)}{2l_2} \left[\frac{1}{3} - \frac{1}{3} \left(\frac{2\tau_2}{t+2\tau_2}\right)^3 \right]. \tag{29}$$

Note that this expression contains an oscillating contribution, thereby reflecting the conservation of the interference effects in a system with impurities. The result (29) was obtained under the assumption that $|x| \ll l_2$ and $t \gg \Delta t$. Actually, however, the oscillating term indicated above is present also at larger x. Altogether, for the distribution function of the electron density in a localized state [6,7] we can obtain

$$p(x) = \rho(x, t \to \infty)$$
$$= p_0(x)\{1 + \tfrac{1}{2} \cos(2k_F x) \exp[-|x|(2/l_1 + 1/l_2)]\}, \tag{30}$$

where an expression for $p_0(x)$ was indicated in Ref. 17. Equation (30) can be obtained by recognizing that for the density-density correlator (see Refs. 6–8) it is always possible to add diagrams with rearranged outer vertices (an example of such a rearrangement is shown in Fig. 3, graphs a and b). The equation for the central part corresponding to a sum of diagrams with permuted outer vertices coincides then with S_m from (15). According to (16), the function $S_m(z)$ differs from the Berezinskiĭ central part $Z_m(z)$ only by a factor. Recognizing that permutation of the vertices gives rise to an exponential factor, we arrive directly at
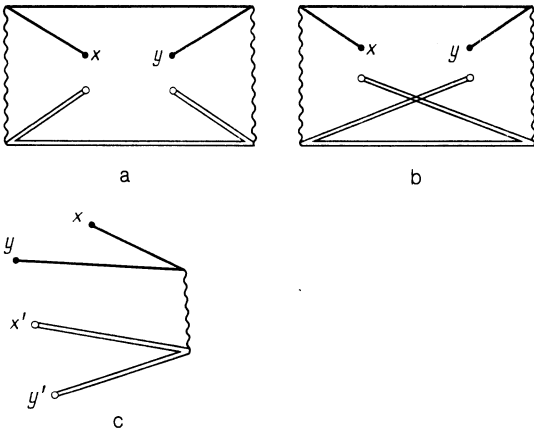
FIG. 3.

expression (30). Clearly, if we are interested in the integral characteristics of $p(x)$ with a scale larger than or equal to l_2, the oscillating contribution to (30) turns out to be negligible in terms of the parameter $1/k_F l$. However, for quantities of order Δx, such that $1/k_F \ll \Delta x \ll l_2$, the oscillatory increment becomes important. Such a situation arises, for example, if we describe localization processes in terms of Gaussian packets of size $\Delta x \ll l_2$. The corresponding matrix elements of the function K can then be interpreted, according to (4), as transition probabilities. Using (4), (7), and (17) we get

$$W_{i \to f}(t) = \chi_a A(\omega) + \chi_b B(\omega), \tag{31}$$

$$\chi_a = \frac{1}{v_F} \int \frac{dq}{2\pi} \left[\varphi_i(k_F + q) \varphi_f(k_F + q) + \varphi_i(-k_F - q) \varphi_f(-k_F - q) \right]^2, \tag{32}$$

$$\chi_b = \frac{1}{v_F} \int \frac{dq}{2\pi} \left[\varphi_i^2(k_F + q) \varphi_f^2(-k_F - q) + \varphi_i^2(-k_F - q) \varphi_f^2(k_F + q) \right]. \tag{33}$$

Choosing $\psi_i(x) = \psi_f(x) = \psi_+(x)$ from (11), we get

$$W_{k_F \to k_F}(t) = \chi_a A(t) \tag{34}$$

and for $\psi_i(x) = \psi_+(x)$, $\psi_f(x) = \psi_-(x)$ we have

$$W_{k_F \to -k_F}(t) = \chi_b B(t), \tag{35}$$

where $\chi_a = \chi_b = (2\pi)^{1/2}/\alpha v_F$. In the limit as $t \to \infty$ we have

$$W_{k_F \to \pm k_F} = W_0 = \chi_a/6\tau_2 = (2\pi)^{1/2}/6\alpha l_2,$$

which has a clear meaning if it is recognized that the width of the packet is $\Delta x = 1/\alpha$.

