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Relativistic impact on the Landauer resistance of Thue–Morse lattices

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Abstract. We have reported a comparative study of the relativistic and non-relativistic Landauer resistances (LR) of Thue–Morse (TM) lattices. The TM lattice treated by us consists of rectangular potential barriers, with their centres distributed according to TM sequence. The purpose behind our study is to examine how the relativistic impact on the LR of TM lattice depends on the energy of the electrons and various parameters related to the TM lattice. Among other things, we find that the relativistic impact increases with increase in the number of barriers in the TM lattice and reduction in the width of barriers.

1. Introduction

Relativistic study of the electronic states and allied properties of aperiodic systems has attracted the attention of many researchers during the last decade or so. The aperiodic cases treated so far in this regard are disordered systems [1–6] and quasi-periodic (QP) systems [7]. The primary aim of these studies was to achieve relativistic generalizations of non-relativistic treatments of various aspects of electron motion in one-dimensional (1D) disordered and QP systems and to gather thereby some knowledge about the extent of relativistic impacts on these aspects, quantitatively [1–7] as well as qualitatively [6]. On the whole, these studies [1–7] are likely to be of considerable importance with regard to electron motion in aperiodic systems consisting of heavy atoms.

Compared with the relativistic study of electron motion in disordered systems, the relativistic study of electron motion in QP systems has received much less attention. It appears that the work in [7] is, so far, the only study to consider relativistic electrons in QP systems. This work dealt with the relativistic transmission coefficient of the Fibonacci lattice. The Fibonacci lattice, which is a 1D version of a quasicrystal [8], has been extensively studied theoretically on a non-relativistic footing as an example of QP systems [9–14] and has also been realized experimentally in the form of systems such as GaAs–AlAs [15]. The exhaustive and meaningful studies of the Fibonacci lattice stimulated efforts towards exploration of QP systems of other types, and the system which has received considerable attention in this respect is the well known Thue–Morse (TM) lattice [16–24]. All studies reported so far about electron motion in the TM lattice have been carried out on a non-relativistic footing. We feel that a relativistic treatment of electrons in motion in the TM lattice would considerably broaden our knowledge with regard to relativistic impacts on electrons in QP systems, and the purpose of this paper is to report a study in this direction. Specifically, we have carried out a relativistic study of the Landauer resistance (LR) [25] of the TM lattice.

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The study of the LR of various 1D systems started to attract substantial attention during the last decade or so. The cases treated so far in this regard are, broadly speaking,

(i) non-relativistic electrons in disordered systems [26–28],
(ii) non-relativistic electrons in periodic systems [26],
(iii) non-relativistic electrons in the Fibonacci lattice [13],
(iv) relativistic electrons in periodic systems and
(v) relativistic electrons in disordered systems [5].

To our knowledge, no study of the LR has so far been reported with regard to the TM lattice. In view of this situation and the fact that the LR provides valuable information about electrical conduction, we have undertaken the relativistic treatment of the LR of the TM lattice and also obtained the non-relativistic LR of such a lattice for comparison between relativistic and non-relativistic results.

The model and some essential features of the TM lattice are discussed in section 2. Section 3 deals with some aspects of relativistic transfer matrices which are required for our relativistic treatment of the LR of the TM lattice. The derivation of the relativistic LR of the TM lattice and related issues are indicated in section 4. The essential aspects of our numerical analysis appear in section 5. Finally, a critical discussion of our results and findings is presented in section 6.

2. Model and some features of Thue–Morse lattices

Our model consists of a system of N rectangular potential barriers, with height V_0 and width b, which are placed along a 1D two-tile QP lattice. The separation between the centres of two consecutive barriers takes one of the two values f and g and such centres are arranged (figure 1) in a TM sequence which is given by [21]

$$S_{n+1} = \{S_n, \overline{S}_n\} \qquad n \geqslant 0 \qquad S_0 = \{f, g\}. \tag{1}$$

$\overline{S}_n$ is the complement of S_n obtained by interchanging f and g. Denoting the total number of tiles in sequences S_{n+1} and S_n by G_{n+1} and G_n, respectively, we obtain

$$G_{n+1} = 2G_n. \tag{2}$$

Equation (2) leads to the following result:

$$G_n = 2.2^n. \tag{3}$$

In our model, the total number N of barriers is the TM number G_n. The reason why we choose the barrier-type potential lies in the fact that they are fairly realistic on the one hand and amenable to exact treatment on the other hand [5, 29–31].

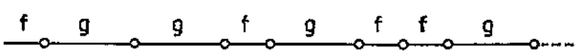

Figure 1. TM lattice: two tiles f and g represent distances between two consecutive points characterizing the centres of two consecutive barriers: these two tiles are arranged in the TM sequence.

