Relativistic study of electrical conduction in disordered systems

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We have reported a relativistic treatment of electrical conduction in a one-dimensional disordered system consisting of a finite number of potential barriers. Our treatment is based on (i) a relativistic generalization of a nonrelativistic approach of Landauer [R. Landauer, Philos. Mag. **21**, 863 (1990)] for electrical resistance of a one-dimensional disordered system and (ii) an averaging procedure due to Erdös and Herndon [P. Erdös and R. C. Herndon, Adv. Phys. **31**, 65 (1983)]. We have carried out exhaustive quantitative analyses of our analytical results and indicated, thereby, the circumstances under which the relativistic effects on electrical resistance in disordered systems may be quite significant.

I. INTRODUCTION

Electronic states and related properties of condensed matter consisting of heavy atoms need to be studied relativistically. Several authors have studied the relativistic features of the electronic properties of condensed matter during the past three decades or so. The aspects which have so far received relativistic (R) treatments are the following: (1) bulk states of three-dimensional (3D) crystalline systems;[1–6] (2) bulk states of one-dimensional (1D) crystalline systems;[7–11] (3) surface states;[12,13] (4) interface states;[14] (5) electronic states of disordered systems.[11,15–21]

The relativistic studies concerning electron motion in disordered systems are recent in comparison with those related to aspects (1)–(4) mentioned above. The works which have appeared so far with regard to relativistic electrons in disordered systems are those mentioned in connection with aspect (5). All these works have treated only the nature of relativistic electronic states in 1D disordered systems. Some of them[11,15–19] have dealt with the exploration of methods while others[20,21] have focused on both methods and the quantitative analysis of the relativistic effects. Now, a worthwhile display of relativistic effects on electron motion in disordered systems can be well provided by relativistic treatment of electrical conduction through such systems. As we indicated earlier, the works Refs. 11 and 15–21 have remained confined only to (relativistic) electronic states in 1D disordered systems without any attention to relativistic effects on electrical conduction in such systems. A relativistic treatment of the phenomenon of electrical conduction in disordered systems is thus very desirable. The purpose of the present paper is to report our work in this direction. It may be noted here that, although several nonrelativistic (NR) works[22–24] have been reported about electrical conduction in disordered systems, we know of no relativistic study to have been reported so far.

For our analysis of relativistic effects on electrical conduction in disordered systems, we have derived the relativistic resistance of a finite 1D disordered system. Our treatment is essentially based on (i) relativistic generalization of Landauer's NR approach[25] toward resistance of a finite 1D disordered system, and (ii) application of an averaging procedure due to Erdös and Herndon.[26] For our treatment, we require some essential features of a 1D Dirac equation and related transfer matrices; these issues are discussed in Sec. II. The aspects related to the model of our study are presented in Sec. III. First, we formulate a generalized model for the treatment of relativistic resistance; then we reduce this model to a special form for the purpose of quantitative analysis. The basic formulas pertaining to relativistic resistance are derived in Sec. IV. The averaged form of relativistic resistance is obtained in Sec. V and the NR forms of the main results of this section are presented in Sec. VI. The numerical analyses pertinent to our important analytical issues are elucidated in Sec. VII. Finally, the results are discussed critically in Sec. VIII; this discussion primarily focuses its attention on (i) exposing the circumstances under which relativistic effects on electrical conduction in disordered systems can be quite significant, (ii) comparison between relativistic resistance of ordered and disordered systems, (iii) indicating the utility of the form of potential chosen for our quantitative analyses, and (iv) discussing the relevance of our results to systems we come across in practice.

II. SOME FEATURES OF 1D DIRAC EQUATIONS AND RELATED TRANSFER MATRICES

A. 1D Dirac equation

The starting point of the relativistic treatment of electron motion in 1D condensed matter is the following time-independent Dirac equation for an electron of mass m moving in a potential $V(x)$:

$$\left[-i\hbar c\sigma_x\frac{d}{dx}+mc^2\sigma_z+V(x)\right]\phi(x)=E_R\phi(x)\ , \quad (1)$$

where σ_x is the component of the Pauli spin matrix

$$\sigma_x=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\ ,$$

σ_z is the z component of the Pauli spin matrix

$$\sigma_z=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\ ,$$

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E_R is the relativistic energy eigenvalue, c is the velocity of light, and ϕ is a two-component spinor

$$\phi=\begin{bmatrix}\phi_1\\ \phi_2\end{bmatrix}.$$

The general solution of Eq. (1) for a constant potential V appears as[7,12,15]

$$\phi=A\begin{bmatrix}1\\ \gamma\end{bmatrix}\exp(i\beta x)+B\begin{bmatrix}1\\ -\gamma\end{bmatrix}\exp(-i\beta x)\ , \tag{2}$$

where

$$\beta^2=\frac{(\varepsilon-V)(\varepsilon-V+2mc^2)}{(\hbar c)^2}\ ,$$

$$\gamma=\frac{\varepsilon-V}{\hbar c\beta}\ ,$$

$$\varepsilon=E_R-mc^2\ .$$

The constants A and B are the amplitudes of spinors moving along the directions of positive and negative x axes, respectively.

B. Relativistic transfer matrix for a single barrier

We consider a potential $V(x)$ which is real, symmetric, and single valued, and has the following properties:

$$V(x)=0 \quad \text{for } x<x_1 \text{ and } x>x_2\ ,$$

$$\neq 0 \quad \text{for } x_1\le x\le x_2\ ,$$

where $-\infty<x_1\le x_2<\infty$. A potential of this kind is called a localized potential. The relativistic transfer matrix W_R is defined as

$$\begin{bmatrix}A_{\rm II}\\ B_{\rm II}\end{bmatrix}=W_R\begin{bmatrix}A_{\rm I}\\ B_{\rm I}\end{bmatrix},$$

where $A_{\rm II}$ and $B_{\rm II}$ are the amplitudes of spinors in the region to the right of x_2, and $A_{\rm I}$ and $B_{\rm I}$ are the amplitudes of spinors in the region to the left of x_1.

