[3] For more accurate estimates, it is necessary to take into account the change in r_c due to the anharmonic interaction of the lattice with the niobium dipoles. When $T \ll T_c$, r_c can be found approximately from the permittivity ε in potassium tantaloniobate.[10]

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Transmission coefficient of an electron traveling across a one-dimensional random potential

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A method of calculating the density of states and resistance of finite one-dimensional chains without determining the eigenfunctions is developed for arbitrary potentials.

INTRODUCTION

We shall derive a formula for the resistance and density of states of one-dimensional chains of random delta-function potentials (Secs. 1 and 2) which can be used in numerical calculations as well as in the investigation of electron localization in the one-dimensional case in an applied field. This expression for the resistance is valid for chains of arbitrary lengths and with an arbitrary type of disorder. The knowledge of the exact electron wave functions in this potential is not required.

The results summarized in the Introduction are contained in Ref. 1.

We consider a potential in the form

$$V(x)=\sum_{l=1}^{N} V_l \delta(x-x_l), \quad x_l < x_{l+1}, \tag{1}$$

where V_l and x_l are arbitrary. The electron Green function in such a system $G(x, x')$ is related to the Green function of free electrons $G_0(x, x')$ by

$$G(x, x')=G_0(x, x')-R_1\frac{G_0(x, x_1)G_0(x_1, x')}{G_0(x_1, x_1)}, \quad x, x' \leqslant x_1, \tag{2}$$

$$G_0(x, x')=\frac{i}{2k}\exp(ik|x-x'|), \quad k=\sqrt{E+i\delta}$$

($\hbar = 1$ and $m_0 = 1/2$ is the electron mass). We shall show that the coefficient of reflection from such a chain can be written in the form

$$R\equiv|R_1|^2=1-|D_N|^{-2}, \tag{3}$$

where

$$D_N=\det\left|\delta_{nl}+\frac{iV_l}{2k}\exp(ik|x_l-x_n|)\right|, \tag{4}$$

and the transmission coefficient for such a chain thus has the form

$$T=1-R=|D_N|^{-2}.$$

According to Landauer,[2] the resistance of such a chain is given by

$$\rho_N=R/T=|D_N|^2-1. \tag{5}$$

The density of states for $N \to \infty$ can also be expressed in terms of D_N:

$$\nu\equiv-(\pi|x_N-x_1|)^{-1}\int_{x_1}^{x_N} dx \operatorname{Im} G(x, x) \xrightarrow[N\to\infty]{} \nu_0-(\pi|x_N-x_1|)^{-1}\frac{\partial}{\partial E}\ln D_N, \tag{6}$$

where $\nu_0 = 1/2\pi k$ is the density of states of free electrons.

A similar expression for the density of states in a one-dimensional chain consisting of delta-function potentials with equal amplitudes (i.e., $V_l = V$) was obtained in Ref. 3. The Green function $G(x, x)$ (and, therefore, also D_N) is an analytic function of the energy $E = k^2$. Using Eqs. (5) and (6), we can derive a dispersion relationship similar to that obtained by Thouless [4]

$$|x_N-x_1|^{-1}\frac{\partial}{\partial E}\ln(\rho_N(E)+1) \xrightarrow[N\to\infty]{} 2\int dE' \frac{\nu_{E'}-\nu_0}{E'-E}, \tag{7}$$

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which links the resistance of a given one-dimensional chain to the density of states.

The dispersion relationship (7) is valid not only for exponentially increasing $\rho_N(E)$ (as $N \to \infty$)[4], but also for finite values of $\rho_N(E)$ [see Eq. (14)].

The determinant D_N of a random chain consisting of delta-function potentials satifies the following recurrence relation:

$$D_N = A_N D_{N-1} - B_N D_{N-2}, \tag{8}$$

where

$$A_N = 1 + \frac{V_N}{V_{N-1}} \exp(2ika_{N-1}) + \frac{iV_N}{2k}[1 - \exp(2ika_{N-1})], \quad N > 1, \tag{9a}$$

$$A_1 = 1 + \frac{iV_1}{2k}, \quad B_N = \frac{V_N}{V_{N-1}} \exp(2ika_{N-1}), \tag{9b}$$

and D_{N-1} (D_{N-2}) is a determinant in the form (4), where the N-th (and also (N − 1)-th) row and column have been omitted

$$a_{N-1} = |x_N - x_{N-1}|, \quad D_{-1} = 0, \quad D_0 = 1.$$

In the Kronig–Penney model when $V_\ell = V$ and the potentials are distributed periodically with a period a, the electron spectrum is given by

$$\cos \beta a = \mathrm{Re}\,[e^{-ika}(1 + iV/2k)], \tag{10}$$

where β plays the role of quasimomentum. The condition $|\cos \beta a| < 1$ determines states in an allowed band.