3. Some aspects of relativistic transfer matrices

As pointed out earlier, we consider a system of N rectangular potential barriers, where N is a TM number. The barriers are placed along the X axis, with their centres at X_n which lie on the axis of symmetry of the barriers. The 1D Dirac equation for the system is

$$\left(-i\hbar c\sigma_x \frac{d}{dx} + mc^2\sigma_z - [E_R - W(x)]\right)\psi(x) = 0 \tag{4}$$

where E_R, c and m are the relativistic energy eigenvalue, the velocity of light in vacuum and the rest mass of the electron, respectively. σ_x and σ_z are the x and z components of the Pauli spin matrix.

$$W(x) = \sum_{n=1}^{N} V(x - x_n) \tag{5}$$

$$V(x - x_n) = \begin{cases} V_0 \\ 0 \end{cases} \qquad \text{for} \begin{cases} x_n - \frac{1}{2}b \leqslant x \leqslant x_n + \frac{1}{2}b \\ x < x_n - \frac{1}{2}b \text{ or } x > x_n + \frac{1}{2}b. \end{cases}$$

The solution of equation (4) yields the following spinor with reference to the nth barrier:

$$\psi_n(x) = p_n \begin{bmatrix} 1 \\ \gamma \end{bmatrix} \exp[i\rho(x - x_n - \tfrac{1}{2}b)] + q_n \begin{bmatrix} 1 \\ -\gamma \end{bmatrix} \exp[-i\rho(x - x_n - \tfrac{1}{2}b)]$$
$$x_n + \tfrac{1}{2}b < x < x_{n+1} - \tfrac{1}{2}b \tag{6}$$

$$\psi_{In}(x) = r_n \begin{bmatrix} 1 \\ i\lambda \end{bmatrix} \exp(-\eta x) + t_n \begin{bmatrix} 1 \\ -i\lambda \end{bmatrix} \exp(\eta x) \qquad x_n - \tfrac{1}{2}b \leqslant x \leqslant x_n + \tfrac{1}{2}b \tag{7}$$

$$\psi_{n-1}(x) = p_{n-1} \begin{bmatrix} 1 \\ \gamma \end{bmatrix} \exp[i\rho(x - x_{n-1} - \tfrac{1}{2}b)] + q_{n-1} \begin{bmatrix} 1 \\ -\gamma \end{bmatrix} \exp[-i\rho(x - x_{n-1} - \tfrac{1}{2}b)]$$
$$x_{n-1} + \tfrac{1}{2}b < x < x_n - \tfrac{1}{2}b \tag{8}$$

where

$$\rho = \frac{1}{c\hbar}\epsilon^{1/2}(\epsilon + 2mc^2)^{1/2} \tag{9}$$

$$\gamma = \epsilon / c\hbar\rho \tag{10}$$

$$\eta = \frac{1}{\hbar c}(V_0 - \epsilon)^{1/2}(\epsilon + 2mc^2 - V_0)^{1/2} \tag{11}$$

$$\lambda = \frac{1}{c\hbar\eta}(V_0 - \epsilon) \tag{12}$$

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

In writing the spinors (6)–(8) we have used the following inequalities:

$$\epsilon < V_0 < \epsilon + mc^2. \tag{13}$$

The right-hand inequality in (13) ensures the absence of the Klein paradox.

Introducing the (2×2) relativistic transfer matrix $\mathbf{M}^{\mathrm{R}}(n)$, we can obtain

$$\begin{bmatrix} p_n \\ q_n \end{bmatrix} = \mathbf{M}^{\mathrm{R}}(n) \begin{bmatrix} p_{n-1} \\ q_{n-1} \end{bmatrix}. \tag{14}$$

The spinors (6)–(8) must conform to the following boundary conditions:

$$\psi_n(x)\,|_{x=x_n+b/2} = \psi_{\mathrm{I}n}(x)\,|_{x=x_n+b/2} \tag{15a}$$

$$\psi_{\mathrm{I}n}(x)\,|_{x=x_n-b/2} = \psi_{n-1}(x)\,|_{x=x_n-b/2}\,. \tag{15b}$$

