Electron tunneling through indirect single barriers

P. A. Schulz
Max-Planck-Institut für Festkörperforschung, D-7000 Stuttgart 80, Federal Republic of Germany
(Received 7 June 1991)

Electron tunneling through single barriers, taking into account the coupling between two different band-edge profiles, is studied by means of a heuristic two-band tight-binding model. The tunneling probabilities, as well as the spectral weights of the tunneling states, are analyzed. This indirect-barrier system directly addresses the issue of Γ-X coupling in GaAs-(Al,Ga)As heterostructures. A relation between this physical system and the resonant tunneling through double-barrier quantum wells and also the atomic-potential scattering is established. The nature of the resonances in the transmission probabilities is discussed and it is shown under which conditions the shape of these resonances can change.

Tunneling through epitaxially grown semiconductor barrier systems has already been extensively studied. Remarkable are the resonance effects that can be detected in current-voltage characteristics of double-barrier quantum well (DBQW) structures. Experimental data are usually analyzed in the effective-mass-approximation (EMA) framework.[1] However, the EMA does not treat the important effect of the coupling between different conduction-band minima. This effect should be of importance in (Al,Ga)As-based systems with barriers having high Al concentrations, where the fundamental gap becomes indirect.[1] An analysis of this effect brings the attention back to single-barrier structures, where the direct (Γ) band-edge profile shows a real barrier, while the indirect (longitudinal X) one is a quantum well.[2] Realistic microscopic calculations,[3] showing the complex coupling effects between the quasibound states in indirect quantum well profiles and the ones in the barrier contacts, leave several open questions. Extensions of the EMA to deal with these systems in a realistic way show a striking problem of nonconservation of tunneling unitarity,[4] while more simplified approaches neglect important interference effects.[5] The aim of this paper is to refer to the tunneling through indirect barriers by means of a simple heuristic model, that can be solved exactly. The tunneling unitarity is conserved and interferences between the Γ and X tunneling "channels" are taken into account. A picture for the qualitative features of the problem is established, relating it to the well-known problem of resonant tunneling in DBQW's and with some aspects of three-dimensional atomic scattering. The unique nature of the tunneling asymmetric resonances is discussed, and we point out the fact that they show up in a large class of semiconductor systems due to very different mechanisms.

The model Hamiltonian consists of an atomic chain with two s-like orbitals (s and s^*) per site, treated in the tight-binding approximation, with nearest-neighbor interactions only. Intrasite hopping is not considered. In order to simulate a barrier (enclosed by semi-infinite contacts) structure, we consider two different sets of parameters, $J=B$, C, where B (C) stands for barrier (contact). Each set of parameters determines the following two-band dispersion relation for an infinite chain [dotted line in Fig. 1(a)]:

$$\begin{aligned}2E_J(k)= {} & E_J^s+E_J^{s^*}+(V_J^{s,s}+V_J^{s^*,s^*})\cos(ka)\\ & \pm\{[E_J^s-E_J^{s^*}+2(V_J^{s,s}-V_J^{s^*,s^*})\cos(ka)]^2\\ & +[4V_J^{s,s^*}\cos(ka)]^2\}^{1/2}\ ,\end{aligned} \tag{1}$$

where k is the one-dimensional wave number and a the chain lattice parameter. E_J^s and $E_J^{s^*}$ are the orbital energies and $V_J^{i,j}$ are the hopping elements; where $i,j=s,s^*$.

