Transmission of an electron through a finite chain of periodic disordered random scatterers

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The transmission of an electron through a chain of disordered equidistant scatterers has heretofore been considered under the assumption that the amplitude for scattering by the center is real. It was established in particular that the average transmission coefficient $\langle T \rangle$ of an electron of energy corresponding to the band center decreases very slowly with increase of the chain length L, like $L^{-1/2}$. At other energies it decreases exponentially, i.e., the electron is localized. It is shown that allowance for the randomness of the phase of the forward-scattering amplitude leads to an exponential decrease of $\langle T \rangle$ also at the band center. The characteristic spatial scale of the localization is determined in this case not by the phase mean free path alone (just as away from the band center), but depends also on the phase relaxation length l_φ. The latter can in general differ strongly from l. The electron is localized at the length l if $l_\varphi \ll l$ and at the length l_φ if $l_\varphi \gg l$.

INTRODUCTION

The transmission of electrons through a chain of disordered equidistant scattering centers has been discussed in the literature many times (see, e.g., Refs. 1 and 2, as well as Refs. 3 and 4, which contain detailed bibliographies). It was established that the equal spacing of the scatterers leads to anomalies in the average density of states, in the average transmission coefficient $\langle T \rangle$ through the chain, and in a number of other quantities. These anomalies are most strongly pronounced when the electron energy corresponds to the center of the band. The density of states at this point diverges, and the transmission coefficient decreases anomalously slowly (like $L^{-1/2}$) with increase of the chain length. At other electron energies the coefficient decreases exponentially. The calculations were performed as a rule under the assumption that the amplitude of the scattering by the centers is real. Exceptions are Refs. 1 and 5, in which the density of states and the closely related wave-function phase distribution were investigated. It was found there that allowance for the random phases of the forward scattering amplitudes eliminates the divergence of the state density at the band center.

The present paper deals in detail with the influence of the forward-scattering phase randomness on the kinetic characteristics of the chain, such as the average transmission coefficient, the average resistance, and others. It is shown that the relation $\langle T \rangle \sim L^{-1/2}$ for the band center is due entirely to the assumption that the scattering amplitude is real. Allowance for randomness of the scattering phase leads to an exponential decrease of $\langle T \rangle$ with increase of the chain length.

An equation essential for further analysis is derived in Sec. 1. A relation is obtained between the solution of this equation and the distribution function of the chain transmission coefficient. Two exactly solvable examples are considered in the next section. The first is the case of a real scattering amplitude for an electron energy corresponding to the band center. The transmission-coefficient distribution function is found and the known result $\langle T \rangle \sim L^{-1/2}$ is derived anew. The second example deals with the opposite limiting case, when the distribution of the phase of the maximum transmission coefficient (or of the reflection coefficient) for scattering by the centers is uniform in the interval from 0 to 2π. The distribution functions of T and an expression for $\langle T \rangle$ are obtained for an arbitrary electron energy. There are no anomalies whatever at the band center, and $\langle T \rangle$ decreases exponentially at all energies.

The calculations in the succeeding sections are carried out for the band center under weak-scattering conditions. The distribution function of the wave-function phase is investigated in Sec. 3, where the phase-relaxation length l is introduced. The distribution coefficient of the transmission coefficient and its mean values for the two limiting cases $l_\varphi \ll l$ and $l_\varphi \gg l$ (l is the mean free path). It is shown that in both cases $\langle T \rangle$ decreases exponentially as the chain length increases. The characteristic scale of the decrease is l for $l_\varphi \ll l$ and $l_\varphi \gg l$.

In Secs. 5–7 are discussed the cases of small-radius scattering centers, of the tight-binding model, and of the substitutional disorder model.

1. DERIVATION OF BASIC EQUATION

The method used in this section is similar to that proposed in Ref. 6 for disordered centers.

Consider a chain consisting of disordered scatterers spaced d apart. Let the potentials of the neighboring centers be nonoverlapping. The wave function in the spaces between them can then be written in the form

$$\Psi_n = a_n^+ e^{ik(z-nd)} + a_n^- e^{-ik(z-nd)} = \Psi_n^+(z) + \Psi_n^-(z). \quad (1)$$

The amplitudes a_n and a_{n+1} are connected by the linear transformation:

$$a_{n+1}^+ = \alpha_{n+1} e^{ikd} a_n^+ + \beta_{n+1} e^{-ikd} a_n^-,$$
$$a_{n+1}^- = \beta_{n+1}^* e^{ikd} a_n^+ + \alpha_{n+1}^* e^{-ikd} a_n^-, \quad (2)$$
$$|\alpha_n|^2 - |\beta_n|^2 = 1.$$

The relations between the random quantities α_n and β_n in terms of the amplitude transmission and reflection coefficients t_n and r_n for scattering by the nth center are given by

$$\alpha_n = 1/t_n^*, \quad \beta_n = -r_n^*/t_n^*. \quad (3)$$

We denote by $W(a^+, a^-, n)$ the probability density for the amplitudes a^+ and a^- to take on specified values in the inter-

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val between the centers n and $n+1$. The function W satisfies the equation

$$W(a^+, a^-, n+1) = \langle W(\tilde{a}^+, \tilde{a}^-, n)\rangle, \quad (4)$$

where the $\tilde{a}^\pm$ are connected with $a^\pm$ by a transformation inverse to (2), and the angle brackets denote averaging over the parameters of this transformation.

