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Perturbation expansion of the transfer matrix for tunnelling problems

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Abstract. A perturbative procedure is used to calculate the transfer matrix and the tunnelling transmission coefficient through a structured potential barrier. The potential is first approximated by a steplike function constructed from a partition procedure. The rate of convergence is only l^2 (l is the step size). Then a Peano perturbative solution is used to achieve an l^4 convergence rate. The accuracy of the procedure is illustrated with the following examples: the trapezoidal barrier, the exactly soluble $15\,\mathrm{sech}^2(z)$ barrier and the biased quantum well.

1. Introduction

Submicron physical systems involving tunnelling are currently studied in view of signal processing applications: quantum wells (Chang *et al* 1974), superlattices (Payne 1985), in the interpretation of scanning tunnelling transmission microscopy images (Lang 1986) and also in the open field of molecular electronics (Carter 1984).

The understanding of these systems requires the calculation of the electron transmission coefficient $T(E)$ through barriers which can have a rather simple structure (the single quantum well, for instance) or a complicated one as in the Aviram-Ratner molecular diode (Aviram and Ratner 1974). For one-dimensional systems, Landauer (1970) has related $T(E)$ to the conductance and generalisations have recently appeared for multichannel systems (Buttiker *et al* 1985).

The WKB approximation gives a good evaluation of $T(E)$ for thick structureless barriers when a low polarising voltage is applied (Simmons 1963). But for more complicated structures, resonances (Ricco and Azbel 1984) are not well reproduced by WKB since matching of the wavefunction in different regions is required.

The transfer matrix, $M(z, z_0)$, has been used in the theory of tunnelling to solve the Schrödinger equation, mostly for square potentials (see, for example, Mora *et al* 1985 and references therein). It provides a good numerical way of computing $T(E)$ as soon as the obstacle has a repeated structure; for instance, random chains in localisation theory (Stone *et al* 1981) and superlattices (Tsu and Esaki 1973).

In this paper, we go further by developing the transfer matrix in a Peano perturbative series (Reed and Simon 1975). Even in the finite voltage case, it leads to a $T(E)$ calculation with perturbative corrections. In § 2, we review the transfer matrix technique; in § 3, a Peano development of $M(z, z_0)$ is given in the 'interaction picture' and the convergence rate analysed; in § 4, we present numerical results for two potentials, the biased quantum well and the barrier $U(z) = 15\,\mathrm{sech}^2(z)$, as tests of the accuracy of our perturbative technique.

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2. The transfer matrix $M(z, z_0)$

Let us consider, for a fixed real E, the initial value problem

$$(-\mathrm{d}^2/\mathrm{d}z^2 + U(z) - E)\varphi(z) = 0 \qquad z_0 \leqslant z \leqslant Z \tag{1a}$$

$$\varphi(z_0) = g_1 \qquad (\mathrm{d}\varphi/\mathrm{d}z)(z_0) = g_2 \tag{1b}$$

where $U(z)$ is a real-valued bounded function with its compact support $\mathrm{supp}(V)$ included in the interval $I = [z_0, Z]$. Equation (1a) is the Schrödinger eigenvalue problem for a particle of mass m and energy $\hbar^2 E/2m$ in a potential $\hbar^2 U(z)/2m$.

On the set $\mathbb{C}^1(I) \cap L^2(I)$ of continuous square integrable functions on I with continuous derivatives, the solutions of (1) are the connection geodesics on the manifold $A_I = \{y \in \mathbb{C}^2;\ y = (\varphi(z), \mathrm{d}\varphi(z)/\mathrm{d}z),\ z \in I\}$ (see, for example, Dieudonné 1971) and the dual problem of (1) is the initial value problem

$$(\mathrm{d}\psi/\mathrm{d}z)(z) = P(z)\psi(z) \tag{2a}$$

$$\psi(z_0) = {}^t(g_1, g_2) \tag{2b}$$

with $\psi(z) = {}^t(\varphi(z), \mathrm{d}\varphi(z)/\mathrm{d}z)$. For each $z \in I$, $P(z)$ is an operator on $L^2(I) \oplus L^2(I)$ defined by

$$P(z)\psi(z) = \begin{bmatrix} 0 & 1 \\ U(z) - E & 0 \end{bmatrix} \psi(z). \tag{3}$$

