RESISTANCE OF ONE-DIMENSIONAL CHAINS IN KRONIG–PENNY-LIKE MODELS

V.M. GASPARIAN, B.L. ALTSHULER, A.G. ARONOV and Z.A. KASAMANIAN
Leningrad Nuclear Physics Institute, Gatchina, Leningrad 188350, USSR

Received 1 July 1988; accepted for publication 15 July 1988
Communicated by V.M. Agranovich

We give the formula for the resistance of one-dimensional chains of arbitrary δ-potentials without finding electron eigenfunctions. We have analyzed the main consequences of this formula, and the distribution functions of resistances are also determined.

In the present paper we give the formula for the resistance of one-dimensional chains with arbitrary δ-potentials, which is convenient for numerical calculations and for the investigation of the electron localization in the one-dimensional case and in an external field. This expression for the resistance is valid for chains with an arbitrary length at any disorder.

Thouless [1] has shown that a relation like that of the dispersion exists between the density of states $\nu(E)$ and $\ln|\psi(x)|$ $(x\to\infty)$ where $\psi(x)$ is the electron wave function. In other words, this relation is one between the density of states and the electron localization radius. It can be written as a relation between the resistance of the sample $\rho_L(E)$ and the density of states

$$\ln[\rho_L(E)+1] = 2L \int dE' \, [\nu_0 - \nu(E')] \ln|E-E'| \, . \quad (1)$$

Here L is the sample length, ν_0 is the density of states of a free electron. On the other hand the density of states in the one-dimensional chain with the same arbitrarily situated δ-potentials $V(x)=V\sum_n \delta(x-x_n)$ is determined by the expression [2]

$$\nu(E) = -\frac{1}{\pi L}\int_0^L dx \, \mathrm{Im}\, G(x,x) = \nu_0 - \frac{1}{\pi L}\mathrm{Im}\frac{\partial}{\partial E}\ln D_L(E) \, , \quad (2)$$

where

$$D_L(E) = \det D_{jl} \, , \quad (3)$$

$$D_{jl} = \delta_{jl} + (\mathrm{i}V/2k)\exp(\mathrm{i}k|x_j - x_l|), \quad E=k^2 \quad (4)$$

and $G(x,x')$ is the retarded electron Green function in the potential $V(x)$.

Using eqs. (1) and (2) and integrating eq. (1) by parts, we obtain

$$\rho_L(E) = |D_L(E)|^2 - 1 \, . \quad (5)$$

We have also made use of the fact that the density of states is proportional to the imaginary part of the retarded Green function which satisfies the usual dispersion relation. Eq. (5) is the main result of our paper. It can be proved in the general case of arbitrary values and arbitrarily arranged δ-potentials in a chain which has the finite length L and is situated in the external potential $u(x)$:

$$U(x) = u(x) + \sum_{n=1}^{N} V_n \delta(x-x_n) \, . \quad (6)$$

In this case

$$D_{jl} = \delta_{jl} + V_j G_0(x_j, x_j) \exp[\Theta(x_j, x_l)] \, , \quad (7)$$

where $G_0(x,x')$ is the retarded electron Green function in the external potential $u(x)$. $\Theta(x,x')$ is determined by [3]

$$\Theta(x,x') = -\tfrac{1}{2}\int_{\min(x,x')}^{\max(x,x')} \frac{dx_1}{G_0(x_1,x_1)} \, . \quad (8)$$