We introduce now in place of $a^\pm$ the new variables

$$I=|a^+|^2+|a^-|^2,\ J=|a^-|^2-|a^+|^2,\ \varphi=\varphi_+-\varphi_-,\ \chi=\varphi_++\varphi_-, \quad (5)$$

where φ_+ and φ_- are respectively the phases of the amplitudes a^+ and a^-, I is the wave intensity, and J is the flux. With the aid of a transformation inverse to (2) we obtain the law of transformation of these quantities when scattered by the center:

$$\tilde{I}=(|\alpha|^2+|\beta|^2)I-2(I^2-J^2)^{1/2}\,\mathrm{Re}(\alpha\beta e^{-i\varphi}),$$
$$(\tilde{I}^2-J^2)^{1/2}e^{i\tilde{\varphi}}=(I^2-J^2)^{1/2}(\alpha^{*2}e^{i(\varphi-2kd)}+\beta^2e^{-i(\varphi+2kd)})-2I\alpha^*\beta e^{-2ikd},$$
$$\tilde{J}=J,\ \tilde{\chi}=\chi+\Delta\chi(I, J, \varphi, \alpha, \beta). \quad (6)$$

Since $\Delta\chi$ is independent of χ, Eq. (4) does not change form when integrated with respect to χ. The new function W depends only on three variables. Conservation of the flux means that J enters in the equation for W only as a parameter. If we put now

$$W(I, \varphi, J, n)=\delta(J-J_0)W(I, \varphi, J_0, n),$$

we obtain for the function $W(I, \varphi, J_0, n)$

$$W(I, \varphi, J_0, n+1)=\langle W(\tilde{I}, \tilde{\varphi}, J_0, n)\rangle. \quad (7)$$

Our aim is to obtain the distribution function $w(\gamma, n)$, where γ is the wave intensity at the end of a chain of length $L=nd$, if its value at the beginning of the chain is equal to the flux $J_0=1$. The intensity γ defined in this manner is connected with the chain's intensity transmission coefficient T by the relation

$$T=2/(\gamma+1). \quad (8)$$

In fact, under these conditions the intensity of a wave incident on the chain from the right is $|a_n^-|^2=(\gamma+1)/2$, and the intensity of the transmitted wave is equal to unity.

The quantity $w(\gamma, n)$ satisfies the equation (see Appendix 1)

$$W(I, n)=\frac{1}{2\pi}\int_1^\infty d\gamma\int_0^{2\pi}d\theta\, w(\gamma, n)\,\delta(I-(\gamma+(\gamma^2-1)^{1/2}\cos\theta)), \quad (9)$$

where $W(I, n)$ is the solution, integrated with respect to φ, of Eq. (7) with $J_0=0$ and the boundary condition $W(I, \varphi, 0)=(1/2\pi)\delta(I-1)$. To solve this equation with respect to $w(\gamma,n)$ we introduce the distribution function $W(s,n)=W(e^s,n)e^s$ of the quantity $s=\ln I$, and denote by $W(p,n)$ its Fourier transform. We obtain then from (9)

$$W(p, n)=\int^\infty d\gamma\, w(\gamma, n)P_{-ip}(\gamma), \quad (10)$$

where $P_{-ip}(\gamma)$ is a Legendre function:

$$P_{-ip}(\gamma)=\frac{1}{2\pi}\int_0^{2\pi}[\gamma+(\gamma^2-1)^{1/2}\cos\theta]^{-ip}\,d\theta.$$

Equation (10) is solved with the aid of the Møller–Fock transformation[7]

$$w(\gamma, n)=\int_0^\infty P_{-1/2-it}(\gamma)\,t\,\mathrm{th}(\pi t)\,W\left(-t-\frac{i}{2}, n\right)dt. \quad (11)$$

To obtain $w(\gamma, n)$ we must thus know the function $W(p, n)$. It is impossible in general to obtain for it a closed equation. This can be done, however, for the function $W(p, \varphi, n)$, which is the Fourier transform of $W(s, \varphi, J, n)$ with $J=0$ and is connected with $W(p, n)$ in obvious fashion. Indeed for a zero flux the equations in (6) are transformed into

$$\tilde{s}=s+\ln|\alpha^*-\beta e^{-i\varphi}|^2, \quad (12a)$$

$$e^{i\tilde{\varphi}}=e^{i(\varphi-2kd)}\frac{\alpha^*-\beta e^{-i\varphi}}{\alpha-\beta^*e^{i\varphi}}, \quad (12b)$$

and we obtain from (7)

$$W(s, \varphi, n+1)=\langle e^{s-\tilde{s}}W(\tilde{s}, \tilde{\varphi}, n)\rangle. \quad (13)$$

Substituting now (12a) in (13) and taking the Fourier transform of the result with respect to s, we get

$$W(p, \varphi, n+1)=\langle|\alpha^*-\beta e^{-i\varphi}|^{2ip-2}W(p, \tilde{\varphi}, n)\rangle. \quad (14)$$

This equation [together with (11)] is the basis of the analysis that follows.

2. EXACT SOLUTIONS

As already noted, the problem of electron transmission through a chain of equidistant disordered scatterers was discussed in the literature under the assumption that the quantities α and β, which describe the scattering by the centers, are real. The scattering was furthermore assumed to be weak. It was shown, in particular, that for $2kd=\pi$ (i.e., at the band center), the average transmission coefficient $\langle T\rangle$ decreases with increase of chain length like $L^{-1/2}$. If, however, $2kd\neq\pi$, the coefficient decreases exponentially.

In Appendix 2 we obtain an exact (without the weak-scattering condition) expression for $w(\gamma, n)$ at $2kd=\pi$ and with real α and β:

$$w(\gamma, n)=\frac{1}{\pi(\gamma^2-1)^{1/2}}\int_{-\infty}^{+\infty}dq\exp\{iq\ln[\gamma+(\gamma^2-1)^{1/2}]+n\ln\langle\cos qv\rangle_v\}. \quad (15)$$

Here v is connected with α and β by the relations $\alpha^2+\beta^2=\cosh v$ and $2\alpha\beta=\sinh v$. In the limit of weak scattering ($|\beta|\ll 1$ and α close to unity) Eq. (15) coincides with the expression obtained for w in Ref. 2. To find $\langle T\rangle$ we must, according to (8), calculate the mean value of $2/(\gamma+1)$:

$$\langle T\rangle=2\int_{-\infty}^{+\infty}\frac{q\,dq}{\mathrm{sh}\,\pi q}\exp(n\ln\langle\cos vq\rangle_v).$$

As $n\to\infty$ the value of this integral is governed by the region of small q and it can be easily calculated:

$$\langle T\rangle\approx(8d/\langle v^2\rangle\pi L)^{1/2}. \quad (16)$$

The relation $\langle T\rangle\propto L^{-1/2}$ holds therefore for scattering of arbitrary strength.