$P(z)$ is a bounded non-self-adjoint operator with a spectrum $\sigma(P(z)) = \{\pm(U(z) - E)^{1/2}\}$ and a norm $\|P(z)\| = \sup_{z \in I}(|(U(z) - E)^{1/2}|)$. Notice that because $P(z)$ is bounded it is sufficient to add a fixed real number $b \geqslant \|P(z)\|$ so that $P(z) + b$ can be inverted on the whole interval: $M(z, z_0)$ is the propagator generated by $P(z)$ which gives the solution of (2) (Reed and Simon 1975):

$$\psi(z) = M(z, z_0)\psi(z_0). \tag{4}$$

This operator $M(z, z_0)$, sometimes called a monodromy transformation (Arnold 1980), has the following properties:

$$M(z_0, z_0) = \mathbb{1} \tag{5a}$$

$$M(z, z_0) = M(z, z_1)M(z_1, z_0) \tag{5b}$$

$$M(z, z_0) \text{ is jointly continuous in } z,\ z_0 \tag{5c}$$

$$\det M(z, z_0) = 1. \tag{5d}$$

The first three properties come from the existence of a propagator for (2) and (5c) guarantees the continuity of $\varphi(z)$ and $\mathrm{d}\varphi(z)/\mathrm{d}z$ as a solution of (1). The property (5d) comes from the real valuedness of $U(z)$ and from the conservation of the probability current density: because (1a) is an eigenvalue equation, one obtains for $z \in I$, $j(z) = j(z_0)$ with

$$j(z) = \frac{\hbar}{2m\mathrm{i}}\left(\varphi^*(z)\frac{\mathrm{d}\varphi}{\mathrm{d}z}(z) - \varphi(z)\frac{\mathrm{d}\varphi^*}{\mathrm{d}z}(z)\right) \tag{6}$$

and this leads to (5d) because from (4)

$$j(z) = \det M(z, z_0) j(z_0). \tag{7}$$

The physical properties of a barrier with a shape $U(z)$ are obtained through a non-unitary transformation of $M(z, z_0)$. Using (5*b*) and the calculated $M(z, z_0)$ for $U(z)=0$, $M(z, z_0)$ can be written

$$M(z, z_0)=[\exp(P(Z)z)X(Z)]S(Z, z_0)[\exp(P(z_0)z_0)X(z_0)]^{-1} \tag{8}$$

where $X(z)$ is an invertible operator independent of z if $\mathrm{d}U(z)/\mathrm{d}z=0$ and

$$S(Z, z_0)=[\exp(P(Z)b)X(Z)]^{-1}M(Z, z_0)[\exp(P(z_0)a)X(z_0)] \tag{9}$$

with $[a, b]$ the smaller interval including the whole $\mathrm{supp}(\mathrm{d}U/\mathrm{d}z)$. The characterisation of the transmission properties of the barrier for a particle of wavevector $k(z)=(E-U(z))^{1/2}$ is achieved by the choice

$$X(z)=\begin{bmatrix} 1 & 1 \\ \mathrm{i}k(z) & -\mathrm{i}k(z) \end{bmatrix} \tag{10}$$

in the non-unitary transformation (9) of $M(b, a)$. On A_I, this choice is equivalent to decomposing locally $\psi(z)$ into $\exp(\pm\mathrm{i}k(z)z)$. The $S(Z, z_0)$ matrix elements satisfy $S_{22}=S_{11}^*$ and $S_{12}=S_{21}^*$ according to the real valuedness of $U(z)$ and $|S_{11}|^2-|S_{12}|^2=k(a)k(b)^{-1}$ from the current conservation: only a modulus and a phase characterise the barrier. Notice that $k(a)k(b)^{-1}\neq 1$ for a biased barrier. From (4), (8) and (10), the current (6) becomes

$$j(z)=(\hbar k(a)/m)|A|^2T(E) \tag{11}$$

where

$$T(E)=k(a)k(b)^{-1}|S_{11}|^{-2} \tag{12}$$

and A is the incident amplitude.