It is surprising that according to (34) and (35) $W_{k_F \to \pm k_F}(t)$ turns out to be of the order of W_0 already at $t \ll \tau_2$. It is therefore of interest to trace the manner in which the other terms are produced. Clearly, perturbation theory can be used for times $t \ll \tau_2$, so that we can confine ourselves here to first orders in the impurity scattering. We consider by way of example transformation of a packet with k_F into a packet with $-k_F$. The first-order graph corresponding to this process is shown in Fig. 3c. It is possible to determine directly from it the entire coordinate dependence of the function K, no longer assuming that $p = p'$. After integration with respect to the coordinates in (4) we find that χ_b in (35)

depends now on ω. Omitting the details, we present the results for a Gaussian packet:

$$\chi_b = \frac{2(2\pi)^{1/2}}{\alpha v_F} \left[\int_{-\infty}^{\infty} \frac{d\xi}{2\pi i} \frac{\exp[-\xi^2/2(\alpha v_F)^2]}{\omega - \xi - i0} \right]^2. \tag{36}$$

Using the convolution theorem, we can write for $W_{k_F \to -k_F}(t)$ an expression that is valid in the entire time range $t \gg 1/\varepsilon_F$.

$$W_{k_F \to -k_F}(t) = \frac{\alpha v_F}{2(2\pi)^{1/2}} \left\{ \int_0^t dt' \exp\left[-\left(\frac{\alpha v_F t'}{2} \right)^2 \right] \right\}^2 B(t), \tag{37}$$

with $B(t)$ from (24). Similar expressions follow also for other transitions, particularly for $k_F \to k_F$. It is necessary here to add one more term that describes a pure ballistic decay. As a result we can establish that the initial stage of the $W_{k_F \to k_F}(t)$ fall-off will follow a ballistic law [see (10)] all the way to $t \approx t_c = \Delta t (\ln \alpha l_2)^{1/2} \ll \tau_2$, and only at $t > t_c$ is the behavior of $W_{k_F \to k_F}(t)$ described by Eq. (34). We assume here that $t_c < \bar{t}$, where $\bar{t}$ is the upper bound of the validity of (10), or that $1 \ll \alpha l_2 \ll \exp[(k_F/\alpha)^2]$.

It follows from (37) that $W_{k_F \to -k_F}(t)$ reaches values of order W_0 over ballistic-decay times and remains constant all the way to t. The cause of this behavior is that for transformation of a packet with k_F into a packet with $-k_F$ a single reflection from the impurity is sufficient. Were we to consider the actual impurity distribution, the probability of such a transition, as a function of the time at $t \lesssim \tau_2$, would exhibit only a spike at times corresponding to an electron negotiating the path to the nearest impurity and returning to the starting point. This probability, averaged over the positions of the impurities, turns out to be constant so long as $t \lesssim \tau$, and its order of magnitude is $\Delta x/l_2 = \Delta t/\tau_2$.

5. CONSEQUENCES FOR OBSERVABLE QUANTITIES

The function K can be used to analyze a number of effects. Consider for example the influence of electron-electron interaction on the density of states (see also Refs. 18 and 19). In first order in d the interaction, the correction to the density of states, averaged over the length L, is equal to

$$\frac{\delta N(\varepsilon)}{N(0)} = \pm \frac{1}{L} \mathrm{Im} \int dx \int dy\, u(x-y) T$$
$$\times \sum_{\varepsilon'} \frac{\partial}{\partial \varepsilon} [K(x,y;x,y;\varepsilon,\varepsilon') -2K(x,x;y,y;\varepsilon,\varepsilon')]. \tag{38}$$