Using the time-reversal symmetry and the space-reversal symmetry of the Dirac equation for a symmetric potential, we obtain the following properties of the elements of W_R.

(i) W_R is independent of $A_{\rm I}$, $B_{\rm I}$, $A_{\rm II}$, and $B_{\rm II}$.

(ii) We have

$$W_R(2,2)=[W_R(1,1)]^*\ , \tag{3a}$$

$$W_R(2,1)=[W_R(1,2)]^*\ , \tag{3b}$$

$$\det W_R=1\ . \tag{3c}$$

(iii) With the help of W_R, we can obtain the transfer matrix W_R' in the coordinate system $x'=x-x_0$, as follows:

$$W_R'=D(x_0)W_RD^{-1}(x_0)\ , \tag{4}$$

where

$$D(x_0)=\begin{bmatrix}\exp(i\beta_1x_0) & 0\\ 0 & \exp(-i\beta_1x_0)\end{bmatrix}.$$

(iv) With proper choice of x_0, we can obtain a form M_R for W_R', where M_R has the following properties:

$$M_R(2,2)=[M_R(1,1)]^*\ , \tag{5a}$$

$$M_R(2,1)=[M_R(1,2)]^*\ , \tag{5b}$$

$$\det M_R=1\ , \tag{5c}$$

$$\mathrm{Re}M_R(1,2)=0\ . \tag{5d}$$

M_R is given by (4), with the condition that x_0 is chosen so as to make (5a)–(5d) valid. Thus, we have

$$M_R=D(x_0)W_RD^{-1}(x_0)\ . \tag{6}$$

In general, x_0 is dependent on β_1. However, for symmetric potential, x_0 is independent of β_1 and is the same as the position of the line of symmetry of the nonzero region of $V(x)$. For a symmetric potential, the elements of M_R can be expressed in terms of two independent parameters λ and ν, as follows:

$$M_R(1,1)=(\cosh\lambda)\exp(-i\nu)\ , \tag{7}$$

$$M_R(1,2)=-i\sinh\lambda\ . \tag{8}$$

The properties of W_R and M_R are formally the same as those of the corresponding NR matrices.[26]

C. Relativistic transfer matrix for a rectangular potential barrier

As we shall see later, our relativistic treatment of resistance is concerned with a chain consisting of a finite number of rectangular barrier-type potentials. Consequently, we require some features of a relativistic transfer matrix for this type of potential, shown in Fig. 1. The spinors $\phi_{\rm I}$, $\phi_{\rm II}$, and $\phi_{\rm III}$ in the regions I, II, and III in Fig. 1 can be obtained from (2), with use of relevant forms of γ and β. In order that the relativistic probability density may be continuous, these spinors are required to satisfy the boundary condition given by (9) and (10):

$$\phi_{\rm I}(x_1)=\phi_{\rm II}(x_1)\ , \tag{9}$$

$$\phi_{\rm II}(x_2)=\phi_{\rm III}(x_2)\ . \tag{10}$$

With the help of (9) and (10) we obtain

$$M_R(1,1)=\exp(-i\beta_1b)\left[\cosh(\chi b)+\frac{\gamma_1^2-\alpha^2}{2\gamma_1\alpha}\sinh(\chi b)\right], \tag{11}$$

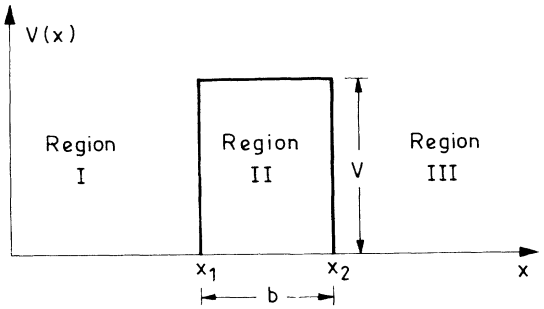

FIG. 1. Model of rectangular potential barrier.

$$M_R(1,2)=-i\frac{\gamma_1^2+\alpha^2}{2\gamma_1\alpha}\sinh(\chi b)\ , \tag{12}$$

where

$$\chi^2=\frac{(V-\varepsilon)(\varepsilon-V+2mc^2)}{(\hbar c)^2}\ ,$$

$$\alpha=\frac{(V-\varepsilon)}{(\hbar c\chi)}\ ,$$

$$\beta_1^2=\frac{\varepsilon(\varepsilon+2mc^2)}{(\hbar c)^2}\ ,$$

$$\gamma_1=\frac{\varepsilon}{(\hbar c\beta_1)}\ .$$

III. THE MODEL

We consider a chain of N lattice points $x_1,x_2,\ldots,x_N$, where $x_1<x_2<\cdots<x_N$. We place N symmetric, nonoverlapping potential barriers $V(x-x_n)$ around x_n. The system, in general, has both shape and position disorder, the latter being only short ranged. We denote the combined distribution function for shape and position by F. F is dependent on the locations x_n and the two parameters λ_n and ν_n for the nth potential barrier; the parameters λ_n and ν_n are defined by (7) and (8). We thus have

$$F=F(x_1,\lambda_1,\nu_1;\ \ldots\ ;x_N,\lambda_N,\nu_N)\ .$$

We now make the following assumptions.