When two or more barriers are put together, the phase shift $\arg(S_{11})-\arg(S_{12})$ must be used to estimate $T(E)$, because in this case there is no superposition rule for $T(E)$ (Saso *et al* 1985) and the final value must be calculated with (5*b*). This phase shift can also be used to evaluate the density of states (Avishai and Band 1985). In the following, $M(z, z_0)$ is evaluated in order to compute $T(E)$ from (9) and (12).

3. Perturbation expansion of $M(z, z_0)$

From (2) and (4), $M(z, z_0)$ is the solution of the initial value problem

$$\mathrm{d}M(z, z_0)/\mathrm{d}z=P(z)M(z, z_0) \tag{13a}$$

$$M(z_0, z_0)=\mathbb{1}. \tag{13b}$$

The solution of (13) can be obtained as a finite or infinite product of exponentials of operators (Magnus *et al* 1966), as a series involving the multiple commutators of $P(z)$ (Bialynicki-Birula *et al* 1969) or as a Peano series (Reed and Simon 1975). The second method is useful for the $P(z)$ operator which leads to a vanishing multiple commutator in finite order. The first reduces to the second after factorisation of the exponentials. Only the last one will be considered in the following:

$$M(z, z_0)=\mathbb{1}+\sum_{m=1}^{\infty}\int_{z_0}^{z}\mathrm{d}z_1\int_{z_0}^{z_1}\mathrm{d}z_2\ldots\int_{z_0}^{z_{m-1}}\mathrm{d}z_m P(z_1)P(z_2)\ldots P(z_m). \tag{14}$$

For $P(z)$ given by (3), the Peano series can be summed for specific $U(z)$, for instance a steplike function $U(z)$, as follows.

Let $\{a_i\}_{i=1,n}$ be the positions of the discontinuities of a steplike function $U(z)$ on I, and $a_0 = z_0$. Because $\mathrm{d}U(z)/\mathrm{d}z$ for $z \in]a_{i-1}, a_i[$, we obtain from (14):

$$M(z, z_0) = \mathbb{1} + \sum_{m=1}^{\infty} \left(\int_{a_0}^{a_1} + \int_{a_1}^{a_2} + \ldots + \int_{a_n}^{z} \right) \mathrm{d}z_1 \int_{a_0}^{z_1} \mathrm{d}z_2 \ldots \int_{a_0}^{z_{m-1}} \mathrm{d}z_m$$
$$\times P(z_1)P(z_2)\ldots P(z_m). \tag{15}$$

By repeating this procedure for the other integrals, the $P(z)$ product will be constant on every m-dimensional integration domain, leading to

$$M(z, z_0) = \exp[(z - a_n)P(a_n)] \prod_{i=0}^{n-1} \exp\left[(a_{i+1} - a_i) P\left(\frac{a_{i+1} + a_i}{2} \right) \right]. \tag{16}$$

This is a useful expression for computing $T(E)$ for a random or periodic succession of barriers like a superlattice (Tsu and Esaki 1973).

For a more general bounded $U(z)$, (16) can also be used but with $U(z)$ approximated by a steplike function $U^{(N)}(z)$, as suggested by Mora *et al* (1985) where N is the approximation order.

To construct $U^{(N)}(z)$, $[z_0, Z]$ is divided in 2^N subintervals of length $l_{(N)} = (Z - z_0)2^{-N}$ and boundaries $a_{(N)}(j) = z_0 + jl_{(N)}$ for $j = 0, 2^N$. The amplitude of each 2^Nth step can be, for example,

$$V^{(N)}(j) = \frac{1}{l^{(N)}} \int_{a_{(N)}(j)}^{a_{(N)}(j+1)} \mathrm{d}z\, U(z) \qquad \text{or} \qquad U^{(N)}(j) = U\left(\frac{a_{(N)}(j) + a_{(N)}(j+1)}{2} \right).$$

Only the second choice will be considered, to avoid the 2^N integrals.