We show now, with a simple example, that the $\langle T\rangle\propto L^{-1/2}$ law is by far not universal for the band center, but is due entirely to the fact that amplitudes for scattering by the centers are real. It must be emphasized that the model proposed below is hypothetical and can hardly correspond to a real physical situation. Its advantage, however, is that it admits of an exact solution for arbitrary k.

Let one of the phases φ_α or φ_β of α and β be distributed independently (of $\mu = |\alpha|^2 + |\beta|^2$, and of the other phase) and uniformly in the interval from 0 to 2π. The mean value $\langle |\alpha^* - \beta e^{-i\varphi}|^{2ip-2}\rangle$ is then independent of φ and is equal to $\langle P_{ip-1}(\mu)\rangle_\mu$. The solution of Eq. (14) with initial condition $W(p,\varphi,0) = 1/2\pi$ is

$$W(p,\varphi,n)=\frac{1}{2\pi}\exp\{n\ln\langle P_{ip-1}(\mu)\rangle_\mu\}.$$

Substituting this expression in (11), we get

$$w(\gamma,n)=\frac{1}{2\pi}\int_0^\infty dt\, t\, \mathrm{th}(\pi t) P_{-1/2+it}(\gamma)\exp\{n\ln\langle P_{-it-1/2}(\mu)\rangle_\mu\}.$$

From this, taking (8) into account, we get

$$\langle T\rangle=\int_0^\infty dt\, t\frac{\mathrm{th}(\pi t)}{\mathrm{ch}(\pi t)}\exp\{n\ln\langle P_{-it-1/2}(\mu)\rangle_\mu\}.$$

At large n this integral is determined by the region of small t, where

$$P_{-it-1/2}(\mu)\approx P_{-1/2}(\mu)-t^2g(\mu),$$

$$g(\mu)=\frac{1}{2\pi}\int_0^\lambda \frac{x^2\,dx}{[2(\mathrm{ch}\,\lambda-\mathrm{ch}\,x)]^{1/2}},\qquad \mathrm{ch}\,\lambda=\mu,$$

so that

$$\langle T\rangle\approx\frac{1}{4}\left[\frac{\pi d\langle P_{-1/2}(\mu)\rangle_\mu}{L\langle g(\mu)\rangle_\mu}\right]^{3/2}\exp\left\{-\frac{L}{d}\ln\frac{1}{\langle P_{-1/2}(\mu)\rangle_\mu}\right\}.$$

Thus, for arbitrary k, the average transmission coefficient decreases exponentially with increase of the chain length. There are no anomalies whatever at the band center. The dependence on the wave vector is only via the parameters of the amplitude (i.e., μ) of the scattering by the centers.

3. PHASE DISTRIBUTION FUNCTIONS AND PHASE SCATTERING LENGTH

It was shown in the preceding section that allowance for the randomness of the scattering-amplitude phases leads, at all energies, to an exponential decrease of $\langle T\rangle$ with decrease of the chain length, rather than to the power-law (16) of the case of real amplitudes and $2kd=\pi$. In this and following sections we consider one more model, which permits a more detailed analysis of the role of the randomness of the phases φ_α and φ_β. It will be shown that at an electron energy close to the band center an important role is played by a new length—the phase relaxation length l_φ. The exponential dependence of $\langle T\rangle$ gives way to an exponential one at $l_\varphi=\infty$. The results will be used in Secs. 5–7, where more realistic situations are discussed.

We designate $\beta = ve^{i\chi}$, $\alpha = (1+v^2)^{1/2}e^{i\varphi_\alpha}$ and put $2kd=\pi, \langle\varphi_\alpha\rangle = \langle\chi\rangle = \langle v\rangle = 0$, $\langle\chi\varphi_\alpha\rangle = \langle\chi v\rangle = \langle\varphi_\alpha v\rangle = 0$; $\langle\chi^2\rangle \ll 1$, $\langle\varphi_\alpha^2\rangle\ll 1$, $\langle v^2\rangle = d/l \ll 1$ (the weak-scattering conditions); l has the meaning of the mean free path. We expand (14) in powers of the small quantities v, χ, and φ_α up to quadratic terms, and average. We obtain then the equation[1)]

$$\frac{\partial W}{\partial x}=-\{p^2\cos^2\varphi+ip\sin^2\varphi\}W$$
$$+\frac{\partial}{\partial\varphi}\left\{(\varepsilon+\sin^2\varphi)\frac{\partial W}{\partial\varphi}-(2ip-1)\sin\varphi\cos\varphi W\right\},\qquad (17)$$

where $x=2nd/l$, $\varepsilon=\langle\varphi_\alpha^2\rangle\, l/d$. In addition, we put $W(n+1)-W(n)\approx\partial W/\partial n$, for owing to the weakness of the scattering the characteristic scale of variation of W is large compared with d.