In the generalized Kronig–Penney model when a unit cell contains not a single delta-function potential but m such potentials with arbitrary amplitudes V_m localized at arbitrary points x_m, the transmission coefficient for a single unit cell has the following form in our notation:

$$t_m = e^{ikd} D_m^{-1}, \quad T = |t_m|^2, \tag{11}$$

where d is the period of the structure. A relationship between the transmission coefficient t_m and the electron spectrum was obtained in Ref. 5. Using Eq. (11), we can write the spectrum in the form

$$\mathrm{Re}\,(e^{-ikd} D_m) = \cos \beta d. \tag{12}$$

For n = 1, Eq. (12) reduces to Eq. (10). After substitution of Eq. (4) in Eq. (12) for n = 2 we obtain the result given in Ref. 6.

Considering a finite Kronig–Penney chain consisting of N identical potentials V, we obtain from Eq. (4)

$$D_N = e^{iNka}\left[\cos N\beta a + i\left(\frac{V}{2k}\cos ka - \sin ka\right)\frac{\sin N\beta a}{\sin \beta a}\right]. \tag{13}$$

As expected, it follows from Eqs. (6) and (13) that

$$\nu = \frac{1}{\pi}\frac{\partial \beta}{\partial E}\Big|_{\mathrm{Im}\,\beta \to +0}$$

as $N \to \infty$.

Substituting Eq. (13) in Eq. (5), we find that the resistance of such a chain has the form

$$\rho_N = \left(\frac{V}{2k}\right)^2 \frac{\sin^2 \beta a N}{\sin^2 \beta a} = \rho_1 \frac{\sin^2 \beta a N}{\sin^2 \beta a}. \tag{14}$$

This expression describes the resistance of the interface between a periodic structure and a perfect conductor (ρ_1 is the "resistance" of a single unit cell).

It can be seen from Eq. (14) that the resistance of the chain does not increase with increasing N and, therefore, the resistivity (per unit cell) for states in the allowed band when $|\cos \beta a| < 1$ tends to zero as $N \to \infty$. For states in the band gap when $\cos(i\beta a) = \cosh \beta a > 1$, the resistance increases exponentially with increasing N.

We shall now consider the case when the delta-function potentials are distributed periodically with a period a, but have different amplitudes V_ℓ. If ka = πn (n is an integer), i.e., in the resonance case, we find from Eq. (4) that

$$D_N = 1 + i\sum_{l=1}^{N}\frac{V_l}{2k}, \quad \rho_N = \left(\sum_{l=1}^{N}\frac{V_l}{2k}\right)^2 = N^2\frac{\bar{V}^2}{4k^2}, \tag{15}$$

where $\bar{V} = N^{-1}\sum_{l=1}^{N} V_l$ is the average value of the potential in the sample. It can be seen from Eq. (15) that for $\langle V \rangle \neq 0$ the quantity ρ_N increases proportionally to the square of the sample length. The meaning of Eq. (15) for ρ_N is quite obvious. It shows that the exact resonance condition ka = πn is equivalent to the situation when all the potentials V_ℓ are located at the same point.

Equation (15) yields the following expression for the resistance averaged over an ensemble of samples:

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

(⟨...⟩ denotes averaging over the ensemble). For $\langle V \rangle = 0$, we have $\rho_N \propto N$, so that the mean free path is proportional to $k^2/\langle V^2 \rangle$.

The recurrence relationship (8) can be used conveniently in numerical solution of the problem of a one-dimensional chain with arbitrary potential. We obtain an asymptotic expression for ρ_N for large values of the random potential. Let us assume that $A_1 \approx iV_1/2k$ and $A_{N>1} \approx V_N k^{-1} \sin ka e^{ika}$. The recurrence relation can then be easily solved since $D_{N-2} \ll D_N$

$$D_N = \frac{i}{2}\frac{\exp[i(N-1)ka]}{\sin ka}\left(\frac{\sin ka}{ka}\right)^N \prod_{l=1}^{N}(V_l a). \tag{17}$$

Using Eq. (17), we obtain an expression for the resistance of a chain similar to the result of Ref. 7

$$\rho_N + 1 = \frac{1}{4\sin^2 ka}\left(\frac{\sin^2 ka}{k^2a^2}\right)^N \prod_{l=1}^{N} V_l^2 = \frac{1}{4\sin^2 ka}\exp\left(\frac{N}{\xi}\right),$$

where the localization length is given by

$$\xi^{-1}(k) = \ln \langle V \rangle^2 a^2 \frac{\sin^2 ka}{k^2a^2} + N^{-1}\sum_{l=1}^{N} \ln \frac{V_l^2}{\langle V \rangle^2}.$$

This formula is valid even in the limit ka → 0, where

$$\xi^{-1}(0) = N^{-1} \sum_{l=1}^{\Lambda} \ln \frac{V_l^2}{\langle V \rangle^2},$$

and $\langle V \rangle$ is the average value of the potential.

