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Relativistic impacts on tunnelling through multi-barrier systems

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Abstract. We have studied relativistic effects on the tunnelling of electrons through a multi-barrier system (MBS) consisting of rectangular barrier potentials, by deriving, for the purpose, relativistic formulae for the transmission coefficient and associated relativistic conditions for resonant tunnelling. Among other things, we have discussed critically the quantitative extents of relativistic impacts on tunnelling through MBSs, especially in the context of their measurability.

1. Introduction

During many past decades, several workers have carried out relativistic studies of electron motion in one-dimensional (1D) condensed matter in the context of

(i) bulk states of crystalline systems [1–3],
(ii) bulk states and related properties of disordered systems [4–9] and
(iii) surface states [10, 11].

These studies have provided much information on the relativistic impacts of the relevant issues, which is very valuable from qualitative as well as quantitative viewpoints. Now, studies of tunnelling through multi-barrier systems (MBSs), especially in the context of resonant tunnelling, constitute an important facet of condensed-matter physics, theoretically [12–15] as well as experimentally [16, 17]. So far, the studies of tunnelling through MBSs have been carried out on a non-relativistic (NR) footing. In view of the fact that relativistic studies of aspects such as (i)–(iii) have proved quite useful, investigation of relativistic impacts on tunnelling through MBSs seems worthwhile, and the purpose of this article is to report an effort in this direction.

The models treated by us consist of an arbitrary number of rectangular-barrier-type potentials as shown in figure 1 and the δ-function equivalent of the model in figure 1. In the context of these models, we have derived

(I) the relativistic transmission coefficient (RTC) and the associated conditions for resonant tunnelling, making use of some aspects (section 2) of the 1D Dirac equation and the relativistic transfer matrix,
(II) the shape of the relativistic transmission spectrum (section 3) and
(III) the NR counterparts (section 4) of aspects (I) and (II).

To explore the quantitative extents of relativistic impacts on tunnelling through MBSs, we have carried out (section 5) a numerical analysis in regard to the essential features of relativistic and NR tunnelling through them. Finally, we have discussed (section 5) critically our findings in respect of relativistic impacts on tunnelling through MBSs.

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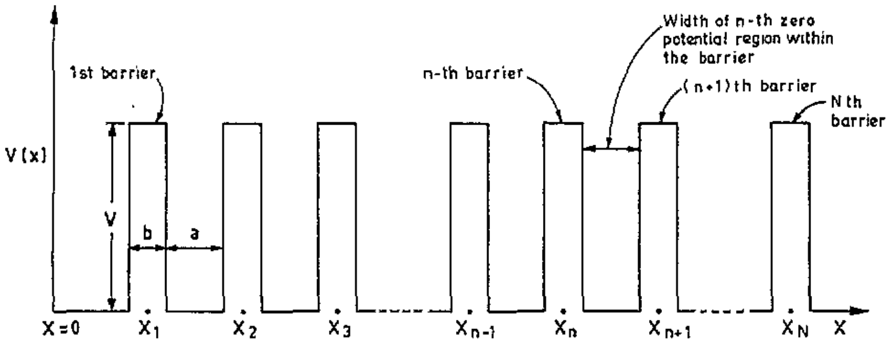

Figure 1. Model of an N-barrier system.

2. Some aspects of the 1D Dirac equation and relativistic transfer matrix

The relativistic treatment of the tunnelling of electrons (with a rest mass m) through a system such as that in figure 1 requires the two-component spinor solutions ψ to the 1D Dirac equation for a constant potential V. Assuming that the electron moves along the x-axis, one obtains ψ as [18]

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

where

$$\beta^2 = (\epsilon - V)(\epsilon - V + 2mc^2)/\hbar^2c^2 \qquad \epsilon = E_{\mathrm{R}} - mc^2 \qquad \gamma = (\epsilon - V)/\hbar c\beta.$$

E_{R} is the relativistic eigenvalue of energy, and A and B are arbitrary constants. In the light of (1), the spinor ψ_n in the nth zero-potential region of figure 1 can be written as

$$\psi_n = A_n\begin{bmatrix}1\\ \gamma_1\end{bmatrix}\exp(\mathrm{i}\beta_1 x) + B_n\begin{bmatrix}1\\ -\gamma_1\end{bmatrix}\exp(-\mathrm{i}\beta_1 x) \qquad n = 0, 1, \ldots, N \tag{2}$$

where

$$\beta_1^2 = \epsilon(\epsilon + 2mc^2)/\hbar^2c^2 \qquad \gamma_1 = \epsilon/\hbar c\beta_1.$$