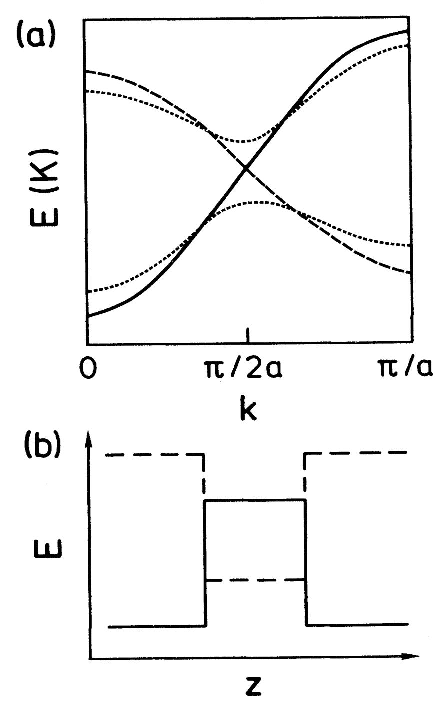

FIG. 1. (a) A schematic bulk dispersion relation for the two s-like orbital tight-binding chain (dotted lines). The model dispersion relation considered throughout the paper is given by the two cosine-like bands, continuous and dashed lines, whose corresponding band-edge (minima) profiles constitute the barrier potential profile shown in (b).

By setting $E^s = E^{s^*}$ the band structure reduces to two crossed cosinelike bands, the direct one, "Γ-like" [continuous line in Fig. 1(a)] and the indirect one, "X-like" [dashed line, Fig. 1(a)]. This is the simplest way to simulate a semiconductor conduction-band dispersion with two different minima. Now the hopping elements can be varied along the chain (the orbital energies are kept constant) in order to simulate the band-edge profiles shown in Fig. 1(b). The interface hopping elements are taken as the geometric average of those for the barrier (B) and the contact (C). This is an usual choice[6] that conserves the unitarity of the tunneling probability.[4] Since $E^s = E^{s^*}$, the Bloch functions for the states in each band are energy-independent linear combination of the atomic orbitals:

$$\Psi_J^{\pm}(k) = \sum_n e^{ikna}(|s\rangle + a_J^{\pm}|S^*\rangle) = \sum_n e^{ikna}\phi_J^{\pm} , \qquad (2)$$

$$a_J^{\pm} = 2V_J^{s,s^*}\{(V_J^{s^*,s^*} - V_J^{s,s}) \mp [(V_J^{s^*,s^*} - V_J^{s,s})^2 + 4(V_J^{s,s^*})^2]^{1/2}\}^{-1} , \qquad (3)$$

where + (−) stands for the direct (indirect) band and n is the chain site index. The hopping elements can be changed in a way that lets the band-edge profile remain constant, while the linear combination of atomic orbitals (ϕ's) of the direct (indirect) -like states in the contact region are changed from orthogonal ($\gamma = \langle \phi_C^+ | \phi_B^- \rangle = 0$) to slightly nonorthogonal ($\gamma \neq 0$) with respect to the indirect (direct) -like states in the barrier. For the parameters used here the effective masses for both minima in both materials are approximately the same ($m^* \approx 0.1 m_0$, for $a = 5.65$ Å). This choice eliminates effects from our results which depend on the differences of the effective masses. The zero of energy is the bottom of the direct conduction band in the contact. Referring to Fig. 1(b), the indirect and the direct barriers are, respectively, 0.1 and 0.3 eV high. The indirect minimum in the contacts is 0.4 eV above the zero of energy. The transmission probabilities, for zero applied bias, are calculated by means of a procedure based on the transfer-matrix technique described elsewhere.[7]

We are going to consider the energy range up to 0.4 eV, so there are only "Γ-like" propagating states in the contacts. The calculated transmission probabilities, as a function of incident electron energies, for barriers with increasing thicknesses are shown in Fig. 2. The resonances where the transmission probability reaches unity are associated with the quantized states in the quantum well defined by the indirect band-edge profile. The resonances can be either Lorentzian-like or asymmetric, showing even dips in the transmission. The dashed curves show the transmission probabilities when the quantized states are not allowed to couple with the propagating states in the contacts ($\gamma = 0$, pure direct barrier). The coupling between the incident electron wave function to the otherwise bound states in the barrier region is achieved when the indirect (direct) Bloch orbital of the barrier material is "tuned" to be slightly nonorthogonal to the direct (indirect) one in the contacts. All the results