(i) The shape and location of potential barriers are independent. Thus,

$$F(x_1,\lambda_1,\nu_1;\ \ldots\ ;x_N,\lambda_N,\nu_N)$$
$$=F_1(x_1,\ \ldots,\ x_N)F_2(\lambda_1,\nu_1;\ \ldots;\ \lambda_N,\nu_N)\ .$$

(ii) There exists no shape correlation between potentials, so that we have

$$F_2(\lambda_1,\nu_1;\ \ldots\ ;\lambda_N,\nu_N)=h_1(\lambda_1,\nu_1)\cdots h_N(\lambda_N,\nu_N)\ .$$

(iii) The function $h_n(\lambda_n,\nu_n)$ is spatially homogeneous. This means

$$h_n(\lambda_n,\nu_n)=h(\lambda_n,\nu_n);\ n=1,2,\ \ldots\ ,N\ .$$

(iv) The short-range order is such that $(x_{n+1}-x_n)$ is an independent random variable. This gives

$$F_1(x_1,\ \ldots\ ,x_N)=g_2(x_2-x_1)\cdots g_N(x_N-x_{N-1})\ .$$

(v) The space is homogeneous, so that

$$g_n(x_n-x_{n-1})=g(x_n-x_{n-1});\ \ n=1,2,\ \ldots\ ,N\ .$$

We have mentioned above some general features of our model.[26] We shall first carry out our relativistic treatment in terms of these general features. For quantitative analysis, we shall, however, follow additional assumptions.

(a) There is no shape disorder.

(b) The potentials are represented by rectangular barriers of height V and width b.

(c) The position disorder corresponds to a rectangular distribution, $g(l\mu_n)$, as given below:

$$g(l\mu_n)=\frac{1}{2\delta}\ \text{ for }\ -\delta\le(l\mu_n)\le\delta\ , \tag{13}$$

$$=0\ \text{ for }\ |l\mu_n|\ge\delta\ , \tag{14}$$

where δ is the maximum disorder,

$$(l+l\mu_n)=(x_n-x_{n-1})\ ,$$

and l is the mean interpotential distance.

IV. BASIC RELATIVISTIC FORMULA FOR RESISTANCE

Our relativistic treatment of resistance consists of two stages, namely (i) derivation of a formula for relativistic resistance (Q_R) of N potential barriers located at specific positions, and (ii) an ensemble average of Q_R. In this section, we derive the formula for Q_R, while its ensemble average is carried out in Sec. V.

In deriving the formula for Q_R, we follow the NR approach discussed by Erdös and Herndon.[26] To begin, let us consider a beam of electrons incident on the first barrier to the left of the system of N potential barriers. The following equations obviously hold true:

$$n_0=\frac{J_i^R+J_r^R}{ve}\ , \tag{15}$$

$$n_t=\frac{J_t^R}{ve}\ , \tag{16}$$

$$\rho_R=\frac{J_r^R}{J_i^R}\ , \tag{17}$$

$$\tau_R=\frac{J_t^R}{J_i^R}\ , \tag{18}$$

$$\rho_R+\tau_R=1\ , \tag{19}$$

where J_i^R, J_r^R, and J_t^R are the incident, reflected, and transmitted (relativistic) currents, respectively. n_0 is the density of electrons on the left of the system, n_t is the density of electrons on the right of the system, v is the velocity of electrons, e is the electronic charge, ρ_R is the (relativistic) reflectance, and τ_R is the (relativistic) transmittance.

From (15)–(19), we obtain

$$\delta n=(n_t-n_0)=(2\rho_R J_i^R)/ve\ . \tag{20}$$

If the electrons change their energy by $\delta\varepsilon$ while passing through the system, we have

$$\delta\varepsilon=e\,\delta v\ , \tag{21}$$

where δv is the potential difference across the system. Using (20) and (21), we have

$$\delta v=\frac{2\rho_R j_i^R}{ev\dfrac{dn}{d\beta_1}\dfrac{d\beta_1}{d\varepsilon}}\ . \tag{22}$$

Subjecting the spinors ϕ to periodic-boundary condition, we obtain

$$\frac{dn}{d\beta_1}=\frac{1}{\pi} . \tag{23}$$

Combining (22) and (23) and taking note of the form of β_1 given earlier, we obtain the resistance Q_R of the system as follows:

$$Q_R=\frac{\delta V}{J_t^R}=\frac{2\pi\hbar}{e^2}S_R , \tag{24}$$

where

$$S_R=\frac{\rho_R}{\tau_R} . \tag{24a}$$

The factors before S_R are all constants and it is customary to take S_R itself as a measure of the resistance of the system.[25,26]

V. ENSEMBLE-AVERAGED RESISTANCE

The formula for resistance given by (24) corresponds to specific locations of potential barriers. Following the usual practice, we now carry out an ensemble averaging of this formula. The procedure we follow for this purpose is that of Erdös and Herndon;[26] this procedure is quite general in the sense that it accommodates arbitrary distribution of atoms in the disordered system.

We first discuss some features of the relativistic transfer matrix, $W_R^{(N)}$, for N barriers at specific positions. Then we obtain S_R in terms of a particular element of $W_R^{(N)}$. Finally, we carry out an ensemble average of S_R by carrying out an averaging of the element of $W_R^{(N)}$ relevant to S_R. The ensemble-averaged form of S_R, which will be denoted as $\langle S_R \rangle$, is taken to be the ensemble-averaged resistance of the system.

A. Some aspects of $W_R^{(N)}$

$W_R^{(N)}$ is defined as

$$\begin{bmatrix} A_N \\ B_N \end{bmatrix}=W_R^{(N)}\begin{bmatrix} A_0 \\ B_0 \end{bmatrix} . \tag{25}$$

In (25), A_0 and B_0 are the amplitudes of the incident and reflected spinors at the first barrier on the left while A_N and B_N are the corresponding entities after the last (Nth) barrier on the right. We obviously can write

$$W_R^{(N)}=P\prod_{n=1}^{N} W_{Rn} , \tag{26}$$

where W_{Rn} is the transfer matrix for the nth barrier and $(P\prod)$ denotes the ordered product of matrices (W_{Rn}), with n decreasing from left to right.

The elements of W_{Rn} satisfy the properties given by (3a)–(3c). Also, the elements of $W_R^{(N)}$ would satisfy these properties. Hence, we have

$$W_R^{(N)}(2,2)=[W_R^{(N)}(1,1)]^* ,$$

$$W_R^{(N)}(2,1)=[W_R^{(N)}(1,2)]^* ,$$

$$\det(W_R^{(N)})=1 .$$

Further, in view of (6) and (26), we can obtain the matrix $W_R^{(N)}$ as

$$W_R^{(N)}=P\prod_{n=1}^{N} D^{-1}(x_n)M_{Rn}D(x_n) ,$$

where

$$M_{Rn}=D(x_n)W_{Rn}D^{-1}(x_n) ,$$

and x_n is the point of symmetry of the nth barrier.

