Scattering-assisted tunneling in double-barrier diodes: Scattering rates and valley current

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We describe the valley current of double-barrier diodes as a scattering-assisted tunneling current. Scattering processes are included by using Fermi's golden rule between the unperturbed states of the tunneling structure, in a true three-dimensional calculation, without adjustable parameters. Intrinsic processes (optical and acoustic phonons, alloy disorder) are treated as well as the contribution of interface roughness. We apply it to several situations (geometry, doping, temperature, materials) and demonstrate that the calculated valley current agrees well with observation both with regard to structure in the valley current and peak-to-valley ratios.

I. INTRODUCTION

The interest in tunneling has been renewed in solid-state physics[1] with electron-tunneling microscopy and quantum semiconductor devices. The advent of epitaxial growth techniques has made possible the Esaki-Tsu proposal of band-structure engineering[2] in order to obtain new transport properties, in particular, the resonant tunneling effect:[3] a structure consisting of two almost identical thin potential barriers (large gap material) separated by a narrow quantum well (small gap material) exhibits resonant transmission of electrons, once described by Bohm.[4] This quantum effect manifests itself macroscopically as negative differential conductivity (NDC) in the current-voltage characteristics (I-V), as observed by Chang, Esaki, and Tsu.[5] The double-barrier diode was becoming the first electronic device whose operating principle relies entirely on a quantum size effect.

It was only ten years later, when Sollner *et al.*[6] obtained significant resonant current and associated NDC that interest was stimulated by potential applications: very high frequency microwave devices and new functional logic devices.[7,8]

Apart from applications, this system has been extensively studied with a view to understanding quantum tunneling. Qualitatively the I-V characteristics of resonant tunneling structures are well understood[3,9] by the direct quantum-mechanical calculation of tunneling transmission through a double-barrier potential. For most energies the transmission probability is essentially the very low product of the transmission probabilities of each of the barriers; for energies close to the energy for which a bound state in the quantum well exists, the transmission increases dramatically and may even become unity if the two barriers have the same transmission probability at the resonance energy. This is analogous to the resonant transmission through a Fabry-Perot etalon in optics. The structure therefore acts as a strong energy filter and the current is essentially the integral of the distribution of electrons supplied times the transmission probability, so if electrons are supplied around the resonance, current can be strong; when the electrons supplied do not have energies around the resonance, the current is very low. An applied external voltage may sweep the resonance through the whole range of energies for which electrons are supplied leading to the characteristic current peak followed by a minimum obtained when the bound state of the well is below the lowest energy supplied with electrons.

This is the picture in which all current in the structure is carried by coherent tunneling. Electrons are injected from the contacts into coherent states for which the particle has a certain probability of being transmitted or reflected; after transmission or reflection the particle is adsorbed in the emitter or collector contact, respectively, without any other disturbance. The problems of this theory are well known. Tunneling depends exponentially on barrier heights and thicknesses, so that quantitative calculations cannot be expected to give very accurate results, but more importantly the peak-to-valley ratios (one indicator of the quality of the sample) observed experimentally (see a tabulation and references in, e.g., Ref. 10) are much smaller than those predicted by the coherent tunneling theory. A more complete calculation is required for the design of resonant tunneling devices.

Several effects may be invoked to explain these discrepancies: the real band structure, the charge distribution, nonequilibrium effects, and scattering processes. Our goal is to show that in double-barrier diodes the lack of quantitative agreement is almost exclusively due to deviations from the ideal structure that disturb the system. Since the coherent picture works for the main features it is reasonable to base an improved theory on that picture but treating the deviations as perturbations. We shall not deal with macroscopic deviations such as inhomogeneities in layer thicknesses, since they may be described macroscopically by having several diode sections in parallel. What we are interested in here are microscopic deviations: some are intrinsic and unavoidable such as phonons and, if some of the material is a ternary alloy, alloy disorder, and some are dependent on growth conditions such as impurities and interface roughness.

The effects of scattering on the tunneling current have been studied by several authors. Apart from phenomenological analyses,[11–14] there are microscopic models for optical phonons,[15–19] acoustic phonons,[19,20] interface roughness,[21,22] impurity,[23,24] or disorder.[25] The main drawback of those theories is that they are either models containing more or less unknown parameters, or that they are strictly one dimensional, or that they treat only one type of interaction, so that comparison with experiments remains almost qualitative.

Here we propose a simple approach to the problem. We describe the system as an ensemble of tunneling states extended over the whole structure between which transitions can occur due to perturbing interactions. For voltages above the resonant tunneling current peak the valley current is viewed as a sequential process in which an electron from the emitter is first captured into the bound state of the well by a scattering-assisted tunneling process. Once it is in the well it can tunnel to the collector side as easily as in the resonant situation, so that the current is assumed controlled by the capture process.

The theory is then reduced to calculating matrix elements of interactions whose strengths are known from bulk properties of the semiconductors. Our calculation is then three dimensional and quantitative; for extrinsic interactions, which vary from sample to sample, any theory is limited by the lack of precise microscopic knowledge of the system so one still has to resort to parametric models, of course. Without detailed deviation some results of our model have been presented elsewhere.[26–29] Further applications of this model will be studied elsewhere.[30]

The remaining part of the paper is organized as follows. In Sec. II, we describe the theory for scattering-assisted tunneling and give the details of scattering rates. In Sec. III we apply this model to several situations and discuss the effects of various parameters: geometry, doping, temperature, material. Section IV contains our conclusion and a comparison with other models for the tunneling current in double-barrier diodes including scattering processes.

II. THEORY

A. Coherent tunneling

We consider a standard III-V semiconductor heterostructure in which the modulation of chemical composition and doping along the growth axis creates a potential in one direction denoted z (longitudinal or perpendicular). Since the potential does not depend on the directions parallel to the interfaces, wave functions can be separated and the Schrödinger equation becomes essentially one dimensional. In the single-particle, effective-mass approximation,[31] which we shall use everywhere in the following, the component of wave functions in the z direction (envelope wave function) is determined by a BenDaniel-Duke Hamiltonian[32]

$$H^0 = -\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*(z)}\frac{d}{dz} + V(z) , \tag{1}$$

where the potential $V(z)$ is the sum of the band-edge potential due to the modulation of the band edge by the chemical composition of the semiconductors of the heterostructure, and the electrostatic potential due to the distribution of mobile carriers and ionized impurities when an external voltage ΔV_e is applied between emitter and collector. The former potential is fixed for a given heterostructure, whereas the latter has to be calculated more or less self-consistently.[30]

The kinetic-energy operator in Eq. (1) is related to the continuity of $1/m^*(z)d\psi/dz$, which is the connection rule at the interface for material-dependent effective mass[33] and rigorously, a material-dependent effective mass leads to a coupling of longitudinal and parallel motion, which can be described by an effective variation of the potential in Eq. (1):

$$\delta V(\varepsilon_\parallel, z) = \varepsilon_\parallel \delta \tilde{m}(z) , \tag{2}$$

where $\delta\tilde{m}(z)$ is the relative variation of effective mass and $\varepsilon_\parallel$ the parallel energy. We neglect this variation, which at most is about 50% of the Fermi energy, since this coupling of parallel and longitudinal motion would prevent the essentially one-dimensional treatment of the motion in the z direction. For simplicity we assume that emitter and collector are the same material.

We also do not intend to treat the possible mixing of different valleys or bands, but assume that the transport can be described as occurring only in the Γ band of the electrons. This of course excludes X-valley tunneling[34–37] and valence-band mixing of light and heavy holes known to be important in hole tunneling, e.g., see Refs. 38–41.

We consider first the unperturbed system, i.e., coherent tunneling. In Fig. 1 we show the one-dimensional (1D) potential seen by the electrons. All states in the unperturbed system can be written as

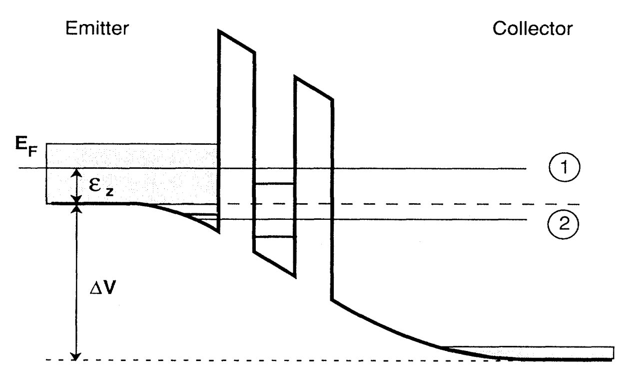

FIG. 1. Potential seen by the electrons in the double-barrier structure. States of type 1 are extended over the whole system, states of type 2 are only connected to the collector. Resonances in the active region indicated by thick lines are possible for both types of states.

$$\psi_k(r)=\frac{1}{\sqrt{\Omega}}\zeta_{k_z}(z)e^{i\mathbf{K}\cdot\mathbf{R}}, \quad \mathbf{k}=(\mathbf{K},k_z) . \tag{3}$$

Here $\Omega=LA$ is the volume of the system; in the directions parallel to the interfaces $(\mathbf{R})$ the free motion is described by plane waves; in the z direction, the longitudinal motion is described by an envelope wave function ζ_{kz}. For most values of k_z, it is essentially a reflected wave on either the emitter or collector side of the barrier; for select values resonant states exist with substantial occupation probability in the well between the two barriers or in the well formed by the accumulation layer in front of the first barrier. Spin is conserved in coherent tunneling and in all scattering processes to be discussed here, so that it will not be specifically introduced.

