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Tunneling and dwell time for one-dimensional generalized Kronig–Penney model

V. Gasparian[a], Ute Gummich[b], E. Jódar[c], J. Ruiz[c,*], M. Ortuño[c]

[a]*Department of Physics, Yerevan State University, 375049, Yerevan, Armenia*
[b]*Fachhochschule Frankfurt, Fachbereich MND, 60318 Frankfurt a.M., Germany*
[c]*Departamento de Fisica, Universidad de Murcia, Murcia, Spain*

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Abstract

We obtain exact expressions for the density of states and the traversal and dwell times of particles travelling through one-dimensional generalized Kronig–Penney models, consisting of periodic arrays of arbitrary sets of δ-potentials. We reduce the problem to the calculation of the properties of one unit cell. For the specific case of two δ-functions per unit cell, we are able to get explicit analytical expressions of the previous magnitudes.

Keywords: Tunneling; Kronig–Penney model

1. Introduction

Tunneling of particles through a barrier is a peculiar phenomena of quantum mechanics. The question of the time required by a particle to cross a given region (or to be reflected from a given region) is a problem that has aroused much interest recently (see, e.g. Refs. [1–3] and references therein). The most direct method to calculate the time during which a transmitted particle interacts with the barrier is to utilize the Larmor clock, for electrons [4, 5] and the optical clock, for photons [6, 7]. In both cases a tunneling process in a magnetic field is considered, but in the first case the magnetic field is perpendicular to the initial direction of the electron and in the second case the magnetic field is parallel to the wavevector of the incident electromagnetic wave. One can explain the results in terms of a complex characteristic time $\tau = \tau_1 - i\tau_2$ [6, 8]. For photons, the real part is proportional to the Faraday rotation and the imaginary part to the degree of ellipticity. Also the Feynman path-integral technique gives rise to a complex time [9, 10]. The physical significance of the complex time has to be discussed more profoundly. It seems, however, that the experiment itself and the size of the wavepacket play an important role in understanding [11]. Beside the traversal and the reflection times, a dwell time can be defined. The dwell time is a measure for the time a particle spends within a barrier, irrespectively whether it is transmitted or reflected. All these characteristic times, i.e. the traversal time τ, the reflection time τ^{R} and the dwell time $\tau^{\mathrm{D}}_{\mp}$, can be expressed in terms of the complex transmission and reflection amplitudes, t and $R_{\pm}$, respectively [5, 12–14]. All these times are also connected with the density of states (DOS) [13–15] and appear in a natural way in the scattering approach to conduction. In a recent series of works on ac transport in mesoscopic conductors, Büttiker and co-authors [17, 18] generalized the concept of the

* Corresponding author.

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DOS, and showed that partial DOS can be defined with full physical significance. These partial DOS are also related to local characteristic times and their relation to the Green Function approach was discussed in Ref. [16].

The dwell time $\tau_{\mp}^{\mathrm{D}}$ is the average number of particles in the barrier divided by the incident flux, i.e.

$$\tau_{\mp}^{(\mathrm{D})} = \frac{1}{2k}\int_0^L |\psi_{\mp}(x)|^2\,\mathrm{d}x. \tag{1}$$

The integral extends over the barrier length L, and $2k$ is the incident flux, where we used the units $e = c = \hbar = 1$, and $m_0 = \frac{1}{2}$ for the electron mass. For electrons, $\psi_{\mp}(x)$ are the steady-state scattering solutions of the time-independent Schrödinger equation. The $\mp$ signs indicate whether the particles incide in the barrier from the left $(-)$ or from the right $(+)$. For photons, $\psi_{\mp}(x)$ correspond to one of the components of the electric or magnetic fields solutions of the Maxwell's equations for a plane wave. $\tau_{\mp}^{\mathrm{D}}$ can also be written in the form of a partial derivative with respect to the energy or, equivalently, to the incident wavevector $k=\sqrt{E}$ [19]:

$$\tau_{\mp}^{(\mathrm{D})} = \pi L \nu(E) + \frac{1}{4k} \times \mathrm{Im}\left\{R\frac{\partial}{\partial k}\ln\frac{R_{\mp}}{R_{\pm}} + \frac{1}{k}(R_{\mp} - R_{\pm})\right\}. \tag{2}$$