We put initially $p=0$ in (17):

$$\frac{\partial W}{\partial x}=\frac{\partial}{\partial\varphi}\left\{(\varepsilon+\sin^2\varphi)\frac{\partial W}{\partial\varphi}+\sin\varphi\cos\varphi W\right\}.\qquad (17a)$$

The solution of this equation is in itself of interest since $W(0,\varphi,x)\equiv W(\varphi,x)$ is the phase distribution function. To solve it, we introduce in place of φ the new variable

$$u=\int_{\pi/2}^{\varphi}\frac{d\psi}{(\varepsilon+\sin^2\psi)^{1/2}}\qquad (18)$$

and replace $W(\varphi,x)$ by the function $\rho(u,x) = (\varepsilon+\sin^2\varphi(u))^{1/2}W(\varphi(u),x)$. It follows then from (17a) that

$$\partial\rho/\partial x=\partial^2\rho/\partial u^2.$$

The condition that $W(\varphi,x)$ be periodic on the segment $(0,\pi)$ leads to periodicity of ρ with a period $2Q(\varepsilon)$, where

$$Q(\varepsilon)=\int_0^{\pi/2}\frac{d\psi}{(\varepsilon+\sin^2\psi)^{1/2}}.$$

Representing ρ by a Fourier series, we get for W

$$W(\varphi,L)=\frac{1}{4Q(\varepsilon)(\varepsilon+\sin^2\varphi)^{1/2}}$$
$$+\sum_{m\neq0}\frac{A_m}{(\varepsilon+\sin^2\varphi)^{1/2}}\exp\left\{\frac{i\pi m}{Q(\varepsilon)}u(\varphi)-\frac{2\pi^2m^2}{Q^2(\varepsilon)l}L\right\}.\qquad (19)$$

For $L\gg l_\varphi = Q^2l/2\pi^2$ the function $W(\varphi,L)$ tends to a stationary value $[4Q(\varepsilon)(\varepsilon+\sin^2\varphi)^{1/2}]^{-1}$ that is independent of the boundary condition. Consequently l_φ is the relaxation length of the phase distribution function. If $\varepsilon\gg1$, then $l_\varphi\ll l$, for in this case $Q\approx\pi/2\varepsilon^{1/2}\ll1$. For $\varepsilon\ll1$, on the contrary, $l\gg l$ inasmuch as now $Q\approx\ln(4/\varepsilon^{1/2})\gg1$. Finally, if $\varepsilon\sim1$ the quantity Q is likewise of the order of unity, so that $l_\varphi\sim l$.

We emphasize that as $L\to\infty$ the phase distribution does not tend to a uniform $W=1/2\pi$. The reason is that φ is the phase difference of counterpropagating waves that are scattered by the same centers, so that their phases are correlated. The distribution of each of the phases φ_+ and φ_- taken separately becomes, of course, uniform when L is increased.

4. ELECTRON PASSAGE AT $l_\varphi \ll l$ AND $l_\varphi \gg l$

We return now to Eq. (17). It is impossible to solve it for arbitrary values of ε. We consider therefore the two limiting cases $\varepsilon\gg1$ and $\varepsilon\ll1$. Let initially $\varepsilon\gg1$. Then, as seen from the equation, the derivative $\partial W/\partial\varphi$ is small. Therefore W is independent of φ in first-order approximation. Integrating (17) with respect to φ we obtain

$$\frac{\partial W}{\partial x}=-\frac{p^2+ip}{2}W.$$

Substituting the solution of this equation in (11) we get

$$w(\gamma,L)=\frac{1}{2\pi}\int_0^\infty P_{-1/2+it}(\gamma)\,t\,\mathrm{th}(\pi t)\exp\left\{-\left(t^2+\frac{1}{4}\right)\frac{L}{l}\right\},$$

which agrees with the expression obtained in Ref. 6 for $w(\gamma,L)$ in the case of weak scattering and disordered scatterers. The average transmission coefficient decreases exponentially:

$$\langle T\rangle \sim (l/L)^{3/2}\exp(-L/4l). \tag{20}$$

The periodicity of the scattering centers is consequently immaterial if the inequality $d/l \ll \langle \varphi_\alpha^2\rangle$ is satisfied.

We turn to the opposite limiting case $\varepsilon \ll 1$. Making the change (18) and substituting

$$W(p,\varphi(u),x)=[\varepsilon+\sin^2\varphi(u)]^{(ip-1)/2}\rho(p,u,x), \tag{21}$$

we obtain the equation

$$\frac{\partial\rho}{\partial x}=\frac{\partial^2\rho}{\partial u^2}-(p^2+ip)\frac{\varepsilon\cos^2\varphi(u)}{\varepsilon+\sin^2\varphi(u)}\rho, \tag{22}$$

the solution of which we seek in the form

$$\rho(p,u,x)=\sum_{m=-\infty}^{+\infty}A_m(p)\rho_m(p,u)\exp[-k_m^2(p)x]. \tag{23}$$

For the functions $\rho_m(p,u)$ we have

$$\frac{\partial^2\rho}{\partial u^2}-(p^2+ip)\frac{\varepsilon\cos^2\varphi(u)}{\varepsilon+\sin^2\varphi(u)}\rho=-k^2\rho. \tag{24}$$

The coefficients $A_m(p)$ are determined by the distribution $\rho(p,u,0)$ at the beginning of the chain. It is easy to verify in the usual way that the periodic solutions of Eq. (24) which correspond to different k^2 are orthogonal (without complex conjugation of one of the functions). Therefore

$$A_m(p)=\left(\int_{-Q}^{Q}\rho(p,u,0)\rho_m(p,u)\,du\right)\left(\int_{-Q}^{Q}\rho_m^2(p,u)\,du\right)^{-1}$$

Integrating $W(p,\varphi,x)$ with respect to φ, we get for $W(-t-i/2,x)$

$$W\left(-t-\frac{i}{2},x\right)=\sum_{m=-\infty}^{+\infty}W_m(t)\exp[-k_m^2(t)x],$$

$$W_m(t)=\left(\int_{-Q}^{Q}[\varepsilon+\sin^2\varphi(u)]^{(2it+1)/4}\rho_m(t,u)\,du\right) \tag{25}$$

$$\times\left(\int_{-Q}^{Q}[\varepsilon+\sin^2\varphi(u)]^{(1-2it)/4}\rho_m(t,u)\,du\right)\left(\pi\int_{-Q}^{Q}\rho_m^2(t,u)\,du\right)^{-1}.$$

