The Landauer resistance of a one-dimensional metal with periodically spaced random impurities

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We find the dependence of the ensemble-averaged resistance, $\langle \rho_L \rangle$, of a one-dimensional chain consisting of periodically spaced random delta-function potentials of the chain length L, the incident-electron energy, and the chain disorder parameter w. We show that generally the $\langle \rho_L \rangle$ vs L dependence can be written as a sum of three exponential functions, two of which tend to zero as $L \to \infty$. Hence the asymptotic expression for $\langle \rho_L \rangle$ is always an exponential function of L. Such an expression for $\langle \rho_L \rangle$ means that the electronic states are indeed localized and makes it possible (which is important) to find the dependence of the localization radius on the incident-electron energy and the force with which an electron interacts with the sites of the chain. We also derive a recurrence representation for $\langle \rho_L \rangle$, which proves convenient in numerical calculations. © *1997 American Institute of Physics.* [S1063-7761(97)01302-4]

1. INTRODUCTION

It is well known that the procedure of averaging and calculating the averages of the physical properties for disordered systems is difficult primarily from the mathematical viewpoint. The phenomenon of electron localization in systems with random interaction potentials makes it possible occasionally to draw certain conclusions about the nature of the possible solutions without actually solving the problem. For instance, in the one-dimensional case, as shown in Refs. 1–4, the dependence of the average resistance of a metal with fixed impurities, where all the electronic states are localized , on the length L of the impurity chain can be expressed, for $L \to \infty$ at absolute zero, by the following formula ($\hbar = e^2 = 1$):

$$\langle \rho_L \rangle = \tfrac{1}{2}(e^{L/\xi} - 1),$$

where ξ is the electronic-state localization radius, which is independent of L. Here the "nonideal region" is assumed to exist between two semi-infinite electrodes in which electrons move freely. It is the fraction of electrons that have passed through the "nonideal region" from one electrode to the other that determines the transmissivity of the system, which is inversely proportional to $\langle \rho_L \rangle$. Thus, such a one-to-one correspondence between the Landauer resistance $\langle \rho_L \rangle$ with $L \to \infty$ and the localization radius ξ of one-electron states, the latter depending only on the electron energy and the force of the electron–impurity interaction, reduces the problem of finding ξ to that of finding $\langle \rho_L \rangle$ with $L \to \infty$, and vice versa.

For instance, for the entire class of random potentials in which the average potential is zero, i.e., potentials of the white-noise type, the localization radii have been calculated both in the presence of an external field and in the absence of such a field.[5] The well-known method of transfer matrices, when applied to the model of short-range potentials,[6] has made it possible to effectively perform numerical calculations but proved ineffective in obtaining analytic results. The determinant method, suggested in Refs. 7 and 8 for one-dimensional systems consisting of random single barriers, made it possible to obtain analytic results only under the assumption of weak or strong scattering of an electron by a single barrier and in the event of resonant passage. Calculations of the localization radius from the behavior of $\langle \rho_L \rangle$ as $L \to \infty$ were also done in Refs. 9–11.

In Ref. 12 it was shown that for the model of periodically spaced delta-function potentials whose amplitudes are independent random quantities with a zero average value, the average Landauer resistance $\langle \rho_L \rangle$ can be represented by a series expansion. In Ref. 13 we were able to sum this series and to derive a finite-difference equation for determining $\langle \rho_L \rangle$. There we also gave solutions for this equation in particular cases, i.e., for electron energies corresponding to the edge and center of the energy band.

In the present paper we find the analytic solution of the finite-difference equation for $\langle \rho_L \rangle$ in the general case. This solution actually gives $\langle \rho_L \rangle$ as a function of the chain length L, the energy of the impinging electron, and the intensity of electron scattering on a single barrier. We show that the solution for $\langle \rho_L \rangle$ with $L \to \infty$ can always be reduced to the form $\langle \rho_L \rangle \propto \exp(L/\xi)$, with ξ independent of L. We also calculate the localization radius.