With the help of spinors (6)–(8) and (15a) and (15b), we can obtain the explicit form of transfer matrix $\mathbf{M}^{\mathrm{R}}(n)$ as follows:

$$(M^{\mathrm{R}}(n))_{11} = \left(\cosh(\eta b) + \frac{\mathrm{i}}{2\gamma\lambda}(\gamma^2 - \lambda^2)\sinh(\eta b)\right)\exp[\mathrm{i}\rho(\Delta x_n - b)] = (M^{\mathrm{R}}(n))^*_{22} \tag{16}$$

$$(M^{\mathrm{R}}(n))_{12} = \left(-\frac{\mathrm{i}}{2\gamma\lambda}(\gamma^2 + \lambda^2)\sinh(\eta b)\right)\exp[-\mathrm{i}\rho(\Delta x_n - b)] = (M^{\mathrm{R}}(n))^*_{21} \tag{17}$$

$$\begin{aligned} &\Delta x_n = x_n - x_{n-1} \\ &\det[\mathbf{M}^{\mathrm{R}}(n)] = 1. \end{aligned} \tag{18}$$

We now introduce another (2×2) transfer matrix $\mathbf{M}^{\mathrm{R}}_n$ with the help of $\mathbf{M}^{\mathrm{R}}(n)$ as follows:

$$\begin{bmatrix} p_N \\ q_N \end{bmatrix} = \mathbf{M}^{\mathrm{R}}_n \begin{bmatrix} p_0 \\ q_0 \end{bmatrix} \tag{19}$$

where

$$\mathbf{M}^{\mathrm{R}}_n = \mathbf{M}^{\mathrm{R}}(N)\mathbf{M}^{\mathrm{R}}(N-1)\mathbf{M}^{\mathrm{R}}(N-2)\ldots\mathbf{M}(1). \tag{20}$$

The elements of $\mathbf{M}^{\mathrm{R}}_n$ have the following properties:

$$(M^{\mathrm{R}}_n)_{11} = (M^{\mathrm{R}}_n)^*_{22} \tag{21}$$

$$(M^{\mathrm{R}}_n)_{12} = (M^{\mathrm{R}}_n)^*_{21} \tag{22}$$

$$\det \mathbf{M}^{\mathrm{R}}_n = 1. \tag{23}$$

By interchanging f and g in a TM sequence, we obtain the complement of this TM sequence. The axis of symmetry of potential barriers in this complement is shifted to the new position $\overline{x}_n$. Consequently, the matrices $\mathbf{M}^{\mathrm{R}}(n)$ and $\mathbf{M}^{\mathrm{R}}_n$ change to $\overline{\mathbf{M}^{\mathrm{R}}}(n)$ and $\overline{\mathbf{M}^{\mathrm{R}}_n}$, respectively as follows:

$$\overline{\mathbf{M}^{\mathrm{R}}}(n) = \mathbf{M}^{\mathrm{R}}(n) \qquad \text{with } \overline{\Delta}x_n = \Delta x_n \qquad \overline{\Delta}x_n = \overline{x_n} - \overline{x_{n1}} \tag{24}$$

$$\overline{\mathbf{M}^{\mathrm{R}}_n} = \overline{\mathbf{M}^{\mathrm{R}}}(N)\overline{\mathbf{M}^{\mathrm{R}}}(n-1)\ldots\overline{\mathbf{M}^{\mathrm{R}}}(1). \tag{25}$$

4. Relativistic Landauer resistance of the Thue–Morse lattice

We consider N potential barriers, where N is the TM number G_n arranged according to the TM sequence. To obtain the relativistic LR of the TM lattice, we require certain entities related to transfer matrices discussed in the previous section and we first indicate these entities.

Using sequence (1), we obtain

$$\mathbf{M}^{\mathrm{R}}_{n+1} = \overline{\mathbf{M}^{\mathrm{R}}_n}\mathbf{M}^{\mathrm{R}}_n \tag{26}$$

$$\overline{\mathbf{M}^{\mathrm{R}}_{n+1}} = \mathbf{M}^{\mathrm{R}}_n\overline{\mathbf{M}^{\mathrm{R}}_n}. \tag{27}$$

Again trace commutative law yields

$$\mathrm{Tr}\mathbf{M}^{\mathrm{R}}_n = \mathrm{Tr}\overline{\mathbf{M}^{\mathrm{R}}_n}. \tag{28}$$

With the help of equations (20) and (25)–(28), we have

$$Y^{\mathrm{R}}_n = \overline{Y^{\mathrm{R}}_n} \tag{29}$$

$$Y^{\mathrm{R}}_n = \tfrac{1}{2}\mathrm{Tr}\mathbf{M}^{\mathrm{R}}_n = \mathrm{Re}(\mathbf{M}^{\mathrm{R}}_n)_{11} \tag{30}$$

$$\overline{Y^{\mathrm{R}}_n} = \tfrac{1}{2}\mathrm{Tr}\overline{\mathbf{M}^{\mathrm{R}}_n} = \mathrm{Re}(\overline{\mathbf{M}^{\mathrm{R}}_n})_{11}. \tag{31}$$