The expression for $W_m(t)$ is given here for the boundary condition $W(p,\varphi,0)=1/2\pi$. We solve Eq. (24) with $\varepsilon\ll1$ successively in three overlapping regions $0\leqslant\varphi\ll1$; $\varepsilon^{1/2}\ll\varphi$ and $\pi-\varphi\gg\varepsilon^{1/2}$, $1\gg\pi-\varphi\geqslant0$.[2)] For $\varphi\ll1$ it follows from (18) and (14) that

$$\varphi\approx\varepsilon^{1/2}\,\mathrm{sh}(u+Q),\ -Q\leqslant u\ll-1,$$

$$\frac{d^2\rho^-}{du^2}-\frac{(p^2+ip)}{\mathrm{ch}^2(u+Q)}\rho^-=-k^2\rho^-. \tag{26a}$$

The solution of this equation is

$$\rho^-(u)=P_{-ip}^{ik}(\mathrm{th}(u+Q))+f^-P_{-ip}^{ik}(-\mathrm{th}(u+Q)), \tag{26b}$$

where P_{-ip}^{ik} is a Legendre function. In the region $\pi-\varphi\ll1$ we obtain similarly

$$\frac{d^2\rho^+}{du^2}-\frac{(p^2+ip)}{\mathrm{ch}^2(u-Q)}\rho^+=-k^2\rho^+,\qquad 1\ll u\leqslant Q, \tag{27a}$$

$$\rho^+=P_{-ip}^{ik}(\mathrm{th}(u-Q))+f^+P_{-ip}^{ik}(-\mathrm{th}(u-Q)). \tag{27b}$$

We consider now the regions $\varphi^2\gg\varepsilon$ and $(\pi-\varphi)^2\gg\varepsilon$. Neglecting compared with $\sin^2\varphi$ in (18) and (24), we have

$$\cos\varphi=-\mathrm{th}\,u,\qquad \sin\varphi=1/\mathrm{ch}\,u,\qquad |u|\ll Q,$$

$$d^2\rho^0/du^2-\varepsilon(p^2+ip)\mathrm{sh}^2u\rho^0=-k^2\rho^0. \tag{28a}$$

This is a Mathieu equation. It can be verified from the sequel that the inequality $|k_m^2(p)|\gg\varepsilon|p^2+ip|\sinh^2u$ is valid for $|u|\ll Q$ and for all p of interest. Therefore

$$\rho^0\approx f_1^0e^{iku}+f_2^0e^{-iku} \tag{28b}$$

It is easily seen that Eq. (28a) coincides with (26a) if $-Q\ll u\ll-1$ and with (27a) if $1\ll u\ll Q$. As a result, the asymptotes of the functions ρ^- and ρ^+ take the form (28b) for $-Q\ll u$ and $u\ll Q$, respectively. Using also the periodicity conditions

$$\rho^-(-Q)=\rho^+(Q),\ d\rho^-/du|_{u=-Q}=d\rho^+/du|_{u=Q},$$

we obtain

$$f^-=f^+=1,\qquad f_1^0=\frac{e^{ikQ}}{\Gamma(1-ik)}\left(1+\frac{\mathrm{sh}\,\pi p}{\mathrm{sh}\,\pi k}\right),$$

$$f_2^0=\frac{e^{-ikQ}\Gamma(-ik)}{\Gamma(1-ik-ip)\Gamma(ip-ik)}$$

and an equation for the spectral parameter k

$$e^{2ikQ}=\frac{\mathrm{sh}((k-p)\pi/2)}{\mathrm{sh}((k+p)\pi/2)}\frac{\Gamma(1-ik)\Gamma(1-ip+ik)}{\Gamma(1+ik)\Gamma(1-ip-ik)}, \tag{29}$$

where $\Gamma(z)$ is the gamma function. This equation cannot be solved for arbitrary values of p. We shall see, however, that to find the mean values (such as $\langle T\rangle$, $\langle\ln T\rangle$, $\langle\gamma\rangle$, $\langle\ln\gamma\rangle$ and others) it is necessary to know $k^2(p)$ only in the vicinity of certain points.

We begin with the calculation of $\langle T\rangle$. Using (11) and (8) we get

$$\langle T\rangle=2\pi\int_0^\infty dt\,t\frac{\mathrm{th}(\pi t)}{\mathrm{ch}(\pi t)}W\left(-t-\frac{i}{2},x\right). \tag{30}$$

It will be shown that for large x this integral is determined by the region of small t. We must therefore solve (29) in the vicinity of $p=-i/2$. For $Q\gg1$ we get

$$k_0^2(t)\approx\frac{\pi^2}{4Q^2}+\frac{\pi^2}{4Q^3}\left(\frac{\pi^2}{8}+14\zeta(3)\right)t^2,$$

where $\zeta(3)\approx1.202$. We have used here only the smallest eigenvalue of Eq. (24), since we are interested in an expression for $\langle T\rangle$ as $x\to\infty$. Calculating now $W_0(t)$ with the aid of Eq. (25), using the functions ρ^+, ρ^-, and ρ^0 taken at $p=-i/2$ (i.e., at $t=0$), we get

$$W\left(-t-\frac{i}{2},x\right)=\frac{2\Gamma^4(1/4)}{\pi^2Q}e^{-k_0^2(t)x}. \tag{31}$$

Substituting (31) in (30) we obtain

$$\langle T\rangle\approx\frac{8\Gamma^4(1/4)(\pi Q)^{1/2}}{[\pi^2/8+14\zeta(3)]^{3/2}}\left(\frac{l_\varphi}{L}\right)^{3/2}e^{-L/4l_\varphi}$$
$$\approx32\left(\ln\frac{4}{\varepsilon^{1/2}}\right)^{1/2}\left(\frac{l_\varphi}{L}\right)^{3/2}e^{-L/4l_\varphi}. \tag{32}$$