In Sec. 2 we formulate the problem and give the results obtained in Ref. 13 that are needed for our present study. In Sec. 3 we find the general solution of the finite-difference equation that the unknown function $\langle \rho_L \rangle$ satisfies. Here we also derive a recurrence relation for $\langle \rho_L \rangle$. Section 4 is devoted to an analysis of the characteristic equation whose roots are used, as shown in Sec. 3, to express the dependence of $\langle \rho_L \rangle$ on L. We also find the solution of the equation for $\langle \rho_L \rangle$, with $L \to \infty$, from which we derive an expression for the electron localization radius. In Sec. 5 we analyze the results.

2. STATEMENT OF THE PROBLEM

We take a chain of N delta-function potentials with arbitrary amplitudes V_n and corresponding coordinates x_n:

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$$V(x)=\sum_{n=1}^{N} V_n\delta(x-x_n), \quad n=1,2,\ldots,N.$$

Let the solution of the Schrödinger equation for an electron with an energy $E=k^2$ ($\hbar=2m_0=1$, with m_0 the electron mass) outside the structure be

$$\psi(k,x)=\begin{cases} e^{ikx}+r_N(k)e^{-ikx}, & x\leqslant x_1, \\ t_N(k)e^{ikx}, & x\geqslant x_N, \end{cases}$$

where $r_N(k)$ and $t_N(k)$ are, respectively, the electron reflection and transmission amplitudes. The Landauer resistance can be expressed in terms of $r_N(k)$ and $t_N(k)$ by the well-known formula

$$\rho_N=\frac{1}{|t_N(k)|^2}-1, \quad |r_N(k)|^2=1-|t_N(k)|^2. \tag{1}$$

This formula holds for any type of scattering potential. In Ref. 13 we found that the quantity ρ_N averaged over the different realizations of the random field for a model in which N delta-function potentials occupy arbitrary points $x_1, x_2, \ldots, x_N$ can be expressed as

$$\langle\rho_N\rangle=1+\sum_{p=1}^{N}\sum_{1\leqslant j_1\leqslant\cdots\leqslant j_p}^{N} 2^{p-1}\alpha^p \times\prod_{l=1}^{p-1}\{1-\cos[2k(x_{j_{l+1}}-x_{j_l})]\}, \tag{2}$$

where

$$\alpha=\frac{1}{w}\int_{-w/2}^{w/2} f(V_j)\frac{V_j^2}{4k^2}dV_j, \quad \frac{1}{w}\int_{-w/2}^{w/2} f(V_j)dV_j=1.$$

Here $f(V_j)$ is the distribution function of the potentials V_j, which is defined in the interval $[w/2,-w/2]$, is assumed equal for all the V_j ($j=1,2,\ldots,N$), and is an arbitrary even function of V_j. In particular, for $f(V_j)=1$ we have $\alpha=w^2/48k^2$.

Direct summation of the series (2), even assuming that the scatterers are positioned equidistantly, runs into unsurmountable difficulties. Equation (2) can be summed only in some particular cases, when the electron energy corresponds either to the center of the energy band or to the edge ($ka=\pi/2$ or $ka=\pi$, where a is the chain period).[12,13] However, as shown in Ref. 13, we can sum over the inner indices in (2). The result is a finite-difference equation for the unknown quantity $\langle\rho_N\rangle$. This equation has the form

$$\langle\rho_N\rangle=\alpha N+\sum_{n=1}^{N} c_{N-n}\langle\rho_n\rangle, \tag{3}$$

where

$$\rho_1=1, \quad c_n=2\alpha[1-\cos(2kan)].$$

Note that Eq. (3) can be interpreted as a system of linear algebraic equations in the unknowns $\langle\rho_1\rangle,\langle\rho_2\rangle,\ldots,\langle\rho_N\rangle$, with the result that $\langle\rho_N\rangle$ can be written in the form of a determinant.

The solution of Eq. (3) for the particular case of $ka=\pi$ can be obtained immediately because $c_n=0$ for all n:

$$\langle\rho_N\rangle=\alpha N. \tag{4}$$

This result corresponds to resonant passage of electrons and was first derived in Ref. 6. In Ref. 13 we found the solution of Eq. (3) for another particular case, where the incident electron energy corresponds to the center of the energy band, $ka=\pi/2$. The solution is

$$\langle\rho_N\rangle=\frac{1}{2}\left[\frac{(a+b)^N+(a-b)^N}{2}+\frac{(a+b)^N-(a-b)^N}{2b}\right], \tag{5}$$

where

$$a=2\alpha, \quad b=\sqrt{1+4\alpha^2}.$$

As the solution (5) shows, for any α and $N\to\infty$ we can write $\langle\rho_N\rangle$ in the form $\langle\rho_N\rangle\propto\exp\{Na/\xi\}$, where ξ is independent of N and is the electron localization radius.