B. Form of S_R in terms of elements of $W_R^{(N)}$

The defining equation for S_R is (24a). ρ_R and τ_R in this equation can be obtained from (17) and (18), keeping in mind the expression for relativistic current density J^R as given below:

$$J^R=\phi^\dagger\sigma_x\phi .$$

Using Eqs. (24a), (17), (18), and (25), the form of J_R, and the fact that there is no reflected spinor beyond the Nth barrier (i.e., $B_N=0$), we have

$$S_R=|W_R^{(N)}(1,2)|^2 . \tag{27}$$

C. Ensemble average of S_R

The matrix $W_R^{(N)}$ and other matrices relevant to it have all the properties similar to their NR counterparts discussed in Ref. 26. Hence, the ensemble average $\langle S_R \rangle$ of S_R can be written straightforwardly in analogy with the corresponding NR entity (result 7.4.3 in Ref. 26). Specifically, we have

$$\begin{aligned}\langle S_R \rangle=-\tfrac{1}{2}+\tfrac{1}{2}(\det T_R)^{-1}[&(\alpha_{R1})^N T_R(1,1)|T_R(2,2)T_R(3,3)-T_R(2,3)T_R(3,2)| \\ &+(\alpha_{R2})^N T_R(1,2)|T_R(2,3)T_R(3,1)-T_R(2,1)T_R(3,3)| \\ &+(\alpha_{R3})^N T_R(1,3)|T_R(2,1)T_R(3,2)-T_R(2,2)T_R(3,1)|] ,\end{aligned} \tag{28}$$

α_{R1}, α_{R2}, and α_{R3}, and three eigenvalues of the 3×3 matrix G_R. $T_R(1,1)$, etc., are elements of the matrix T_R, which diagonalizes G_R to $\bar{G}_R$, say,

$$\bar{G}_R=T_R^{-1}G_R T_R .$$

The elements of G_R are as given below:

$$G_R(1,1)=|q_R(1,1)|^2+|q_R(1,2)|^2 , \tag{29}$$

$$G_R(1,2)=\sqrt{2}q_R(1,1)[q_R(1,2)]^*C_R U_R=[G_R(1,3)]^* , \tag{30}$$

$$G_R(2,1)=-\sqrt{2}q_R(1,1)[q_R(1,2)]^*=[G_R(3,1)]^* , \quad (31)$$

$$G_R(2,2)=q_R(1,1)q_R(1,1)C_R U_R=[G_R(3,3)]^* , \quad (32)$$

$$G_R(2,3)=-|q_R(1,2)|^2 C_R^* U_R^*=[G_R(3,2)]^* , \quad (33)$$

$$C_R=\exp(2i\beta_1 l) ,$$

$$U_R=\int_{-\infty}^{+\infty} g(l\mu_n)\exp(2i\beta_1 l\mu_n)d(l\mu_n) ,$$

$$q_R(i,j)=\int_{-\infty}^{+\infty} M_{Rn}(i,j)h(\lambda_n,\nu_n)d\lambda_n d\nu_n .$$

The eigenvalues α_{Ri} can be either all real or one real and two others a complex-conjugate pair. Within certain ranges of energy ε, all three eigenvalues α_{Ri} are real; these ranges of energy are called overdamped regions. For these regions, we have, from Eq. (28),

$$\langle S_R\rangle=-\frac{1}{2}+\frac{1}{2}\frac{\omega_1(\alpha_{R1})^N+\omega_2(\alpha_{R2})^N+\omega_3(\alpha_{R3})^N}{\omega_1+\omega_2+\omega_3} , \quad N>1 , \quad (34)$$

where

$$\omega_i=T_R(l,i)\mathrm{Im}\{T_R(2,k)[T_R(2,l)]^*\}$$

(i,k,l) is the cyclic permutation of (1,2,3).

If α_{Ri} is real, and α_{R2} and α_{R3} are a complex-conjugate pair, again from Eq. (28) we get

$$\langle S_R\rangle=-\frac{1}{2}+\frac{1}{2}\frac{(\alpha_{R1})^N+\xi_{R2}|\alpha_{R2}|^2\cos(N\xi_{R1}+\xi_{R3})}{1+\xi_{R2}\cos(\xi_{R3})} , \quad N>1 , \quad (35)$$

where

$$\alpha_{R2}=|\alpha_{R2}|\exp(i\xi_{R1}) ,$$

$$\frac{T_R(1,2)\{[T_R(2,1)]^*[T_R(3,2)]^*-T_R(2,1)[T_R(2,2)]^*\}}{T_R(1,1)[|T_R(2,2)|^2-|T_R(3,2)|^2]}=\frac{1}{2}\xi_{R2}\exp(i\xi_{R3}) .$$

ξ_{R1}, ξ_{R2}, and ξ_{R3} are all real. The regions of ε for which Eq. (35) is valid are called underdamped regions.

The results expressed by (28), (34), and (35) all correspond to relativistic resistance of disordered systems under various conditions. It is worthwhile to compare $\langle S_R\rangle$ for disordered systems with the corresponding entity (S_R^0) for periodic systems.