The region for $n = 0$ is the zero-potential region to the left of the first barrier and the region for $n = N$ corresponds to the zero-potential region to the right of the Nth barrier. We now define the (2×2) transfer matrix $\mathbf{W}_N^{\mathrm{R}}$ as

$$\begin{bmatrix}A_N\\ B_N\end{bmatrix} = \mathbf{W}_N^{\mathrm{R}}\begin{bmatrix}A_0\\ B_0\end{bmatrix}. \tag{3}$$

It can be shown [9] that

$$\mathbf{W}_N^{\mathrm{R}} = \mathbf{M}_N^{\mathrm{R}} \ldots \mathbf{M}_1^{\mathrm{R}} : \tag{4}$$

$$\mathbf{M}_n^{\mathrm{R}} = (\mathbf{F}_{\mathrm{R}}^*)^n \mathbf{M}_{\mathrm{R}} (\mathbf{F}_{\mathrm{R}})^n \tag{5}$$

$$\mathbf{F}_{\mathrm{R}} = \begin{bmatrix}\exp(\mathrm{i}\beta_1 f) & 0\\ 0 & \exp(-\mathrm{i}\beta_1 f)\end{bmatrix} \qquad f = a + b. \tag{6}$$

$M_{\rm R}$ is the relativistic transfer matrix for a single barrier with its origin on the line of its symmetry, and it can be obtained as [9, 19]

$$M_{\rm R}(11) = \exp(-\mathrm{i}\beta_1 b)\,[\cosh(\eta b) + [\mathrm{i}(\gamma_1^2 - \sigma^2)/2\gamma_1\sigma]\,\sinh(\eta b) = [M_{\rm R}(21)]^* \tag{7}$$

$$M_{\rm R}(12) = -\mathrm{i}[(\gamma_1^2 + \sigma^2)/2\gamma_1\sigma]\sinh(\eta b) = [M_{\rm R}(21)]^* \tag{8}$$

$$\eta^2 = (V - \epsilon)(\epsilon - V + 2mc^2)/(\hbar c)^2 \qquad \epsilon < V < \epsilon + 2mc^2 \tag{9}$$

$$\sigma = (V - \epsilon)/\hbar c\eta.$$

With the help of (4) and (5), we obtain

$$W_N^{\rm R}(11) = \{[\exp(-\mathrm{i}N\beta_1 f)]/(t_2 - t_1)\}\{t_1^N[t_2 - G_{\rm R}(11)] - t_2^N[t_1 - G_{\rm R}(11)]\} = [W_N^{\rm R}(22)]^* \tag{10}$$

$$W_N^{\rm R}(12) = \{[\exp(-\mathrm{i}N\beta_1 f)]/(t_2 - t_1)\}(t_2^N - t_1^N)G_{\rm R}(12) = [W_N^{\rm R}(21)]^* \tag{11}$$

$$\det W_N^{\rm R} = 1\ldots \tag{12}$$

$$\mathbf{G}_{\rm R} = \mathbf{M}_{\rm R}\mathbf{F}_{\rm R}. \tag{13}$$

t_1 and t_2 are eigenvalues of $\mathbf{G}_{\rm R}$ given by

$$t_1 = 1/t_2 = \exp(\mathrm{i}\theta_{\rm R}) \qquad |d_{\rm R}| < 2 \tag{14}$$

$$t_1 = (1/t_2)\exp(\phi_{\rm R}) \qquad |d_{\rm R}| \geqslant 2 \tag{15}$$

$$d_{\rm R} = \mathrm{Tr}(\mathbf{G}_R) \tag{16}$$

$$\cos\theta_{\rm R} = \tfrac{1}{2}d_{\rm R} \qquad |d_{\rm R}| < 2 \tag{17}$$

$$\cosh\phi_{\rm R} = \tfrac{1}{2}d_{\rm R} \qquad |d_{\rm R}| \geqslant 2. \tag{18}$$