Here $\varepsilon = i\pi T(2n+1)$, $\varepsilon' = i\pi T(2m+1)$ are the Matsubara frequencies, and a nonzero contribution to (38) exists if $\mathrm{Im}\varepsilon\,\mathrm{Im}\varepsilon' < 0$ and the correction has the same sign as $\mathrm{Im}\varepsilon$. The first term of (38) is the contribution of the exchange process, the second of the direct process, and $u(x)$ is the interaction potential. Following an analytic continuation, it is possible to rewrite (38) in the form

$$\frac{\delta N(\varepsilon)}{N(0)} = -\frac{1}{4} \mathrm{Im} \int_{-\infty}^{\infty} dz \left(\mathrm{th}\frac{z-\varepsilon}{2T} + \mathrm{th}\frac{z+\varepsilon}{2T} \right) \times \frac{\partial}{i\partial z} \Phi[-2i\tau_2(z+i0)], \tag{39}$$

$$\Phi(s) = 4A(s)g_2 + 2B(s)g_1 - [A(s)+B(s)]g_2 - A(s)g_1,$$

where we have used the explicit expression for the function K and introduced the dimensionless constants g_1 and g_2, which are used in the theory of one-dimensional interaction of a Fermi gas and correspond to forward and backward scattering:

$$g_1 = N(0) \int dx\, u(x), \qquad g_2 = N(0) \int dx\, u(x) \cos(2k_F x),$$

and the effective radius of the potential $u(x)$ is assumed much smaller than the mean free path l_2. From (39) we can ultimately obtain

$$\frac{\delta N(\varepsilon)}{N(0)} = -\frac{g_1 + 2g_2}{6\tau_2 T}\left(2\,\mathrm{ch}\,\frac{\varepsilon}{2T}\right)^{-2} - \frac{g_1 - g_2}{6\tau_2 T}$$

$$\times \int_0^\infty dy\left[\left(\mathrm{ch}\,\frac{y - \varepsilon\tau_2}{T\tau_2}\right)^{-2} + \left(\mathrm{ch}\,\frac{y + \varepsilon\tau_2}{T\tau_2}\right)^{-2}\right] \int_0^\infty \frac{u^3 e^{-u}\, du}{u^2 + 4y^2}.$$

$$(40)$$

The substantial dependence of δN on T is due to the first term of (40), with δN a maximum at $T \approx \varepsilon$ and equal to $\delta N/N(0) \approx -(g_1 + 2g_2)/\varepsilon\tau_2$. Only the contribution of the second term of (40) remains at lower temperatures.

It should be noted that although the result (40) was obtained in first order in the interaction, the disorder is taken here into account accurately, in contrast to approaches based on diffusion approximation[18] or on the self-consistent scheme.[19]

The function K obtained above enabled us to calculate also a number of the observable characteristics that describe the interaction of the nuclear spin with the conduction electrons. It is important to note that if we are considering in this interaction the scalar part corresponding to a contact term of type $A(I_n, S_n)$, where A is the hyperfine interaction constant, I_n the spin of the nucleus, and S_n the spin density of the electrons at the site n, we must know the local characteristics of the electronic system in atomic scale. The function K calculated above contains in fact such information. In particular, the time T_1 of nuclear spin relaxation via the conduction electrons is given by[20]

$$T_1^{-1} = A^2 \int d\varepsilon\, f(\varepsilon + \omega_e)\,[1 - f(\varepsilon)]\,F_{\omega_e}(0), \qquad (41)$$

where $F_\omega(z)$ is defined in (26), $f(\varepsilon)$ is the Fermi function, and $\omega_e = 2\mu H$ is the Zeeman splitting energy. Substituting (28) in (41) we can find that the rate of nuclear relaxation in the magnetic field, notwithstanding the localization, is described as before by the Korringa formula, just as in the case of free electrons:

$$\frac{1}{T_1} = \frac{1}{T_{1k}}\left[1 + \frac{\pi}{2\tau_2}\delta(\omega_e)\right], \qquad T_{1k} = \frac{1}{2T[AN(0)]^2}. \qquad (42)$$