Below we show, however, that Eq. (3) can also be solved in the general case, i.e., for any values of the incident-electron energy and the parameter α.

3. SOLVING THE FINITE DIFFERENCE EQUATION FOR $\langle\rho_N\rangle$

Let us now solve Eq. (3) in the general case. We seek the solution in the following form:

$$\langle\rho_N\rangle=\sum_{j=1}^{p} A_j x_j^N+A_0, \tag{6}$$

where the x_j, A_j, and A_0 are assumed independent of N. The quantity p, determining the number of terms in (6), will be left undefined for the time being. Substituting the solution (6) in Eq. (3) and requiring that the latter hold for all values of N, we arrive at the necessary relationships determining x_j, A_j, and A_0. These conditions are

$$\sum_{j=1}^{p} A_j x_j=\frac{1}{2}+\alpha, \tag{7}$$

$$\sum_{j=1}^{p}\frac{A_j}{1+x_j}=\frac{1-\alpha}{4}, \tag{8}$$

$$\sum_{j=1}^{p} A_j=\frac{1}{2}, \quad A_0=\frac{1}{2}. \tag{9}$$

Here the x_j are the roots of the characteristic equation

$$x^3-x^2(l+m)+x(l-m)-1=0, \tag{10}$$

where

$$l=1+2\cos(2ka), \quad m=2\alpha[1-\cos(2ka)]. \tag{11}$$

Note that Eq. (10) implies, among other things, that $p=3$ in Eqs. (7)–(9). Simultaneous solution of Eqs. (7)–(9) and Eq. (10) determines the coefficients A_j ($j=1,2,3$):

$$A_1=\frac{1}{2}\frac{(1-\alpha)(1+l)-(1+x_1)(l+m-x_1-2\alpha)}{(x_2-x_1)(x_3-x_1)}. \tag{12}$$

A_2 and A_3 can be obtained from (12) via cyclic permutation of x_1, x_2, and x_3. The quantities x_j, which are the roots of the cubic equation (10), are given by the standard formulas

$$x_1=C+D+\frac{l+m}{3},$$
$$x_{2,3}=-\frac{C+D}{2}\pm i\sqrt{3}\,\frac{C-D}{2}+\frac{l+m}{3}. \tag{13}$$

Here

$$C=\sqrt[3]{-\frac{q}{2}+\sqrt{Q}},\quad D=\sqrt[3]{-\frac{q}{2}-\sqrt{Q}},$$
$$Q=\frac{2l}{3}\,\frac{l^2+3m^2}{9}-\frac{1}{12}\left(\frac{l^2-m^2}{3}\right)^2-\frac{l^2-m^2}{6}+\frac{1}{4}, \tag{14}$$
$$q=-2\left(\frac{l+m}{3}\right)^3+\frac{l^2-m^2}{3}-1.$$

From the general solution given by (6), (12), and (13) we can easily find the particular solution for electrons with an energy corresponding to the center of the energy band. Indeed, for $ka=\pi/2$ Eqs. (11) yield $l=-1$ and $m=4\alpha$. Then the solutions of Eq. (10) are

$$x_1=-1,\quad x_{2,3}=2\alpha\pm\sqrt{1+4\alpha^2}. \tag{15}$$

Plugging (15) into (6) and (12) and noting that the coefficient A_1, corresponding to the root $x_1=-1$, is zero, we arrive at the solution (5) found in Ref. 13.