The approximation $P^{(N)}(z)$ of $P(z)$ is obtained from $U^{(N)}(z)$ just as $P(z)$ is obtained from $U(z)$ in (3). With $P^{(N)}(z)$ substituted in (13), (13) is exactly solvable as has already been demonstrated and its solution $M^{(N)}(z, z_0)$ is given by (16).

From (16) and for large N, $M^{(N)}(z, z_0)$ can be developed up to the third order in $l_{(N-1)}$:

$$M^{(N)}(Z, z_0) = \prod_{j=0}^{2^{N-1}-1} [M^{(N-1)}(a_{(N-1)}(j+1), a_{(N-1)}(j)) + l^3_{(N-1)} C^{(N-1)}(j) + \mathrm{O}(l^4_{(N-1)})] \tag{17}$$

with $C^{(N-1)}(j)$ the bounded operator, defined by

$$C^{(N-1)}(j) = \begin{bmatrix} -\frac{1}{16}U'(j) & 0 \\ \frac{1}{32}U''(j) & \frac{1}{16}U'(j) \end{bmatrix}. \tag{18}$$

A cluster expansion of (17) gives the lowest-order correction to $M^{(N-1)}(Z, z_0)$ in terms of $U(z)$ derivatives:

$$M^{(N)}(Z, z_0) = M^{(N-1)}(Z, z_0) + l^2_{(N-1)} \left(\sum_{i=1}^{2^{N-1}} \sum_{j_1 > \cdots > j_i = 0}^{2^{N-1}-1} \sum_{\alpha=1}^{i} l^i_{(N-1)} P(j_1) \ldots P(j_{\alpha-1}) \right.$$
$$\left. \times C^{(N-1)}(j_\alpha) P(j_{\alpha-1}) \ldots P(j_i) \right). \tag{19}$$

In (19) and for any order N, the term in brackets is majored in norm by $2(Z-z_0)\|C\|\exp[2\|P\|(Z-z_0)]$. Therefore, the series $\Sigma_{j=1}^{\infty} M^{(j)}(Z, z_0) - M^{(j-1)}(Z, z_0)$ is norm convergent to the exact solution of (13) with a $l^2_{(N+1)}$ rate which also, according to (12), is the convergence rate for $T(E)$.

To improve convergence, $M^{(N)}(Z, z_0)$ can be chosen as the zeroth order for a Peano perturbative development of $M(Z, z_0)$ because this series converges like the exponential. As in the interaction picture of time-dependent perturbation theory, the corresponding $P^{(N)}(z)$ gives the non-perturbative part of $P(z)$ in (13a) and $Q^{(N)}(z) = P(z) - P^{(N)}(z)$ the perturbation. (The $Q^{(N)}(z)$ singularity arising from $\det(Q^{(N)}(z)) = 0$ can be removed as was done for $P(z)$ in § 2.) Thus $M^{(N)}(z, z_0)$ defines the transformation from 'the Schrödinger picture' (13) to the 'interaction picture':

$$W(z, z_0) = [M^{(N)}(z, z_0)]^{-1} M(z, z_0) \tag{20}$$

where $W(z, z_0)$ is the solution of the equation

$$(\mathrm{d}W/\mathrm{d}z)(z, z_0) = \{[M^{(N)}(z, z_0)]^{-1} Q^{(N)}(z) M^{(N)}(z, z_0)\} W(z, z_0). \tag{21}$$

As usual, the Peano solution of (21) can be written

$$M(z, z_0) = M^{(N)}(z, z_0) + \sum_{i=1}^{\infty} \int_{z_0}^{z} \mathrm{d}z_1 \ldots \int_{z_0}^{z_{i-1}} \mathrm{d}z_i \times \{M^{(N)}(z, z_1) Q^{(N)}(z_1) M^{(N)}(z_1, z_2) \ldots Q^{(N)}(z_i) M^{(N)}(z_i, z_0)\}. \tag{22}$$