R_- and R_+ are the reflection amplitudes, and R is the modulus of both of them, $R = |R_-| = |R_+|$. t is the transmission amplitude, which is independent of the incident direction as can be deduced from time-reversal and current conservation requirements [21]. $\nu(E)$ is the integrated DOS, which is proportional to the real component of the traversal time. The two components of the traversal time τ can also be expressed in terms of the Green function $G(x,x;E)$ of whole system [13]:

$$\begin{aligned}\tau_1 &= \mathrm{Im}\int_0^L G(x,x)\,\mathrm{d}x \\ &= \frac{1}{2k}\mathrm{Im}\left\{\frac{\partial \ln t}{\partial k} + \frac{1}{2k}(R_- + R_+)\right\}, \\ \tau_2 &= \mathrm{Re}\int_0^L G(x,x)\,\mathrm{d}x \\ &= \frac{1}{2k}\mathrm{Re}\left\{\frac{\partial \ln t}{\partial k} + \frac{1}{2k}(R_- + R_+)\right\}.\end{aligned} \tag{3}$$

Eqs. (2) and (3) are general expressions, independent of the model considered. For a symmetric potential barrier $(R_- = R_+)$ the two dwell times coincide between themselves and are equal to the real component of the traversal time τ_1.

In this paper we show that it is possible to obtain exact analytical expressions for the characteristic times for a complex system, than can incorporate most of the interesting features of the problem.

2. Theory

In order to obtain the characteristic times for periodic systems with complex unit cells, we consider the case where the extent of each individual potential $V(x)$ is small as compared to any other typical length of the system. Therefore a generalised Kronig–Penney (GKP) is discussed, where the unit cell consists of n arbitrary δ-functions. The total potential is of the form:

$$V(x) = \sum_{l=1}^{n} V_l \sum_{m=1}^{M} \delta[x - (x_l + md)], \tag{4}$$

where d is the lattice period, and M is the number of cells.

First of all, we have to determine the transmission and the reflection amplitudes, t and $R_{\pm}$, respectively. This could be done, in principle, using the transfer-matrix technique. We prefer, however, to use the characteristic determinant method [20], which is more convenient for analytical calculations.

The transmission amplitude through a general structure is inversely proportional to the characteristic determinant $D(E)$:

$$t = D^{-1}. \tag{5}$$

The determinant D depends on the potential profile $V(x)$. In the case of N δ-potentials of arbitrary strength V_l and at arbitrary points x_l, D satisfies the following recurrence relationship:

$$D_j = A_j D_{j-1} - B_j D_{j-2}, \tag{6}$$

where the index j runs over the different δ functions $(j = 1, 2, \ldots, N)$. The initial conditions are

$$A_1 = 1 + \frac{\mathrm{i}V_1}{2k}; \qquad D_0 = 1; \qquad D_{-1} = 0, \tag{7}$$

and we have for $j > 1$:

$$A_j = 1 + B_j + \frac{\mathrm{i}V_j}{2k}[1 - \exp(2\mathrm{i}ka_{j-1})], \tag{8}$$

and

$$B_j = \frac{V_j}{V_{j-1}} \exp(2\mathrm{i}ka_{j-1}). \tag{9}$$

Now, let us consider the specific application of the previous general expressions to our system of periodic sets of δ- potentials. The recurrence relation (6) for D_j together with the periodicity of the system allow us to find an analytical expression for the characteristic determinant D_{Mn} (M times n is equal to N, the total number of δ-potentials in GKP model) and so for the inverse of the transmission amplitude:

$$D_{Mn} = \mathrm{e}^{\mathrm{i}Mkd}\left\{\cos(M\beta d) + \mathrm{i}\,\mathrm{Im}\{\mathrm{e}^{-\mathrm{i}kd}D_n\}\frac{\sin(M\beta d)}{\sin(\beta d)}\right\} = t^{-1}, \tag{10}$$

where β plays the role of quasimomentum for the GKP and is given by the equation [22]:

$$\cos(\beta d) = \mathrm{Re}\{\mathrm{e}^{-\mathrm{i}kd}D_n\}, \tag{11}$$

where D_n is the characteristic determinant for one unit cell. When the modulus of the RHS of Eq. (11) turns out to be greater than 1, β has to be taken as imaginary. This situation corresponds to a forbidden energy gap (in an infinite system).