Combining (6) and the characteristic equation (10), we obtain the following recurrence equation for $\langle\rho_N\rangle$:

$$\langle\rho_N\rangle=(l-m)\langle\rho_{N-1}\rangle-(l+m)\langle\rho_{N-2}\rangle+\langle\rho_{N-3}\rangle+m, \tag{16}$$

where the initial values $\langle\rho_1\rangle$, $\langle\rho_2\rangle$, and $\langle\rho_3\rangle$ for (16) can be found from (3):

$$\langle\rho_1\rangle=\alpha,\quad \langle\rho_2\rangle=2\alpha+2\alpha^2[1-\cos(2ka)],$$
$$\langle\rho_3\rangle=3\alpha+2\alpha^2[3-2\cos(2ka)-\cos(4ka)]$$
$$+4\alpha^3[1-\cos(2ka)]^3.$$

The recurrence equation (16) can be used for numerical calculations and for studying $\langle\rho_N\rangle$ for moderate values of N.

We note that, as solution (6) shows, the dependence of the average Landauer resistance of a chain of periodically spaced random delta-function potentials on the chain length $L=Na$ generally has the form of a sum of three exponential functions.

4. LOCALIZATION OF ONE-ELECTRON STATES

Now let us discuss the behavior of $\langle\rho_L\rangle$, the solution (6), as $L\to\infty$. We wish to demonstrate that for all reasonable values of the parameters l and m the quantity $\langle\rho_L\rangle$ increases in the limit $L\to\infty$ according to an exponential law. This means that in our model all the one-electron states are localized. The only exceptions are the edges of the energy bands ($ka=\pi m$, $m=1,2,\ldots$), for which the $\langle\rho_L\rangle$ vs L dependence is linear.[5]

To prove the above statement we must first establish certain properties of the real roots of the characteristic equation (10). This requires writing Eq. (10) in the form

$$l=\frac{x^2+x+1}{x}-\frac{x+1}{x-1}m. \tag{17}$$

Here we allowed for the fact that $x_j\neq 0$ and excluded the solution $x_j=1$, $j=1,2,3$, which corresponds to the edges of the energy bands (see above). If we substitute any real solution x_j of Eq. (10) in (17), then in the plane specified by the coordinates l and m Eq. (17) specifies a straight line containing all the pairs l and m for which x_j is a solution of Eq. (10). This statement provides the key to establishing whether or not a fixed real x_j is a solution of Eq. (10). To this end we need only to plug x_j into Eq. (17) and see whether the straight line (17) passes through the range of possible values of the parameter l and m. If it does, x_j is a solution of Eq. (10).

As the definitions (11) of the parameters l and m imply, the ranges of their allowed values are

$$-1\leqslant l\leqslant 3,\quad m\geqslant 0. \tag{18}$$

Examining the various straight lines in the l, m plane for a fixed x_j, we can easily see that these straight lines pass through the region specified in (18) only if

$$-1\leqslant x_j<0,\quad x_j\geqslant 1. \tag{19}$$

Hence the conditions (19) determine the range of values of the real roots of Eq. (10) for arbitrary values of the electron energy (or ka) and the parameter α.

As is well known, for $Q>0$ Eq. (10) has only one real root. Then the other two roots are complex-valued and $x_2=x_3^*$. This means that we can always write

$$x_2=\rho e^{i\varphi},\quad x_3=\rho e^{-i\varphi}, \tag{20}$$

where ρ and φ are real numbers. According to Viete's theorem, we have the following relationship for the roots of Eq. (10):

$$x_1x_2x_3=1. \tag{21}$$

Plugging (20) into (21) yields

$$x_1\rho^2=1. \tag{22}$$

Since by definition ρ^2 is positive, Eq. (22) implies that the only real root x_1 is positive, so that according to (19) we have

$$x_1\geqslant 1. \tag{23}$$

Then from (22) it follows that $0<\rho^2\leqslant 1$. The real root x_1 in the given case ($Q>0$) can be found from (13). Using (20) and (22), we write the solution (6) in the following form:

$$\langle\rho_N\rangle=A_1x_1^N+2ax_1^{-N/2}\cos(N\varphi+\psi)-\tfrac{1}{2}. \tag{24}$$