With the help of (35) we have the following form of S_R^0 for underdamped regions:

$$S_R^0=-\frac{1}{2}+\frac{1}{2}\frac{1+\xi_{R2}\cos(N\xi_{R1}+\xi_{R3})}{1+\xi_{R2}\cos(\xi_{R3})}, \quad N>1 . \quad (36)$$

For overdamped regions we have, from Eq. (34),

$$S_R^0=-\frac{1}{2}+\frac{1}{2}\frac{\omega_1+\omega_2(\alpha_{R2})^N+\omega_3(\alpha_{R3})^N}{\omega_1+\omega_2+\omega_3}, \quad N>1 . \quad (37)$$

VI. ENSEMBLE-AVERAGED RESISTANCE FOR THE NR CASE

For comparison between $\langle S_R\rangle$ and the corresponding entity, denoted by $\langle S_{\mathrm{NR}}\rangle$, for the NR case, we require the form of $\langle S_{\mathrm{NR}}\rangle$. The general form of S_{NR} was reported by Erdös and Herndon.[26] The $\langle S_{\mathrm{NR}}\rangle$ for our model is obtainable from this general form by incorporating in it the various entities relevant to our model. Specifically, we have $\langle S_{\mathrm{NR}}\rangle$ as given below:

$$\begin{aligned}\langle S_{\mathrm{NR}}\rangle=&-\tfrac{1}{2}+\tfrac{1}{2}\det(T_{\mathrm{NR}})^{-1}[(\alpha_{\mathrm{NR1}})^N T_{\mathrm{NR}}(1,1)|T_{\mathrm{NR}}(2,2)T_{\mathrm{NR}}(3,3)-T_{\mathrm{NR}}(2,3)T_{\mathrm{NR}}(3,2)|\\&+(\alpha_{\mathrm{NR2}})^N T_{\mathrm{NR}}(1,2)|T_{\mathrm{NR}}(2,3)T_{\mathrm{NR}}(3,1)-T_{\mathrm{NR}}(2,1)T_{\mathrm{NR}}(3,3)|\\&+(\alpha_{\mathrm{NR3}})^N T_{\mathrm{NR}}(1,3)|T_{\mathrm{NR}}(2,1)T_{\mathrm{NR}}(3,2)-T_{\mathrm{NR}}(2,2)T_{\mathrm{NR}}(3,1)|], \quad N>1 , \quad (38)\end{aligned}$$

where

$$G_{\mathrm{NR}}(1,1)=|q_{\mathrm{NR}}(1,1)|^2+|q_{\mathrm{NR}}(1,2)|^2 , \quad (39)$$

$$G_{\mathrm{NR}}(1,2)=\sqrt{2}q_{\mathrm{NR}}(1,2)[q_{\mathrm{NR}}(1,2)]^* C_{\mathrm{NR}} U_{\mathrm{NR}}=[G_{\mathrm{NR}}(1,3)]^* , \quad (40)$$

$$G_{\mathrm{NR}}(2,1)=-\sqrt{2}q_{\mathrm{NR}}(1,1)[q_{\mathrm{NR}}(1,2)]^*=[G_{\mathrm{NR}}(3,1)]^* , \quad (41)$$

$$G_{\mathrm{NR}}(2,2)=q_{\mathrm{NR}}(1,1)q_{\mathrm{NR}}(1,1)C_{\mathrm{NR}} U_{\mathrm{NR}}=[G_{\mathrm{NR}}(3,3)]^* , \quad (42)$$

$$G_{\mathrm{NR}}(2,3)=-|q_{\mathrm{NR}}(1,2)|^2 C_{\mathrm{NR}}^* U_{\mathrm{NR}}^*=[G_{\mathrm{NR}}(3,2)]^* , \quad (43)$$

$$C_{\mathrm{NR}}=\exp(2ik_1 l) ,$$

$$U_{\mathrm{NR}}=\int_{-\infty}^{+\infty} d(l\mu_n)\exp(2ik_1 l\mu_n)g(l\mu_n) ,$$

$$q_{\mathrm{NR}}(i,j)=\int_{-\infty}^{+\infty} M_{\mathrm{NR}}(i,j)h(\lambda_n,\nu_n)d\lambda_n d\nu_n ,$$

$$k_1^2=\frac{2m\varepsilon}{\hbar^2} .$$

α_{NR1}, α_{NR2}, and α_{NR3} are the eigenvalues of G_{NR}. T_{NR} is the matrix that transforms G_{NR} to the diagonal form $\overline{G_{\mathrm{NR}}}$:

$$\overline{G_{\mathrm{NR}}}=T_{\mathrm{NR}}^{-1}G_{\mathrm{NR}}T_{\mathrm{NR}} .$$

The form of M_{NR} for the rectangular barrier-type potential appears as[27]

$$M_{\rm NR}(1,1)=\exp(-ik_1b)\left[\frac{k_1^2-k_2^2}{2k_1k_2}\sinh(k_2b)+\cosh(k_2b)\right]=[M_{\rm NR}(2,2)]^*\ ,$$

$$M_{\rm NR}(1,2)=-i\frac{k_1^2+k_2^2}{2k_1k_2}\sinh(k_2b)=[M_{\rm NR}(2,1)]^*\ ,$$

where

$$k_2^2=\frac{2m}{\hbar^2}(V-\varepsilon)\ .$$

The forms of $\langle S_{\rm NR}\rangle$ for overdamped and underdamped regions are given, respectively, by (44) and (45):

$$\langle S_{\rm NR}\rangle=-\frac{1}{2}+\frac{1}{2}\frac{\sigma_1(\alpha_{\rm NR1})^N+\sigma_2(\alpha_{\rm NR_2})^N+\sigma_3(\alpha_{\rm NR3})^N}{(\sigma_1+\sigma_2+\sigma_3)}\ , \tag{44}$$

$$\langle S_{\rm NR}\rangle=-\frac{1}{2}+\frac{1}{2}\frac{(\alpha_{\rm NR1})^N+\xi_{\rm NR2}(\alpha_{\rm NR2})^N\cos(N\xi_{\rm NR1}+\xi_{\rm NR3})}{1+\xi_{\rm NR2}\cos(\xi_{\rm NR3})}\ , \tag{45}$$

where

$$\sigma_i=T_{\rm NR}(1,i)\,{\rm Im}[T_{\rm NR}(2,k)T_{\rm NR}^*(2,l)]\ ,$$

(i,k,l) is the cyclic permutation of (1,2,3),

$$\alpha_{\rm NR2}=|\alpha_{\rm NR2}|\exp(i\xi_{\rm NR1})\ ,$$

and

$$\frac{T_{\rm NR}(1,2)\{[T_{\rm NR}(2,1)]^*[T_{\rm NR}(3,2)]^*-T_{\rm NR}(2,1)[T_{\rm NR}(2,2)]^*\}}{T_{\rm NR}(1,1)[|T_{\rm NR}(2,2)|^2-|T_{\rm NR}(3,2)|^2]}=\tfrac{1}{2}\xi_{\rm NR2}\exp(i\xi_{\rm NR3})\ .$$