The basis of tunneling states ζ_{kz} is not unique. Our choice is imposed by the postulate of ideal contacts, as described in Sec. II B 1. These tunneling states are characterized by their asymptotic behavior far from the quantum structure because of the flat-band boundary conditions imposed by highly doped contacts. They are naturally written in the canonical basis of plane waves. On one side, the state is composed of an incident plane wave plus a reflected wave; on the other side, there is only one transmitted wave. We take the emitter contact band edge as energy zero and use the sign of k_z to distinguish states of equal energy. For $k_z>0$, $\varepsilon_z=\hbar^2k_z^2/2m^*$,

$$\zeta_{k_z}(z)=\sqrt{\alpha_{k_z}}\begin{cases} e^{ik_zz}+r_{k_z}e^{-ik_zz}, & z\to-\infty \\ t_{k_z}e^{i\tilde{k}_zz}, & z\to\infty , \end{cases} \tag{4}$$

and for $k_z<0$, $\varepsilon_z=\hbar^2k_z^2/2m^*-\Delta V$,

$$\zeta_{k_z}(z)=\sqrt{\alpha_{k_z}}\begin{cases} t_{k_z}e^{i\tilde{k}_zz}, & z\to-\infty \\ e^{ik_zz}+r_{k_z}e^{-k_zz}, & z\to\infty , \end{cases} \tag{5}$$

with, respectively,

$$\frac{\hbar^2\tilde{k}_z^2}{2m^*}=\frac{\hbar^2k_z^2}{2m^*}\pm\Delta V , \tag{6}$$

and α_{kz} the normalization factor

$$\alpha_{k_z}=\frac{2}{1+|r_{k_z}|^2+|t_{k_z}|^2} . \tag{7}$$

In the expressions r_{kz} and t_{kz} are complex-valued quantities, which can be calculated only by solving the Schrödinger equation for the Hamiltonian H^0 in Eq. (1). The solutions can be written for each energy as a 2×2 scattering matrix that relates the outgoing to the incoming amplitudes.

A special case is found for $-(2m^*\Delta V)^{1/2}<k_z<0$. Those states (designated type 2 in Fig. 1) are not connected to the emitter:

$$\zeta_{k_z}(z)=\begin{cases} 0, & z\to-\infty \\ e^{ik_zz}+e^{i\varphi_{kz}}e^{-ik_zz}, & z\to\infty , \end{cases} \tag{8}$$

and a particle which enters such a state will end in the collector. In particular, a quasibound state is completely described by the phase shift φ_{kz}; it is a resonance in the energy derivative of the scattering phase shift. The local density of states (DOS) associated to this resonance is given by[42,43]

$$D_r(\varepsilon_z)=\frac{1}{2\pi}\frac{d\varphi}{d\varepsilon_z} , \tag{9}$$

and the lifetime of the quasibound states is $\hbar/\Delta\varepsilon_z$, where $\Delta\varepsilon_z$ is the width of the resonance in Eq. (9).[44]

Being the totality of linearly independent solutions to a Schrödinger equation, the states of type 1 and 2 constitute a complete set of wave functions

$$\int dk_z\zeta_{k_z}(z)\zeta_{k_z^*}(z')=2\pi\delta(z-z') . \tag{10}$$

They are specifically normalized in the sense that

$$\langle\zeta_{k_z}|\zeta_{k_z'}\rangle=2\pi\delta(k_z-k_z') . \tag{11}$$

This is easily shown by direct integration in real space. The orthogonality of two degenerate states ζ_{k_z} and $\zeta_{-\tilde{k}_z}$ poses a fundamental problem. It requires that

$$r_{k_z}t^*_{-\tilde{k}_z}+t_{k_z}r^*_{-\tilde{k}_z}=0 . \tag{12}$$

However, time-reversal symmetry and conservation of probability current implies

$$r_{k_z}t^*_{k_z}+t_{k_z}r^*_{-\tilde{k}_z}=0, \quad \frac{t_{k_z}}{k_z}=\frac{t_{-\tilde{k}_z}}{\tilde{k}_z} . \tag{13}$$

Therefore Eq. (12) is fulfilled only in the case $\Delta V=0$ and the two states cannot be perfectly orthogonal when $\Delta V\neq0$. This result was suggested by Coon and Liu[45] and discussed by Stone and Szafer[46] and is contrary to the claim of Kriman, Kluksdahl, and Ferry,[47] whose extension of a Lippman-Schwinger result is suspect.

It is not difficult to choose two combinations which are orthogonal, of course, but we prefer to neglect the nonorthogonality because use of those combinations would be incompatible with the postulate of ideal contacts which will be used in the following. We want to point out that in most real systems, and in particular for the valley current which is the object of our work, $|t_{kz}|\ll1$, so that the problem is not quite so serious apart from very special cases. In view of this approximation we also neglect the deviation from unity of the normalization factors α_{kz} in Eqs. (4) and (5) in the rest of the paper.

In terms of r_{kz} and t_{kz} the reflection and transmission probabilities are given by

$$R(\varepsilon_z)=|r_{k_z}|^2, \quad T(\varepsilon_z)=\frac{\tilde{k}_z}{k_z}|t_{k_z}|^2 , \tag{14}$$

and the conservation of probability current implies the unitarity relation

$$R(\varepsilon_z)+T(\varepsilon_z)=1 . \tag{15}$$

Around a transmission resonance ε_r, a Breit-Wigner expression applies,[44] i.e., the transmission has Lorentzian shape

$$T(\varepsilon_z)=\frac{T_r}{1+\left[\varepsilon_z-\frac{\varepsilon_r}{\Gamma}\right]^2}\ , \tag{16}$$

in which the broadening and the transmission at resonance are expressed in terms of partial width for decay of the resonant level in the emitter or collector continuum

$$T_r=\frac{4\Gamma_e\Gamma_c}{(\Gamma_e+\Gamma_c)^2},\quad \Gamma=\frac{\Gamma_e+\Gamma_c}{2}\ . \tag{17}$$

In the Oppenheimer formalism[48,49] these parameters are expressed as a function of the coupling through the barrier V_i in a way that resembles Fermi's golden rule:

$$\Gamma_i=2\pi\sum_{k_z}|V_{ik_z}|^2\delta(\varepsilon_z-\varepsilon_w)\ , \tag{18}$$

in which the δ function describes the conservation of energy in direct tunneling from a contact state of energy ε_z to the quasibound state in the well of energy ε_w. This paves the way for a transfer Hamiltonian treatment of resonant tunneling.[12,50,51]

However, the validity of this method is questioned for thin barriers and in our quantitative calculations we rather obtain the basis functions $\zeta_{kz}(z)$ numerically. The structure is divided into subunits (planes of atoms) within which the electric field may be assumed constant and solutions of Schrödinger equation are combinations of Airy functions. The transfer matrix for the whole system as well as the wave functions in the quantum structure are obtained by multiplying the individual transfer matrices of the subunits and using the connection rules at interfaces.[3,52] A material-dependent effective mass is used, since it strongly controls attenuation of wave functions in the barriers.

Scattering states are defined by a wave vector $\mathbf{k}=(\mathbf{K},k_z)$. However, for emitter states, interesting quantities such as transmission probabilities depend only on longitudinal and parallel energy ε_z and $\varepsilon_\parallel$ (due to rotational invariance), so for convenience we can equally well describe an emitter electron by those two energies instead of wave vectors.

B. Scattering-assisted tunneling

1. Current density

The emitter and collector contacts are considered ideal in the sense that any particle that arrives at the contact is absorbed by scattering processes in the contact reservoir; the contact furthermore populates all states that inject particles according to the equilibrium Fermi-Dirac f_{FD} distribution with a temperature and chemical potential determined by the doping of the contact and the external voltage. In particular we will not consider deviations from those equilibrium distributions due to scattering processes in the active region.

In the following we will neglect the small contribution of current injected from collector to emitter (corresponding to a voltage larger than the emitter Fermi energy). The emitter provides electrons $\mathbf{k_e}=(\mathbf{K},k_z)$ with the Fermi-Dirac statistics f_{FD}. The general expression of the current density from emitter to collector, with a factor 2 for spin, is

$$J=2e\sum_{\mathbf{k_e}}f_{\mathrm{FD}}(\mathbf{k_e})j_z(\mathbf{k_e})\ . \tag{19}$$

The z component of the current density of an emitter state may be written as the product of the current injected by the emitter by the probability to reach the collector (transmission probability)

$$j_z(\mathbf{k_e})=\frac{\hbar k_z}{\Omega m^*}T(\mathbf{k_e})=\frac{\hbar k_z}{\Omega m^*}T(\varepsilon_z,\varepsilon_\parallel)\ , \tag{20}$$

so that the current density may be written

$$J=\frac{2e}{h}\int_0^\infty d\varepsilon_z\int_0^\infty d\varepsilon_\parallel D(\varepsilon_\parallel)f_{\mathrm{FD}}(\varepsilon_z+\varepsilon_\parallel)T(\varepsilon_z,\varepsilon_\parallel)\ . \tag{21}$$

In this expression, $D(\varepsilon_\parallel)$ is the parallel DOS without spin degeneracy, which is constant in a 2D system

$$D(\varepsilon_\parallel)=\frac{m^*}{2\pi\hbar^2}=D_0\ . \tag{22}$$

The reason we introduce the parallel DOS is discussed in Ref. 30 where a magnetic field is applied to the structure. Then many expressions will be generalized essentially by considering the Landau-level DOS instead of D_0.