Thus, for $\varepsilon\ll1$ (just as for $\varepsilon\gg1$) the average transmission coefficient decreases exponentially with increase of the chain length. Now, however, the argument of the exponential contains not the mean free path but the much larger phase relaxation length l_φ.[3)]

The average transmission coefficient is determined by the relatively small values $\gamma \gtrsim 1$. The function $w(\gamma,L)$ with such γ can be easily found by substituting (31) in (11):

$$w(\gamma, L) \approx 5{,}1\left(\ln\frac{4}{\varepsilon^{1/2}}\right)^{1/2} P_{-1/2}(\gamma)\left(\frac{l_\varphi}{L}\right)^{3/2} e^{-L/4l_\varphi}.$$

It can be used to calculate mean values of the type $\langle T^\nu\rangle$, where $\nu \gg 1$. It is not suitable, however for finding $\langle \ln \gamma\rangle$, the average chain resistance $\langle(\gamma - 1)/2\rangle$, and other quantities whose values are determined by the region of large γ.

To find $w(\gamma,L)$ for $L \to \infty$ and $\gamma \gg 1$ we use the asymptotic representation[7]

$$P_{-1/2+it}(\gamma) = 2\,\mathrm{Re}\frac{2^{it}\Gamma(it)}{(2\pi\gamma)^{1/2}\Gamma(1/2+it)} e^{it\ln\gamma}.$$

Substituting this expression in (11) and calculating the integral by the saddle-point method we obtain

$$w(\gamma, x) = \frac{\Gamma(it_0)\, t_0\, \mathrm{th}(\pi t_0)\, 2^{it_0}}{\Gamma(1/2+it_0)\,|\Phi''(t_0)|^{1/2}} e^{\Phi(t_0)} W(t_0),$$
$$\Phi(t) = (it - 1/2)\ln\gamma - k^2(t)x, \qquad (33)$$

where t_0 is the saddle point determined from the equation

$$i\ln\gamma - x\frac{dk^2}{dt}\bigg|_{t=t_0} = 0. \qquad (34)$$

Only one term of the series is retained in (33), the one corresponding to the largest $-k^2(t_0)$ at $t = t_0$.

We shall show now that with the aid of (33) we can find the distribution function

$$f(s, x) = w(e^s, x)e^s \qquad (35)$$

of the quantity $s = \ln\gamma$ near its most probable value s_0. Obviously, the value of t_0 corresponding to s_0 is determined by the equation $d(\Phi + s)/ds = 0$, where t_0 must be taken to be a function of s. Recognizing that $(\partial\Phi/\partial t)_{t=t_0} = 0$, we obtain $d(\Phi + s)/ds = it_0 + 1/2$, i.e., $t_0 = i/2$. We can now find s_0 from the equation $(\partial\Phi/\partial t)_{t=i/2} = 0$. To this end we solve (29) in the vicinity of $t = i/2$, (i.e., $p = -i$):

$$k^2(t) = \left(t - \frac{i}{2}\right)^2 + \frac{i}{Q}\left(t - \frac{i}{2}\right). \qquad (36)$$

Substituting this expression in $\Phi(t)$ we obtain $(\partial\Phi/\partial t)_{t=i/2} = i\ln\gamma - ix/Q$, and consequently $s_0 = x/Q$. Using (33)–(36) we obtain the function $f(s,x)$:

$$f(\ln\gamma, x) = \left(\frac{1}{4\pi x}\right)^{1/2}\exp\left[-\frac{(\ln\gamma + x/Q)^2}{4x}\right],$$

$$\langle\ln\gamma\rangle = s_0 = \frac{x}{Q}.$$

Similarly, considering the function $g(s,x) = e^{\nu s}w(e^s, x)$, we can calculate $\langle\gamma\rangle$. It is simpler, however, to use Eq. (10), noting that $P_{-ip}(\gamma) = \gamma$ if $p = i$. Consequently, $\langle\gamma\rangle = W(i,x)$. From (29), at $p = i$, we obtain $k = i(1 + 2e^{-2Q}) \approx i(1 + \varepsilon/8)$. As a result, apart from a numerical factor preceding the exponential, we obtain as $L \to \infty$

$$\langle\gamma\rangle \sim \exp[(2L/l)(1+\varepsilon/4)].$$

Thus $\langle\gamma\rangle$ and with it the average chain resistance increases exponentially with increase of the chain length [just as for real α and β (Ref. 2)].

The main result of the present section is the derivation of Eq. (32) for the average transmission coefficient. Evidently, allowance for the random phases φ_α and χ, even though they are small, leads to a qualitative difference in the cases $\varphi_\alpha, \varphi_\beta = 0, \pi$ [see Eq. (16)]. This important result lends itself to the following illustrative interpretation. It was emphasized in Ref. 6 that the group of transformations (2) which describe the scattering of electrons by centers is isomorphous to a subgroup of a special Lorentz group whose transformations preserve the coordinate Z. The isomorphism is achieved with the aid of the equations $X = 2\,\mathrm{Re}(a^+a^-)$, $Y = 2\,\mathrm{Im}(a^+a^-)$, $\tau = |a^+|^2 + |a^-|^2$. Consequently, the electron motion along the chain corresponds to random walk of a point over the surface of the hyperboloid $\tau^2 - X^2 - Y^2 = J^2 = \mathrm{const}$. It can be shown that for real α and β and for $2kd = \pi$ the coordinate Y only reverses sign at each step (i.e., after each scattering by a center). This means that the diffusion of the point is along two lines on the hyperboloid, such that their projections on the XY plane are two straight lines parallel to the X axis. The diffusion is therefore essentially one-dimensional in this case. Allowance, however for the randomness of the phases β_α and χ, be they even small, makes the diffusion two-dimensional. It is this which leads to the qualitative change of the dependence of $\langle T\rangle$ on the chain length. In real physical situations the scattering amplitude is complex, so that $\langle T\rangle$ should decrease exponentially with the chain length, in accord with equations of the type (20) or (32).