VII. NUMERICAL ANALYSES

Our numerical analyses are pertinent to elucidating the following aspects: (A) relative features of $\langle S_R\rangle$ and S_R^0, (B) general difference between $\langle S_R\rangle$ and $\langle S_{\rm NR}\rangle$, and (C) quantitative impacts of various parameters on the difference between $\langle S_R\rangle$ and $\langle S_{\rm NR}\rangle$.

There are essentially three main stages of our numerical calculations.

(i) *Finding G_R and $G_{\rm NR}$.* We can find G_R from (29)–(33) and $G_{\rm NR}$ from (39)–(43).

(ii) *Finding the eigenvalues α_R and $\alpha_{\rm NR}$.* α_R and $\alpha_{\rm NR}$ are obtained by numerically solving the characteristic equations (46a) and (46b), respectively.

$$|G_R-\alpha_R I|=0\ , \tag{46a}$$

$$|G_{\rm NR}-\alpha_{\rm NR}I|=0\ . \tag{46b}$$

(iii) *Finding $\langle S_R\rangle$, $\langle S_{\rm NR}\rangle$, and S_R^0.* With the help of various entities under (i) and (ii), we obtain $\langle S_R\rangle$ from (34) and (35), for overdamped and underdamped regions, respectively. To get $\langle S_{\rm NR}\rangle$, we use (44) and (45) corresponding, respectively, to overdamped and underdamped regions. Finally, S_R^0 is computed from (36) and (37) for underdamped and overdamped regions, respectively.

Throughout our numerical analyses, we have made use of (13) and (14) for $g(l\mu_n)$ and the two assumptions [(a) and (b)] preceding them. Our results are shown in Tables I and II and the graphs of Figs. 2–6. The values we have adopted for various parameters are shown in the tables, as well as in the graphs and their captions; these values are close to the ones employed previously by many authors.[7,13]

VIII. RESULTS AND DISCUSSION

The graphs and tables throw light on all three aspects (A), (B), and (C), mentioned in the following section.

(A) *Relative features of $\langle S_R\rangle$ and S_R^0.* $\langle S_R\rangle$ and S_R^0 for underdamped and overdamped regions are shown in the graphs of Figs. 2 and 3, respectively. Looking at the graphs in Fig. 2, we see that, for underdamped regions, S_R^0 oscillates with N; these oscillations are due to the presence of oscillatory terms in S_R^0. On the other hand, $\langle S_R\rangle$ for underdamped regions oscillates with N only for low values of N, the amplitudes of oscillations diminishing with increase of N and increasing almost exponentially with N for high values of N.

The solution of (46a) leads to the following criterion in order for ε to lie in the underdamped regions:

$$-1<t_R<1\ , \tag{47}$$

where

$$t_R=\cosh(\chi b)\cos[\beta_1(l-b)]+\left[\frac{\gamma_1^2-\alpha^2}{2\gamma_1\alpha}\right]\sinh(\chi b)\sin[\beta_1(l-b)]\ .$$

TABLE I. Shown in this table are results that correspond to the following values of various parameters: $l=5\times10^{-10}$ m, $\delta=5\times10^{-11}$ m, $N=500$. These results are concerned with the difference between $\langle S_{NR}\rangle$ and $\langle S_R\rangle$ for various energies.

V (eV)	b (m)	E or ε (eV)	$\langle S_{NR}\rangle$	$\langle S_R\rangle$	Δ
30	1×10^{-12}	10	0.7872×10^{-1}	0.7873×10^{-1}	0.1783×10^{-2}
		15	0.2978	0.2977	-0.2143×10^{-1}
		20	0.9331×10^{-1}	0.9331×10^{-1}	0.7836×10^{-2}
30	5×10^{-12}	10	0.1705×10^{2}	0.1706×10^{2}	0.3291×10^{-2}
		15	0.5740×10^{6}	0.5727×10^{6}	-0.2396
		20	0.2990×10^{2}	0.2991×10^{2}	0.2500×10^{-1}
30	10×10^{-12}	10	0.7321×10^{6}	0.7321×10^{6}	0.5501×10^{-4}
		15	0.2787×10^{29}	0.2762×10^{29}	-0.9026
		20	0.3571×10^{7}	0.3574×10^{7}	0.7118×10^{-1}

Criterion (47) corresponds to allowed regions of an ordered system with potential barriers of width b and periodicity l. Erdös and Herndon[26] reported earlier the NR criterion for underdamped regions for an ordered system with δ-function potentials; the inequalities in (47) correspond to a generalization of this criterion in two respects, namely, (i) they are relativistic and (ii) they are involved with (rectangular) barrier-type potentials.

The minimum value of S_R^0 is seen to be zero or nearly zero for certain N values. These N values correspond to total transmission. From (36), we can obtain the following criterion for total transmission:

$$\xi_{R1}=\left[\frac{2\pi}{N}\right](\text{integer});\quad N>1\ .$$

Coming to the graphs of Fig. 3, we note the following features of $\langle S_R\rangle$ and S_R^0 for overdamped regions.

(i) Both $\langle S_R\rangle$ and S_R^0 increase with N, nearly exponentially.

(ii) $\langle S_R\rangle$ is generally higher than S_R^0.

(iii) $\langle S_R\rangle$ increases quite substantially with increase of δ, the disorder parameter.