In the light of the elements of $\mathbf{M}^{\mathrm{R}}_n$ and $\overline{\mathbf{M}^{\mathrm{R}}_n}$, we obtain

$$I^{\mathrm{R}}_n = \mathrm{Im}(M^{\mathrm{R}}_n)_{11} = \frac{1}{2\mathrm{i}}[(M^{\mathrm{R}}_n)_{11} - (M^{\mathrm{R}}_n)^*_{11}] \tag{32}$$

$$\overline{I^{\mathrm{R}}_n} = \mathrm{Im}(\overline{M^{\mathrm{R}}_n})_{11} = \frac{1}{2\mathrm{i}}[(\overline{M^{\mathrm{R}}_n})_{11} - (\overline{M^{\mathrm{R}}_n})^*_{11}]. \tag{33}$$

With the help of equations (26), (27) and (29)–(31), we obtain the following relativistic dynamical trace map:

$$Y^{\mathrm{R}}_{n+1} = 4(Y^{\mathrm{R}}_{n-1})^2 Y^{\mathrm{R}}_n - 4(Y^{\mathrm{R}}_{n-1})^2 + 1 \qquad n \geqslant 1. \tag{34}$$

Equation (34) leads to the relativistic energy spectrum of an infinite periodic lattice with the periodicity S_{n+1}; the allowed energies of this spectrum satisfy the following criteria:

$$\lim_{n\to\infty} |Y^{\mathrm{R}}_n| \leqslant 1. \tag{35}$$

Using equations (26), (27), (29), (32) and (33), we can obtain the recursion relations for I^{R}_n and $\overline{I^{\mathrm{R}}_n}$ as given below:

$$I^{\mathrm{R}}_{n+1} = 4Y^{\mathrm{R}}_n Y^{\mathrm{R}}_{n-1} I^{\mathrm{R}}_{n-1} - 2Y^{\mathrm{R}}_{n-1}(I^{\mathrm{R}}_{n-1} - \overline{I^{\mathrm{R}}_{n-1}}) \qquad n \geqslant 1 \tag{36}$$

$$\overline{I^{\mathrm{R}}_{n+1}} = 4Y^{\mathrm{R}}_n Y^{\mathrm{R}}_{n-1} \overline{I^{\mathrm{R}}_{n-1}} + 2Y^{\mathrm{R}}_{n-1}(I^{\mathrm{R}}_{n-1} - \overline{I^{\mathrm{R}}_{n-1}}) \qquad n \geqslant 1. \tag{37}$$

Now, as is well known, the LR for a chain of barriers is defined as the ratio of the reflection coefficient to the transmission coefficient [25]. This definition means that the relativistic LR is equal to the squares of the modulus of $\mathbf{M}^{\mathrm{R}}_{n+1}(12)$ for a chain of barriers [5]. We thus have

$$\rho^{\mathrm{R}}_{n+1} = |\mathbf{M}^{\mathrm{R}}_{n+1}(12)|^2. \tag{38}$$

ρ^{R}_{n+1} is the relativistic LR for the TM sequence S_{n+1}. Using equations (26), (27), (29)–(34), (36) and (37) and the fact that $\det \mathbf{M}^{\mathrm{R}}_{n+1} = \det \overline{\mathbf{M}^{\mathrm{R}}_{n+1}} = 1$, equation (38) can be written as

$$\rho^{\mathrm{R}}_{n+1} = 4(Y^{\mathrm{R}}_{n-1})^2(A^{\mathrm{R}}_n + B^{\mathrm{R}}_n) \qquad n \geqslant 1 \tag{39}$$

where

$$A^{\mathrm{R}}_n = 2(Y^{\mathrm{R}}_n - 1)[2(Y^{\mathrm{R}}_{n-1})^2(Y^{\mathrm{R}}_n - 1) + 1] + (I^{\mathrm{R}}_{n-1} - \overline{I^{\mathrm{R}}_{n-1}})^2 \tag{40}$$

$$B^{\mathrm{R}}_n = 4Y^{\mathrm{R}}_n I^{\mathrm{R}}_{n-1}[\overline{I^{\mathrm{R}}_{n-1}} + I^{\mathrm{R}}_{n-1}(Y^{\mathrm{R}}_n - 1)]. \tag{41}$$

4.1. Relativistic Landauer resistance for the δ-function equivalent of our model

While studying electron motion in a 1D chain of barriers, it often appears worthwhile to compare the results obtained for the chain of barriers with those for the δ-function equivalent of this chain [30]. In view of this, we would now obtain the δ-function equivalent of ρ^{R}_{n+1}.