3. Relativistic treatment of tunnelling

3.1. Formulae for the relativistic transmission coefficient

To derive the formulae for the RTC, we assume the electrons to be incident at the left-hand end of the chain of barriers in figure 1 along the positive direction of the x axis and to be transmitted beyond the right-hand end of the chain. The RTC $T_N^{\rm R}$ is defined as the ratio of the transmitted relativistic current density $J_{\rm t}^{\rm R}$ to the incident relativistic current density $J_{\rm i}^{\rm R}$, which correspond respectively to the A_n- and B_n-dependent parts of (2). If we make use of these spinors, the formula $C\psi^+\sigma_x\psi$ for the relativistic current density, the fact that there is no reflected current beyond the Nth barrier (i.e. $B_N = 0$), and equations (10), (14) and (15), we obtain the following two forms $T_{N\rm I}^{\rm R}$ and $T_{N\rm II}^{\rm R}$ of $T_N^{\rm R}$:

$$T_{N\rm I}^{\rm R} = 1/\{1 + |M_{\rm R}(12)|^2[U_r(\cos\theta_{\rm R})]^2\} \qquad |d_{\rm R}| < 2 \tag{19}$$

$$T_{N\rm II}^{\rm R} = 1/\{1 + |M_{\rm R}(12)|^2[h_r(\phi_{\rm R})]^2\} \qquad |d_{\rm R}| \geqslant 2 \tag{20}$$

$$U_r(\cos\theta_{\rm R}) = \sin[(r+1)\theta_{\rm R}]/\sin\theta_{\rm R} \qquad r = N - 1 \tag{21}$$

$$h_r(\phi_{\rm R}) = \sinh[(r+1)\phi_{\rm R}]/\sinh\phi_{\rm R} \qquad r = N - 1 \tag{22}$$

and $U_r(\cos\theta_{\rm R})$ is the well known Chebyshev polynomial of the second kind [20].

3.2. Relativistic condition for resonant tunnelling

As is well known, the transmission coefficient across any system of potential barriers becomes unity when resonant tunnelling occurs. We can see that relativistic resonant tunnelling cannot occur at all for $|d_R| \geqslant 2$, a condition which is related to $T^R_{N\text{II}}$; this is because the entity $|M_R(12)|^2[h_r(\phi_R)]^2$ in the denominator of $T^R_{N\text{II}}$ is always greater than zero. Relativistic resonant tunnelling can occur only for $T^R_{N\text{I}}$ which corresponds to $|d_R| < 2$. The condition for resonant tunnelling due to $T_{N\text{I}}$ appears as

$$U_r(\cos\theta_R) = 0. \tag{23}$$

The energies satisfying (23) are those which correspond to $|d_R| < 2$. This condition corresponds to energies in the allowed bands of an infinite crystal with rectangular-barrier-type potentials, having $a+b$ as the periodicity, while the condition $|d_R| \geqslant 2$ corresponds to energies in the forbidden regions of the relativistic band structure of such a system [18, 21]. Hence, the energies for which relativistic resonant tunnelling can occur for the model in figure 1 must necessarily lie within allowed regions of relativistic band structure of the infinite crystal just mentioned.

3.3. Relativistic transmission coefficient for the δ-function equivalent of the model in figure 1

It seems worthwhile to compare the RTC of the model in figure 1 with that for its δ-function equivalent, which is obtained by setting $V \to \infty$, $b \to 0$, such that Vb remains finite and equals p (say). For this purpose, we need the values $T^{R0}_{N\text{I}}$ and $T^{R0}_{N\text{II}}$ assumed by $T^R_{N\text{I}}$ and $T^R_{N\text{II}}$, respectively, under the just-mentioned limits with regard to V and b. Explicitly, we have

$$T^{R0}_{N\text{I}} = 1/\{1 + |M_{R0}(12)|^2[U_r(\cos\theta_{R0})]^2\} \tag{24}$$

$$T^{R0}_{N\text{II}} = 1/\{1 + |M_{R0}(12)|^2[h_r(\phi_{R0})]^2\} \tag{25}$$

$$\cos\theta_{R0} = \tfrac{1}{2}d_{R0} \qquad |d_{R0}| < 2 \tag{26}$$

$$\cos(h\phi_{R0}) = \tfrac{1}{2}d_{R0} \qquad |d_{R0}| \geqslant 2 \tag{27}$$

$$M_{R0}(12) = \delta\text{-function limit of } M_R(12) = -\tfrac{1}{2}\,\mathrm{i}[(1-\gamma_1^2)/\gamma_1]\sin(p/\hbar c) \tag{28}$$

$$d_{R0} = \delta\text{-function limit of } d_R = 2\cos(\beta_1 a)\cos(p/hc) + \{(1+\gamma_1^2)/\gamma_1\}\sin(\beta_1 a)\sin(p/\hbar c). \tag{29}$$