The coefficients A_2 and A_3 of the solution (6) can be written as

$$A_2=ae^{i\psi},\quad A_3=ae^{-i\psi},$$

since $A_3=A_2^*$. If we let N go to infinity and allow for the condition (23), from (24) we obtain the following asymptotic expression for $\langle\rho_N\rangle$:

$$\langle\rho_N\rangle=A_1x_1^N-\tfrac{1}{2}. \tag{25}$$

Reducing this expression to the form $\langle\rho_L\rangle\propto\exp\{L/\xi\}$, we arrive at a simple formula for the localization radius ξ:

$$\xi=\frac{a}{\ln x_1}. \tag{26}$$

Let us now examine another case, where $Q\leqslant 0$. Equation (10) then has three real roots. As Eq. (21) shows, all three roots cannot be greater than unity simultaneously, since in this case their product would be greater than unity, which contradicts (21). The case where all three roots are equal to unity, $x_1=x_2=x_3=1$ $(Q=0)$, corresponds to the edge of the energy band and is a feature of this model; it has been repeatedly discussed in the literature.[8,9] The case when one of the roots is negative and the other two are positive is also impossible, since $x_1x_2x_3$ would be negative, which contradicts condition (21). Hence the only variant that does not contradict conditions (19)–(21) is the one in which $x_1\geqslant 1$ and $-1\leqslant x_{2,3}<0$. In this case one of the negative roots, say x_3, can be found from (13) by using the formula

$$x_3=C+D+\frac{l+m}{3}, \tag{27}$$

with $C=D^*$. The other two roots are also determined by (13) and can be written as

$$x_{1,2}=a\pm b, \tag{28}$$

with a and b expressed in terms of x_3 in the following manner:

$$a=\frac{l+m-x_3}{2},$$
$$b=\sqrt{\frac{3}{4}\left(\frac{l+m}{2}+x_3\right)(l+m-x_3)+m-l}. \tag{29}$$

Instead of a and b we introduce other variables, ρ and x, by the formulas

$$a=\rho\sinh x,\quad b=\rho\cosh x. \tag{30}$$

Then $b^2-a^2=\rho^2=-x_3^{-1}$. Plugging (30) and (29) into the solution (6) for $\langle\rho_N\rangle$, we arrive at the following expressions:

$$\langle\rho_N\rangle=\begin{cases}\frac{1}{2}\{(-1)^NA_3\rho^{-2N}+\rho^N[K_1\sinh(xN)\\ +K_2\cosh(xN)]\}-1, & N=2n+1,\\ \frac{1}{2}\{(-1)^NA_3\rho^{-2N}+\rho^N[K_1\cosh(xN)\\ +K_2\sinh(xN)]\}-1, & N=2n,\end{cases} \tag{31}$$

where

$$K_{1,2}=\frac{A_1\pm A_2}{2},\quad n=1,2,\ldots.$$

As noted earlier, for the electron energy corresponding to the center of the energy band, $ka=\pi/2$, we have $A_3=0$. For this particular case we can easily see that $K_1=\rho=1$ and $K_2=1/\cosh x$ hold, and the solutions (31) become the solutions (53) and (54) of Ref. 13. If we take N to infinity, as in the case $Q>0$, the solutions (31) become the solutions (25), in which $x_1=a+b>1$. Hence in this case too the localization radius is determined by formula (26).

We have proved that the solution (6) with $L\to\infty$ always leads to an exponential dependence of the average Landauer resistance $\langle\rho_L\rangle$ on L. This means, in particular, that all the one-electron states are localized, with the localization radius given by formula (26).

5. THE LOCALIZATION RADIUS OF ONE-ELECTRON STATES

Before proceeding with the calculation of the localization radius of one-electron states we would like to mention several general properties of the solution obtained for $\langle\rho_N\rangle$.

As noted earlier, the average Landauer resistance $\langle\rho_N\rangle$, expressed by (24) and (31), in the asymptotic case $N\to\infty$ is a power function of N, i.e., $\langle\rho_N\rangle\propto x_1^N$, with $x_1>1$, and is independent of N. The nature of the transition to such a dependence is determined by the values of the roots x_2 and x_3 of the characteristic equation (10). The farther the electron energy is from the edges of the energy bands, the closer the absolute values of x_2 and x_3 are to zero, and hence the more rapidly the solutions (24) and (31) acquire the form (25) as N grows. The dependence of $\langle\rho_L\rangle$ on L is oscillatory for any electron energy, but such behavior becomes less and less evident as L increases. The average Landauer resistance $\langle\rho_L\rangle$ depends on the incident-electron energy in a similar way, provided that L and w are fixed.