(iv) ε for S_R^0 in the overdamped region falls within the forbidden region of an ordered system with potential barriers of width b and periodicity l, the criterion relevant to the case being

$$|t_R|>1\ .$$

(B) *General difference between* $\langle S_R\rangle$ *and* $\langle S_{NR}\rangle$. The general differences between $\langle S_R\rangle$ and $\langle S_{NR}\rangle$ for underdamped regions are shown in the graphs of Figs. 4 and 5, while the corresponding general differences for overdamped regions are shown in the graphs of Fig. 6.

Looking at Fig. 5, we see that the difference between $\langle S_R\rangle$ and $\langle S_{NR}\rangle$, manifested through Δ, oscillates for underdamped regions up to some critical value (N_c) of N; beyond N_c, the difference between $\langle S_R\rangle$ and $\langle S_{NR}\rangle$ assumes a constant value. With increase of δ, the value of N_c slightly decreases, and the amplitudes of oscillations increase noticeably.

The graphs in Fig. 6 show the following features for overdamped regions: (i) Δ has no oscillations with N; (ii) $|\Delta|$ shows a minimum for some value (N_m) of N; (iii) with increase of δ, Δ increases; (iv) with increase of δ, N_m slightly decreases.

(C) *Quantitative effects of various parameters on* $\langle S_R\rangle$ *and* $\langle S_{NR}\rangle$. In order to demonstrate the relative quantitative effects of various parameters on $\langle S_R\rangle$ and $\langle S_{NR}\rangle$ more clearly than the graphs in Figs. 2–6 can do, we have computed Tables I and II. The results in these

TABLE II. Shown in this table are results that correspond to the following values of various parameters: $l=5\times10^{-10}$ m, $\delta=5\times10^{-11}$ m, $N=500$. These results are similar to those of Table I for a different value of V.

V (eV)	b (m)	ε or E (eV)	$\langle S_{NR}\rangle$	$\langle S_R\rangle$	Δ
40	1×10^{-12}	15	0.6616	0.6615	-0.2543×10^{-1}
		20	0.1770	0.1771	0.8230
		30	0.1598	0.1591	-0.2321×10^{-2}
40	5×10^{-12}	15	0.1668×10^{12}	0.1661×10^{12}	-0.4385
		20	0.6692×10^{3}	0.6695×10^{3}	0.3954×10^{-1}
		30	0.5375×10^{3}	0.5373×10^{3}	-0.2235×10^{-1}
40	10×10^{-12}	15	0.3872×10^{53}	0.3826×10^{53}	-0.1175×10^{1}
		20	0.4591×10^{12}	0.4596×10^{12}	0.9769×10^{-1}
		30	0.8305×10^{12}	0.8294×10^{12}	-0.1287

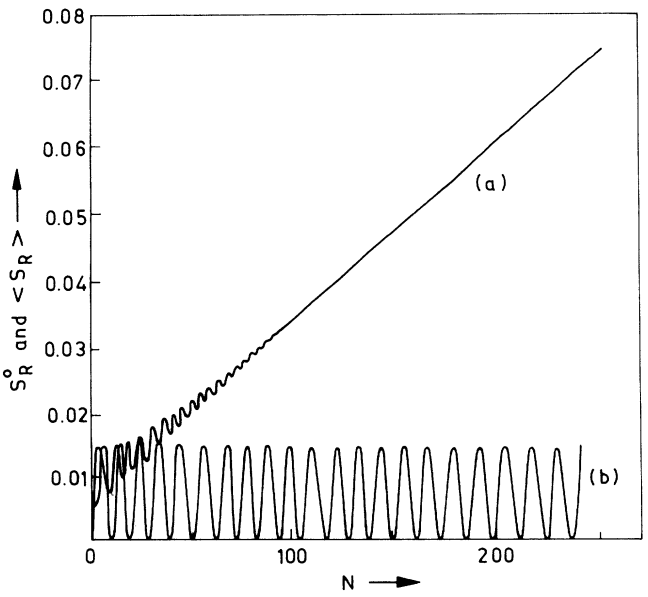

FIG. 2. Variation of S_R^0 and $\langle S_R \rangle$ with N in the underdamped region. (a) Corresponds to $\langle S_R \rangle$ with $\delta = 2.5 \times 10^{-11}$ m; (b) refers to S_R^0. For both (a) and (b), other parameters are as follows: $l = 1.0 \times 10^{-10}$ m; $b = 1.0 \times 10^{-11}$ m; $\varepsilon = 10$ eV; $V = 50$ eV.

tables indicate the following features.

(i) Dependence of $\langle S_R \rangle$ and $\langle S_{NR} \rangle$ on ε: Both $\langle S_R \rangle$ and $\langle S_{NR} \rangle$ are seen to show oscillations generally with ε.

(ii) Effect of b: Both $\langle S_R \rangle$ and $\langle S_{NR} \rangle$ increase rapidly with b. The magnitude of Δ also increases with b. In conformity with Figs. 4 and 5, Δ, however, may be positive or negative; this observation indicates that $\langle S_R \rangle$ may be larger or smaller than $\langle S_{NR} \rangle$.

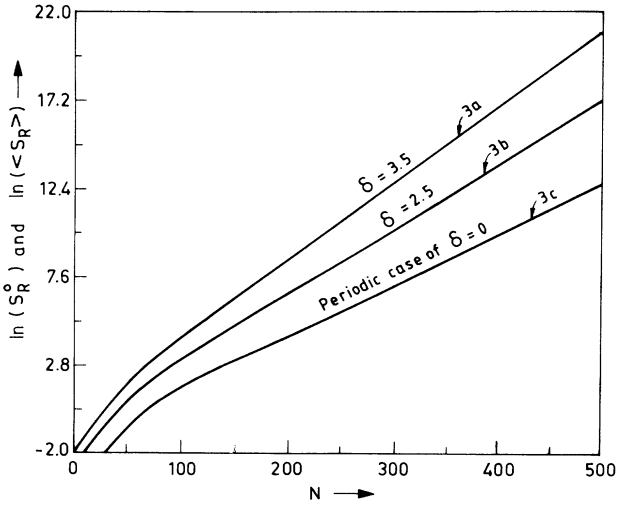

FIG. 3. Variation of S_R^0 and $\langle S_R \rangle$ with N in the overdamped region. (a) and (b) correspond to $\langle S_R \rangle$, and (c) corresponds to S_R^0, which is concerned with the periodic case. For all three graphs, the values of other parameters are the same as those in Fig. 2.

