Resonant Tunneling and Band Mixing in Multichannel Superlattices

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Compact and closed expressions for the evaluation of n-cell transmission amplitudes, in superlattices with N open channels, are written in terms of the single-cell transmission amplitudes and a set of noncommutative polynomials, which, in the one-channel case, reduce to the Chebyshev polynomials. Interesting and nontrivial features, due to channel mixing and multiple interference phenomena occurring along the n-cell system, emerge when applying to specific potential profiles. [S0031-9007(98)05557-4]

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The evaluation of transmission amplitudes through finite periodic systems with finite cross section is not only of interest in quantum mechanics and scattering theory, but is also relevant to the understanding of band mixing processes and resonant transmission of traveling modes in heterostructures, superlattices, quantum-dot arrays, etc. [1–3]. Although transmission probabilities for finite one-dimensional potentials have been routinely calculated since the early days of quantum mechanics [4], few analytic expressions for finite periodic chains are known [5,6]. Although these expressions are valuable, they are restricted to one-channel, transversely invariant or strictly 1D systems.

The purpose of this Letter is to report rigorous new formulas for an easy evaluation of transmission amplitudes in *multichannel* superlattices. Using transfer matrices, which relate wave vectors at two sides of the scattering region, the n-cell transmission amplitude t_n can be expressed as a simple function of the single-cell reflection and transmission amplitudes r and t, and well defined orthogonal polynomials $p_{N,n}$.

By open channels we mean, as usual, the physically allowed propagating modes. In general they depend on the quantum or optical model envisioned. In the scattering approach to the electronic transport processes, each of the nonevanescent transversal quantum states define a channel. For definiteness, we will be concerned with mulitchannel transport properties through heterostructures with cross section $W = w_x w_y$, periodic in the growing coordinate z, with time-reversal invariant and spin-independent interactions, i.e., periodic 3D systems of the so called orthogonal universality class [7]. In general, we consider potential functions $V(x,y,z)$, which contain, at least, two parts: $V_T(x,y)$,, infinite for $|x| > w_x/2$ and $|y| > w_y/2$; and the function $V_L(x,y,z)$, periodic in z. Using N eigenfunctions $\varphi_i(x,y)$ of (see, for example. Ref. [8])

$$\left[-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V_T(x,y)\right]\varphi_i(x,y) = \varepsilon_i \varphi_i(x,y),$$

one obtains the coupled equations

$$\left[\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + \left(E - \frac{k_{Tj}^2\hbar^2}{2m^*}\right)\right]\phi_j(z) = \sum_{i=1}^{N} V_{ji}(z)\phi_i(z)$$

with $k_{Tj} = \pi(n_x^2/w_x^2 + n_y^2/w_y^2)^{1/2}$ and

$$V_{ji}(z) = \frac{1}{W}\int_0^{w_x}\int_0^{w_y} V_L(x,y,z)\varphi_j^*(x,y)\varphi_i(x,y)\,dx\,dy$$

the channel couplings. Though N is taken here as the number of open channels, it counts in general the open and some closed channels.

Assume now that the single-cell transfer matrix, denoted by M, has been obtained. It is known that the transfer matrices of the orthogonal class, independently of the particular potential shape, have the general structure

$$M = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} \tag{1}$$

with α and β, $N \times N$ complex matrices. When flux is conserved, these submatrices can be written, in the Bargmann's parametrization, as $\alpha = u \cosh\chi\, v^\dagger$ and $\beta = u \sinh\chi\, v^T$, with u and v, $N \times N$ unitary matrices and χ a diagonal matrix with elements $\chi_{ii} \geq 0$ (see Ref. [7]). Even though we deal with systems of the orthogonal universality class, our calculations extend easily to other universality classes [7].