The knowledge of the characteristic determinant allows us to calculate also the reflection amplitudes from the left and from the right [20] which for the GKP model are given by:

$$R_- = \frac{\mathrm{e}^{\mathrm{i}(M-1)kd}}{D_{Mn}} \frac{\sin(M\beta d)}{\sin(\beta d)} \left(\frac{r_-^{(n)}}{t^{(n)}}\right), \tag{12}$$

$$R_+ = \frac{\mathrm{e}^{\mathrm{i}(M-1)kd}}{D_{Mn}} \frac{\sin(M\beta d)}{\sin(\beta d)} \left(\frac{r_+^{(n)}}{t^{(n)}}\right), \tag{13}$$

where $r_-^{(n)}$ ($r_+^{(n)}$) is the reflection amplitude of a single unit cell when the particle incides from the left (right). t_n is the transmission amplitude for a single unit cell. For a finite number n of δ-potentials, $r_\pm^{(n)}$ and t_n have been calculated in Ref. [20].

3. Two δ-functions per unit cell

For the purpose of illustration, we want to present the results for a diatomic crystal, i.e. for $n = 2$. The determinant for a unit cell, D_2 in this case, becomes:

$$D_2 = \begin{vmatrix} 1 + \mathrm{i}V_1/2k & \mathrm{i}V_2/2k\mathrm{e}^{-\mathrm{i}ka} \\ \mathrm{i}V_1/2k\mathrm{e}^{\mathrm{i}ka} & 1 + \mathrm{i}V_2/2k \end{vmatrix}. \tag{14}$$

Therefore, the equation for the energy spectrum (11) reads

$$\cos\beta d = \cos kd + \left(\frac{V_1}{2k} + \frac{V_2}{2k}\right)\sin kd + 2\left(\frac{V_1}{2k}\right)\left(\frac{V_2}{2k}\right)\sin ka \sin k(d-a), \tag{15}$$

where $a = x_2 - x_1$ is the distance between potentials V_2 and V_1. Substituting $V_1 = V_2$ and $d = 2a$ into (15) we can obtain the energy spectrum for the simple Kronig–Penney model.

The determinant of the whole system is given by Eq. (10), with the factor $\mathrm{Im}\{\mathrm{e}^{-\mathrm{i}kd}D_2\}$ being equal to

$$\mathrm{Im}\{\mathrm{e}^{-\mathrm{i}kd}D_2\} = \left(\frac{V_1}{2k} + \frac{V_2}{2k}\right)\cos kd - \sin kd + 2\frac{V_1}{2k}\frac{V_2}{2k}\sin ka \cos k(d-a). \tag{16}$$

The ratio between the reflection and the transmission amplitudes, which appear in Eqs. (12) and (13), can also be evaluated using D_{M2}. We arrive at:

$$\frac{r_\mp^{(n)}}{t^{(n)}} = -\mathrm{i}(A \mp \mathrm{i}B)\mathrm{e}^{\mathrm{i}ka}, \tag{17}$$

where

$$A = \left(\frac{V_1}{2k} + \frac{V_2}{2k}\right)\cos ka + 2\frac{V_1}{2k}\frac{V_2}{2k}\sin ka, \tag{18}$$

and

$$B = \left(\frac{V_1}{2k} - \frac{V_2}{2k}\right)\sin ka. \tag{19}$$

Furthermore, the transmission coefficient for the GKP model is given by

$$T = |D_{M2}|^{-2} = \left\{ 1 + (|D_2|^2 - 1)\frac{\sin^2(M\beta d)}{\sin^2(\beta d)} \right\}^{-1}. \tag{20}$$

This equation shows that there are two distinct cases for which an incident wave is totally transmitted, i.e. $T=1$. The first case occurs when $\sin(M\beta d)/\sin(\beta d)=0$. It corresponds to destructive interference between path reflected from different unit cells. We have

$$\beta d = \frac{\pi n}{M} \quad (n = 1,\dots,M-1). \tag{21}$$

In the second case, there is no reflected wave from any individual cell and it corresponds to the condition:

$$T_2 = |D_2|^{-2} = 1. \tag{22}$$

In these two resonance cases, the transmission time τ_1 becomes extraordinarily large, as we will see later on.