We shall consider the properties of a one-dimensional chain in Lloyd's model,[8] when the distribution function of potentials is the Cauchy distribution

$$P(V_n) = \pi^{-1} \frac{\gamma}{(V_n - V)^2 + \gamma^2}.$$

According to Ref. 8, we have in this model

$$\langle G(x, x) \rangle = G(x, x)|_{V \to V + i\gamma \operatorname{sign} \operatorname{Im} E},$$

and, therefore, [see Eq. (6)]

$$\langle \ln(\rho_N + 1) \rangle = -2 \operatorname{Re} \left\langle \int_{x_1}^{x_N} dx \int_{-\infty}^{E} dE' G(x, x'; E') \right\rangle = \ln |\bar{D}_N|^2,$$

where $\bar{D}_N$ is the determinant for the Kronig–Penney model where all the potentials are replaced by $V - i\gamma$. It follows from Eq. (13) that $\bar{D}_N$ for periodically distributed potentials is given by

$$\bar{D}_N = \exp(iNka) \left\{ \cos N\bar{\beta}a + i \left[\frac{V - i\gamma}{2k} \cos ka - \sin ka \right] \frac{\sin N\bar{\beta}a}{\sin \bar{\beta}a} \right\}, \quad (18)$$

where $\bar{\beta}$ is described by

$$\cos \bar{\beta}a = \cos ka - \frac{V - i\gamma}{2k} \sin ka.$$

It follows from Eqs. (18) and (5) that the resistance of a chain consisting of N delta-function potentials has the form (L = aN)

$$\langle \ln(\rho_N + 1) \rangle = \ln \left(\beta_1 \frac{\operatorname{sh}^2 yL + \sin^2 \beta L}{\operatorname{sh}^2 ya + \sin^2 \beta a} + 1 \right), \quad (19)$$

where $y = \operatorname{Im} \bar{\beta}, \beta$ is given by Eq. (10), and

$$\beta_1 = \left| 1 + \frac{V + i\gamma}{2k} \right|^2 - 1.$$

Considering the limit $L \to \infty$, we can conclude from Eq. (19) that the average geometric resistance increases exponentially with increasing sample length L and the localization radius for an arbitrary ka is given by[9]

$$\xi^{-1} = \lim_{L \to \infty} L^{-1} \langle \ln(\rho_N + 1) \rangle = \frac{2}{a} \operatorname{Im} \beta = \frac{2}{a} y = \frac{2}{a} \ln(\sqrt{t+1} + \sqrt{t}),$$

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

It can be seen that the localization radius remains finite when $ka \to 0$. On the other hand, if $ka \to \pi n$ ($n = 1, 2, 3\ldots$), then ξ tends to infinity. This is a direct consequence of the model considered, i.e., periodically distributed scatterers forming a simple lattice. In a slightly more general model when a unit cell contains two delta-function potentials[10] or if the original potential is supplemented by a periodic field,[11] the singularities in the density of states and the unbounded increase in ξ disappear.

1. DERIVATION OF THE PRINCIPAL EXPRESSIONS

We shall now derive a relationship between the reflection coefficient of a linear chain consisting of random delta-function potentials and the determinant D_N.

We shall consider a sequence of delta-function potentials with arbitrary amplitudes V_ℓ located at arbitrary points x_ℓ [Eq. (1)]. If the system is subjected, in addition to V(x), also to a regular potential U(x) (an applied electric field, periodic potential, etc.), then the electron Green function should satisfy the Schrödinger equation

$$\left\{ -\frac{\partial^2}{\partial x^2} + U(x) + \sum_{l=1}^{N} V_l \delta(x - x_l) - k^2 \right\} G(x, x'; k) = \delta(x - x'). \quad (20)$$

Equation (20) can be written in the Dyson form

$$G(x, x') + \int dx'' G_0(x, x'') V(x'') G(x'', x') = G_0(x, x'), \quad (21)$$

where $G_0(x, x')$ is the Green function of an electron in the potential U(x).