For the purpose of calculating transmission amplitudes, it is fundamental to recall the relations

$$t = (\alpha^\dagger)^{-1} \quad \text{and} \quad r^* = -\alpha^{-1}\beta \tag{2}$$

between the N-channel transfer and scattering matrix blocks, of a single cell. Similar relations hold, of course, for the n-cell transmission and reflection amplitudes t_n and r_n, and the submatrices α_n and β_n, of the n-cell transfer matrix

$$M_n = \begin{pmatrix} \alpha_n & \beta_n \\ \beta_n^* & \alpha_n^* \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}^n. \tag{3}$$

We shall present simple expressions to obtain α_n and β_n, i.e., to obtain M_n, *without* calculating powers of M. Although the power evaluations may numerically be attained, they become analytically unmanageable, even for small n. The method proposed here allows better numerical calculations, and more physical insights. We obtain α_n and β_n, and thus t_n, as simple functions of α, β, and a set of polynomials $p_{N,n}$, which, for simplicity, will be denoted just as p_n, unless the number of channels N needs to be specified. These polynomials play, for finite periodic systems, a similar role as the Bloch functions in 1D infinite periodic systems.

Using the transfer matrix property $M_n = MM_{n-1}$, it is easy to obtain

$$\alpha_n^* = p_n - \beta^{-1}\alpha\beta p_{n-1} \quad \text{and} \quad \beta_n = \beta p_{n-1}\,. \tag{4}$$

Thus, the n-cell transmission amplitude is given by

$$t_n^T = (p_n - \beta^{-1}\alpha\beta p_{n-1})^{-1} \tag{5}$$

while the *n-cell* four-probe Landauer conductance by

$$G_n = \frac{1}{p_{n-1}}\, G \left(\frac{1}{p_{n-1}}\right)^{\dagger}. \tag{6}$$

These are simple functions of the *matrix polynomials* p_n *and the single-cell transfer matrix blocks*. It is clear that these polynomials are of central importance here. Knowing them, the conductance and transmission coefficients can easily be evaluated, without having to solve explicitly the Schrödinger equation of the whole system. All we need is to solve the single-cell Schrödinger equation.

Despite the importance of the polynomials p_n, and in order to keep the paper readable for the general audience, we shall just mention some of its general properties. The polynomials are solutions of the *matrix recurrence relation* (MRR) [9]

$$p_n - \zeta p_{n-1} + \eta p_{n-2} = 0 \qquad n \geq 1\,, \tag{7}$$

where $\zeta = (\beta^{-1}\alpha\beta + \alpha^*)$, $\eta = (\alpha^*\beta^{-1}\alpha\beta - \beta^*\beta)$, $p_{-1} = 0$, and $p_0 = I_N$ (the unit matrix of dimension N). This relation resembles the well known orthogonal polynomial recurrence relations. In fact, in the one channel case (i.e., for $N = 1$), Eq. (8) reduces to the well known Chebyshev recurrence relation. When the number of channels is larger than one (i.e., $N > 1$), all the factors appearing in (8) become $N \times N$ matrices. This makes the problem complex and interesting [10].

The general solution to the MRR is

$$p_m = \sum_{k=0}^{2N-1}\sum_{l=0}^{k} p_l g_{k-l} q_{m-k} \quad \text{for} \quad m \geq 2N\,. \tag{8}$$

Here, the higher order matrix polynomials are expressed in terms of the first $2N - 1$ lower order polynomials p_l and the invariant functions

$$g_m = \sum_{l_m > \cdots > l_2 > l_1 = 1}^{2N} \lambda_{l_1}\lambda_{l_2}\cdots\lambda_{l_m}$$

and

$$q_n = \sum_{i=1}^{2N} \frac{\lambda_i^{2N+n-1}}{\prod_{j\neq i}^{2N}(\lambda_i - \lambda_j)}\,, \tag{9}$$

where λ_i is the ith eigenvalue of M. The symmetric functions g_m can also, of course, be written in terms of the transfer matrix traces.

For $N = 1$, we have $p_m = q_m$, which, according to the comment after Eq. (8), is just the well known Chebyshev polynomial U_n evaluated at $\mathrm{Tr}\, M/2 = (\lambda_1 + \lambda_2)/2$.

All the interface matchings, required when solving the Schrödinger equation, are implicitly taken into account by solving the MRR. It is clear, from Eqs. (6) and (7), that the polynomial zeros determine the transmission and conductance resonances. While the information on the tunneling processes is provided by the single-cell submatrices α and β, the very complicated quantum interference phenomenon, which gives rise to the band structure, level splittings, band and channel mixings, and other interesting properties, is carried out by the polynomials p_n.