2. Coherent tunneling

In the absence of scattering processes, the current through the structure reduces to the coherent tunneling current carried by the tunneling states. In the following the superscript 0 shall indicate coherent tunneling. The z component of the current density of an emitter state is

$$j_z^0(\mathbf{k})=\frac{\hbar}{m^*}\,\mathrm{Im}\left[\psi_{\mathbf{k}}^*(\mathbf{r})\frac{\partial}{\partial z}\psi_{\mathbf{k}}(\mathbf{r})\right]=\frac{\hbar k_z}{\Omega m^*}T^0(k_z)\ . \tag{23}$$

In their original article, Tsu and Esaki[3] assumed that the current is dominated by coherent tunneling. Then, as the transmission only depends on longitudinal motion, it is possible to group together the states that have the same longitudinal motion

$$J=\frac{e}{h}\int_0^\infty d\varepsilon_z T^0(\varepsilon_z)F(\varepsilon_z)\ , \tag{24}$$

in which the "supply function"[1] describes the statistics of injected electrons:

$$F(\varepsilon_z)=2\int_0^\infty d\varepsilon_\parallel D(\varepsilon_\parallel)f_{\mathrm{FD}}(\varepsilon_z+\varepsilon_\parallel)\ , \tag{25}$$

or

$$F(\varepsilon_z)=\frac{m^*k_BT}{\pi\hbar^2}\log\left[1+\exp\left[\frac{E_F-\varepsilon_z}{k_BT}\right]\right]\ , \tag{26}$$

with E_F the Fermi level in the emitter. According to Eq.

(17) and the analysis of Weil and Vinter,[12] the resonant transmission has a peak of order $T_{\min}/T_{\max}$, where $T_{\min}$ and $T_{\max}$ are the smaller and greater transmissions of the two barriers. In particular, it becomes unity in the symmetry case; the width of the resonant peak is proportional to $T_{\max}$, so that the resonant current is proportional to $T_{\min}$, whereas the off-resonant current is of order $T_{\min}T_{\max}$. Therefore this simple model predicts a peak current to valley current ratio of order $1/T_{\max}$, much higher than experimentally observed, by several orders of magnitude, as will be apparent in the figures of Sec. III.

3. *Valley current*

To go beyond this coherent tunneling approximation, one has to consider scattering processes in the active region which permit transitions between the tunneling states. To calculate the scattering rates we use Fermi's golden rule in the Born approximation,[44] so that if we denote the perturbing Hamiltonians H_j^p, where j can indicate interaction with acoustic phonons, optical phonons via the Fröhlich interaction, alloy disorder scattering in the barriers, interface roughness, or impurity scattering, the scattering rate between state $\mathbf{k}$ and state $\mathbf{k}'$ is given by

$$S(\mathbf{k}\to\mathbf{k}')=\frac{2\pi}{\hbar}\sum_j N_j^{\pm}|\langle\mathbf{k}'|H_j^p|\mathbf{k}\rangle|^2[1-f_{\mathrm{FD}}(\mathbf{k}')]\times\delta(E_{\mathbf{k}'}-E_{\mathbf{k}}\pm\hbar\omega_j) \tag{27}$$

for emission/absorption of a quantum $\hbar\omega_j$, where

$$N_j^-=\frac{1}{\exp\left[\dfrac{\hbar\omega_j}{k_BT}\right]-1},\quad N_j^+=N_j^-+1 \tag{28}$$

are the Bose factors for an inelastic scattering process. In Eqs. (27) and (28) $\hbar\omega_j$ is the energy transferred in the scattering process; for elastic processes $\omega_j=0$ and $N_j^{\pm}=1$; it is assumed as usual that the different interactions do not interfere. It is important to notice that even elastic processes can change k_z, so that they act as inelastic processes if one only considers energy due to motion in the z direction.

The general problem of relating the current through the structure to the scattering rates is very intricate because electrons may suffer multiple scattering events and the zeroth order (coherent tunneling) is already a scattering problem.[29] So here we will use simple approximations.

All scattering processes do not contribute equally to the current through the structure. In resonant tunneling structures there are quasilocalized levels in the structures that give resonances in the coherent tunneling probability as well as scattering probability: The matrix element in the golden rule Eq. (27) requires an overlap of the wave functions in the initial and final states in the region where the interaction takes place. Specific to the double barrier is that nonresonant states have a very small probability in the well and even less beyond the second barrier. We can therefore neglect contributions from scattering processes between nonresonant states of opposite sign of k_z. We can also neglect processes between nonresonant states of the same sign since they both have almost equal probability (either both near 0 or both near 1) of arriving at the collector; their contribution really describes the access resistance between the emitting contact and the barriers. The only scattering processes that are important therefore involve at least one state that has nonnegligible probability in the well, i.e., a resonance.

In the valley region, i.e., for voltages above the resonant tunneling current peak, the resonant state of the well ($\mathbf{k}_w$) is pulled below the emitter conduction band edge. Those states are then resonances of type 2 that have no tunneling connection with the emitter and can only be populated by scattering processes.

The main contribution to the current is then a process by which the electrons in the emitter are trapped into the resonant state in the well, from which they will eventually arrive in the collector contact (sequential tunneling):

$$j_z(\mathbf{k}_e)\approx\frac{1}{A}\sum_{\mathbf{k}'\approx\mathbf{k}_w}S(\mathbf{k}_e\to\mathbf{k}')\ . \tag{29}$$

Dividing by the flow of electrons injected from the emitter into the state $\mathbf{k}_e$ defines the scattering-assisted tunneling probability that an electron starting in state $\mathbf{k}_e$ arrives at the collector:

$$W(\mathbf{k}_e)=W(\varepsilon_z,\varepsilon_\parallel)=\frac{Lm^*}{\hbar k_z}\sum_{\mathbf{k}'\approx\mathbf{k}_w}S(\mathbf{k}_e\to\mathbf{k}')\ . \tag{30}$$

In the valley region the scattering processes then become more important than direct tunneling because there is no transmission state into which to scatter. Direct tunneling from the emitter is entirely switched off and only scattering processes contribute to the current

$$T^0(\varepsilon_z)\ll W(\varepsilon_z,\varepsilon_\parallel)\ll 1\ . \tag{31}$$

The second inequality means that scattering processes can be treated perturbatively. It will be shown to be well satisfied in the quantitative results (Sec. II C 5). The first inequality of Eq. (31) is a very interesting property of double barriers compared to single tunneling barriers in that it becomes possible to study the scattering-assisted tunneling processes without a large background of direct tunneling current.

The scattering processes are then responsible for the valley current in the I-V characteristics of resonant tunneling structures and the final expression for the valley current is given by Eq. (21) with

$$T(\varepsilon_z,\varepsilon_\parallel)\approx W(\varepsilon_z,\varepsilon_\parallel)\ . \tag{32}$$

For scattering process j, we have

$$W_j(\varepsilon_z,\varepsilon_\parallel)=\frac{Lm^*}{\hbar k_z}\sum_{\mathbf{k}'}S_j(\mathbf{k}\to\mathbf{k}')\ . \tag{33}$$

A considerable simplification of the calculation can be obtained by replacing the sum over final states near the resonance by a truly bound state in the well:[29]

$$\psi_{w\mathbf{K}}(\mathbf{r})=\frac{1}{\sqrt{A}}\zeta_w(z)e^{i\mathbf{K}\cdot\mathbf{R}}\ . \tag{34}$$

This will be correct as long as the overlap of the emitter states with the tail of the resonant state on the collector side of the double barrier is negligible compared with the overlap in the well. Numerically this means that we calculate the wave functions in the modified potential illustrated in Fig. 2. The parallel energy in the well $\varepsilon_{\parallel w}$ is defined by energy conservation

$$\varepsilon_{\parallel w}=\frac{\hbar^2 K_w^2}{2m^*}=\varepsilon_z-\varepsilon_w+\varepsilon_{\parallel}\mp\hbar\omega_j , \tag{35}$$

which gives a threshold for the process

$$\varepsilon_z+\varepsilon_{\parallel}>\varepsilon_w\pm\hbar\omega_j . \tag{36}$$

Moreover, in this off-resonance situation, the well states remain nearly empty so that we can replace the Pauli factor $1-f_{\mathrm{FD}}(\mathbf{k}')$ by unity. There remains an integration over the angle θ between emitter and well parallel momentum, as shown in Fig. 3:

$$W_j(\varepsilon_z,\varepsilon_{\parallel})=\frac{2m^*}{\hbar^2 k_z}N_j^{\pm}D(\varepsilon_{\parallel w})\int_0^{\pi}d\theta\, M_j(\mathbf{k},\theta) , \tag{37}$$

with the matrix element

$$M_j(\mathbf{k},\theta)=\Omega|\langle\mathbf{k}|H_j^p|\mathbf{K}_w(\theta)\rangle|^2 . \tag{38}$$

The tunneling wave functions are explicitly included in the matrix elements, so that our model is not restricted to thick barriers as is the transfer Hamiltonian formalism. We have also introduced the parallel DOS of the final level. The Bose factor is equal to unity in case of elastic scattering. For the parallel motion we assume a parabolic dispersion with the emitter material effective mass.

C. Calculation of matrix elements

Quantitative results on the valley current now require the evaluation of the interaction matrix elements. They

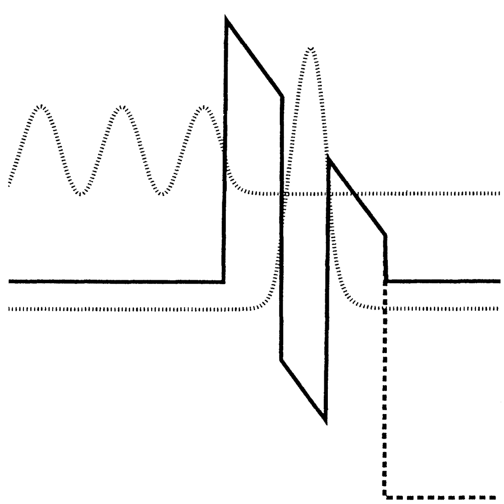

FIG. 2. Idealized double-barrier potential used to calculate the well bound state and any incident electron wave function.