It follows, however, from (42) that it should increase substantially when the field is turned off. To make expression (42) more understandable, we introduce the phenomenological lifetime of the electrons in the localized state, a time that can be identified, under certain assumptions, with the inelastic-interaction time τ_{in}. Equation (42) takes then the form

$$\frac{1}{T_1} = \frac{1}{T_{1k}}\left[1 + \frac{\tau_{in}}{2\tau_2}\frac{1}{1 + (\omega_e \tau_{in})^2}\right], \qquad (43)$$

where now $\tau_{in}(T)$ is the temperature-dependent time, and it is usually assumed that $\tau_{in} \sim 1/T^p\,(p \geqslant 1)$. Note that the same time $\tau_{in}(T)$ enters in the expression for the conductivity[21]

$$\sigma(T) \approx \sigma_0 \tau_2/\tau_{in}(T), \qquad (44)$$

where σ_0 is the Boltzmann value of the conductivity, and it is assumed that $\tau_2 \ll \tau_{in}(T)$. Thus, at low temperatures one can expect a substantial increase of the rate of nuclear relaxation, and the appearance of a noticeable field dependence.

The Knight shift can be similarly considered. It is determined by the value of the spin density of the electrons at the nucleus[20,22]

$$S(x) = \frac{\omega_e}{2}\sum_n \psi_n^2(x)\frac{\partial f}{\partial \varepsilon}\bigg|_{\varepsilon = \varepsilon_n}.$$

This yields

$$\langle S^2(x)\rangle = \left(\frac{\omega_e}{2}\right)^2 \int d\varepsilon \frac{\partial f}{\partial \varepsilon}\int d\varepsilon' \frac{\partial f}{\partial \varepsilon'}F_{\varepsilon - \varepsilon'}(0)$$

$$= \langle S(x)\rangle^2 + \left(\frac{\omega_e}{2}\right)^2 \int d\varepsilon\left(\frac{\partial f}{\partial \varepsilon}\right)^2 \frac{\pi}{3\tau_2},$$

and the variance of the Knight shift k is thus

$$\langle (k - \langle k\rangle)^2\rangle/\langle k\rangle^2 = \pi/12\tau_2 T, \qquad (45)$$

where $\langle k\rangle$ is the Knight shift averaged over the volume. The total distribution function k was approximately calculated in Ref. 22.

6. RELAXATION OF MEAN SQUARED DISPLACEMENT

It is curious to ascertain how other characteristics, such as the mean squared displacement, vary during the spreading process. From the general relations[16] we have

$$\langle x^2\rangle_\omega^{(d)} = -2dD(\omega - i0)/(\omega - i0)^2, \qquad (46)$$

where $D(\omega)$ is the diffusion coefficient and d the dimensionality of the system. The asymptotic behavior of $D(\omega)$ is known in the one-dimensional case for low and high frequencies[6-9]:

$$D(\omega) = \begin{cases} 2v_F^2[-i/\omega + 2/\omega^2\tau_2], & \omega\tau_2 \gg 1, \quad (47) \\ 2l_2^2\{i\omega\zeta(3) + \tau_2[\omega\ln(2\omega\tau_2)]^2\}, & \omega\tau_2 \ll 1, \quad (48) \end{cases}$$

where $\zeta(3)$ is the Riemann zeta function. Hence, inverting (46), we get

$$\langle x^2(t)\rangle = \begin{cases} 2(v_F t)^2[1 - \tfrac{2}{3}v_F t/l_2], & t \ll \tau_2, \quad (49) \\ 4l_2^2[\zeta(3) - (2\tau_2/t)\ln(t/2\tau_2)], & t \gg \tau_2. \quad (50) \end{cases}$$

It is clear that the logarithmic singularity in (48) is due to resonant transitions between localized states having energies that differ by values less than or of the order of ω, and spaced $\sim 2l_2|\ln \omega\tau_2|$ apart. This physical picture of the resonance states was proposed by Mott[1] and verified by direct calculation in Ref. 19. Actually, the asymptotic behavior found above for the autocorrelator [see, e.g., Eq. (34)] can also be interpreted in terms of resonance transitions. In fact, for a given arrangement of the impurities, the function $W_{i \to i}(t)$ can according to (1) be written in the form

$$W(t) \approx (\Delta x)^2 \sum_n |\psi_n(y_0)|^4 + (\Delta x)^2 \sum_{n,m} |\psi_n(y_0)\psi_m(y_0)|^2$$