Let us now discuss some applications. For the one-channel 1D systems, the n-cell transmission amplitude and the four probe Landauer conductance are obtained from

$$t_n = \frac{t^*}{p_n t^* - p_{n-1}} \quad \text{and} \quad G_n = \frac{G}{p_{n-1}^2}\,, \tag{10}$$

where G and t are the single-cell conductance and transmission amplitudes, respectively, and $p_{n-1} = U_{n-1}$. The role of the Chebyshev polynomial in the resonant behavior of $|t_n|^2$ and G_n is clear.

In Fig. 1, the one-channel Landauer conductance and transmission coefficients of $Al_xGa_{1-x}As/GaAs$, with $x = 0.3$, are plotted as functions of the incident energy. The potential profile has been taken as a sequence of square barriers of height 0.23 eV and width 20 Å, separated a distance 100 Å. In Figs. 1(a) and 1(b) we show $T_1 = |t_1|^2$and $T_n = |t_n|^2$. In Fig. 1(a) the system contains three barriers and two wells, i.e., $n = 3$. The trace of M (dotted curve), known to predict band widths and their position, is also plotted. In 1(b) the same parameters have been taken, but now we choose $n = 7$. It is clear that the band structure is better defined when n gets larger. The band positions and widths are the same. In Fig. 1(c) we have G and G_n (these in units of $e^2/\pi\hbar$) and the Chebyshev polynomial p_{n-1} (U_6 in this case).

One can easily play with other possibilities, using the one-channel expressions. For example, band structure tailoring due to impurities can be predicted. In Fig. 2, we plot the transmission probability for a one-channel system with $n = 14$ (i.e., 14 barriers and 13 wells), containing *one* "impurity well" at the center of the system, for the same potential parameters as in Fig. 1, i.e., $V_o =$ 0.23 eV, $a = 20$ Å, and $b = 100$ Å. Taking the impurity width $b_i = z_i b$, impurity levels are produced at will in the energy gaps, varying z_i . In Figs. 2(a) and 2(b), z_i has been taken equal to 0.85 and 1.1, respectively. The impurity levels separate from the bottom or the upper band edges, respectively. Simultaneously, the resonant-band structures are strongly modified.

If we have more than one open channel, all the physical quantities are matrices. It is known from the scattering theory that the matrix element $(t_n)_{ik} \equiv t_{n,ik}$ represents the transmission amplitude from channel k on the left to channel i on the right. Hence, $T_{n,i} = \sum_k |t_{n,ik}|^2$ is the total transmission probability to channel i. To illustrate the use of our method in the calculation of these quantities, with clear channel mixing effects, we need to consider *more than one channel*.

We shall discuss now a simple example with more than one open channel. Let the sequence of layers $ABABA\ldots$, where the A's are finite-cross-section layers of δ-scatterer centers (monatomic layers), and the B's thicker layers of length l_c and constant potential with also finite cross section. In other words, we are dealing with a potential region $V = V_T + V_L$, where V_T is taken as an infinite sequence of square wells, and $V_L = \gamma[\delta(z - \nu l_c)\sum_\mu \delta(x - x_\mu)\delta(y - y_\mu)]$, with $\nu = 1, \ldots, n$, and (x_μ, y_μ) denoting the scattering centers positions.

For a given Fermi energy E_F, the N open channels are those propagating modes with longitudinal wave numbers $k_j^2 = k^2 - k_{Tj}^2 \geq 0$, $(j = 1, \ldots, N)$ and the coupling constants

$$\Gamma_{ij} = \frac{2m^*\gamma}{\hbar^2} \sum_\mu \varphi_i^*(x_\mu, y_\mu)\varphi_j(x_\mu, y_\mu). \qquad (11)$$