We shall derive an explicit expression for $G(x, x')$ as follows. We isolate in the potential V(x) the term corresponding to the point on the right-hand edge x_N:

$$V(x) = V_N \delta(x - x_N) + \sum_{l=1}^{N-1} V_l \delta(x - x_l). \quad (22)$$

Substituting Eq. (22) in Eq. (21), we obtain

$$G(x, x') + \int dx'' G_N(x, x'') \sum_{l=1}^{N-1} V_l \delta(x'' - x_l) G(x'', x') = G_N(x, x'), \quad (23a)$$

where

$$G_N(x, x') \equiv G_0(x, x') - V_N \frac{G_0(x, x_N) G_0(x_N, x')}{1 + V_N G_0(x_N, x_N)} = G_0(x, x') - r_N \frac{G_0(x, x_N) G_0(x_N, x')}{G_0(x_N, x_N)}, \quad -\infty < x, x' < \infty, \quad (23b)$$

$$r_j = V_j G_0(x_j, x_j)[1 + V_j G_0(x_j, x_j)]^{-1}, \quad (23c)$$

and r_N is the complex amplitude of the reflection of an electron from the potential V_N in the absence of the remaining (N − 1) potentials on the left. Separating now the next (N − 1)-th potential from the second term in the expression (22) and repeating this procedure, we obtain

$$G(x, x') + \int dx'' G_{N-1}(x, x'') \sum_{l=1}^{N-2} V_l \delta(x'' - x_l) G(x'', x') = G_{N-1}(x, x').$$

Here,

$$G_{N-1}(x, x') = G_N(x, x') - R_{N-1}^{\leftarrow} \frac{G_N(x, x_{N-1}) G_N(x_{N-1}, x')}{G_N(x_{N-1}, x_{N-1})}, \quad (24)$$

$$x_{N-1} \leqslant x, x' \leqslant x_N,$$

where

$$R_{N-1} = \frac{V_{N-1}^{\leftarrow} G_N(x_{N-1}, x_{N-1})}{1 + V_{N-1} G_N(x_{N-1}, x_{N-1})} = \frac{r_{N-1}(1 - r_N z_{N-1,N})}{1 - r_N r_{N-1} z_{N-1,N}} \quad (25)$$

is the amplitude of reflection from the (N-1)-th center; the arrow indicates the orientation of the incident wave. The quantity $R_{N-1}^{\leftarrow}$ differs from r_{N-1} since it includes a delta-function potential at the point x_N. The quantity $z_{N-1,N}$ in Eq. (25) is given by

$$z_{N-1,N} = \frac{G_0(x_{N-1}, x_N) G_0(x_N, x_{N-1})}{G_0(x_N, x_N) G_0(x_{N-1}, x_{N-1})}. \quad (26)$$

Using a relationship between G(x, x') and the diagonal Green functions (for the same one-dimensional coordinates)[12]

$$G(x, x') = (G(x, x)\, G(x', x'))^{1/2} \exp\left\{ -\int_{\min(x, x')}^{\max(x, x')} \frac{dx_1}{2G(x_1, x_1)} \right\},$$

we obtain

$$z_{N-1, N} = \exp\left\{ -\int_{x_{N-1}}^{x_N} \frac{dx}{G_0(x, x)} \right\} = z_{N, N-1}.$$

We shall now express $G_{N-1}(x, x')$ for $x, x' \leq x_{N-1}$ in terms of the bare Green function $G_0(x, x')$ and $R_{N-1}^{\rightarrow}$

$$G_{N-1}(x, x') = G_0(x, x') - R_{N-1}^{\rightarrow} \frac{G_0(x, x_{N-1})\, G_0(x_{N-1}, x')}{G_0(x_{N-1}, x_{N-1})} \tag{27}$$

and, equating Eq. (24) to Eq. (27) for $x = x' = x_{N-1}$, we obtain for $R_{N-1}^{\rightarrow}$

$$R_{N-1}^{\rightarrow} = [r_{N-1} + r_N(1 - 2r_{N-1})\, z_{N-1, N}][1 - r_N r_{N-1} z_{N-1, N}]^{-1}.$$