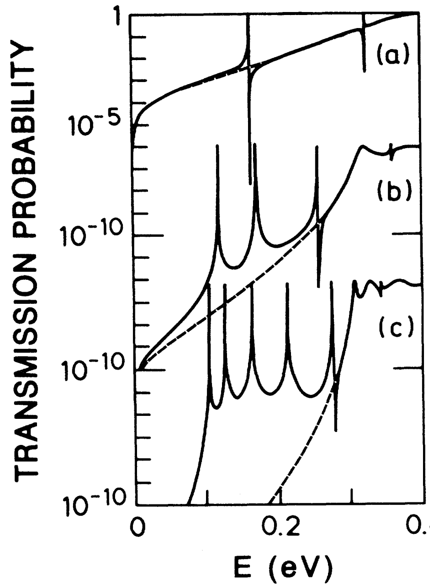

FIG. 2. Transmission probabilities as function of energy for single barriers, like the one shown in Fig. 1, for increasing barrier thickness (L, given in number of lattice parameters), with coupling between different Bloch functions ($\gamma = 0.02$, continuous lines) and for the corresponding direct barriers ($\gamma = 0$, dashed lines): (a) $L = 7a$, (b) $L = 15a$, (c) $L = 25a$.

shown here are for $\gamma = 0.02$. The evolution of the transmission probability can easily be followed when the barrier thickness is increased and new states are bound in the indirect well. Lower resonances change from an asymmetric to a Lorentzian shape when the transmission probability of the direct barrier is sufficiently reduced, with increasing barrier thickness. Quasibound states sufficiently near the direct barrier edge can still give rise to asymmetric resonances, as well as for those above this edge. It is also seen in Fig. 2 that the transmission probability for thin barriers is mainly determined by the direct barrier for the full range of energy, except near resonances. The apparent deviation from this behavior for thicker barriers, at off-resonances energies, is only due to the finite width of the resonances, that start to overlap, when bound states are sufficiently near to each other. Indeed, only near resonances the tunneling state has a large spectral weight for states near the indirect minimum of the Brillouin zone. Off resonance the tunneling states show essentially the same spectral weight distribution as a tunneling state at the same energy for $\gamma = 0$. In Fig. 3 we show the spectral weights[6] of the Fourier transform of the wave function inside the barrier region, where the barrier is the same as in Fig. 2(c), at different energies: at the first resonance (continuous line) and in the middle between the first and second resonances (dashed line). The equivalence to the second case for $\gamma = 0$ is shown by the dotted line.

The problem addresses the resonant tunneling in DBQW's in the EMA. There the presence of the well has also scarcely any effect off resonance, but can dramatically change the tunneling probability throughout the global barrier at the energies of the quasibound states.[8] In

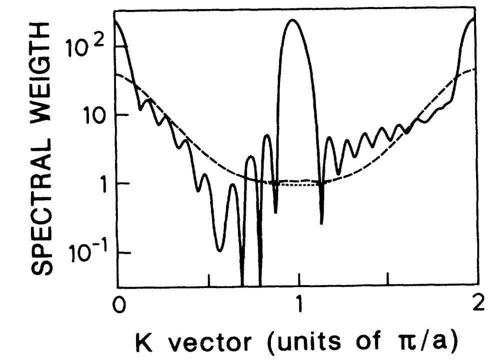

FIG. 3. Spectral weights of the Fourier transforms of tunneling states shown in Fig. 2(c) at different energies: at the first resonance (continuous line) and at the middle between the first and second resonance (dashed line). The dotted line shows the equivalent to the dashed one for the case of a pure direct barrier.

DBQW's the widths of the resonances are determined by the barrier thicknesses: the thinner the barriers the broader the resonances.[9] For the indirect single barrier, the symmetric resonance widths, although influenced by the direct barrier in the same way as in DBQW's, are principally determined by the Bloch-function coupling: the stronger the coupling, the wider the resonances. So it is possible, unlike in DBQW'S, to *make the direct barrier more transparent keeping the resonance width approximately constant.*

The width of the asymmetric resonances is also directly proportional to the Bloch-function coupling, but its dependence on the direct barrier is the opposite one as for Lorentzian resonances: the more transparent the direct barrier, the thinner the asymmetric resonances. This behavior can be observed in Figs. 2 and 4. In Fig. 4(a) we see that for a given indirect barrier, the shape of the resonance can be changed by modifying the Bloch-function coupling: $\gamma=0.02$ (continuous line) and 0.005 (dashed line). Experimentally this effect could be envisaged by applying hydrostatic pressure in order to lower the indirect [X in (Ga,Al)As systems] band profile, relative to the direct one, and bring the bound states to energies where the direct barrier transparency is low enough to permit Lorentzian resonances instead of asymmetric ones for the same coupling, $\gamma=0.02$, Fig. 4(b). It should be noticed here that new tunneling channels are opened, since the X-like propagating states in the contacts now become available in this energy range [dot-dashed line in Fig. 4(b)].