For large N, the Taylor expansion of $M^{(N)}(Z, z_0)$ and $M^{(N)}(Z, z_1) Q^{(N)}(z_1) M^{(N)}(z_1, z_0)$ as in (17) leads, after integration, to an l^4 rate of convergence for $M(Z, z_0)$, calculated

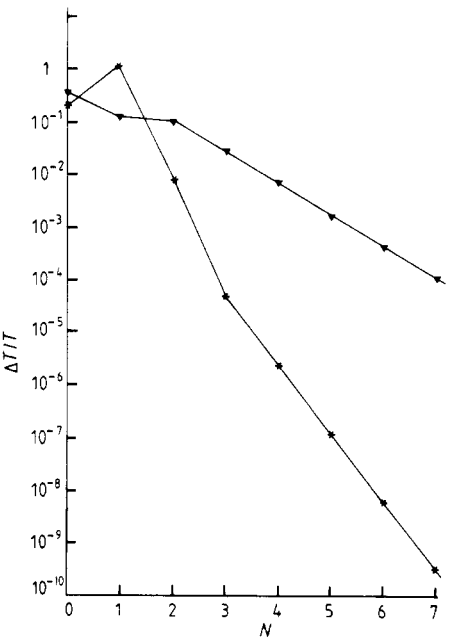

Figure 1. Comparison of the relative error for the zeroth (▼) and first (★) order in the Peano expansion for a trapezoidal barrier (width 20 Å, height 0.5 eV, applied voltage 10 V, effective mass 0.1 m_e, incident energy 0.1 eV).

to first order in (22). The resulting explicit expression for $M(z, z_0)$ can be written

$$M(z, z_0) = M^{(N)}(z, z_0) + \sum_{i=0}^{2^N-1} M^{(N)}(z, a_{i+1}) I_i M^{(N)}(a_i, z_0) \tag{23}$$

where $M^{(N)}(z, z_0)$ is given by (16) and

$$I_i = \int_{a_i}^{a_{i+1}} [V(x) - \tfrac{1}{2}V(a_{i+1} + a_i)] A_i(x)\, dx \tag{24a}$$

with

$$A_i(x) = \begin{bmatrix} (1/k_i)\sin(x_{i+1})\cos(x_i) & -(1/k_i^2)\sin(x_{i+1})\sin(x_i) \\ \cos(x_{i+1})\cos(x_i) & -(1/k_i)\cos(x_{i+1})\sin(x_i) \end{bmatrix} \tag{24b}$$

$$k_i = \left\{ \frac{2m}{\hbar^2} \left[E - V\left(\frac{a_i + a_{i+1}}{2} \right) \right] \right\}^{1/2} \qquad x_i = k_i(x_i - x)_{i=0,2^N-1}.$$

Equation (23) was tested with a trapezoidal barrier: zeroth and first order $T(E)$ given by (12) are plotted in figure 1. (Note that the first-order expression (23) for $N = 5$ is equivalent to the zeroth-order one for $N = 11$.)

4. Examples

First we consider the potential $U(z) = 15\,\mathrm{sech}^2(z)$ in order to test the accuracy of the proposed method for a continuous potential. The exact $T(E)$ is given by the formula (Landau and Lifshitz 1967):

$$T(E) = \frac{\sinh^2(\pi\sqrt{E})}{\sinh^2(\pi\sqrt{E}) + \cosh^2(\pi\sqrt{59/2})}. \tag{25}$$

Vigneron and Lambin (1980) have developed an algorithm for calculating $T(E)$ based on a finite-difference approximation of the Schrödinger equation. A comparison between this algorithm and ours is given in figure 2 ($U(z)$ has been taken to vanish for $z < 0$ and $z > 20$ in performing the numerical computations). Our zeroth order gives results with a similar relative error to the Vigneron and Lambin method but the first-order correction greatly improves the results.