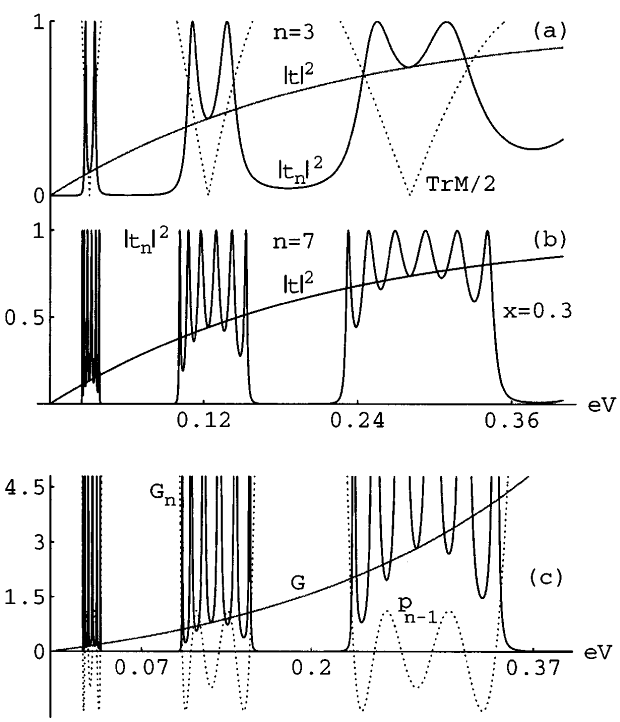

FIG. 1. Four probe Landauer conductance and transmission probabilities as functions of the energy in one-channel systems. In (a) and (b) we plot $|t|^2$ and $|t_n|^2$ for a $Al_{0.3}Ga_{0.7}As/GaAs$ superlattice, represented by square barriers of hight $V_o = 0.23$ eV, and width $a = 20$ Å, separated a distance $b = 100$ Å (the well width). We also plot in (a) the real part of α (dashed line), which predicts band widths and their position. In (c), the single-cell and the n-cell conductances G and G_n (in units of $e^2/\pi\hbar$) are plotted for the same system, together with the Chebyshev polynomial.

For $N = 2$, the transfer matrix is given by

$$\alpha = I_2 + \beta \quad \text{and} \quad \beta = -\frac{i}{2k_1k_2}\begin{pmatrix} k_2\Gamma_{11} & k_2\Gamma_{12} \\ k_1\Gamma_{21} & k_1\Gamma_{22} \end{pmatrix},$$

with $k_2\Gamma_{12} = k_1\Gamma_{21}$ when flux is conserved. In this case, t and t_n are 2×2 matrices. This is the simplest extension beyond the one-channel systems, which already exhibits channel mixing effects. Equations (6) and (9) allow direct calculations of transmission amplitudes for any number of cells. In Fig. 3, we plot transmission probabilities for the system $ABABABA$ (with four δ-barrier layers A and three wells B, i.e., $n = 4$). In Figs. 3(a) and 3(c), uncoupled-channels ($\Gamma_{12} = 0$) transmission probabilities $T_{11} = |t_{4,11}|^2$ and $T_{22} = |t_{4,22}|^2$ are shown. In this uncoupled-channels limit, well defined resonances are seen. Their particular positions and widths depend, of course, on the specific choice for the underlying parameters. When the channel coupling is turned on, channel mixing takes place, as can be seen in Fig. 3(b), where $|t_{4,11}|2$ is plotted again for $\Gamma_{12} = -0.904$. Depending on the coupling parameter, interference effects or new resonances, proper of the uncoupled-channel 2, may appear indicating, as suggested in Ref. [11] for hole transport, propagation via transformation from channel 1 to channel 2 and back to channel 1. Because of channel interference, some of the uncoupled-channel resonances remain, while others disappear. In Fig. 3(d), the total conductance $g = \mathrm{Tr}(tt^\dagger)$ is plotted when the channels are coupled and interfere. The behavior of the total conductance differs from the well defined resonant-band structures, seen for uncoupled or one-channel transmission amplitudes. Frequently, experimental conductances, with *resonance broadenings*, suppressions, and other effects of primary importance, can be explained in terms of *interchannel and interlayer interfering couplings*.