Repeating this procedure N times, we obtain the Green function for an interval $[x_1, x_2]$ which includes all the delta-function potentials:

$$G(x, x') = G_1(x, x') - R_1^{\leftarrow} \frac{G_1(x_1, x_1)\, G_1(x_1, x')}{G_1(x_1, x_1)}, \tag{28}$$

where $R_1^{\leftarrow}$ is the amplitude of reflection from the first center in the presence of all the other centers:

$$R_1^{\leftarrow} = \frac{r_1(1 - R_2 z_{1,2})}{(1 - r_1 R_2 z_{1,2})},$$

$$G_1(x, x') = G_0(x, x') - R_2 \frac{G_0(x, x_2)\, G_0(x_2, x')}{G_0(x_2, x_2)}.$$

On the other hand, we obtain for $x, x' \leq x_1$,

$$G(x, x') = G_0(x, x') - R_1 \frac{G_0(x, x_1)\, G_0(x_1, x')}{G_0(x_1, x_1)}. \tag{29}$$

Equating Eqs. (28) and (29) for $x = x' = x_1$, we obtain

$$R_1^{\rightarrow} = \frac{r_1 + z_{1,2} R_2 (1 - 2r_1)}{1 - z_{1,2} r_1 R_2} = -\frac{A}{B}. \tag{30}$$

The quantity $R_1^{\rightarrow}$ is the amplitude of reflection of an electron from a chain of potentials which is directly related to the resistance by the Landauer formula.[2]

The numerator and denominator in Eq. (30) can be written as the determinants

$$B = \det \hat{B} = \begin{vmatrix} 1 & R_2 \\ r_1 & z_{1,2}^{-1} \end{vmatrix}, \quad A = \det \hat{A} = \begin{vmatrix} 0 & r_1 & R_2 \\ 1 & 1 & R_2 \\ 1 & r_1 & z_{1,2}^{-1} \end{vmatrix}. \tag{31}$$

It can be seen from Eq. (31) that the matrix $\hat{A}$ is obtained from the matrix $\hat{B}$ by augmenting it on the left and on top. Substituting again in Eq. (31) an expression for $R_1^{\leftarrow}$ similar to Eq. (30) and repeating this procedure N times, we obtain expressions for $\hat{A}$ and $\hat{B}$ in terms of r_j and $z_{j,j+1}$

$$R_1 = -\frac{\det \hat{D}_{N+1}}{\det \hat{D}_N} = -\frac{\tilde{D}_{N+1}}{D_N}, \tag{32}$$

where the matrix $\hat{D}_N$ is given by

$$(\hat{D}_N)_{nl} = \delta_{nl} + V_l G_0(x_l, x_l)\, z_{n, l}^{1/2}, \tag{33}$$

and the matrix $\hat{\tilde{D}}_{N+1}$ is again obtained from $\hat{D}_N$ by bordering on the left and at the top

$$(\hat{\tilde{D}}_{N+1})_{n+1,\, l+1} = (\hat{D}_N)_{n, l}, \quad (\hat{\tilde{D}}_{N+1})_{1,1} = 0, \tag{34a}$$

$$(\hat{\tilde{D}}_{N+1})_{n, 1} = z_{n-1, 1}^{1/2}, \quad (\hat{\tilde{D}}_{N+1})_{1, n} = V_{n-1} G_0(x_{n-1}, x_{n-1})\, z_{n-1, 1}^{1/2}. \tag{34b}$$

We shall now prove the validity of Eq. (3) by mathematical induction. It is easy to verify that, for N = 1,

$$R \equiv |R_1|^2 = |r_1|^2 = 1 - |D_1|^{-2}.$$

We shall assume now that the relationship

$$R = 1 - |D_N|^{-2}, \quad T = |D_N|^{-2} \tag{35}$$

holds for some N and we shall show that this implies its validity when N is replaced by N + 1. When we isolate the potential of the first center $V_1 \delta(x - x_1)$, then the determinants D_{N+1} and $\tilde{D}_{N+2}$ can be expressed in terms of D_1 corresponding to the first center and the determinants D_N and $\tilde{D}_{N+1}$ corresponding to the remaining chain consisting of N potentials $V_l \delta(x - x_l)$, $2 \leq l \leq N + 1$

$$D_{N+1} = D_1 D_N \begin{vmatrix} 1 & R_2 z_{1,2}^{1/2} \\ r_1 z_{1,2}^{1/2} & 1 \end{vmatrix}, \quad \tilde{D}_{N+2} = D_1 D_N \begin{vmatrix} 0 & r_1 & R_2 z_{1,2}^{1/2} \\ 1 & 1 & R_2 z_{1,2}^{1/2} \\ z_{1,2}^{1/2} & r_1 z_{1,2}^{1/2} & 1 \end{vmatrix} \tag{36}$$