Next the $T(E)$ for a quantum well has been calculated from (23) for several applied voltages and compared to the Tsu-Esaki (1973) approximation, which, for a single quantum well, is equivalent to replacing $U(z)$ by $\overline{U(z)} = \frac{1}{2}eV$ inside the well with V the applied voltage (see figure 3).

For low voltages compared to the barrier height, the Tsu-Esaki approximation agrees well with our calculation (see figures 4(a) and (b)). For large voltages, the barriers are thicker in the Tsu-Esaki approximation, so the bound states are better defined and the resonances are less broadened than in our approach (see figures 4(c) and (d)). The potential $U(z)$ of the biased quantum well (figure 3) is a piecewise continuous function with first-order discontinuities. Our calculation therefore uses the following partition procedure for each continuous part of $U(z)$: $N = 2$ for the barriers and $N = 4$ for the well, and the complete transfer matrix is obtained from (16). The resulting $T(E)$ is stable against an increase in N.

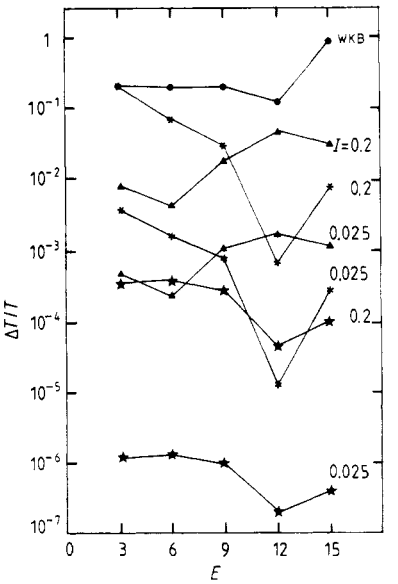

Figure 2. Comparison of the relative errors for the calculated transmissivity $T(E)$ of the barrier $V(z) = 15\,\mathrm{sech}^2(z)$ from the transfer-matrix technique in zeroth order (▲) and first order (★) and for the Vigneron-Lambin technique (*) and the WKB value (●). Two different values of the step size have been used. Only the points need to be considered, the connecting lines being arbitrary ($\hbar^2 E/2m = 3.81\ E$ is the energy in eV).

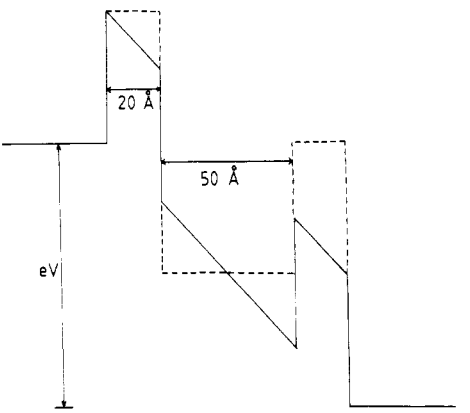

Figure 3. Model potential (full line) and Tsu-Esaki approximation (broken line) for a quantum well (widths 20 Å, separation 50 Å, height 0.5 eV, applied voltage 1.0 V, effective mass 0.1 m_e).

5. Conclusion

The one-dimensional stationary Schrödinger equation has been replaced by its dual equation for the transfer matrix $M(z, z_0)$. The general solution $M(z, z_0)$ is given, after a discretisation of the potential, as a Peano series. $M(z, z_0)$ is related to the transmission coefficient $T(E)$, leading to a numerical algorithm for a calculation of $T(E)$ for a potential of arbitrary shape. Work is in progress to extend this method to a non-local