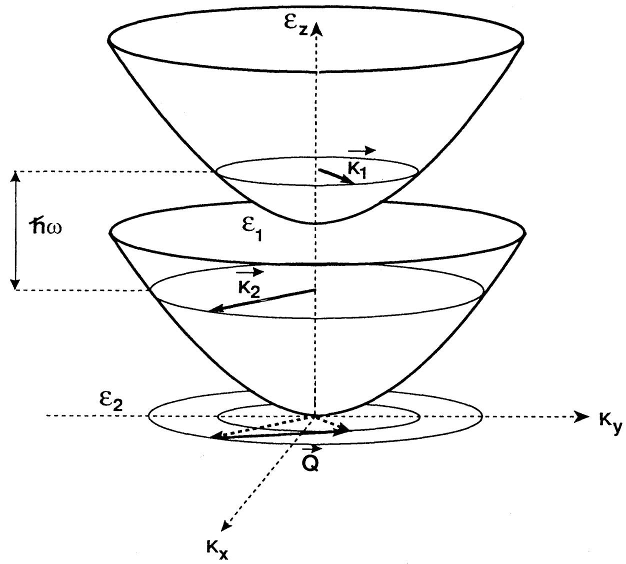

FIG. 3. Scattering process between a state $(\varepsilon_1,\mathbf{K}_1)$ and $(\varepsilon_2,\mathbf{K}_2)$ involving a transfer of energy $\hbar\omega$ and a transfer of momentum $\mathbf{Q}$.

are perfectly analogous to intersubband scattering matrix elements in two-dimensional systems.[31,53] We start with longitudinal-optical (LO) phonon scattering which, in polar semiconductors, is expected to be the dominant scattering process allowing the transfer of a carrier from the emitter to the well. Then we evaluate matrix elements for the other intrinsic processes: acoustic phonons and alloy disorder. These processes are unavoidable. Among extrinsic processes (elastic scatterers), we neglect impurity scattering,[23,54,55] since usually undoped spacers are added to limit this scattering mechanism.[30] We rather concentrate on interface roughness scattering, which has been recently suggested to be dominant in the fall of the resonant current after the resonant peak[56] and which is unavoidable in all present epitaxial growth techniques.

The phonon modes interacting with electrons are considered to be the same as those of bulk material (contacts and well). Only the polar optical-phonon (LO) and deformation-potential acoustic-phonon (AC) interactions are taken into account; other kinds of electron-phonon coupling, such as the piezoelectric interaction, are much weaker and not considered here. More refined models for the coupling with phonon modes associated with the multilayered structure, such as interface or slab modes, exist in the literature,[57] but for simplicity we keep only the bulk modes. The sum rule on form factors derived by Mori and Ando[58] gives some support for the validity of the approximation. We also ignore screening.

The electron-phonon interaction is described by the following Hamiltonian[59] for phonons of wave vector $\mathbf{q}=(\mathbf{Q},q_z)$ and of frequency ω_q:

$$H_{e\text{-ph}}=\frac{1}{\sqrt{\Omega}}\sum_{\mathbf{q}}\alpha_{\mathbf{q}}[e^{i}(\mathbf{q}\cdot\mathbf{r}-\omega_q t)+\mathrm{H.c.}] . \tag{39}$$

The interaction is delocalized in all the structure and not restricted to the well. The first term leads to emission (+) and the second to absorption (−). Assuming the phonon dispersion is much smaller than the electronic dispersion we find the matrix element of Eq. (38) as

$$M^{\pm}(\mathbf{k},\theta)=\sum_{\mathbf{q}}|\alpha_{\mathbf{q}}|^2\,|\langle\mathbf{k}|e^{\pm i\mathbf{q}\cdot\mathbf{r}}|\mathbf{K}_w(\theta)\rangle|^2 \ . \qquad (40)$$

The $\exp(i\mathbf{Q}\cdot\mathbf{R})$ dependence of the phonon potential leads, upon integration in the plane parallel to the interfaces, to conservation of parallel momentum:

$$\mathbf{Q}_\theta=\pm[\mathbf{K}-\mathbf{K}_w(\theta)],\quad Q_\theta=(K^2+K_w^2-2KK_w\cos\theta)^{1/2} \ . \qquad (41)$$

Only the summation over q_z remains:

$$M^{\pm}(\varepsilon_z,\mathbf{Q}_\theta)=\frac{1}{2\pi}\int dq_z\,\alpha^2_{q_z,\mathbf{Q}_\theta}|\langle\zeta_{k_z}|e^{\pm iq_z z}|\zeta_w\rangle|^2 \ . \qquad (42)$$

The lack of definite momentum for the electrons in the z direction leads to the dependence of the matrix element on Q_θ, a dependence not considered in one-dimensional models, e.g., by Cai *et al.*[17] Note the cancellation of the normalization factor of extended states over the whole structure ($1/\sqrt{L}$).

1. LO phonons

A LO phonon creates in a polar, crystal, like GaAs, a polarization wave. Associated to this polarization wave is an electric potential on which electrons can be scattered. For LO phonons (dispersionless Einstein band), we use the Fröhlich interaction strength[59]

$$\alpha_{\mathbf{q}}=\frac{\alpha_{\mathrm{LO}}}{q},\quad \alpha_{\mathrm{LO}}=\left[\frac{e^2\hbar\omega_{\mathrm{LO}}}{2\varepsilon_p}\right]^{1/2} , \qquad (43)$$

where $1/\varepsilon_p=1/\varepsilon_\infty-1/\varepsilon_s$, $\varepsilon_s,\varepsilon_\infty$ being the static and high-frequency limit permittivities, respectively. The summation over q_z in Eq. (42) gives[12,55,60]

$$M^{\mathrm{LO}\pm}(\varepsilon_z,Q_\theta)=\frac{\alpha^2_{\mathrm{LO}}}{2}\frac{F^{\mathrm{LO}}(\varepsilon_z,Q_\theta)}{Q_\theta} , \qquad (44)$$

where we have introduced the form factor for LO phonon scattering:

$$F^{\mathrm{LO}}(\varepsilon_z,Q)=\int_{-\infty}^{\infty}dz\int_{-\infty}^{\infty}dz'\zeta^*_{k_z}(z)\zeta_w(z)e^{-Q|z-z'|}\times\zeta_{k_z}(z')\zeta^*_w(z') \ . \qquad (45)$$

Above the threshold $\varepsilon_z+\varepsilon_\parallel>\varepsilon_w\pm\hbar\omega_{\mathrm{LO}}$, the capture is possible with the probability

$$W^{\mathrm{LO}\pm}(\varepsilon_z,\varepsilon_\parallel)=\frac{e^2\omega_{\mathrm{LO}}m^*}{2\hbar\varepsilon_p}N^{\pm}_{\mathrm{LO}}\frac{1}{k_z}D(\varepsilon_{\parallel w})\times\int_0^\pi d\theta\frac{F^{\mathrm{LO}}(\varepsilon_z,Q_\theta)}{Q_\theta} \ . \qquad (46)$$

This expression accounts for the 3D interaction process, involving a transfer of parallel momentum, as described in Fig. 3.

2. Acoustic phonons

In case of acoustic phonons,

$$\alpha_{\mathbf{q}}=\alpha_{\mathrm{AC}}\sqrt{q} ,\quad \alpha_{\mathrm{AC}}=\left[\frac{\hbar\Xi^2}{2\rho v_s}\right]^{1/2} , \qquad (47)$$

where Ξ is the acoustic deformation potential, ρ is the density, and v_s is the sound velocity. As well as the interacting electrons, the phonons which take part in the scattering process are near the zone center. Hence acoustic phonon scattering is quasielastic and we may use the Debye approximation $\omega_q=v_s q$. For a sufficiently high temperature ($k_BT>1$ meV), acoustic-phonon statistics may be approximated by

$$N^{\pm}_{\mathbf{q}}\cong\frac{k_BT}{\hbar\omega_q}\Longrightarrow\alpha^2_{\mathbf{q}}N^{\pm}_{\mathbf{q}}\cong\alpha^2_{\mathrm{AC}}\frac{k_BT}{\hbar v_s} \ . \qquad (48)$$

Then integration over q_z is straightforward, and summing over absorption and emission, we get

$$M^{\mathrm{AC}}(\varepsilon_z)=2\frac{k_BT}{\hbar v_s}\alpha^2_{\mathrm{AC}}F^{\mathrm{AC}}(\varepsilon_z) , \qquad (49)$$

with the form factor for acoustic-phonon scattering:

$$F^{\mathrm{AC}}(\varepsilon_z)=\int_{-\infty}^{\infty}dz|\zeta_{k_z}(z)|^2|\zeta_w(z)|^2 \ . \qquad (50)$$

Above the threshold $\varepsilon_z+\varepsilon_\parallel>\varepsilon_w$, the capture probability due to acoustic phonons is then

$$W^{\mathrm{AC}}(\varepsilon_z,\varepsilon_\parallel)=\frac{2\pi m^*\Xi^2k_BT}{\hbar^2\rho v_s^2}D(\varepsilon_{\parallel w})\frac{F^{\mathrm{AC}}(\varepsilon_z)}{k_z} \ . \qquad (51)$$