The system of equations (32) and (36) is equivalent to Eq. (31). Evaluating the determinants (36) for D_{N+1} and $\tilde{D}_{N+2}$, we obtain

$$|D_{N+1}| = |(1 - r_1 R_2 z_{1,2})\, t_1^{-1} T_2^{-1}|,$$
$$|\tilde{D}_{N+2}| = |[r_1 + R_2(1 - 2r_1) z_{1,2}]\, t_1^{-1} T_2^{-1}|. \tag{37}$$

It follows from the expression (23) for r_1 and from the fact that the Green function $G_0(x, x)$ is imaginary in the continuous spectrum that

$$r_1 + r_1^* = 2|r_1|^2.$$

We can then write the expression (37) for $|\tilde{D}_{N+2}|^2$ in the form

$$|\tilde{D}_{N+2}|^2 = -1 + |D_{N+1}|^2. \tag{38}$$

It follows directly from Eqs. (38) and (32) that Eq. (35) is satisfied for a chain consisting of N + 1 scattering centers. Equations (33) and (34) yield the following recurrence relationship:

$$D_N = A_N D_{N-1} - B_N D_{N-2}, \tag{39}$$

$$\tilde{D}_{N+1} = \frac{1 - V_1 G_0(x_1, x_1)}{V_1 G_0(x_1, x_1)} D_N - \frac{D_{-1+N}}{V_1 G_0(x_1, x_1)}, \tag{40}$$

where

$$A_N = 1 + \frac{V_N G_0(x_N, x_N)}{V_{N-1} G_0(x_{N-1}, x_{N-1})} z_{N-1, N} + V_N G_0(x_N, x_N)(1 - z_{N-1, N}), \quad N > 1,$$

$$A_1 = 1 + V_1 G_0(x_1, x_1), \quad B_N = \frac{V_N G_0(x_N, x_N)}{V_{N-1} G_0(x_{N-1}, x_{N-1})} z_{N-1, N}.$$

and $D_{N-1}(N-2)$ is the determinant (33) where the N-th (and N − 1-th) row and column have been omitted; D_{-1+N} is the determinant (33) where the first row and column have been omitted; $D_0 = 1$ and $D_{-1} = 0$. In particular, in the case $G_0(x, x) = i/2k$, i.e., when $V(x) = 0$, Eq. (39) yields the recurrence relationship (8).

2. LOCAL DENSITY OF STATES

It is of interest to obtain an explicit expression for the local density of states $\nu(E, x)$ of electrons with an energy E at a point x in a one-dimensional chain of random delta-function potentials with an arbitrary type of disorder. The density of states is important because the fluctuations of the local electron density of states lead to fluctuations of the Knight shift, i.e., to inhomogeneous broadening of a nuclear magnetic resonance line.

To evaluate the local density of states in a chain of finite length, we require an explicit expression for the Green function $G(x, x')$ satisfying Eq. (2) within each cell $x_n \leq x, x' \leq x_{N+1}$ for a given number of scatterers N. To obtain this expression, we shall repeat the procedure described earlier isolating, in the potential $V(x)$ defined by Eq. (1), the delta-function potentials no longer in decreasing order as in the derivation of Eqs. (28) and (20), but in such a way that we approach in the last N-th step the given n-th potential from the right. We then obtain the following expression for the Green function [see Eq. (28)]:

$$G(x, x') = G_n(x, x') - \tilde{R}_n \frac{G_n(x, x_n) G_n(x_n, x')}{G_n(x_n, x_n)}, \tag{41}$$

where

$$G_n(x, x') = G_0(x, x') - R_{n+1} \frac{G_0(x, x_{n+1}) G_0(x_{n+1}, x')}{G_0(x_{n+1}, x_{n+1})}. \tag{42}$$

Setting $x = x'$ and using Eq. (42), we obtain from Eq. (41) an expression for the Green function of equal coordinates

$$G(x, x) = \frac{G_0(x, x)}{1 - R_n \overleftarrow{R}_{n+1} z_{n, n+1}} \{1 + R_n \overleftarrow{R}_{n+1} z_{n, n+1} - R_{n+1} z_{x, n+1} - R_n z_{n, x}\}. \tag{43}$$

Here, $z_{x,n+1}$ ($z_{n,x}$) is given by Eq. (26) with a variable lower (upper) limit; $\tilde{R}_n$ is the amplitude of reflection from the left-hand block containing n centers in the presence of the right-hand block containing (N − n) centers, i.e.,

$$\tilde{R}_n = \frac{R_n (1 - R_{n+1} z_{n, n+1})}{1 - R_n \overleftarrow{R}_{n+1} z_{n, n+1}}, \tag{44}$$