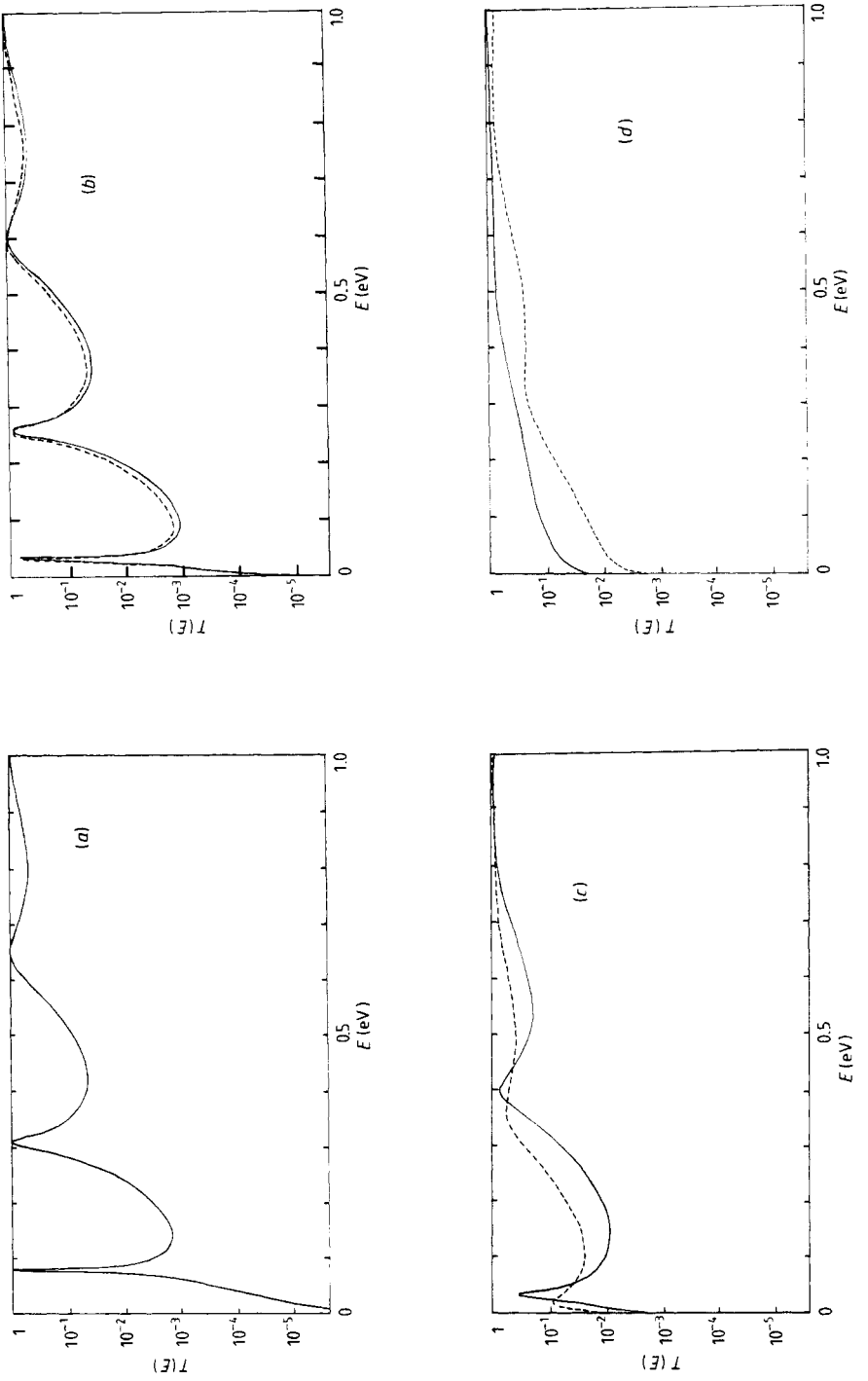

Figure 4. Transmission coefficient $T(E)$ of the quantum well (width 20 Å, separation 50 Å, height 0.5 eV, effective mass 0.1 m_e) calculated with the transfer-matrix technique (broken curve) and Tsu–Esaki approximation (full curve) for four different applied voltages: (*a*) 0 V; (*b*) 0.1 V; (*c*) 1.0 V; (*d*) 1.8 V.

potential in order to calculate $T(E)$ for structures such as the Aviram–Ratner diode using the pseudopotential technique.

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