3.4. Shape of the relativistic transmission spectrum

As we shall see later, $T^R_{N\text{I}}$ falls sharply with increasing ϵ around the energies ϵ_s at which resonant tunnelling occurs. Using this fact, we obtain [14] the RTC $T^{Rs}_{N\text{I}}$ around ϵ_s as given below:

$$T^{Rs}_{N\text{I}} = 1/\{1 + [(\epsilon - \epsilon_s)/\Delta\epsilon_s]^2\} \tag{30}$$

$$\Delta\epsilon_s = \{|M_R(12)|^2(\mathrm{d}/\mathrm{d}\,d_R)[U_r(\cos\theta_R)](\mathrm{d}/\mathrm{d}\epsilon)(d_R)\}_{\epsilon=\epsilon_s}. \tag{31}$$

As can be seen from (30), the shape of the relativistic transmission spectrum is Lorentzian near the energies ϵ_s with $2\Delta\epsilon_s$ as the full width of $T^{Rs}_{N\text{I}}$ at ϵ_s.

4. Non-relativistic tunnelling

The results for tunnelling of NR electrons through our models can be obtained, without using an *ab-initio* treatment, by subjecting our relativistic results to the condition that the velocity c of light goes to infinity. The NR limits $T_{N\mathrm{I}}$ and $T_{N\mathrm{II}}$, of $T^{\mathrm{R}}_{N\mathrm{I}}$ and $T^{\mathrm{R}}_{N\mathrm{II}}$, respectively, are given by

$$T_{N\mathrm{I}} = 1/\{1 + |M(12)|^2[U_r(\cos\theta)]^2\} \tag{32}$$

$$T_{N\mathrm{II}} = 1/\{1 + |M(12)|^2[h_r(\phi)]^2\} \tag{33}$$

$$\cos\theta = \tfrac{1}{2}d \qquad |d| < 2$$

$$\cosh\phi = \tfrac{1}{2}d \qquad |d| \geqslant 2.$$

$$d = \text{NR limit of } d_{\mathrm{R}} = 2\{\cosh(k_2b)\cos(k_1a) + [(k_2^2 - k_1^2)/2k_1k_2]\sinh(k_2b)\sin(k_1a)\} \tag{34}$$

$$M(12) = \text{NR limit of } M_{\mathrm{R}}(12) = -\mathrm{i}[(k_1^2 + k_2^2)/2k_1k_2]/\sinh(k_2b) \tag{35}$$

$$k_1 = (1/\hbar)(2mE)^{1/2} \qquad k_2 = (1/\hbar)[2m(V-E)]^{1/2} \qquad V > E$$

where E is the NR eigenvalue of the energy of the electron.

The NR condition for resonant tunnelling is the NR limit of (23), and it is given by

$$U_r(\cos\theta) = 0. \tag{36}$$

The shape of the NR transmission spectrum around the energies E_s at NR resonant tunnelling is the NR limit $T^s_{N\mathrm{I}}$ of $T^{\mathrm{R}s}_{N\mathrm{I}}$, and it is given by

$$T^s_{N\mathrm{I}} = 1/\{1 + [(E - E_s)/\Delta E_s]^2\} \tag{37}$$

$$\Delta E_s = \{|M(12)|^2(\mathrm{d}/\mathrm{d}d)[U_r(\cos\theta)](\mathrm{d}/\mathrm{d}E)(d)\}_{E=E_s} \tag{38}$$

$$2\Delta E_s = \text{full width of } T^s_N \text{ at } E_s.$$

The NR limits $T^0_{N\mathrm{I}}$ and $T^0_{N\mathrm{II}}$ of $T^{\mathrm{R}0}_{N\mathrm{I}}$ and $T^{\mathrm{R}0}_{N\mathrm{II}}$, respectively, appear as