$\overleftarrow{R}_n$ is the reflection amplitude from the left block containing n centers in the absence of the right-hand block; $\overrightarrow{R}_{n+1}$ is the amplitude of reflection from the right-hand block containing (N − n) centers in the absence of the left-hand block. The amplitude $\overrightarrow{R}_{n+1}$ can be obtained from Eq. (32) by omitting the first n rows and n columns in D_N

$$R_{n+1} = -\frac{\det \hat{D}_{-n+N+1}}{\det \hat{D}_{-n+N}} = -\frac{D_{-n+N+1}}{D_{-n+N}}. \tag{45}$$

The structure of $\overleftarrow{R}_n$ is similar to Eq. (32), i.e.,

$$R_n = -\frac{\det \hat{D}^0_{n+1}}{\det \hat{D}_n} = -\frac{D^0_{n+1}}{D_n}. \tag{46}$$

However, the matrix $\hat{D}^0_{n+1}$ is obtained by bordering D_n on the right and at the bottom

$$(\hat{D}^0_{N+1})_{n, l} = (\hat{D}_N)_{n, l}, \quad (\hat{D}^0_{N+1})_{N+1, N+1} = 0,$$
$$(\hat{D}^0_{N+1})_{N+1, n} = V_n G_0(x_n, x_n) z^{1/2}_{N+1, n+1}, \quad (\hat{D}^0_{N+1})_{n, N+1} = z^{1/2}_{n+1, N+1}.$$

The following recurrence relationship is obtained for D^0_{n+1} :

$$D^0_{n+1} = \frac{1 - V_n G_0(x_n, x_n)}{V_n G_0(x_n, x_n)} D_n - \frac{D_{n-1}}{V_n G_0(x_n, x_n)}. \tag{47}$$

Although Eqs. (41)-(46) hold in a given interval $[x_n, x_{n+1}]$, we can apply them formally to obtain the Green functions also for $x, x' \leq x_1$ and for $x, x' \geq x_N$: a) for n = 0, we obtain from Eq. (41) using Eqs. (42) and (44) the relationship (29) since $R_0 \equiv 0$, $\tilde{R}_0 = 0$; b) for n = N, Eq. (41) together with Eqs. (42), (44) and (45) yield

$$G(x, x') = G_0(x, x') - R_N \frac{G_0(x, x_N) G_0(x_N, x)}{G_0(x_N, x_N)},$$

since $R_{N+1} \equiv 0$ and $\tilde{R}_N = R_N$.

The local density of states is by definition given by

$$\nu(E, x) = \frac{1}{\pi} \operatorname{Im} G(x, x) = \frac{1}{\pi} \operatorname{Im} \frac{G_0(x, x)}{D_N V_n^2 G_0^2(x_n, x_n)} \left\{ (D_n - D_{n-1}) \right.$$
$$(D_{-(n-1)+N} - D_{-n+N}) - V_n G_0(x_n, x_n) \left[\left(1 - \cos \int_{x_n}^{x} \frac{idt}{G_0(tt)} \right) [2 V_n G_0 \right.$$
$$\times (x_n, x_n) D_n D_{-n+N} - (D_n - D_{n-1}) D_{-n+N} - (D_{-(n-1)+N} - D_{-n+N}) D_n]$$
$$\left. \left. - i \sin \int_{x_n}^{x} \frac{idt}{G_0(tt)} [(D_n - D_{n-1}) D_{-n+N} - (D_{-(n-1)+N} - D_{-n+N}) D_n] \right] \right\}. \tag{48}$$

We derived Eq. (48) from Eq. (43) making use of the recurrence relationships (39), (40), and (47). In particular, for $G_0(x, x) = i/2k$, we find that in the resonance case, i.e., for D_n defined by Eq. (15), Eq. (48) yields for $x = x_n$

$$\nu(E, x_n) = \frac{1}{2\pi k} \frac{1}{1 + \left(\sum_{l=1}^{N} \frac{V_l}{2k} \right)^2}.$$

It can be seen that the local density of states at an exact resonance point, i.e., for $ka = \pi n$ is independent of the number of the site.