We calculated the dependence of ξ on ka and w numerically, with the results depicted in Fig. 1. Clearly, at a fixed w the value of the localization radius increases as a function of the electron energy within the first energy band $(0\leqslant ka\leqslant\pi)$, tending to infinity as $ka\to\pi$. Note that the localization radius has a minimum when the electron energy varies within the second band $(\pi\leqslant ka\leqslant 2\pi)$, and the value of this minimum tends to the center of the energy band as w increases. The diagram in Fig. 1 clearly demonstrates a natural physical result: at fixed electron energies the localization radius monotonically decreases as the chain disorder parameter w increases. Figure 1 also depicts the curves of equal values of the localization radius of electronic states. The universal result obtained here is that the electron energy must grow with w for the localization radius to remain unchanged.

In conclusion we note that in the cases of weak and strong electron scattering, simple analytic expressions can be obtained for the dependence of the localization radius on the electron energy and the chain disorder parameter w.

Let us start with weak electron scattering, i.e., $\alpha\ll 1$. In this limit the root of Eq. (10) determining the localization radius can be found in the form

$$x_1=1+\Delta x, \tag{32}$$

where $0<\Delta x\ll 1$. Plugging (32) into (10) and keeping only terms linear in α, we arrive at the following expression for Δx:

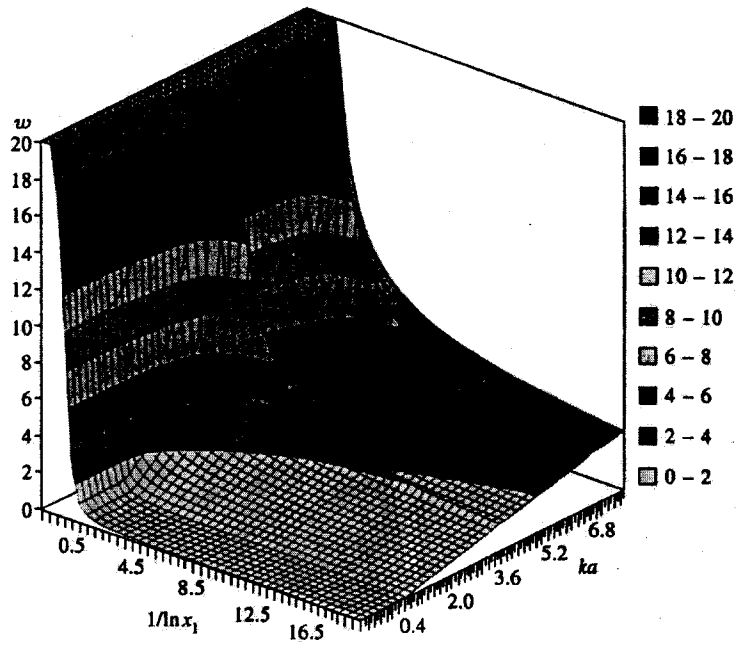

FIG. 1. Dependence of the electron localization radius $\xi/a=1/\ln x_1$ on ka and w.

$$\Delta x=\frac{3m}{3-l}=2\alpha. \tag{33}$$

Plugging (32) and (33) into (26) and taking $\ln(1+2\alpha)\approx 2\alpha$, we finally obtain

$$\xi=96\left(\frac{k}{w}\right)^2 a. \tag{34}$$

Here the value of ξ exceeds by a factor of two the value obtained by Perel' and Polyakov.[9] The reason is that in Ref. 9 the localization radius was determined from the value of $\langle \ln \rho\rangle$, which for $\alpha \ll 1$ is two times the value of $\ln\langle\rho\rangle$.

In the limit of strong electron scattering, i.e., $\alpha \gg 1$, and with the additional requirement that

$$\alpha \sin^2(ka) \gg 1, \tag{35}$$

we arrive at the following simple expression for the electron localization radius:

$$\xi=\frac{a}{\ln[4\alpha \sin^2(ka)]}. \tag{36}$$

The same result was obtained in Ref. 13 for $\alpha \gg 1$. We see that to derive formula (36) we need a stronger requirement than $\alpha \gg 1$, namely, condition (35) must be met.

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