$$T^0_{N\mathrm{I}} = 1/\{1 + |M_0(12)|^2[U_r(\cos\theta_0)]^2\} \tag{39}$$

$$T^0_{N\mathrm{II}} = 1/\{1 + |M_0(12)|^2[h_r(\phi_0)]^2\} \tag{40}$$

$$M_0(12) = \text{NR limit of } M_{\mathrm{R}0}(12) = -\mathrm{i}q \tag{41}$$

$$\cos\theta_0 = \tfrac{1}{2}d_0 \qquad |d_0| < 2 \tag{42}$$

$$\cosh\phi_0 = \tfrac{1}{2}d_0 \qquad |d_0| \geqslant 2 \tag{43}$$

$$d_0 = 2\cos(k_1a) + 2q\sin(k_1a)$$

$$q = mp/\hbar^2k_1.$$

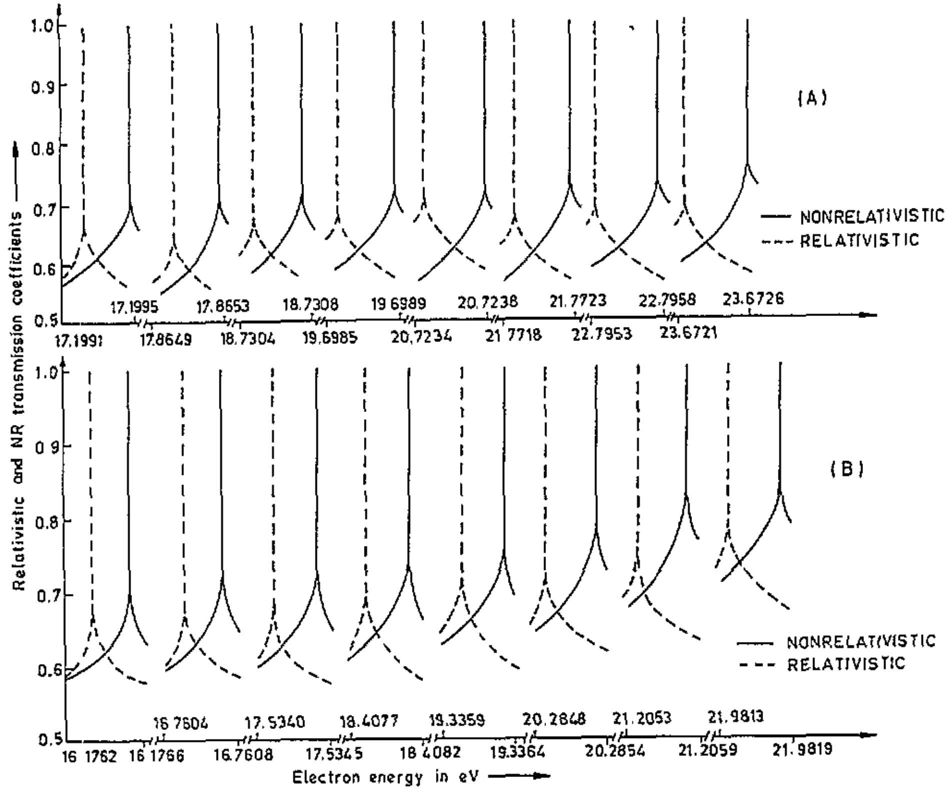

Figure 2. Relativistic and NR transmission spectra for (a) δ-function potentials and (b) barrier-type potentials. The graphs in both (a) and (b) correspond to $N = 9$, $a = 5$ Å, $V = 50$ eV and the fourth allowed band. For graphs in (b), $b = 0.2$ Å. For graphs in (a), the parameter p is the product Vb with the values of V and b just mentioned. Resonant tunnelling occurs when the transmission coefficients become unity.

5. Results and discussion

As mentioned earlier, we have carried out a numerical analysis to elucidate the quantitative extents of relativistic impacts on the tunnelling of electrons through MBSs. The results of our numerical analyses are displayed in figures 2–4.

The graphs in figure 2 show that, for both barrier-type and δ-function-type potentials, the energies ϵ_s at which relativistic resonant tunnelling occurs are lower than the corresponding NR energies E_s. Figure 3 shows that the difference $\Delta W_s = E_s - \epsilon_s$ increases with increasing order s at which resonant tunnelling occurs; this figure also shows that the increase in ΔW_s with increasing s occurs more for the δ-function potential than for the barrier-type potential.