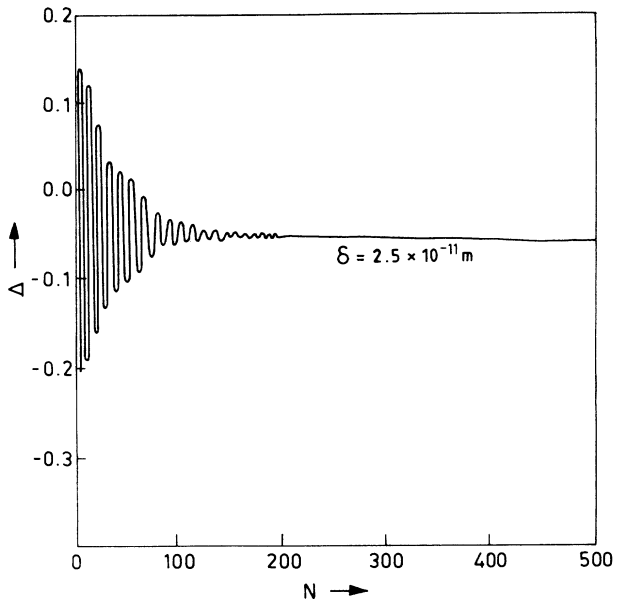

FIG. 4. Variation of Δ with N for the underdamped region. The values of l, b, V, and ε are the same as those in Figs. 2 and 3.

(iii) Effect of V: Both $\langle S_R \rangle$ and $\langle S_{NR} \rangle$ increase significantly with V. The magnitude of Δ also increases with V; Δ may be positive or negative, indicating again that $\langle S_R \rangle$ may be larger or smaller than $\langle S_{NR} \rangle$.

To end the paper, we would like to make the following comments.

(a) The quantitative results of Erdös and Herndon[26] were obtained for δ-function potentials. In our relativistic, as well as associated nonrelativistic, treatments, we have considered rectangular barrier-type potentials,

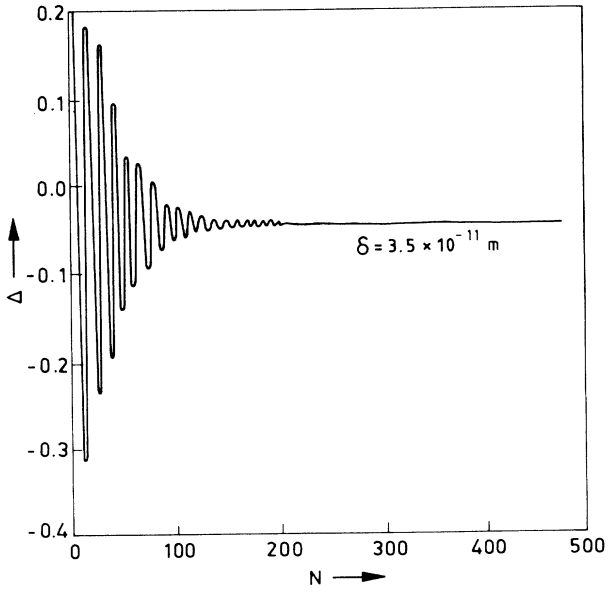

FIG. 5. Variation of Δ with N for a higher value of δ than that in Fig. 4. Other parameters are the same as those in Figs. 2–4.

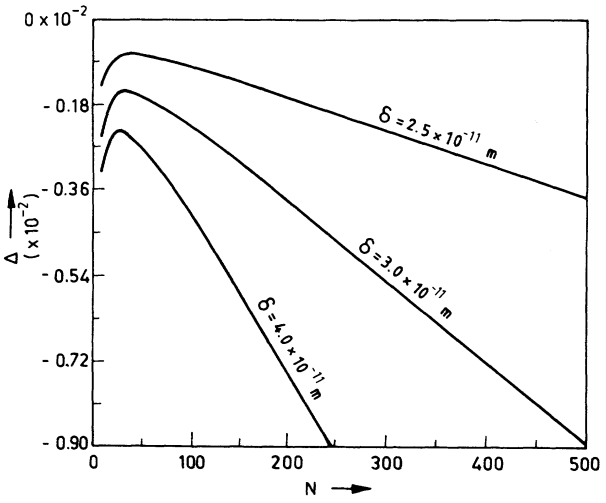

FIG. 6. Variation of Δ with N for overdamped regions. The values of δ are shown alongside the graphs and other parameters are the same as those in Figs. 2–5.

which are more realistic than δ-function potentials[28] and are being used in recent times.[29] Hence, our results for both $\langle S_R \rangle$ and $\langle S_{NR} \rangle$ are likely to conform more to realistic systems than the NR results of Erdös and Herndon[26] or the form of $\langle S_R \rangle$ with δ-function potentials.

(b) Finite disordered systems like the model we have treated are close to "thin films." Hence, our results are likely to be of importance in regard to the properties of thin films.

(c) The magnitudes of Δ shown in Tables I and II are generally comparable to, and sometimes higher than, the relativistic impacts on aspects like band structures[7] and surface states.[13] Hence, the study of relativistic impacts on electrical conduction in disordered systems deserves serious attention.

(d) The model we have treated is essentially a finite disordered system and this kind of model is of considerable importance in regard to electrical conduction in disordered systems.[30]

(e) The present study is an effort towards exploration of relativistic effects on electrical conduction in disordered systems. The primary objective behind this study is to bring forth some results which will pave the way for studies about the problem that are more realistic than ours.

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