The δ-function limit of ρ^{R}_{n+1} can be obtained, as usual, by setting $V_0 \to \infty$, $b \to 0$, such that $V_0 b = \text{finite} = \alpha$ (say). With these conditions, we have

$$(M^{\mathrm{R0}}(n))_{11} = \left[\cos(\alpha/c\hbar) - \frac{\mathrm{i}}{2}\frac{1+\gamma^2}{\gamma}\sin(\alpha/c\hbar)\right]\exp(\mathrm{i}\rho\Delta x_n) = (M^{\mathrm{R0}}(n))^*_{22} \tag{42}$$

$$(M^{\mathrm{R0}}(n))_{12} = \left[-\frac{\mathrm{i}}{2}\frac{1-\gamma^2}{\gamma}\sin(\alpha/c\hbar)\right]\exp(-\mathrm{i}\rho\Delta x_n) = (M^{\mathrm{R0}}(n))^*_{21} \tag{43}$$

$$\overline{\mathbf{M}^{\mathrm{R0}}}(n) = \mathbf{M}^{\mathrm{R0}}(n) \qquad \text{with } \overline{\Delta x_n} = \Delta x_n. \tag{44}$$

$\mathbf{M}^{\mathrm{R0}}(n)$ and $\overline{\mathbf{M}^{\mathrm{R0}}}(n)$ are δ-function equivalents of $\mathbf{M}^{\mathrm{R}}(n)$ and $\overline{\mathbf{M}^{\mathrm{R}}}(n)$. If $\mathbf{M}^{\mathrm{R0}}_n$ and $\overline{\mathbf{M}^{\mathrm{R0}}_n}$ are δ-function equivalents of $\mathbf{M}^{\mathrm{R}}_n$ and $\overline{\mathbf{M}^{\mathrm{R}}_n}$, we have

$$\mathbf{M}^{\mathrm{R0}}_n = \mathbf{M}^{\mathrm{R0}}(N)\mathbf{M}^{\mathrm{R0}}(N-1)\ldots\mathbf{M}^{\mathrm{R0}}(1) \tag{45}$$

$$\overline{\mathbf{M}^{\mathrm{R0}}_n} = \overline{\mathbf{M}^{\mathrm{R0}}}(N)\overline{\mathbf{M}^{\mathrm{R0}}}(N-1)\ldots\overline{\mathbf{M}^{\mathrm{R0}}}(1). \tag{46}$$

The δ-function equivalent ρ^{R0}_{n+1} of ρ^{R}_{n+1} now appears as

$$\rho^{\mathrm{R0}}_{n+1} = 4(Y^{\mathrm{R0}}_{n-1})^2(A^{\mathrm{R0}}_n + B^{\mathrm{R0}}_n) \qquad n \geqslant 1 \tag{47}$$

where

$$A^{\mathrm{R0}}_n = 2(Y^{\mathrm{R0}}_n - 1)[2(Y^{\mathrm{R0}}_{n-1})^2(Y^{\mathrm{R0}}_n - 1) + 1] + (I^{\mathrm{R0}}_{n-1} - \overline{I^{\mathrm{R0}}_{n-1}})^2 \tag{48}$$

$$B^{\mathrm{R0}}_n = 4Y^{\mathrm{R0}}_n I^{\mathrm{R0}}_{n-1}[\overline{I^{\mathrm{R0}}_{n-1}} + I^{\mathrm{R0}}_{n-1}(Y^{\mathrm{R0}}_n - 1)] \tag{49}$$

$$Y^{\mathrm{R0}}_n = \tfrac{1}{2}\mathrm{Tr}\mathbf{M}^{\mathrm{R0}}_n = \mathrm{Re}(M^{\mathrm{R0}}_n)_{11} \tag{50}$$

$$I^{\mathrm{R0}}_n = \mathrm{Im}(M^{\mathrm{R0}}_n)_{11} = \frac{1}{2\mathrm{i}}[(M^{\mathrm{R0}}_n)_{11} - (M^{\mathrm{R0}}_n)^*_{11}] \tag{51}$$

$$\overline{I^{\mathrm{R0}}_n} = \mathrm{Im}(\overline{M^{\mathrm{R0}}_n})_{11} = \frac{1}{2\mathrm{i}}[(\overline{M^{\mathrm{R0}}_n})_{11} - (\overline{M^{\mathrm{R0}}_n})^*_{11}]. \tag{52}$$

It may be noted that the δ-function equivalent of (34) appears as

$$Y^{\mathrm{R0}}_{n+1} = 4(Y^{\mathrm{R0}}_{n-1})^2 Y^{\mathrm{R0}}_n - 4(Y^{\mathrm{R0}}_{n-1})^2 + 1 \qquad n \geqslant 1. \tag{53}$$