An analogy between the present one-dimensional scattering problem and the three-dimensional resonance scattering in atomic physics[10] is conceivable. Indeed, we can define a "potential scattering," the transparency of the direct barrier; and a "resonance scattering," the effect of the quasibound states in the indirect quantum-well profile of the barrier. It is well known that the interference between both scattering terms in atomic physics leads to asymmetric resonances in the scattering cross section, as discussed by Fano in the context of atomic au-

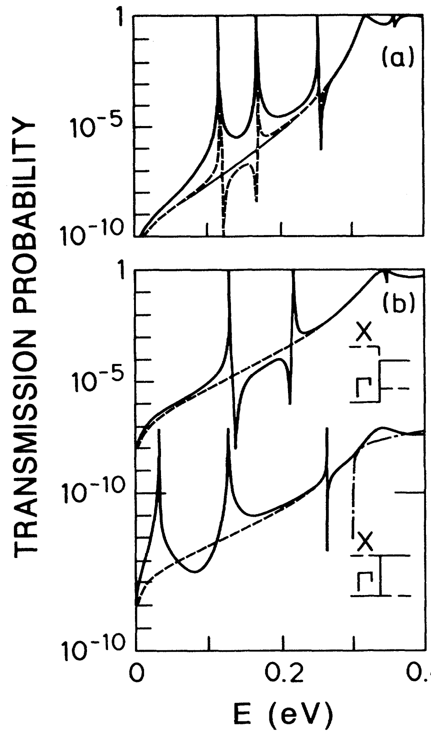

FIG. 4. (a) Transmission probability as a function of energy for the barrier of Fig. 2(b) for $\gamma=0.02$ (continuous line) and 0.005 (dashed line). (b) Transmission probability for a single barrier with $L=11a$ and $\gamma=0.02$ (dashed lines are for $\gamma=0$) for the two different band alignments shown as insets. The dot-dashed line is for tunneling probabilities associated with X-like propagating states in the contacts.

toionization processes[11] (discrete states coupled to a continuum of states). Keeping this picture in mind, we argue that the resonances in the transmission probabilities of the indirect barrier are Fano-like resonances, *irrespective of the barrier thickness.* Whenever $\gamma\neq0$, the X-like quantized states are always coupled to the continuum of Γ-like states in the contacts. In Fig. 5 we show transmis-

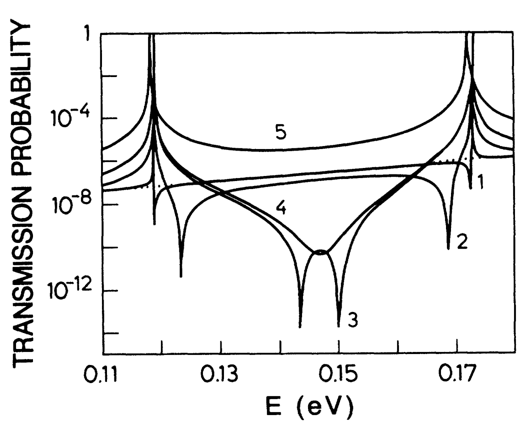

FIG. 5. Transmission probabilities for the single barrier of Fig. 2(b), in the energy range of the two first resonances, with increasing γ, from 1 to 5: $\gamma=0.001$, 0.005, 0.009 125, 0.009 25, 0.2, respectively.