$$\times \exp[i(\varepsilon_n - \varepsilon_m)t], \qquad (51)$$

where use is made of the fact that Δx (the spatial dimension of the wave packet with center y_0) is much less than l_2 (the scale of the eigenfunctions of the total Hamiltonian). The first term in (51) corresponds to the value to which $W(t)$ tends as $t \to \infty$, and the second describes the law in accordance with which this takes place. At large t the contribution to (51) ensures only states with close energy: $|\varepsilon_n - \varepsilon_m| = \omega \ll 1/t$. If it is assumed that these states are randomly distributed over the energy scale, their number as a function of the time decreases like $1/t$. States with different energies correspond to wave functions with different positions of the center, so that according to Ref. 15 we have

$$\psi_n^2(y) \approx l_2^{-1} \exp\left[-(y-R_n)/2l_2\right].$$

On the other hand, as indicated in Refs. 1 and 15, states with close energies are located at a distance larger than or of the order of $|R_n - R_m| = 2l_2 \ln(1/\omega\tau_2)$. As a result, the term under the second summation of sign in (51) turns out to be proportional to $1/t^2$, and on the whole this ensures a decrease of $W(t) - W_0$ like $1/t^3$, as follows from (34).

A conclusion that can be drawn from the presented analysis of the time dependence of the localization in the one-dimensional case is that in this case there is no time region corresponding to diffuse spreading, and the transition proceeds directly from ballistic spreading to localization. The reason is that the localization radius L_{loc} can substantially exceed the mean free path l and a diffusive spreading regime should be observed. The corresponding time interval can be estimated at $\tau < t < T_{loc}$, where $T_{loc} = L_{loc}^2/2dD_0$, and $D_0 = v_F^2\tau/d$ is the diffusion coefficient.

For a two-dimensional system[23] we have $L_{loc} \approx l \exp(\pi\varepsilon_F\tau)$, and consequently $T_{loc} \approx \tau\exp(2\pi\varepsilon_F\tau)$. The behavior of $\langle x^2(t) \rangle$ at a time $t < T_{loc}$ can be determined by perturbation theory. According to Ref. 24, the diffusion coefficient, with account taken of the first correction in the parameter $1/\varepsilon_F\tau$, is equal to

$$D(\omega) = D_0\left[1 - \frac{1}{2\pi\varepsilon_F\tau}\ln\left(-\frac{1}{i\omega\tau}\right)\right]$$

and accordingly

$$\langle x^2(t) \rangle = 4D_0 t\left[1 - \frac{1}{2\pi\varepsilon_F\tau}\ln\frac{t}{\tau}\right]. \tag{52}$$

We can similarly find for the autocorrelator in the two-dimensional case at $t \ll T_{loc}$

$$W(t) = \frac{\tau}{t}\left(1 + \frac{1}{2\pi\varepsilon_F\tau}\ln\frac{t}{\tau}\right). \tag{53}$$

The character of the approach of $\langle x^2(t) \rangle$ to a stationary value after a time $t \gg T_{loc}$ can be determined by using the Mott picture of resonance states. According to Mott,

$$D(\omega) = -i\omega L_{loc}^2(\varepsilon)\left[1 + i\omega\tau_c\left(\ln\frac{1}{\omega\tau_c}\right)^{d+1}\right], \tag{54}$$

where $\tau_c(\varepsilon) = N(\varepsilon)[L_{loc}(\varepsilon)]^d$ and $N(\varepsilon)$ is the density of states. For $d = 2$ we have $\tau_c \approx \varepsilon_F\tau T_{loc}$. This yields for the mean squared displacement

$$\frac{\langle x^2(\infty) \rangle - \langle x^2(t) \rangle}{\langle x^2(\infty) \rangle} \approx \frac{\tau_c}{t}\left(\ln\frac{t}{\tau_c}\right)^d, \tag{55}$$

where $\langle x^2(\infty) \rangle \approx L_{loc}^2$. An attempt can be made to obtain, from similar considerations, the character of the approach of $W(t)$ to its stationary value $W_0 \approx (1/k_F L_{loc})^d$ at $t \gg T_{loc}$. The foregoing analysis of Eq. (51) can be repeated also for $d > 1$ by making the substitution $2l_2 \to L_{loc}$. The distance between resonance states with energies that differ by $\omega = \varepsilon_n - \varepsilon_m$ turns out to equal in this case $R = |R_n - R_m| \approx L_{loc}|\ln \omega\tau_c|$. Estimating the factor $|\psi_n(y_0)\psi_m(y_0)|^2$ from its maximum value, equal to $\exp(-R/L_{loc})$, we can conclude that $W(t)$ is transformed into W_0 again in proportion to $1/t^3$ or possibly faster because of the logarithmic factor.