3. Alloy disorder

In an alloy $A_xB_{1-x}C$ with atomic potentials V_A and V_B, alloy disorder scattering (AL) is usually treated[31] by a contact potential

$$V^{\mathrm{AL}}(\mathbf{r})=\Delta V\delta x(\mathbf{r})\quad\text{where }\Delta V=V_A-V_B , \qquad (52)$$

with the following assumption on the concentration fluctuation δx:

$$\langle\delta x(\mathbf{r})\delta x(\mathbf{r}')\rangle=\Omega_0x(1-x)\delta(\mathbf{r}-\mathbf{r}') , \qquad (53)$$

where Ω_0 is the primitive cell volume. Configurational average leads to the same term as for acoustic phonons

$$\langle|\langle\mathbf{k}|\delta x(\mathbf{r})|\mathbf{k}'\rangle|^2\rangle_{\mathrm{av}}=\Omega_0x(1-x)\frac{1}{\Omega}\sum_{\mathbf{q}}|\langle\mathbf{k}|e^{i\mathbf{q}\cdot\mathbf{r}}|\mathbf{k}'\rangle|^2 , \qquad (54)$$

so that the square matrix element becomes

$$M^{\mathrm{AL}}(\varepsilon_z)=\Omega_0\Delta V^2x(1-x)F^{\mathrm{AL}}(\varepsilon_z) , \qquad (55)$$

with the following form factor for alloy disorder scattering:

$$F^{\mathrm{AL}}(\varepsilon_z)=\int_{\mathrm{alloy}}dz|\zeta_{k_z}(z)|^2|\zeta_w(z)|^2 \ . \qquad (56)$$

Above the threshold $\varepsilon_z+\varepsilon_\parallel>\varepsilon_w$, the capture probability due to alloy disorder is then

$$W^{\mathrm{AL}}(\varepsilon_z,\varepsilon_\parallel)=\frac{2\pi m^*\Omega_0\Delta V^2 x(1-x)}{\hbar^2}D(\varepsilon_{\parallel w})\frac{F^{\mathrm{AL}}(\varepsilon_z)}{k_z} . \quad (57)$$

4. *Interface roughness*

The usual model for interface roughness is a distribution of terraces of monolayer thickness Δ and of lateral size described by a Gaussian distribution with a characteristic correlation length Λ.[53,61] The perturbing potential can therefore be described by

$$V^{\mathrm{IR}}(\mathbf{r})=V_b\Delta\delta(z-z_i)F(\mathbf{R}) , \quad (58)$$

with the correlation function for the fluctuations

$$\langle F(\mathbf{R})F(\mathbf{R}')\rangle=\exp\left[-\frac{|\mathbf{R}-\mathbf{R}'|^2}{\Lambda^2}\right] , \quad (59)$$

where V_b is the barrier height and z_i is the average position of the interface. The configurational average gives

$$\langle|\langle\mathbf{K}|F(\mathbf{R})|\mathbf{K}_w(\theta)\rangle|^2\rangle_{\mathrm{av}}=\frac{1}{A}\int d^2\mathbf{R}e^{i\mathbf{Q}_\theta\cdot\mathbf{R}}\exp\left[-\frac{R^2}{\Lambda^2}\right] , \quad (60)$$

where $\mathbf{Q}_\theta=\mathbf{K}-\mathbf{K}_w(\theta)$, so that the square matrix element becomes

$$M^{\mathrm{IR}}(\varepsilon_z,Q_\theta)=\pi\Lambda^2V_b^2\Delta^2F^{\mathrm{IR}}(\varepsilon_z)\exp\left[-\frac{Q_\theta^2\Lambda^2}{4}\right] , \quad (61)$$

with the form factor for interface roughness scattering

$$F^{\mathrm{IR}}(\varepsilon_z)=|\zeta_{k_z}(z_i)|^2\,|\zeta_w(z_i)|^2 . \quad (62)$$

We define

$$G_\Lambda^{\mathrm{IR}}(\varepsilon_z,\varepsilon_\parallel)=\Lambda^2\int_0^\pi d\theta\exp\left[-\frac{Q_\theta^2\Lambda^2}{4}\right] \quad (63)$$

$$=\pi\Lambda^2\exp\left[-\frac{(K^2+K_w^2)\Lambda^2}{4}\right]I_0\left[\frac{KK_w\Lambda^2}{2}\right] , \quad (64)$$

where I_0 is the modified Bessel function of order zero.

Above the threshold $\varepsilon_z+\varepsilon_\parallel>\varepsilon_w$, the capture probability due to interface roughness is

$$W^{\mathrm{IR}}(\varepsilon_z,\varepsilon_\parallel)=\frac{2\pi m^*\Delta^2V_b^2}{\hbar^2}D(\varepsilon_{\parallel w})\frac{F^{\mathrm{IR}}(\varepsilon_z)}{k_z}G_\Lambda^{\mathrm{IR}}(\varepsilon_z,\varepsilon_\parallel) . \quad (65)$$

This is the contribution of one interface, the quality of which is characterized by Λ. Then the contributions of all the interfaces must be added, with their respective qualities. Despite the usual asymmetry in growth quality between top ($Al_xGa_{1-x}As$ on GaAs) and bottom interfaces,[62] we have taken the same value for all interfaces.

It is worth comparing this expression with that obtained by Leo and MacDonald.[22] They treat the disorder as a perturbation to the tunneling wave-function basis in the general Lippman-Schwinger formalism, but at the end they keep only the first-order term, which gives exactly our result; in their Eq. (11) the integral over E_z' can be identified as $2\pi|\zeta_w(z_i)|^2$ in our notation, when the resonant state is narrow, so the two expressions are identical if one takes

$$\frac{N_T}{A}A_T^2=G_\Lambda^{\mathrm{IR}} , \quad (66)$$

where the notation on the left-hand side is that of Leo and MacDonald. The two models therefore closely resemble each other. However, if we take the small Q limit in our expression for G^{IR}, the right-hand side of Eq. (66) becomes $\pi\Lambda^2$. The value of Λ is usually determined by fitting mobilities obtained with the full correlation function to experimental data, so the value of 40 nm^2 for the coupling constant in Eq. (66) used by Leo and MacDonald seems lower than one would expect from the experimental value of $\Lambda\approx6.5$ nm.[63,64]

5. *Comparison of capture probability*

In Fig. 4 we show as an example the total (summed over $\mathbf{K}'$) scattering rates into the resonant state of the well in a situation where the well level is 20 meV below the emitter conduction band edge in a standard structure of two $Al_{0.4}Ga_{0.6}As$ barriers of 5-nm thickness and a well of 5 nm. The abscissa is the component of energy in the z direction of the incoming state ε_z. We stress that the

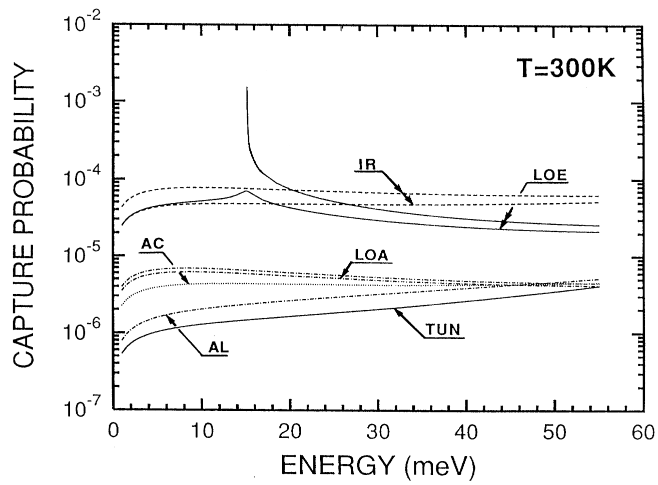

FIG. 4. Example of scattering transmission rates via the resonant state for the different interactions as a function of ε_z, at 300 K. Scattering by optical-phonon emission (LOE) and absorption (LOA), by interface roughness (IR), by alloy disorder (AL), and by acoustic phonons (AC), as well as the direct tunneling transmission (TUN) are shown. The structure has a 5-nm well, 5-nm $Al_{0.4}Ga_{0.6}As$ barriers and the contact doping is $10^{18}/cm^3$. The resonant state is 20 meV below the emitter conduction-band edge, and the transmission rates are shown for $\varepsilon_\parallel=0$ (upper curves) and 25 meV (lower curves); only LO and IR processes depend on $\varepsilon_\parallel$.

TABLE I. Parameters used in present computation.

	GaAs/ $Al_xGa_{1-x}As$	$Ga_{0.47}In_{0.53}As$/ $Al_{0.48}In_{0.52}As$
m^* (m_e)	$0.067+0.083x$[a]	0.041/0.075[b,c]
ΔE_c (eV)	$0.8x$[d]	0.53[e]
ε_s (ε_0)	12.9[f]	13.73[b]
ε_∞ (ε_0)	10.9[f]	11.36[b]
$\hbar\omega_{LO}$ (meV)	36.6[f]	32.7[b]
Ξ (eV)	12.0[g]	5.89[b]
ρ (kg/m^3)	5320[f]	5590[b]
V_s (m/s)	5220[f]	4810[b]
$\Omega_0\Delta V_{Al}^2$(Å^3 eV^2)	175	175

[a]S. Adachi, J. Appl. Phys. **58**, R1 (1985).
[b]T. P. Pearsall, *GaInAsP Alloy Semiconductors* (Wiley, New York, 1982).
[c]D. Olego *et al.*, Appl. Phys. Lett. **41**, 476 (1982).
[d]H. Kroemer, Surf. Sci. **174**, 299 (1986).
[e]Y. Sugiyama *et al.*, Jpn. J. Appl. Phys. **25**, L648 (1986).
[f]J. Blakemore, J. Appl. Phys. **53**, R123 (1982).
[g]B. Vinter, Phys. Rev. B **33**, 5904 (1986).

scattering probability due to acoustic phonons or alloy disorder does not depend on parallel motion. For optical phonon scattering and interface roughness scattering the two curves correspond to a kinetic energy parallel to the interfaces of 0 and 25 meV, respectively. It can be seen that all the scattering processes are more important than the direct tunneling probability, but they are all much smaller than 1 as claimed in Eq. (31), leading to the first-order approximation Eq. (32). Thus the valley current is primarily controlled by the capture rate from the emitter into the well and is given by the sum over the trapping rates of populated initial states.