The determinant $D_N = \det D_{jl}$ satisfies the following recurrence relation, which can be derived from definition (7). This is the generalization of eq. (3) by Bychkov and Dyhne [2] in the general case:

$$D_N = A_N D_{N-1} - B_N D_{N-2}, \tag{9}$$

where

$$B_N = \frac{V_N G_0(x_N, x_N)}{V_{N-1} G_0(x_{N-1}, x_{N-1})} \exp[2\Theta(x_N, x_{N-1})], \quad N>1, \tag{10}$$

$$A_N = 1 + B_N - V_N G_0(x_N, x_N)\{1 - \exp[2\Theta(x_N, x_{N-1})]\}, \quad N>1, \tag{11}$$

$$A_1 = 1 + V_1 G_0(x_1, x_1), \quad D_0 = 1, \quad D_{-1} = 0. \tag{12}$$

D_{N-1} (D_{N-2}) is the determinant of matrix (7) with the Nth ($(N-1)$th) column and line removed. The transmittance amplitude t_N of N δ-potentials is related to D_N by

$$t_N = D_N^{-1}. \tag{13}$$

Therefore, the equation for the resistance eq. (5) can be rewritten in the Landauer form [4]

$$\rho_N(E) = |D_N|^2 - 1 = \frac{1-T_N}{T_N}, \tag{14}$$

where $T_N = |t_N|^2$. The expression for the density of states is related to D_N by an equation which is the generalization of eq. (2) for δ-potentials with arbitrary amplitudes V_j and an arbitrary external potential $u(x)$:

$$\nu = \nu_0 - \frac{1}{\pi L}\frac{\partial}{\partial E} \operatorname{Im} \ln D_N, \quad \nu_0 = \operatorname{Im} \int_0^L \frac{dx}{\pi L} G_0(x,x). \tag{15}$$

If the external potential $u(x)$ is absent, then $G_0(x, x) = i/2k$ and matrix D_{jl} has the form

$$D_{jl} = \delta_{jl} + (iV_j/2k) \exp(ik|x_j - x_l|). \tag{7a}$$

In this case A_N and B_N are determined by

$$B_N = (V_N/V_{N-1}) \exp(2ik|x_N - x_{N-1}|),$$

$$A_N = 1 + B_N + (iV_N/2k)[1 - \exp(2ik|x_N - x_{N-1}|)], \quad N>1, \tag{10a}$$

$$A_1 = 1 + iV_1/2k. \tag{11a}$$

Eqs. (5) and (7a) allow one to obtain both well known and new results.

(1) For the Kronig–Penny chain consisting of N identical and periodically arranged potentials V, the electron spectrum is determined thus:

$$\cos \beta a = \operatorname{Re}[(1 + iV/2k) \exp(ika)]. \tag{16}$$

Here a is the period of the structure and β plays the role of quasimomentum. The condition $|\cos \beta a| < 1$ determines the states in the allowed energy band. In this case one can obtain the expression for D_N (e.g., by making use of the recurrence relation eq. (9)):

$$D_N = e^{iNka}\left[\cos N\beta a + i\left(\frac{V}{2k}\cos ka - \sin ka\right)\frac{\sin N\beta a}{\sin \beta a}\right]. \tag{17}$$

After the substitution of eq. (17) in eq. (14) the resistance of this chain has the form

$$\rho_N = \frac{\sin^2 N\beta a}{\sin^2 \beta a}\left(\frac{V}{2k}\right)^2 = \rho_1 \frac{\sin^2 N\beta a}{\sin^2 \beta a}. \tag{18}$$

This formula describes the resistance of the interface between an ideal conductor and the periodic structure. ρ_1 is the resistance of the elementary cell.

Resistance ρ_N does not increase monotonically with N and at $|\cos \beta a| < 1$ the resistivity goes to zero at $N \to \infty$. At the same time the resistance increases exponentially with N for the states in the energy gap (where $\cos \beta a = \operatorname{ch}(i\beta a) > 1$).