Using all this information, we find for the characteristic times the following expressions:

$$\tau_1 = -\frac{(d-a)}{2k} - \frac{1}{2k}\left\{ \frac{\partial}{\partial k}\phi + \frac{1}{k}\sqrt{R}\cos\varphi \times \cos(\phi + k(d-a)) \right\},$$

$$\tau_2 = \frac{1}{2k}\left\{ \frac{1}{2}\frac{\partial}{\partial k}\ln T - \frac{1}{k}\sqrt{R}\cos\varphi \times \sin(\phi + k(d-a)) \right\},$$

$$\tau_{\mp}^{\mathrm{D}} = -\frac{(d-a)}{2k} - \frac{1}{2k}\left\{ \frac{\partial}{\partial k}\phi \pm R\frac{\partial}{\partial k}\varphi + \frac{1}{k}\sqrt{R}\cos(\phi + k(d-a) \mp \varphi) \right\}, \tag{23}$$

where $\tan\phi$ and $\tan\varphi$ are given by

$$\tan\phi = \Omega\frac{\tan(M\beta d)}{\sin(\beta d)}, \qquad \tan\varphi = \frac{B}{A}. \tag{24}$$

In a forbidden gap, β becomes imaginary and therefore Eq. (24) reads

$$\tan\phi = \Omega\frac{\tanh(M\beta d)}{\sinh(\beta d)}. \tag{25}$$

Near the resonance energy, E_0 Eqs. (23) for the characteristic times reduce to

$$\tau_1^{\mathrm{res}} = -\frac{(d-a)}{2k} - \frac{1}{2k}\left\{ \frac{\Omega M d}{\sin(\beta d)}\frac{\partial}{\partial k}\beta - |E - E_0|\Gamma(E_0)\cos\varphi\cos k(d-a) \right\},$$

$$\tau_2^{\mathrm{res}} = \frac{1}{2k^2}|E - E_0|\Gamma(E_0)\cos\varphi\sin k(d-a),$$

$$\tau_{\mp}^{\mathrm{D}} = \tau_1 \mp \frac{1}{2k}|E - E_0|\Gamma(E_0)\sin\varphi\sin k(d-a), \tag{26}$$

where $\Gamma(E_0) = (\frac{1}{2}\partial^2 T/\partial E^2)^{1/2}$

Exactly in the resonance, the dwell times both from the right and from the left are equal to τ_1.

4. Numerical results

We have used Eqs. (23) to calculate the characteristic times as a function of the energy of the incident particle for systems with two δ-potentials per unit cell. For more complex systems, we have obtained numerically the characteristic determinant corresponding to the unit cell and then we have used Eqs. (10), (12) and (13) to calculate the characteristic times. The following graphs show the plots of these times as a function of energy for electrons and for various choices of the parameters.

In Fig. 1, we show τ_1 and τ_2 as a function of energy for a simple KP model consisting of five unit cells with $V_1 = V_2 = 3$ and $d = 2$. The first allowed band extends between approximately 1.5 and π. In this range, we observe nine oscillations in τ_1 and τ_2, each one corresponding to a resonance level, in accordance with Eq. (21). τ_1, which is proportional to the DOS, reproduces the characteristic features of the Kronig–Penney DOS, i.e. τ_1 presents two van Hove singularities at the band edges. The strength of these singularities shows a well known asymmetry [23]. In the forbidden gap, that extends between π and 4 approximately, the DOS becomes drastically small (it would be zero for an infinite system) and so does τ_1. For large energies (not shown in the figure), τ_1 tends to the traversal time of a free particle

$$\tau_0 \equiv \frac{(M-1)d + a}{2k}. \tag{27}$$

τ_0 is smaller than τ_1 in the allowed bands, and bigger in the forbidden gaps. τ_1 is proportional to $E^{1/2}$ at

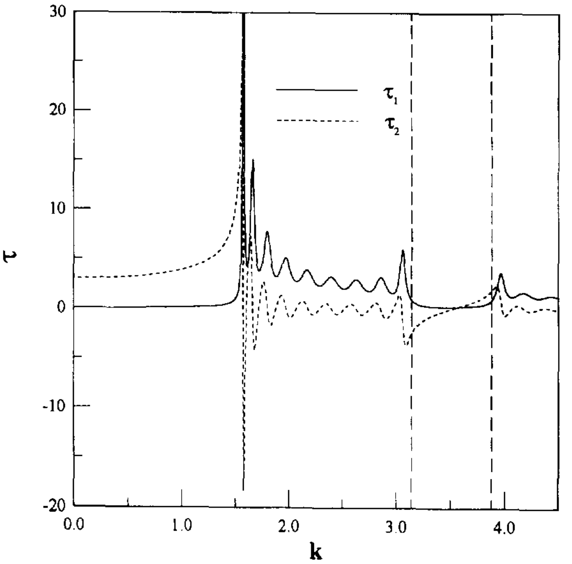

Fig. 1. Two components of the tunneling time τ_1 and τ_2, as a function of incident wavevector, for a Kronig–Penney chain consisting $N = 10$ identical potentials. The values of the parameters are $V = 3$, $a = 1$ and $d = 2a = 2$.