5. Non-relativistic Landauer resistance of the Thue–Morse lattice

The results of any relativistic treatment should reduce to the corresponding non-relativistic results when the velocity of light c is allowed to become infinite compared with the velocity of the particle under consideration. Hence, the non-relativistic LR of the TM lattice can be obtained, without using an *ab-initio* treatment, by subjecting our relativistic results to the condition $c \to \infty$. Using these situations, the non-relativistic LR of the TM lattice with barrier-type potentials, denoted as ρ_{n+1}, can be obtained as

$$\rho_{n+1} = 4Y_{n-1}^2(A_n + B_n) \qquad n \geqslant 1 \tag{54}$$

where

$$A_n = 2(Y_n - 1)[2Y_{n-1}^2(Y_n - 1) + 1] + (I_{n-1} - \overline{I}_{n-1})^2 \tag{55}$$

$$B_n = 4Y_n I_{n-1}[\overline{I}_{n-1} + I_{n-1}(Y_n - 1)] \tag{56}$$

$$Y_n = \tfrac{1}{2}\mathrm{Tr}\mathbf{M}_n = \mathrm{Re}(M_n)_{11} \tag{57}$$

$$I_n = \mathrm{Im}(M_n)_{11} = \frac{1}{2\mathrm{i}}[(M_n)_{11} - (M_n)_{11}^*] \tag{58}$$

$$\overline{I}_n = \mathrm{Im}(\overline{M}_n)_{11} = \frac{1}{2\mathrm{i}}[(\overline{M}_n)_{11} - (\overline{M}_n)_{11}^*]. \tag{59}$$

The matrix $\mathbf{M}_n$ is the non-relativistic equivalent of $\mathbf{M}_n^{\mathrm{R}}$ and it is given by

$$\mathbf{M}_n = \mathbf{M}(N)\mathbf{M}(N-1)\ldots\mathbf{M}(1). \tag{60}$$

$\mathbf{M}(n)$ is the non-relativistic equivalent of $\mathbf{M}^{\mathrm{R}}(n)$. The elements of $\mathbf{M}(n)$ are as follows:

$$(M(n))_{11} = \left[\cosh(\beta b) + \frac{\mathrm{i}}{2k\beta}(k^2 - \beta^2)\sinh(\beta b)\right]\exp[\mathrm{i}k(\Delta x_n - b)] = (M(n))_{22}^* \tag{61}$$

$$(M(n))_{12} = \left[-\frac{\mathrm{i}}{2k\beta}(k^2 + \beta^2)\sinh(\beta b)\right]\exp[-\mathrm{i}k(\Delta x_n - b)] = (M(n))_{21}^*. \tag{62}$$

$\overline{\mathbf{M}_n}$ is the non-relativistic equivalent of $\overline{\mathbf{M}_n^{\mathrm{R}}}$ and it can be written as

$$\overline{\mathbf{M}}_n = \overline{\mathbf{M}}(N)\overline{\mathbf{M}}(N-1)\ldots\overline{\mathbf{M}}(1) \tag{63}$$

$$\overline{\mathbf{M}}(n) = \mathbf{M}(n) \qquad \text{with } \overline{\Delta}x_n = \Delta x_n \tag{64}$$

$$k^2 = \frac{2mE}{\hbar^2} \qquad \beta^2 = \frac{2m}{\hbar^2}(V_0 - E) \qquad V_0 < E. \tag{65}$$

E is the non-relativistic eigenenergy value and is equivalent to the entity ϵ in the relativistic treatment.

The δ-function equivalent ρ_{n+1}^0 of ρ_{n+1} appears as

$$\rho_{n+1}^0 = 4(Y_{n-1}^0)^2(A_n^0 + B_n^0) \qquad n \geqslant 1 \tag{66}$$

where

$$A_n^0 = 2(Y_n^0 - 1)[2(Y_{n-1}^0)^2(Y_n^0 - 1) + 1] + (I_{n-1}^0 - \overline{I_{n-1}^0})^2 \tag{67}$$

$$B_n^0 = 4Y_n^0 I_{n-1}^0[\overline{I_{n-1}^0} + I_{n-1}^0(Y_n^0 - 1)] \tag{68}$$

$$Y_n^0 = \tfrac{1}{2}\mathrm{Tr}M_n^0 = \mathrm{Re}(M_n^0)_{11}$$

$$I_n^0 = \mathrm{Im}(M_n^0)_{11} = \frac{1}{2\mathrm{i}}[(M_n^0)_{11} - (M_n^0)_{11}^*]$$