Let us consider the generalized Kronig–Penny model in which the elementary cell consists of n rather than one δ-like potential (fig. 1). The amplitudes V_i of these potentials and their positions are arbitrary. The transmittance amplitude through the elementary cell in our notation has the form:

$$t_n = e^{ika} D_n^{-1}, \quad T_n = |t_n|^2. \tag{19}$$

The relation between the transmittance amplitude t_n and the electron spectrum was obtained earlier [5]. According to ref. [5] the electron spectrum in this case is

$$\operatorname{Re} 1/t_n = \operatorname{Re}(e^{-ika} D_n) = \cos \beta a. \tag{20}$$

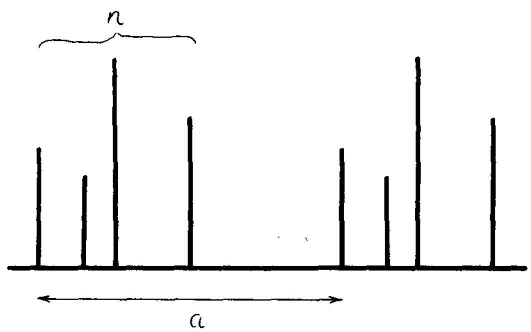

Fig. 1. Generalized Kronig–Penny model with n centers in the elementary cell; the period of the structure is denoted a.

At $n=1$ eq. (20) coincides obviously with eq. (10), while at $n=2$ it leads to the result obtained in ref. [6].

For the generalized Kronig–Penny model the resistance is determined by eq. (18).

(2) If arbitrary δ-like potentials are arranged periodically ($x_n=na$), the recurrence relation can be solved, because at $V_i(\sin ka)/k \gg 1$ (i.e. if the resonance is absent, $ka \neq \pi n$) the values A_1 and $A_{N>1}$ are equal,

$$A_1 \simeq \mathrm{i} V_1/2k, \quad A_{N>1} \simeq (V_N/k)\mathrm{e}^{\mathrm{i}ka} \sin ka$$

and

$$D_{N-2} \ll D_N .$$

As a result we obtain

$$D_N = \mathrm{i}\frac{\exp[\mathrm{i}(N-1)ka]}{\sin ka}\left(\frac{\sin ka}{k}\right)^N \prod_{i=1}^{N} V_i$$

and the resistance of the chain is [7]

$$\rho_N + 1 = \frac{1}{4\sin^2 ka}\left(\frac{\sin^2 ka}{k^2}\right)^N \prod_{i=1}^{N} V_i^2 . \tag{21}$$

From eq. (21) it follows that

$$\rho_N + 1 \simeq \exp[\langle \ln(\rho_N+1)\rangle] = \frac{1}{4\sin^2 ka}\exp(L/\xi) , \tag{22}$$

where the inverse localization length is equal to

$$\xi^{-1}(k) = \xi^{-1}(0) + a^{-1}\ln\frac{\sin^2 ka}{(ka)^2} , \tag{23}$$

$$\xi^{-1}(0) = a^{-1}\langle \ln V_j^2 a^2\rangle . \tag{24}$$

One can easily extend eqs. (21)–(24) in case of a chain of arbitrary arranged strong potentials.

Let us consider the distribution of the resistances in the case of periodically arranged δ-like potentials with random magnitudes.

In a nonresonance case $\ln \rho_N \propto \sum_i V_i^2$ and according to the central limit theorem $\ln(\rho_N+1)$ is distributed normally

$$W(\rho_N) = \frac{1}{(\rho_N+1)\sqrt{2\pi N\sigma}} \times \exp\left(-\frac{[\ln(\rho_N+1) - N\ln(\rho_0+1)]^2}{2N\sigma}\right) , \tag{25}$$

where

$$\rho_0 + 1 = \sin^2 ka \exp[\langle \ln(V_i/k)^2\rangle] ,$$
$$\sigma = \langle \ln^2(V_i/k)^2 - \langle \ln(V_i/k)^2\rangle^2\rangle . \tag{26}$$

This distribution function coincides with the resistance distribution in an ensemble of 1D chains with identical scattering centers randomly located, which was obtained earlier in refs. [8–10].