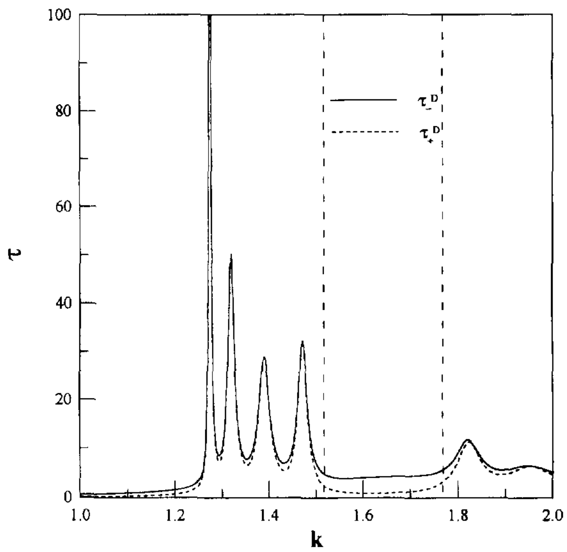

Fig. 2. Two components of the tunneling time τ_1 and τ_2, as a function of incident wavevector, for a GKP for a diatomic crystal. The values of the parameters are $V_1 = 1$, $V_2 = 3$, $N = 10$, $a = 1$ and $d = 3a = 3$.

very low energies. This behaviour of τ_1 reflects the fact that the system is *open and finite*, as was discussed in the literature [8].

If the δ-potential were attractive, we would see similar features in the behaviour of τ_1 and τ_2 than in the case of repulsive potentials. The only relevant difference is that the value of τ_1 would always be smaller than τ_0 in the allowed bands, except for energies close to resonances. τ_2 shows the same number of resonances as τ_1, but the peaks of the resonances are shifted to lower energies.

In Fig. 2, we represent τ_1 and τ_2 for an asymmetric GKP model corresponding to the following choice of the parameters: $V_1 = 1$, $V_2 = 3$, $M = 5$ and $d = 3$. The separations between allowed bands and forbidden gaps are marked by vertical dashed lines. Since $V_1 \neq V_2$ there is no resonance level due to reflections within an individual cell. Only remain the four resonance levels associated with intercell reflection. The other features are similar to those in the previous case. We have also represented (dashed curve) the expression for the resonance time, given by Eqs. (26). We can check that this curve is tangent to the curve corresponding to τ_1 in each resonance, and constitutes a good approximation for the resonance times.

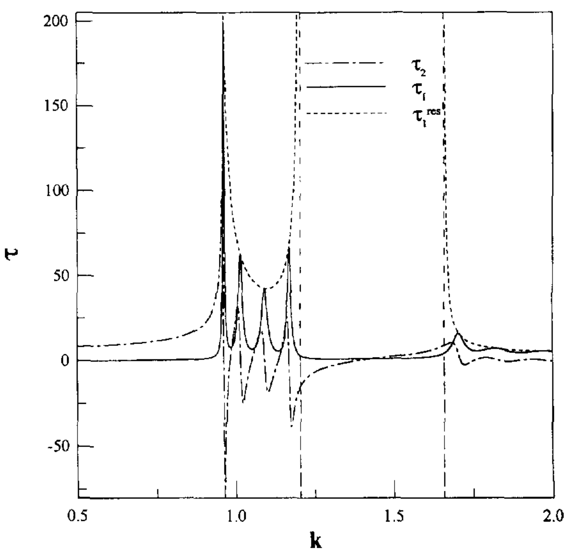

Fig. 3. The dwell times for a particle incident from the left (dotted curve) and from the right (dashed curve) for the GPK model. The value of the parameters are $V_1 = 1$, $V_2 = 2$, $V_3 = 3$, $M = 5$ and $d = 3$.

In Fig. 3, we show the dwell times for a particle incident from the left (dotted curve) and from the right (dashed curve) for the GKP model with parameters $V_1 = 1$, $V_2 = 2$, $V_3 = 3$, $M = 5$ and $d = 3$. These times are given by Eq. (1). The difference between the two dwell times is considerably large in the forbidden gap. τ_1 is equal to the average value of the two dwell times.

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