The graphs in figure 4 show that the relativistic full width is smaller than the NR full width, for all orders s of energies at resonant tunnelling. As a result, the relativistic transmission spectrum around energies for relativistic resonant tunnelling is sharper than the corresponding NR spectrum. In view of this situation, the total current transmitted via relativistic tunnelling is likely to be less than the corresponding current due to NR tunnelling. We feel that the features shown in figures 2–4, with regard to relativistic impacts on tunnelling, are likely to be important in connection with solid state devices. The graphs in figure 2 show that relativistic impacts on energies at resonant tunnelling appear in about

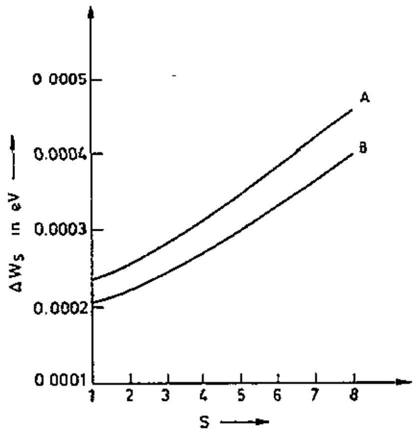

Figure 3. The variation in the difference $\Delta W_s (= E_s - \epsilon_s)$ between the energies corresponding to NR and relativistic resonant tunnelling, with the order s: curve A, δ-function potential; curve B, barrier-type potential.

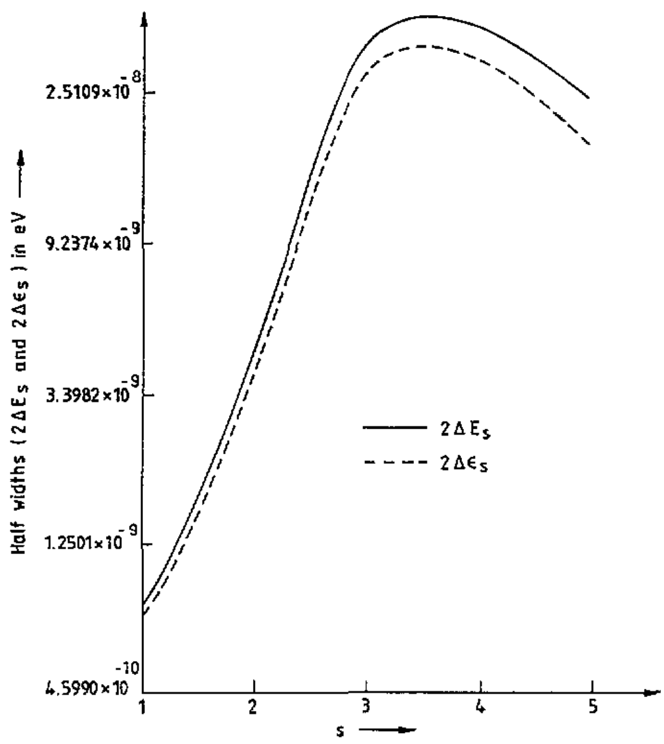

Figure 4. Variation in $2\,\Delta E_s$ and $2\,\Delta\epsilon_s$ with the order s of energies at resonant tunnelling for barrier-type potentials. Both curves correspond to $N = 6$ and the fourth band. Other parameters for both curves are the same as those for figure 2(*b*).

the fifth digit. Consequently, the experimental detection of such impacts would be possible if the barriers are fabricated with high precision and if the energy dependence of resonant tunnelling is measured with an ultra-high accuracy.

Finally, we would like to highlight our qualitative findings about the domains of energies at which resonant tunnelling would occur. We consider the case of barrier-type potentials for that purpose. As elucidated earlier, these domains for barrier-type potentials are the allowed regions of band structures of an infinite crystal with rectangular-barrier-type potentials, having the part $a + b$ of the finite system as its periodicity, the allowed regions for NR and relativistic cases corresponding to $|d| < 2$ and $|d_R| < 2$, respectively. These features of resonant tunnelling essentially establish that the tunnelling of electrons through a finite system has an important linkage with the propagation of electrons through an associated infinite system.

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