5. TRANSMISSION THROUGH A CHAIN OF CENTERS WITH SMALL-RADIUS POTENTIALS

In this case $\beta = i\eta$ and $\alpha = 1 + i\eta$, where $\eta = k_0/k$. We put, as above, $2kd = \pi$ and assume the scattering to be weak, so that $k_0 d \ll 1$. Expanding the right-hand side of (14) in powers of η, we obtain a differential equation whose coefficients have a period 2π. Its left-hand side contains the function $W(p,\varphi,x)$ and the right-hand side $W(p,\varphi + \pi,x)$. The ensuing difficulty can be eliminated by considering in place of (14) an equation that relates $W(p,\varphi,n + 2)$ with $W(p,\varphi,n)$. The averaging in this case should be over the parameters of the two centers, putting $\langle\eta_1\eta_2\rangle = 0$. Making next the substitution $\varphi \to \varphi + \pi/2$, we obtain Eq. (17) with $\varepsilon = 1$. It does not contain a small parameter, and cannot be solved analytically. As before, however, we can solve exactly an equation for the phase distribution function. The corresponding phase relaxation length is $l_\varphi = lQ^2(1)/2\pi^2$, with $Q(1) = 2^{-1/2}K(1/2) \approx 1.31$, where $K(1/2)$ is a complete elliptic integral of the first kind. Consequently $l_\varphi \approx 0.1l$. Clearly, the average transmission coefficient decreases exponentially. The argument of the exponential contains a length that differs only numerically from the mean free path.

6. TIGHT-BINDING MODEL WITH DIAGONAL DISORDER

In this model, the Schrödinger equation takes the form

$$E\Psi_n = E_n\Psi_n + V(\Psi_{n-1} + \Psi_{n+1}), \qquad (37)$$

where Ψ_n and E_n are the wave-function amplitude and the electron energy in the site numbered n, while V is the overlap integral between neighboring sites. If the sites are identical ($E_n = E_0$), the electron can propagate freely along the chain. The corresponding eigenfunctions are the plane waves

$$\Psi_n = a^+ e^{iknd} + a^- e^{-iknd} \tag{38}$$

with a dispersion law

$$E(k) = E_0 + 2V \cos kd. \tag{39}$$

Assume now that on some section of the chain the energies E_n differ from one another and are random: $E_n = E_0$ for $n \leqslant 0$ and $n \geqslant N+1$, $E_n = E_0 + \varepsilon_n$ for $1 \leqslant n \leqslant N$, and the mean value $\langle \varepsilon_n \rangle = 0$. Consider the passage of an electron with a quasimomentum k through this segment. From (37) and (39) it follows that

$$2V \cos kd \Psi_n = \varepsilon_n \Psi_n + V(\Psi_{n-1} + \Psi_{n+1}), \tag{40}$$

where $\varepsilon_n = 0$ for $n \leqslant 0$ and $n \geqslant N+1$. Using this equation, we can find consistently Ψ_n for any n if, for example Ψ_{-1} and Ψ_0 are known. More convenient for our purposes, however, are the variables a_n^+ and a_n^- introduced with the aid of the relations

$$\Psi_n = a_n^+ + a_n^-, \quad \Psi_{n+1} = e^{ikd} a_n^+ + e^{-ikd} a_n^-. \tag{41}$$

The difference $|a_n^-|^2 - |a_n^+|^2$ has the meaning of the probability flux J. From (40) and (41) we obtain

$$a_{n+1}^+ = e^{ikd}(1 + i\eta_{n+1}) a_n^+ + i e^{-ikd} \eta_{n+1} a_n,$$
$$a_{n+1}^- = -i e^{ikd} \eta_{n+1} a_n^+ + e^{-ikd}(1 - i\eta_{n+1}) a_n^-,$$

where $\eta_n = \varepsilon_n / 2V \sin kd$. These equations agree with relations (2) if we put $\alpha_n = 1 + i\eta_n$ and $\beta_n = i\eta_n$. These are precisely the forms of α_n and β_n for scattering by small-radius potentials (see Sec. 5).

Consequently, the problem considered is equivalent to the problems of passage of an electron through a chain of scattering centers with small-radius potential. At $2kd = \pi$ and $\varepsilon_n \ll V$ the electron is localized over a length on the order of $d \cdot 4^2 / \langle \varepsilon_n^2 \rangle$, which plays in this case the role of the mean free path l.

7. MODEL OF SUBSTITUTION DISORDER

We write the Schrödinger equation in the form

$$-\Psi''(z) + \sum_n V_n(z - nd)\Psi = k^2 \Psi,$$

where $V_n(z - nd)$ takes on values $V_a(z - nd)$ with probability q and $V_b(z - nd)$ with probability $1 - q$. We subtract from this potential the periodic (average) potential

$$\sum \{ qV_a(z - nd) + (1 - q) V_b(z - nd) \}.$$

This does not influence the manner in which such quantities as $\langle T \rangle$, the average resistance, and others depend on the chain length. The result is a chain of scattering centers with potentials $(1 - q)V$ and $-qV$, respectively (here $V = V_a - V_b$), with probabilities q and $1 - q$.

The decrease of $\langle T \rangle$ (at $2kd = \pi$) with increase of the chain length depends on the properties of the potential V. If its scattering amplitude is real, we have $\langle T \rangle \sim L^{-1/2}$. Allowance for the randomness of the phases φ_α and φ_β leads, as above, to an exponential decrease of $\langle T \rangle$. Let, for example, V be a small-radius potential. We have then $\alpha_n = 1 + i\eta_n$ and $\beta_n = i\eta_n$, where $\eta_n = (1 - q) k_0 / k$ with probability q and $\eta_n = -qk_0/k$ with probability $1 - q$. Obviously, $\langle \eta_n \rangle = 0$ and $\langle \eta_{n+1} \eta_n \rangle = 0$. This is precisely the situation discussed in Sec. 5.