In the case of a three-dimensional system, localized states correspond to the energy region $\varepsilon < \varepsilon_c$, where ε_c is the mobility edge, estimated at $\varepsilon_c \approx 1/\tau$. Interest attaches here to states near the threshold, where $L_{loc}(\varepsilon) \approx l|\varepsilon_c/(\varepsilon - \varepsilon_c)| \gg l$. The law according to which $\langle x^2(t) \rangle$ increases to values of order L_{loc}^2 can be found from scaling considerations[25]:

$$D(\omega) = D_0(i\omega\tau)^{1/3}.$$

Consequently

$$\langle x^2(t) \rangle \approx l^2(t/\tau)^{2/3}, \quad W(t) \approx (\tau/t)^{2/3}.$$

The present results are valid so long as $\tau \ll t \ll \tau_c \approx \tau|\varepsilon_c/(\varepsilon - \varepsilon_c)|^3$, and for $t \gg \tau_c$, while Eq. (55) holds for $\langle x^2(t) \rangle$.

7. CONCLUDING REMARKS

Thus, using as an example a one-dimensional system with weak disorder we succeeded in obtaining, for the first time ever, exact analytic expressions for the functions $\rho(x,t)$ [see (29)] and $W_{k_F \to \pm k_F}(t)$ [see (34, 35, 37)], which describe the time evolution of the localization process. Incidentally, such a power-law dependence on the time cannot be obtained in the self-consistent approach in the spirit of Vollhardt and Wölfle[23]. As $t \to \infty$ these functions characterize the properties of the stationary localized state. For example, Eq. (30) for $p(x)$ is a specific expression for the distribution of the electron density in the region $1/k_F < x < l$, i.e., where the quantity $2lp(x)$ changes from 1 to 2/3 (see, e.g., the figure in Ref. 15). Similarly, Eq. (28) for the correlator of the density of states $F_\omega(z)$ describes in the same region the transition from $n^2(0)$ to $(2/3)N^2(0)$ (see the figure in Ref. 15).

Note that the presence of a δ-function contribution to Eq. (28) for $F_\omega(z)$ is not a property unique to the one-dimensional model. In fact, using Eqs. (5), (5') and (7), (7') from the paper of Berezinskiĭ and Gor'kov,[16] which are suitable for any dimensionality d of the space, and recognizing that the dependence on q should enter in the form of the dimensionless combination qL_{loc}, we reach the conclusion that

$$F_\omega(0) = \int \langle\!\langle \rho_\varepsilon\rho_{\varepsilon+\omega}(q) \rangle\!\rangle \frac{d^dq}{(2\pi)^d}$$

$$= N^2(\varepsilon)b(\varepsilon)\left[1 + C\frac{1}{\tau(\varepsilon)}\delta(\omega)\right],$$

where C is a certain constant, $b(\varepsilon)$ is a function of ε, and $\tau(\varepsilon) = N(\varepsilon)[L_{loc}(\varepsilon)]^d$. The obtained scale $\tau(\varepsilon)$ accords therefore with the one used by us in the framework of Mott's

phenomenological approach to discuss the relaxation of the mean squared displacement.

For $z \neq 0$ and a δ-function contribution, the constant C should be replaced by some dimensionless function $f(z/L_{\text{loc}})$. Comparing (28) and (30) of the present paper with Eq. (11) of Ref. 15 we find that in the one-dimensional case at arbitrary z the singular contribution (as $\omega \to 0$) should be written in the form

$$F_\omega(z) \to \delta(\omega) N(0) p(z),$$

where $p(z)$ is described by Eq. (30).

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