$$\overline{I_n^0} = \mathrm{Im}(\overline{M_n^0})_{11} = \frac{1}{2\mathrm{i}}[(\overline{M_n^0})_{11} - (\overline{M_n^0})_{11}^*]$$

$$\mathbf{M}_n^0 = \mathbf{M}^0(N)\mathbf{M}^0(N-1)\ldots\mathbf{M}^0(1)$$

$$(M^0(n))_{11} = (1 - \mathrm{i}\tau)\exp(\mathrm{i}k\Delta x_n) = (M^0(n))_{22}^*$$

$$(M^0(n))_{12} = -\mathrm{i}\tau\exp(-\mathrm{i}k\Delta x_n) = (M^0(n))_{21}^*$$

$$\overline{\mathbf{M}_n^0} = \overline{\mathbf{M}^0}(N)\overline{\mathbf{M}^0}(N-1)\ldots\overline{\mathbf{M}^0}(1)$$

$$\overline{\mathbf{M}^0}(n) = \mathbf{M}^0(n) \qquad \text{with } \overline{\Delta x_n} = \Delta x_n$$

$$\tau = \frac{m\alpha}{\hbar^2 k}.$$

6. Numerical analysis

In order to elucidate the circumstances under which relativistic impacts on the LR of the TM lattice can become significant, we have carried out some quantitative analysis, with regard to the relativistic and non-relativistic LRs for both barrier-type potentials and δ-function-type potentials. The formulae used for barrier-type potentials are (39) and (54), denoting the relativistic and non-relativistic cases, respectively. The formulae for δ-function potentials are given by (47) and (66), corresponding to the relativistic and non-relativistic cases, respectively. For effective elucidation of the difference between the relativistic and non-relativistic LRs, we have computed the values of two entities defined below:

$$\Delta\rho_{n+1} = \frac{\rho_{n+1} - \rho_{n+1}^{\mathrm{R}}}{\rho_{n+1}} \times 100$$

$$\Delta\rho_{n+1}^0 = \frac{\rho_{n+1}^0 - \rho_{n+1}^{\mathrm{R0}}}{\rho_{n+1}^0} \times 100.$$

The results or our numerical analysis are shown in figures 2–5.

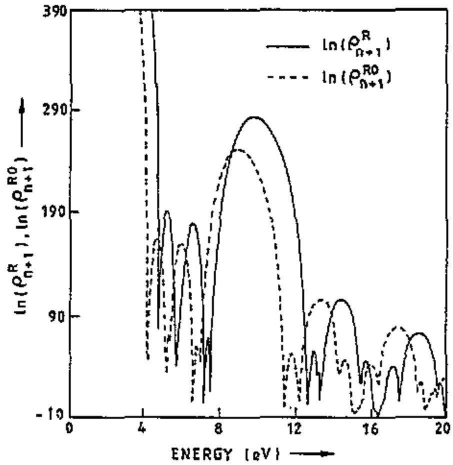

Figure 2. Variation in the relativistic LR with energy, for both barrier-type potentials and δ-function potentials. The parameters are as follows: $f = 1$ Å, $g = 2$ Å, $b = 0.5$ Å, $V_0 = 20$ eV and $N = 256$.

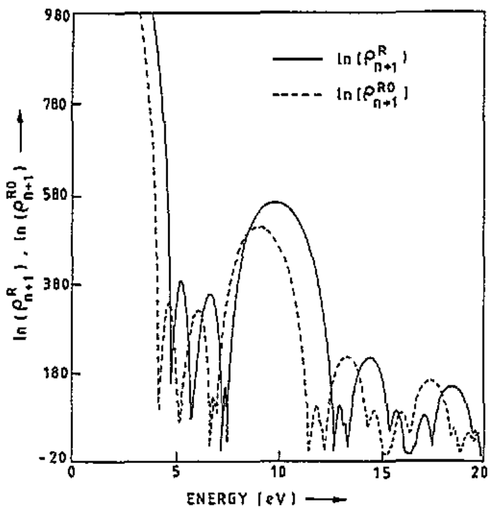

Figure 3. Same type of plots as in figure 3, with $N = 512$; the other parameters are the same as those in figure 2.

7. Discussion of results and conclusions

Figures 2 and 3 show the variation in relativistic LR with energy, for both the barrier potential (ρ^{R}_{n+1}) and the δ-function potential (ρ^{R0}_{n+1}). These figures lead to the following observations.

(i) Both ρ^{R}_{n+1} and ρ^{R0}_{n+1} show some oscillations with energy, with one peak considerably larger than the peaks on both sides of it.