In the results shown the parameters used for phonon and alloy disorder scattering are given in Table I and for interface roughness we have used the values $\Lambda=6.5$ nm and $\Delta=0.3$ nm (one atomic layer of GaAs) found by mobility measurements.[63,64]

III. RESULTS

In this section we show some characteristic quantitative results of our theory, in particular on the structure and magnitude of the current beyond the resonant peak. The parameters used in the calculations are listed in Table I.

A. Intrinsic scattering processes

We first consider the case of a "standard" structure with 5-nm $Al_{0.4}Ga_{0.6}As$ barriers, a 4-nm well (so that there is only one resonant level in the well), and a contact doping of 10^{18} cm^{-3}. In Fig. 5 we show the coherent tunneling current in the resonant regime and compare coherent tunneling current and scattering current in the off-resonant regime, at low temperature (4 K) in Fig. 5(a) and at room temperature in Fig. 5(b). At room temperature, coherent tunneling current beyond the resonance is mainly thermoionic. We have included only intrinsic scattering processes (LO and acoustic phonons, alloy disorder). The peak-to-valley ratio becomes 40 at 4 K (rather than 235 when no scattering is taken into account) and 6 at 300 K (rather than 19).

Alloy disorder scattering and LO phonon emission (LOE) increase only little with temperature. On the contrary, acoustic phonon scattering and LO phonon absorption are very sensitive to the temperature. The scattering currents decrease with increasing voltage, whereas the tunnel current increases. Therefore, the valley voltage is shifted from the termination of resonant tunneling to a higher value. Between these two voltages, the tunnel current increases approximately from 5% to 50% of the total current. As for the rest of the current, it is shared at low temperature between LOE (90% to 75%) and alloy disorder scattering. At room temperature, the ratios become 70% for LOE and around 10% for each of alloy disorder scattering, acoustic-phonon scattering, and LO phonon absorption.

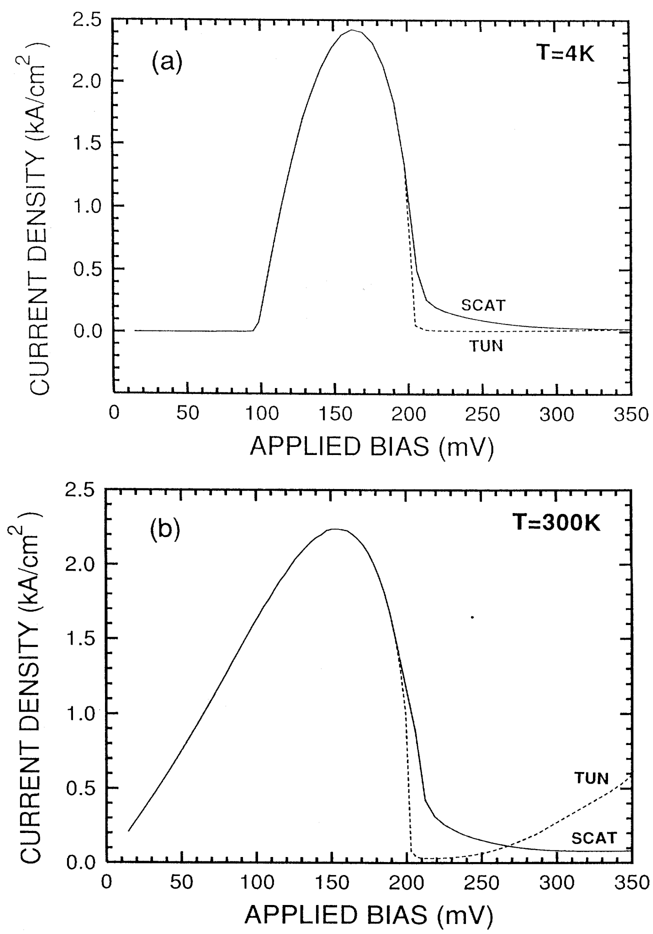

FIG. 5. Calculated characteristics of a double-barrier diode (4-nm well, 5-nm $Al_{0.4}Ga_{0.6}As$ barrier, doping: 10^{18}/cm^3) at 4 K (a) and 300 K (b). The coherent tunnel valley current is shown by the dashed line (TUN) and the contribution of scattering processes by the solid line (SCAT).

B. Interface roughness scattering

In Fig. 6 we show results for the contribution of interface roughness to the valley current calculated for the same structure as in Fig. 5 at 4 and 300 K. We show the dependence on the correlation length Λ for 2, 5, and 10 nm. Two features are noteworthy. The contribution to the nonresonant part of the current from interface roughness is mainly important in the fall after the resonant peak and is comparable in magnitude with the LO phonon emission contribution, and the dependence with Λ is not trivial because of the function $G^{\mathrm{IR}}(\Lambda)$ defined in Eq. (63). Experimentally, values of Λ of 5–7 nm are found for the GaAs/$Al_xGa_{1-x}As$ system,[63,64] so we see that the interface roughness can be expected to roughly double the valley current determined by intrinsic processes. In all the following simulations a value of 6.5 nm has been used for the interface roughness correlation length.

The most systematic investigation of *I-V* characteristics has been carried out by Guéret *et al.*[56] on double-barrier structures of varying barrier thickness but a constant rather low barrier height. They conclude, based on a simplified diffraction model, that the most likely cause for the observed large valley current should be interface roughness. From our study we believe it is mainly in the fall of the resonant current that interface roughness is dominant, and Guéret's deduction of a reasonable correlation length of $\Lambda \approx 8$ nm is indeed based on the broadening of the resonance peak. One should not conclude, however, that the nonresonant current is always dominated by interface roughness scattering; the relative importance of the different scattering mechanisms depends on structure, voltage, and temperature in a nontrivial way.

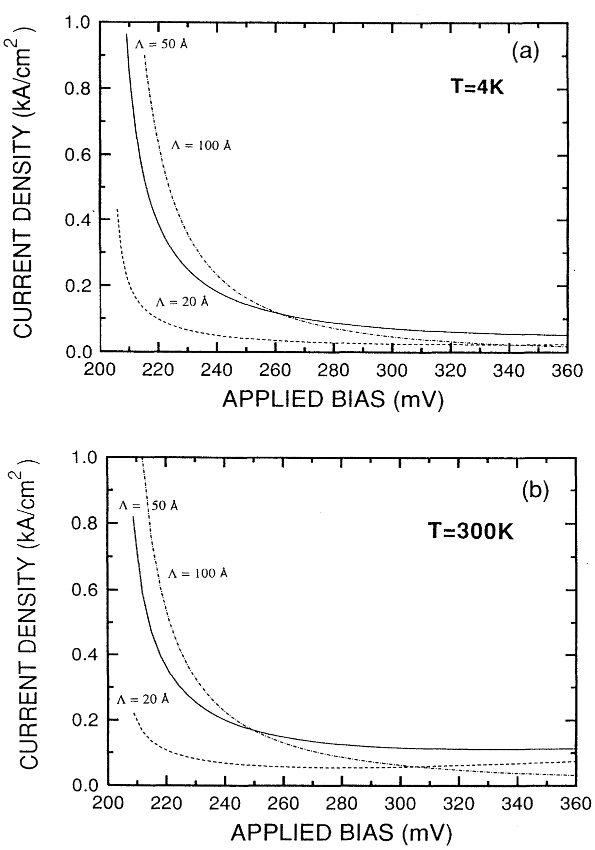

FIG. 6. Interface roughness scattering in the same structure as in Fig. 5, at 4 K (a) and 300 K (b). Three values of the correlation length are compared: 20 Å (dashed line), 50 Å (solid line), and 100 Å (dash-dotted line). The monolayer thickness is 3 Å.

C. LO phonon satellite

The direct signature of the LO phonon interaction in the double-barrier structures is the appearance of phonon replicas of the main elastic peaks in the valley region. In comparison, the phonon effect is extremely difficult to observe in single barriers where it is masked by much larger elastic tunneling.[65] In fact, it is not a direct replica of the resonance but rather the manifestation of the threshold for LO phonon emission found in Eq. (46): LO phonon emission only begins for voltages such that $E_F > \varepsilon_w + \hbar\omega_{\mathrm{LO}}$. The coupling then gives a maximum just after the threshold when $E_F - \varepsilon_w = \hbar\omega_{\mathrm{LO}}$ followed by a more slowly decreasing tail. In the cases described above with a highly doped emitter and a Fermi energy larger than the phonon energy this threshold occurs during the resonant process so that we just get the tail of the LOE satellite. In order to resolve the phonon peak it is therefore necessary to have a lower doping near the emitter barrier: $E_F < \hbar\omega_{\mathrm{LO}}$.