(3) If $ka=\pi n$, a resonance transmission takes place. From eq. (4) we obtain

$$D_N = 1 + \mathrm{i}\sum_{l=1}^{N}\frac{V_l}{2k} , \tag{27}$$

$$\rho_N = \left|\sum_{l=1}^{N}\frac{V_l}{2k}\right|^2 . \tag{28}$$

Eq. (28) is natural: it manifests the fact that our chain is equivalent to the single potential $\sum_{l=1}^{N} V_l$ provided the resonance condition $ka=\pi n$ is valid. The ensemble averaged resistance at $ka=\pi n$ according to eq. (28) is equal to

$$\langle \rho_N\rangle = \left(\frac{N}{2k}\right)^2 \langle V\rangle^2 + N\frac{\langle V^2\rangle - \langle V\rangle^2}{4k^2} \tag{29}$$

($\langle\ \rangle$ means ensemble averaging) at $\langle V\rangle = 0$, $\langle \rho_N\rangle \propto N$, the resistivity is finite and the mean free path is proportional to $k^2/\langle V^2\rangle$.

The distribution function in the resonance case differs from eq. (25). According to the central limit theorem $\sum_{i=1}^{N} V_i$ is distributed normally at $N \gg 1$. Therefore in the resonance case when the resistance is determined by eq. (28) the distribution function of the resistance at $\langle V\rangle = 0$ has the form

$$W(\rho)=2(\rho\langle\rho\rangle\pi)^{-1/2}\exp(-\rho/\langle\rho\rangle)\,. \tag{30}$$

At $\langle V\rangle\neq 0$ the expression for $W(\rho)$ differs from eq. (30) only by the change of ρ for $(\rho^{1/2}-\langle V\rangle/2k)^2$, and $\langle\rho\rangle$ is determined by eq. (29).

(4) We can calculate the Thouless energy shift δE: the shift of energy levels at the variation of the phase of the boundary conditions. By definition [11] $\delta E=\partial^2 E/\partial(\beta L)^2$. The second derivation from eq. (28) with respect to β is equal to

$$\delta E=\left.\frac{\partial^2 E}{\partial(\beta L)^2}\right|_{\beta=0}$$

$$=-\left(\mathrm{Re}\,\frac{\mathrm{d}}{\mathrm{d}E}D_N\,\mathrm{e}^{-\mathrm{i}kL}\right)^{-1}_{\beta=0}. \tag{31}$$

According to ref. [11] the product of $L\delta E$ and the density of states (15) is equal to the conductance of the sample. The comparison of this product with eq. (14) shows that this relation is not exactly correct.

(5) The dispersion relation (1) takes place not only for the localized states but in arbitrary cases, for example, in the periodic Kronig–Penny model or in the electric field, when the delocalized states can appear.

(6) Let us consider the periodic potential arrangement when the potential distribution function is the Cauchy distribution (Lloyd model):

$$P(V_i)=\frac{1}{\pi}\frac{\gamma}{(V_i-V)^2+\gamma^2}, \tag{32}$$

where V and γ are the parameters of the distribution. According to ref. [12] under this assumption

$$\langle G(x,x)\rangle=G(x,x)\,|_{V_i}-V+i\gamma\,\mathrm{sign}\,E\,.$$

Hence, using eq. (15) we obtain

$$\langle\ln(\rho_N+1)\rangle=-2\,\mathrm{Re}\left\langle\int_{x_1}^{x_N}\mathrm{d}x\int_{-\infty}^{E}\mathrm{d}E'\;G_{E'}(x,x)\right\rangle$$

$$=\ln|\bar{D}_N(E)|^2\,, \tag{33}$$

where $\bar{D}_N$ is the determinant (17) after the substitution of all the potentials V_i by $V-\mathrm{i}\gamma$. Provided the centers are arranged periodically, $\bar{D}_N$ is determined by eq. (17),

$$\bar{D}_N=\exp(\mathrm{i}Nka)\Bigg[\cos N\bar{\beta}a$$

$$+\mathrm{i}\left(\frac{V-\mathrm{i}\gamma}{2k}\cos ka-\sin ka\right)\frac{\sin N\bar{\beta}a}{\sin\bar{\beta}a}\Bigg]. \tag{34}$$