CONCLUSION

We have shown that allowance for even an arbitrarily small random phase φ_α of the amplitude transmission coefficient in scattering by centers is of principal importance if the scatterer arrangement is periodic and the electron energy corresponds to (or is close to) the band center. The chain transmission coefficient decreases in this case exponentially when the chain length increases, in contrast to the cases $\varphi_\alpha, \varphi_\beta = 0, \pi$, when it decreases like $L^{-1/2}$. The argument of the exponential is determined not only by the mean free path (as, for example, for disordered scatterers or far from the band center[2]), but depends also on a more subtle property—the phase relaxation length l_φ. It contains the quantity $1/4l$ if $l_\varphi \ll 1$ and $1/4l_\varphi$ if $l_\varphi \gg l$.

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APPENDIX 1

Consider the transformation

$$\Psi_n^+ = A\Psi_0^+ + B\Psi_0^-, \quad \Psi_n^- = B^* \Psi_0^+ + A^* \Psi_0^-, \quad |A|^2 - |B|^2 = 1.$$

which relates the wave function at the beginning of the chain to its values in an interval between centers n and $n+1$. We choose its three independent parameters to be the phases φ_A and φ_B of the quantities A and B and the quantity $|A|^2 + |B|^2$, which coincides with quantity γ introduced in the main text. We introduce the distribution function $w(\gamma, \varphi_A, \varphi_B, \eta)$, and denote by $g(\gamma, \varphi_A, \varphi_B, I, \varphi, J_0)$ the probabilities of the values I and φ for given $\gamma, \varphi_A, \varphi_B$, and J_0. We have then

$$W(I, \varphi, J_0, n) = \int_0^{2\pi} d\varphi_A \int_0^{2\pi} d\varphi_B \int_1^{\infty} d\gamma \, w(\gamma, \varphi_A, \varphi_B, n) g(\gamma, \varphi_A, \varphi_B, I, \varphi, J_0). \tag{A1}$$

The function g is defined as

$$g = \int_0^{2\pi} d\varphi' \int_0^{\infty} dI' W(I', \varphi', J_0, 0) \delta(I - I(\gamma, \varphi_A, \varphi_B, I', \varphi', J_0)) \delta(\varphi - \varphi(\gamma, \varphi_A, \varphi_B, I', \varphi', J_0)). \tag{A2}$$

The intensity I' and the phase φ' at the beginning of the chain are connected with the values at the end of the chain by relations similar to (6). For $J_0 = 0$, in particular, we have

$$I = I'(\gamma + (\gamma^2 - 1)^{1/2} \cos(\varphi' + \varphi_A - \varphi_B)). \tag{A3}$$

We substitute now (A2) in (A1), integrate the result with respect to φ, and then put $J_0 = 0$ and $W(I', \varphi', 0, 0) = (1/2\pi)\delta(I' - 1)$. Taking (A3) into account, we obtain Eq. (9).

APPENDIX 2

For real α, β, and $2kd = \pi$ we can rewrite (12b) in the form

$$\cos \tilde{\varphi} = -\frac{\operatorname{ch} v \cos \varphi - \operatorname{sh} v}{\operatorname{ch} v - \operatorname{sh} v \cos \varphi}. \tag{A1'}$$

Let $0<\varphi<\pi$. We introduce the variables u and $\tilde{u}$ defined by

$$\cos\varphi=-\mathrm{th}\,u,\quad \sin\varphi=1/\mathrm{ch}\,u,$$
$$\cos\tilde{\varphi}=-\mathrm{th}\,\tilde{u},\quad \sin\tilde{\varphi}=1/\mathrm{ch}\,\tilde{u}. \tag{A2'}$$

It follows then from (A1′) that $u = -u - v$, and from (14) we have

$$G(p,u,n+1)=\langle G(p,-u-v,n)\rangle_v, \tag{A3'}$$
$$G(p,u,n)=W(p,\varphi(u),n)\,\mathrm{ch}^{ip-1}u.$$

Equation (A3′) is solved using a Fourier transformation (it must be recognized here that $G(p,u,n)$ is even in u because $G(p,u,0) = (2\pi)^{-1}\cosh^{ip-1}u$ is even). For W we have

$$W\left(-t-\frac{i}{2},\varphi,n\right)=\frac{1}{4\pi^2}\int_{-\infty}^{+\infty}dq\int_0^\pi\frac{d\theta}{\sin\theta}\left(\frac{\sin\theta}{\sin\varphi}\right)^{it+1/2}$$
$$\times\left(\frac{\mathrm{tg}(\varphi/2)}{\mathrm{tg}(\theta/2)}\right)^{iq}\exp(n\ln\langle\cos qv\rangle_v). \tag{A4'}$$

The expression for W in the region $\pi\leqslant\varphi\leqslant 2$ is obtained similarly and coincides with (A4). Integrating (A4) with respect to φ and substituting the result in (11), we obtain (15).

[1)] Equation (17) is obtained under the condition $W(p,\varphi,n) = W(p,\varphi+\pi,n)$. These are precisely the solutions we need. In the general case the period of the function W is 2π.

[2)] Note that (24) can be transformed into a Lamé equation of general form, for which no solutions are known.

[3)] Note that Eq. (32) with $\varepsilon\to 0$ ($l_\varphi\to\infty$) does not go over into expression (16) which is valid at $\varepsilon = 0$. The reason is that (32) is only the leading term of the series. For a correct transition to the limit it is necessary to sum the entire series before putting $\varepsilon = 0$.

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