The local density of states for large values of the random potential V_n and for $x = x_n$, when D_n is given by Eq. (17) has the form

$$\nu(E, x_n) \approx 2k/\pi V_n^2.$$

3. RESISTANCE OF BLOCKS CONNECTED IN SERIES

Consider now two chains (I and II) which contain, respectively, n and m arbitrary delta-function potentials and are connected in series. Assume

that the phase the wave acquires between these chains is ϕ. We obtain [Eq. (36)]

$$D_{n+m} = D_n D_m \begin{vmatrix} 1 & R_{\tilde{I}\tilde{I}} e^{i\varphi} \\ R_{\tilde{I}} e^{i\varphi} & 1 \end{vmatrix},$$

where $R_{I(\tilde{I})}$ is the amplitude of reflection from the region containing n (m) scatterers

$$\frac{1}{T_{n+m}} = |D_{n+m}|^2 = \frac{1 + |R_{\tilde{I}}|^2 |R_{\tilde{I}\tilde{I}}|^2 - 2|R_{\tilde{I}}||R_{\tilde{I}\tilde{I}}|\cos\theta}{|T_{\tilde{I}}||T_{\tilde{I}\tilde{I}}|},$$

$\theta = 2\phi + \theta_I + \theta_{II}$; $\theta_{I(II)}$ is the phase acquired by the wave after passing across the region I (II).

We shall evaluate the quantity $\langle \ln(\rho_{I+II} + 1) \rangle$, where $\langle \ldots \rangle$ denotes averaging over the phase θ within the interval $[0, 2\pi]$

$$\langle \ln(\rho_{I+II} + 1) \rangle = \langle \ln T_{n+m} \rangle = \langle \ln T_I \rangle + \langle \ln T_{II} \rangle - \\ - \langle \ln(1 + |R_{\tilde{I}}|^2 |R_{\tilde{I}\tilde{I}}|^2 - 2|R_{\tilde{I}}||R_{\tilde{I}\tilde{I}}|\cos\theta) \rangle,$$

the last term vanishes and, therefore, (see Ref. 13)

$$\langle \ln(\rho_{I+II} + 1) \rangle = \langle \ln(\rho_I + 1) \rangle + \langle \ln(\rho_{II} + 1) \rangle. \quad (49)$$

Considering the resistance $\tilde{\rho}_n$ of a block containing n centers which is included in a total chain of N scatterers, we can use Eq. (44) since $\tilde{R}_n$ is amplitude of reflection from the left-hand block in the presence of the right-hand block

$$|\tilde{R}_n|^2 \equiv \frac{\tilde{\rho}_n}{1 + \tilde{\rho}_n} = \frac{\rho_n(\rho_{-n+N} + 1)\left(1 + \frac{\rho_{-n+N}}{1 + \rho_{-n+N}} - 2\sqrt{\frac{\rho_{-n+N}}{1 + \rho_{-n+N}}}\cos\theta\right)}{1 + \rho_N} \quad (50)$$

Here, ρ_n and ρ_{-n+N} are the resistances of the individual blocks; ρ_N is the resistance of the whole chain; $\theta = 2\phi + \theta_1$; θ_1 is the phase the wave acquires having travelled across the left-hand block; ϕ is the phase of the wave between the left-hand and right-hand blocks. Applying the method used in the derivation of Eq. (49) to Eq. (50), we obtain

$$\langle \ln(\rho_N + 1) \rangle = \langle \ln \rho_n \rangle + \langle \ln(\rho_{-n+N} + 1) \rangle - \left\langle \ln \frac{\tilde{\rho}_n}{1 + \tilde{\rho}_n} \right\rangle.$$

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Kinetic models of clusterizaton of point defects in solids

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A system of nonlinear equations with a new type of kernel is used to study the process of coagulation. This system of equations describes clusterization of point defects in solids. Systems with and without a source are studied. Long-term asymptotic solutions are obtained for a class of model transport coefficients. The resultant dependences for a system with a source have the "scaling" form.

1. INTRODUCTION. FORMULATION OF THE MODEL

Various problems of coagulation dynamics are encountered in solid-state physics. They may include problems of radiation physics concerning clusterization of intrinsic defects, i.e., interstices and vacancies, problems of segregation dynamics, etc. Clusters of various sizes, shapes, and internal structure are formed in the process of growth of defect aggregates, which may be regarded as diffusion-limited. It is rather difficult to study the general case and, therefore, the investigation is often restricted to a spatially homogeneous case when the average concentration of k-particle clusters $c_k(t)$ over the volume is calculated. The classical equations of coagulation dynamics have the following form in this case [1,2]:

$$\frac{dc_k}{dt} = \frac{1}{2}\sum_{i+j=k} K_{ij} c_i c_j - c_k \sum_{j=1}^{\infty} K_{kj} c_j. \quad (1)$$

The transport coefficients K_{ij} for diffusion-limited effects [i] + [j] → [i + j] can be expressed

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