sion probabilities for the same structure of Fig. 2(b), in the energy range of the two first resonances, for different values of γ. For very weak coupling, the resonances are asymmetric and very sharp. By increasing the coupling, the resonances become wider, with the dips moving toward each other, up to a point where they overlap, giving rise to symmetric resonances. This resonance shape flip occurs only for pairs of resonances, where the transmission dips approach each other by rising γ. Unpaired resonances, below the direct band edge in the barrier, remain asymmetric, *independent of the barrier thickness or coupling strength.* This pairing depends on the symmetry of the quasibound states and of the chain: for barriers with even number of sites, it is the first resonance that remains unpaired. With increasing barrier thickness, the coupling strength necessary to have pairs of Lorentzian resonances, instead of asymmetric ones, diminishes. So, for a given coupling between Bloch functions, the number of symmetric resonances rises (in pairs) with increasing barrier thickness.

In summary, for tunneling through an indirect (symmetric) barrier profile, the transmission probability always reaches unity at resonance and the important quantity to be considered is the resonance width. Off resonance, it is the direct barrier that determines the tunneling probability for all energy ranges, *irrespective of the effective masses associated with each minimum.* The problem immediately addresses resonant tunneling in the usual DBQW's, keeping in mind the striking feature that the resonance widths are now determined by microscopic (Bloch-function coupling) and mesoscopic (band-edge profile) physical properties. We have seen that the relationship between these properties determines the shape of the resonance and we suggest that this relationship *could be tuned experimentally.* An important insight given here is on the origin of the change from asymmetric to Lorentzian-like resonances when the barrier thickness is increased, while the microscopic description of the band structure is kept constant.

We would like to mention that asymmetric resonances in transmission probabilities in the context of vertical transport in semiconductor heterostructures seem to be a general effect. It happens always that one has a high off-resonance transmission probability together with a "resonance coupling" mechanism. This mechanism can be either elastic, as in the present case; or inelastic, as in phonon-assisted resonances in transmission probabilities for energies above a quantum-well profile.[12] The present system shows these asymmetric resonances due to a *coupling between single bands related to different layers in* the heterostructure. Another "elastic case" is the resonant tunneling of holes in DBQW's, where asymmetric resonances are introduced in the transmission probability, when different hole bands in the same heterostructure layer are coupled.[13]

The author would like to acknowledge Professor Dr. R. R. Gerhardts for helpful discussions and M. Rossmanith for a critical reading of the manuscript. Early suggestions on the model by Professor C. E. T. Gonçalves da Silva are also acknowledged. The author is grateful to the Brazilian agency Fundação de Amparo à Pesquisa do Estado de São Paulo for financial support.

[1]E. E. Mendez, in *Physics and Applications of Quantum Wells and Superlattices,* edited by E. E. Mendez and K. von Klitzing (Plenum, New York, 1987), p. 159.
[2]E. E. Mendez, W. I. Wang, E. Calleja, and C. E. T. Gonçalves da Silva, Appl. Phys. Lett. **50**, 1263 (1987).
[3]D. Y. K. Ko and J. C. Inkson, Semicond. Sci. Technol. **3**, 791 (1988).
[4]T. Ando and H. Akera, Phys. Rev. B **40**, 11 619 (1989).
[5]H. C. Liu, Appl. Phys. Lett. **51**, 1019 (1987).
[6]P. A. Schulz and C. E. T. Gonçalves da Silva, Phys. Rev. B **35**, 8126 (1987).
[7]P. A. Schulz, D. S. Galvão, and M. J. Caldas, Phys. Rev. B (to be published).
[8]B. Ricco and M. Ya. Azbel, Phys. Rev. B **29**, 1970 (1984).
[9]M. Büttiker, IBM J. Res. Dev. **32**, 63 (1988).
[10]L. D. Landau and E. M. Lifshitz, *Quantum Mechanics,* 3rd ed. (Pergamon, New York, 1977), Vol. III. p. 553.
[11]U. Fano, Phys. Rev. **124**, 1860 (1961).
[12]W. Cai, P. Hu, T. F. Zheng, B. Yudain, and M. Lax, Phys. Rev. B **41**, 3513 (1990).
[13]Calvin Yi-Ping Chao and Shun Lien Chuang, Phys. Rev. B **43**, 7027 (1991); R. Wessel and M. Altarelli, *ibid.* **39**, 12 802 (1989).