We presented here a method for the evaluation of multichannel-multilayer tunneling properties. This

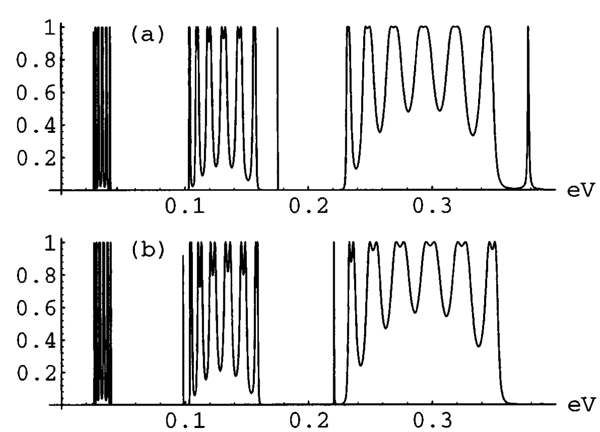

FIG. 2. Gap levels produced by one impurity well at the center of a $Al_xGa_{1-x}As/GaAs$ superlattice, with $n = 14$ and $x = 0.3$, i.e., twice as large as the system of Fig. 1(b). In (a), the impurity width $b_i = z_i b$ is taken with $z_i = 0.85$, while in (b), we choose $z_i = 1.1$. Clearly, level positions depend on z_i.

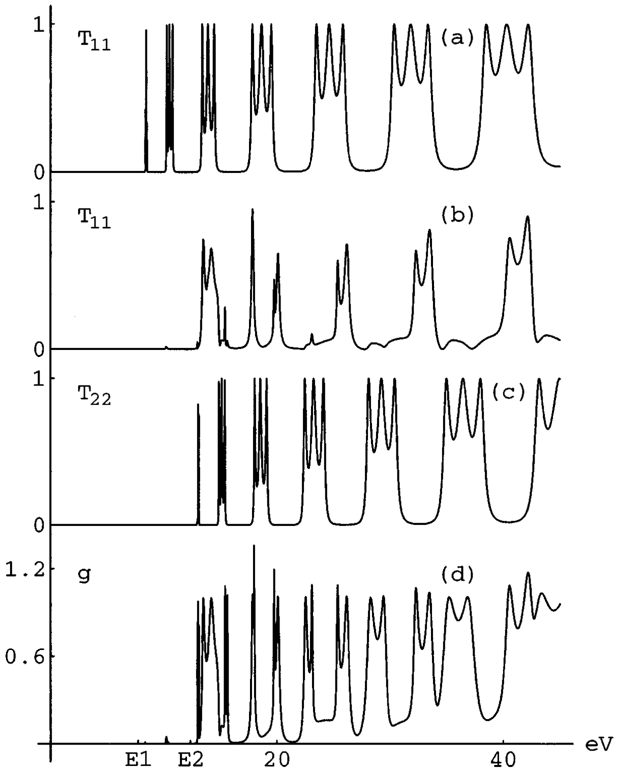

FIG. 3. Coupled and uncoupled two-channel transmission probabilities in a 3D superlattice. Transversely confined propagating modes are scattered by δ-potential centers located in planes A of a sequence $ABAB\ldots$. In the uncoupled channels limit (i.e., $\Gamma_{12} = 0$), the transmission coefficients $T_{11} = |t_{n,11}|^2$ and $T_{22} = |t_{n,22}|^2$ are shown in (a) and (c). They behave, of course, as in the one-channel case. In the coupled case [see (b) and (d)], channel mixing effects are seen for T_{11} and the conductance $g = \mathrm{Tr}(tt^\dagger)$. In this example, the transversal width is ≈30 Å, the cell length $l_c \approx 30$ Å, and $n = 4$. The one- and two-channel thresholds are ≈7.71 eV and ≈12.34 eV, respectively.

method allows easier numerical calculations, and provides simple analytic formulas for the n-cell transmission amplitudes t_n, entirely expressed in terms of the single-cell amplitude t, and a set of noncommutative polynomials $p_{N,n}$, reported here. Interesting and nontrivial features come out for the transmission probabilities and the Landauer conductance. As one should expect in a quantum process of this kind, which generalizes the 1D behavior, the multichannel superlattice tunneling contains information of the single-barrier tunneling, embodied by t, and the complicated interference phenomena and channel mixings described by $p_{N,n}$. It will be of interest to extend this method to include electric fields.

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