(ii) The peaks of ρ^{R0}_{n+1} are seen to occur at lower energies than those for the corresponding peaks of ρ^{R}_{n+1}.

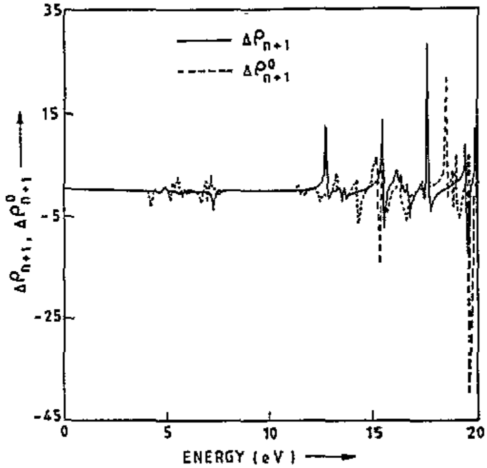

Figure 4. Variation in the difference between the relativistic and non-relativistic LRs with energy. All parameters are the same as those in figure 3.

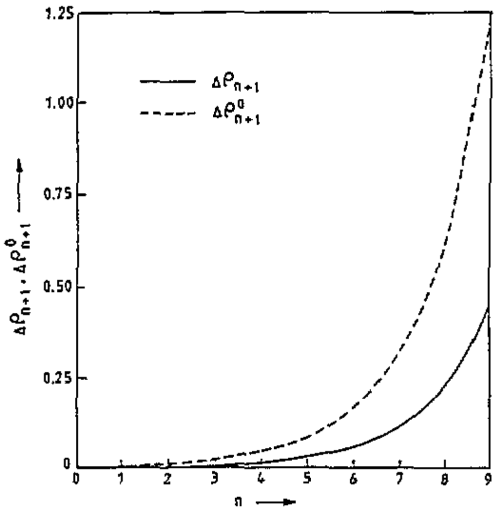

Figure 5. Variation in difference between the relativistic and non-relativistic LRs with n. Both plots correspond to a fixed energy of 8 eV. The values of f, g, b and V_0 are the same as those in figure 2.

(iii) Both ρ^{R}_{n+1} and ρ^{R0}_{n+1} increase with increase in N.

The variations in ρ_{n+1} and ρ^0_{n+1} with energy are seen to be of the same nature qualitatively. There are, however, quantitative differences between the non-relativistic and the relativistic LRs. To see the origin of these quantitative differences, we recollect that the LR of our TM lattice is defined as the ratio of the reflection coefficient to the transmission coefficient of the whole chain of barriers in the TM lattice. As a function of energy, these coefficients are quantitatively different for the relativistic and the non-relativistic cases. Consequently quantitative differences arise in the variations in the non-relativistic and relativistic LRs with energy.

We find it convenient to elucidate the quantitative differences between the relativistic and non-relativistic LRs of the TM lattice by means of figures 4 and 5. Figure 4 shows that both $\Delta\rho_{n+1}$ and $\Delta\rho^0_{n+1}$ (defined in section 6) remain almost constant at low energies, while they show oscillations at high energies corresponding to about 12–20 eV. The peak values of $\Delta\rho^0_{n+1}$ in the oscillating region are seen to occur at lower energies than those for the corresponding peak of $\Delta\rho_{n+1}$. The oscillations of $\Delta\rho_{n+1}$ and $\Delta\rho^0_{n+1}$ show that, at some energies, the relativistic LR is more than the non-relativistic LR, while at some other energies the reverse is the case. The oscillations of $\Delta\rho_{n+1}$ and $\Delta\rho^0_{n+1}$ in the energy interval 10–20 eV indicates that, for this energy interval, the ranges of energies corresponding to substantial relativistic and non-relativistic values of the LR are not coincident. On the other hand, the nearly constant values of $\Delta\rho_{n+1}$ and $\Delta\rho^0_{n+1}$ in the energy interval from very low values to about 10 eV suggest that the ranges concerned with significant relativistic and non-relativistic values of the LR are nearly coincident.

Figure 5 shows the variations in $\Delta\rho_{n+1}$ and $\Delta\rho^0_{n+1}$ with n for a fixed energy. n is related to the number N of barriers as $N = 2 \times 2^n$. The plots in figure 5 indicate that the difference between the relativistic and non-relativistic LRs increases with increasing n and, hence, with increasing N. Further, the increase in this difference with increasing N is seen to be more for the δ-function potential than for the barrier-type potential.

To conclude, we can say that the relativistic impact on the LR of the TM lattice is quite substantial when

(i) the energy of the electron is high,
(ii) the number of the barriers in the chain is large and
(iii) the width of the barriers is very small.

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