Here $\bar{\beta}$ is determined by the relation

$$\cos\bar{\beta}a=\cos ka+\frac{V-\mathrm{i}\gamma}{2k}\sin ka\,. \tag{35}$$

Using eqs. (33) and (34) one can show that the resistance of the chain consisting of N δ-like potentials is equal to $(L=Na)$

$$\langle\ln(\rho_N+1)\rangle=\ln\left(1+\bar{\rho}_1\,\frac{\mathrm{sh}^2 yL+\sin^2\beta L}{\mathrm{sh}^2 ya+\sin^2\beta a}\right), \tag{36}$$

$$\bar{\rho}_1=\left|1+\frac{\gamma+\mathrm{i}V}{2k}\right|^2-1\,.$$

Here $y=\mathrm{Im}\,\bar{\beta}$.

From eq. (36) one can see that at $L\to\infty$ the geometric mean resistance increases exponentially with the sample length L. At arbitrary ka the inverse localization radius

$$\xi^{-1}\equiv\lim_{L\to\infty}\frac{1}{L}\langle\ln(\rho_N+1)\rangle=\frac{2}{a}\,\mathrm{Im}\,\bar{\beta} \tag{37}$$

is determined from eqs. (34), (35)

$$\xi^{-1}=2a^{-1}\ln(\sqrt{y+1}+\sqrt{y})\,, \tag{38}$$

$$2y=\left(\frac{\gamma}{2k}\right)^2\sin^2 ka-\sin^2\beta a$$

$$+\left\{\left[\left(\frac{\gamma}{2k}\right)^2\sin^2 ka-\sin^2\beta a\right]^2+\frac{\gamma^2}{k^2}\sin^2 ka\right\}^{1/2}.$$

Here β is determined by eq. (16). This result was obtained earlier by Hirota and Ishii [13].

We wish to thank Dr. L.I. Glasman and Dr. M.I. Raikin for helpful discussions. We thank especially Dr. S.A. Gredeskul and Dr. L.A. Pastur, who subjected our paper to a benevolent critical analysis.

References

[1] D.J. Thouless, J. Phys. C 5 (1972) 77.

[2] Yu.A. Bychkov and A.M. Dyhne, Pis'ma Zh. Eksp. Teor. Fiz. 3 (1966) 313.
[3] Z.A. Kasamanian, Izv. Fiz. 11 (1980) 20.
[4] R. Landauer, Phys. Lett. A 85 (1981) 91.
[5] V. Heine, The pseudopotential concept, in: Solid state physics: advances in research and applications, Vol. 24, eds. H. Ehrenreich, F. Seitz and D. Turnbull (Academic Press, New York, 1970).
[6] A.M. Eldib, H.F. Hassan and M.A. Mokamed, J. Phys. C 20 (1987) 3011.
[7] I.F. Ichkovich, I.O. Kulik and R.I. Shehter, Fiz. Nizk. Temp. 13 (1987) 1166.
[8] A.A. Abrikosov, Solid State Commun. 37 (1981) 997.
[9] V.I. Mel'nikov, Fiz. Tverd. Tela 23 (1981) 782.
[10] V.I. Perel' and D.G. Polyakov, Zh. Eksp. Teor. Fiz. 86 (1984) 352; Pis'ma Zh. Eksp. Teor. Fiz. 37 (1983) 535.
[11] D.J. Thouless, Phys. Rep. 136 (1974) 94.
[12] I.M. Lifshitz, G.A. Gredeskul and L.A. Pastur, Wedenie v teoriu neupoviadochih sistem (Nauka, Moscow, 1982).
[13] I. Hirota and K. Ishii, Prog. Theor. Phys. 45 (1971) 1713.