This was precisely the case in a structure studied by Goldman, Tsui, and Cunningham.[66] Their observation of a LO phonon satellite was the first experimental proof of scattering processes in the valley current [see the inset of Fig. 7(a)]. In Fig. 7 we have tried to recover their observation using the same parameters (barrier width 8.5 nm with 40% Al, well width = 5.6 nm, doping = 2×10^{17} cm^{-3}). The difference from our earlier result[26] is that the influence on the potential shape has been taken into account in a Thomas-Fermi-like manner.[30] The resonant current is calculated as purely coherent and the current beyond resonance includes interface roughness scattering. It can be seen that excellent agreement with the experiment is obtained for the shape of the characteristics (particularly the sudden drop of the resonant current) and for the relative intensity of the peaks: 4% experimentally, 4.5% theoretically. We find a much lower current scale, by a factor of 40 (the calculated resonant level width is 10^{-4} meV). Our simulations (varying the barrier thickness and height and the effective mass in the barriers) show that, contrary to the current scale, the general form of the characteristic is not very sensitive to the transparency of the barrier. Although Goldman, Tsui, and Cunningham,[66] (and Leadbeater *et al.*[67]) conclude that they observed AlAs LO phonons (47 meV), our calculation has been done for the GaAs LO phonon, since our model is not adapted to localized phonon modes. In Fig. 7(b) the logarithmic scale allows the comparison of the various contributions to the valley current and their dependence with the bias. This figure shows that there is no general rule for the valley current. In the fall of the resonant current, interface roughness dominates among elastic scattering processes. At higher voltage, LOE dominates. But for intermediate voltages, there may be a strong contribution of alloy disorder.

Our result is very similar to the one of Wingreen, Jacobsen, and Wilkins.[15] However, they have considered a very large width of the resonant level (7.2 meV) and hence obtain a very large current density 2000 times larger than observed experimentally. Our result is also comparable with the simulation of Rudberg[18] as far as the amplitude of the phonon replica is concerned, but we note that he obtains a "shoulder" to the main peak rather than the expected threshold for phonon emission. Con-

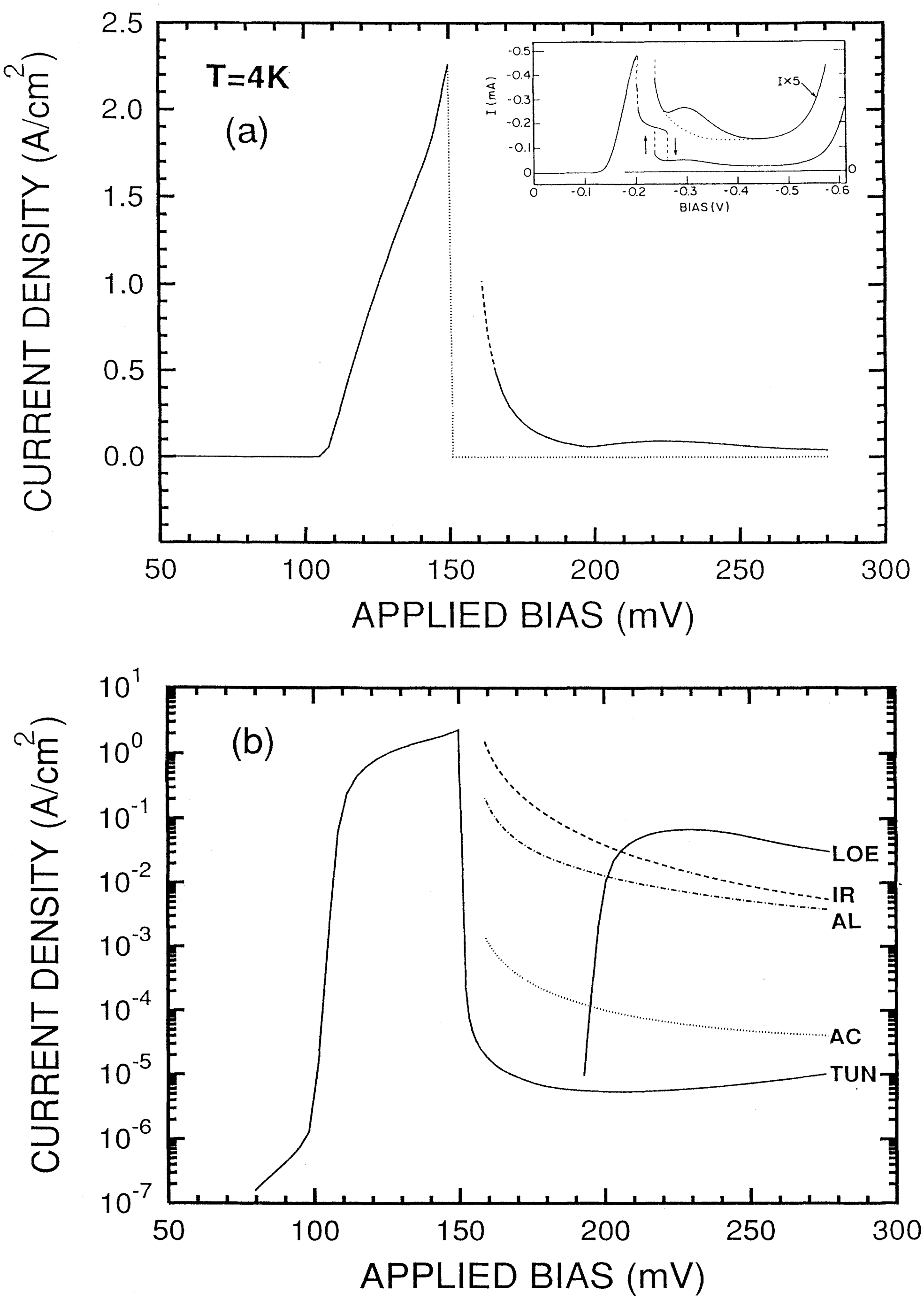

FIG. 7. (a) Calculated current-voltage characteristic for the structure studied by Goldman, Tsui, and Cunningham (Ref. 66) (5.6-nm well, 8.5-nm $Al_{0.4}Ga_{0.6}As$ barriers, doping: $2\times10^{17}/cm^3$, 4 K), showing the satellite peak due to LO phonon emission. Inset: experimental curve of Goldman, Tsui, and Cunningham (reverse bias). (b) Detail of the scattering contributions to the current in a logarithmic scale.

cerning the phonon active in the tunneling we mention the model calculation of Jauho on resonant tunneling in the presence of inelastic scattering,[68] in which it seems that barrier phonons are of minor importance.

D. Comparison of material performance

Starting from the structure described in Sec. III A, we discuss the influence of the intrinsic scattering processes on the peak-to-valley ratio at room temperature, as a function of the thickness of the two identical barrier layers. This ratio is calculated in Fig. 8(a) with (i) and without (ii) scattering. Apart from the quasilinear dependence of the ratio (i), it is interesting to note that it is not proportional to the ratio (ii), that is to say not simply governed by the overlap of wave functions. The peak current (also shown) is another essential parameter for the design but we see that optimization of such a device requires proper account of the scattering processes. The reduction of peak-to-valley ratio is remarkable, and since those curves are calculated without interface roughness scattering, we see that our results describe very well the fact that peak-to-valley ratios of more than 4 in the GaAs/Al_xGa_{1-x}As system have rarely been observed, the highest ratio to date being 4.9 in a structure with 3-nm barriers and 60% Al concentration.[69]

Other materials containing indium have been shown to give much higher peak-to-valley ratios.[70–72] The smaller effective masses allow a better contrast between the width of the resonant level and the off-resonant transmission. Moreover, for a given transparency of the barriers, higher barriers practically eliminate the thermoionic component of the valley current up to room temperature. Let us illustrate these points in the case of the $Al_{0.48}In_{0.52}As/Ga_{0.47}In_{0.53}As$ system, where we have studied a structure described by Lakhani *et al.*[71] (barriers of 7.2 nm, well of 4.3 nm, doping 10^{18} cm^{-3}). At 77 K, we find a peak-to-valley ratio of 123 instead of 9000 without scattering; at 300 K, this ratio becomes 19 instead of 144. Experimentally, these ratios are 39 and 7 at 77 K and 300 K, respectively. Using 530 meV for the barrier height, the calculated peak current density is 17A/cm^2, a factor of 20 lower than the experimental value. In Fig. 8(b), we compare the performances of this material with GaAs/Al_xGa_{1-x}As for comparable current densities. Scattering currents are reduced as well as coherent tunnel current, but in addition the ratio between thee contributions depends strongly on the material.

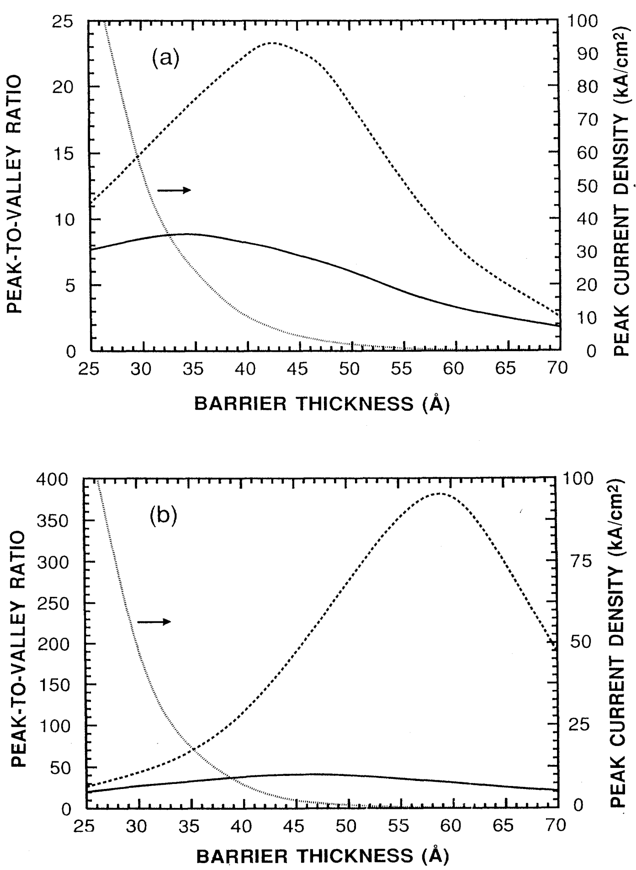

FIG. 8. (a) Effect of the barrier thickness on the peak-to-valley ratio at room temperature. Dashed line, coherent tunneling only; full line, intrinsic scattering processes included (phonon and alloy disorder). The materials are GaAs/$Al_{0.4}Ga_{0.6}As$; the well width is 4 nm; the doping is $10^{18}/cm^3$. The peak current density (dotted line) is also shown. (b) Same figure for $Ga_{0.47}In_{0.53}As/Al_{0.48}In_{0.52}As$ (well width 4.3 nm) in the same range of current density.

E. Intersubband scattering

We now focus on another situation occurring in a double-barrier structure with at least two levels, for voltages such that resonant tunneling is possible through the second level (see Fig. 9). Then there is competition between the resonant tunneling and scattering processes between the two levels in the well. Figure 10 shows on logarithmic scale a case where this intersubband scattering dominates. The detail of the different scattering contri-

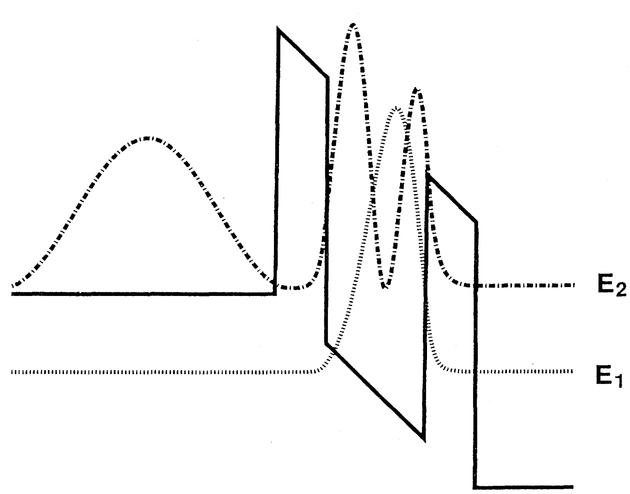

FIG. 9. Potential and wave functions squared in the situation of resonant tunneling through the second level.

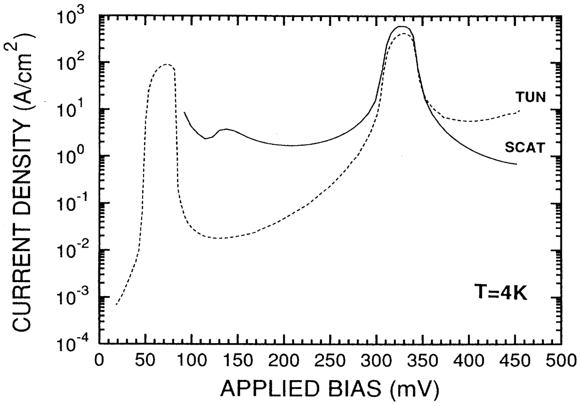

FIG. 10. Comparison of scattering currents (SCAT) and coherent tunneling current (TUN) in a double-barrier diode with two resonant levels (8-nm well, 5-nm $Al_{0.4}Ga_{0.6}As$ barriers, doping: $2\times10^{17}/cm^3$, 4 K). These curves show the LO-phonon satellite after the first resonance and the dominance of scattering around the second resonance.

butions is published elsewhere.[27] Then, the transport mechanism is truly sequential: electrons tunnel through the first barrier into the second level of the well, then are scattered down to the first level from which they tunnel out of the well into the collector. Note that the calculated case corresponds to a low doping in the mitter so that the LO phonon satellite is visible between the two resonant peaks. Evidence of such sequential tunneling was reported by Payling *et al.*[73] from magnetotunneling measurements (see Sec. III) and confirmed by Skolnick *et al.*[74] using a photoluminescence experiment. Both techniques show a large charge buildup on the lower well subband during second-level resonance.

IV. CONCLUSION

We have described the valley current of a double-barrier system as a scattering-assisted tunneling current. The major calculational work is in the evaluation of matrix elements of the perturbing interactions and the integrations over initial and final states. The theory shows very satisfactory quantitative agreement with experimental valley current in several systems of different geometry, materials, doping, and temperature.

As mentioned earlier other theories for transport including scattering in resonant tunneling structures have been published, so it is worth pointing out the similarities and differences with the other main models. In fact phonon-assisted tunneling (or hopping) has earlier been described for superlattices several years ago by Tsu and Döhler[75] in the high-field case and more recently by Palmier and Chomette[76] for the low-field situation. It should also be mentioned that our work is a fairly natural extension of calculations of phonon-assisted tunneling between two coupled quantum wells,[77] enlarged to treat other scattering processes by Ferreira and Bastard.[78]

For resonant tunneling structures the influence of the coupling to optical phonons has been studied in various Green's-function formalisms by Wingreen, Jacobsen, and Wilkins,[15] Jonson,[16] Rudberg,[18] and Cai *et al.*[17] Those models are all essentially one dimensional and the transfer of momentum between perpendicular and parallel motion is at most considered in estimating the one-dimensional effective coupling. On the other hand, the models can be completely solvable and show multiphonon processes.

Another difference from our model is also in the description of the electron-phonon coupling, which in some models is restricted to the well. This means that the spectrum of the well state is changed to contain phonon satellites; this enhances the density of final states for emitter electron to tunnel into, but the tunneling matrix element remains unchanged and the escape rate of the electron initially in the well is unchanged by the coupling to the phonon. A coupling between emitter states and the well state through phonon interaction in the barriers seems to open up an additional channel for tunneling into and out of the well and some estimates have been made by Wu and McGill.[19] Apart from these specific differences it seems that, as in the case of interface roughness scattering, the first-order approximations to the models are equivalent to our approach.

In the case of elastic-scattering processes it is clear that a 3D model is necessary in order to obtain a contribution to the valley current. Such models have been described for impurity scattering in the well by Fertig, He, and Das Sarma[23] and (for the broadening of the transmission resonance) by Gu *et al.*[24] We have already shown the equivalence between our model and that of Leo and MacDonald[22] for the interface roughness scattering in Sec. II C; results without configurational average have been published by Liu and Coon.[21] For completeness we also mention the phenomenological description of 1D double barriers including quasielastic scattering by Büttiker.[14]

As for less perfect barriers, phonon-assisted resonant tunneling via a pointlike state in the barrier has been studied by Glazman and Shekter[20] and strongly disordered barriers have been modeled by Schulz and Gonçalves da Silva.[25]

It can be seen that our method is related on many points with those described above. The main contribution of our work is therefore the complete quantitative treatment of all the scattering processes. This is the only way to be able to show that the valley current is not dominated but rather controlled by interface roughness scattering in some voltage intervals and by optical phonon scattering for other voltages. It is also the only way to verify if the usual scattering processes suffice to explain the characteristics of double-barrier diodes.

We believe the results we have obtained indeed show that for most resonant tunneling structures the valley current, peak-to-valley ratios are well described even quantitatively by our first-order Born approximation in the basis of the transmission wave functions imposed by the contacts so that the double-barrier diode is an interesting system to study scattering processes.

On the other hand, we are well aware that our method has its limitations. The first-order Born approximation excludes contributions due to virtual transitions or interference effects. The effect of multiple-scattering processes might well be important in the resonant regime. Then an assumption of uncorrelated successive scattering processes may allow to study the broadening of the resonant transmission.[28,29]

The second limitation comes from the fact that the system is treated as if the electrons were completely independent with equilibrium Fermi-Dirac distributions on emitter and collector states. This is the case for all the theories that only discuss the transmission probabilities. The Pauli exclusion principle introduces a factor $1-f_{\mathrm{FD}}(\mathbf{k}')$ in the scattering term of Eq. (27). In the off-resonance situation, the well states remain nearly empty, so that the factor can be neglected. The main effect on the current will therefore come from *nonequilibrium* population of the resonant states. Furthermore, the assumption of independent electrons excludes genuine many-body effects, such as screening of the interactions, exchange, and correlation. Those effects are beyond the scope of the present theory.

It is clear that only dc characteristics have been described, and an extension to dynamic problems is not obvious; also the specific nature of resonant tunneling structures with a quite well-defined resonant state in the well in which the current is controlled by the double-barrier structure rather than access regions has been utilized at many points. For shrinking barriers this becomes gradually invalid and then it is necessary to apply a theory that allows a description of quantum transport far from equilibrium. Many aspects of this problem are discussed extensively by Frensley[79] but we believe that the scattering processes are a more important ingredient in ordinary double-barrier diodes than the quantum correlations totally neglected by the Born approximation in Fermi's golden rule.

In Ref. 30, the scattering-assisted tunneling formalism is applied in the situation of two-dimensional injection and extended to the case where a magnetic field is applied parallel to the current.

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