Tight-binding approach to resonant tunneling with electron-phonon coupling

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We consider resonant tunneling through a double barrier when the electrons interact with longitudinal-optical phonons in the double-barrier well. We use a tight-binding model for the electron Hamiltonian, with a linear coupling to the phonon modes. Phonon-mediated scattering amplitudes for the double-barrier structure are efficiently obtained by a recursive Green-function technique. This technique allows us to go beyond the unrealistic assumption of Lorentzian line shapes, used in previous treatments. Our results are in qualitative agreement with earlier calculations, but quantitatively the phonon peaks are enhanced typically by 50%.

I. INTRODUCTION

In idealized theoretical treatments of resonant tunneling through a double-barrier potential structure (DBS) one assumes a perfectly clean and periodic crystal through which the electrons move without being scattered. An epitaxially grown DBS prevents free particle motion and gives rise to a transmission spectrum with peaks at certain resonance energies, corresponding to quasibound states in the well between the two barriers. A common semiconductor structure, made up of $Al_xGa_{1-x}As$ barriers enclosing a GaAs well, with the corresponding transmission spectrum is shown in Fig. 1. Note that there is perfect transmission, $T=1$, on resonance in this idealized symmetric example.

In a real sample the situation is much more complex than depicted in the figure. This is due to the various scattering mechanisms causing deviations from a nice, predictable one-dimensional (1D) electronic motion. These scattering mechanisms are of two kinds, *elastic*, in which the electron preserves its energy and phase memory, and *inelastic*, in which the electron energy is changed and the phase memory lost. Scattering off impurity atoms is an elastic process, whereas electron-electron and electron-phonon interaction are examples of inelastic processes. The absolute and relative importance of the different scattering mechanisms depend strongly on which physical system one investigates. We shall not go into any detail on this subject, but refer the reader to the literature[1] for calculations of the various scattering matrix elements. At this point, let us simply state that in polar semiconductors like GaAs the *dominant* scattering process is due to coupling to longitudinal-optical (LO) phonons.[2]

The first experimental observation of LO-phonon-assisted resonant tunneling was reported by Goldman, Tsui, and Cunningham.[3] In addition to the well-known elastic resonance peak, they observed a replica peak in the I-V curve of an $Al_xGa_{1-x}As$-GaAs DBS. At a certain voltage across the DBS the Fermi level of the emitter contact is lined up with the resonant level in the well, and electrons can tunnel resonantly through the DBS. Increasing the bias further, one eventually brings the resonant level below the emitter conduction-band edge, and the current is strongly reduced. However, when the resonant level is pulled sufficiently below the conduction-band edge, resonant tunneling is again made possible, now via emission of a LO phonon. The inelastic replica peak occurs at a voltage such that the energy difference

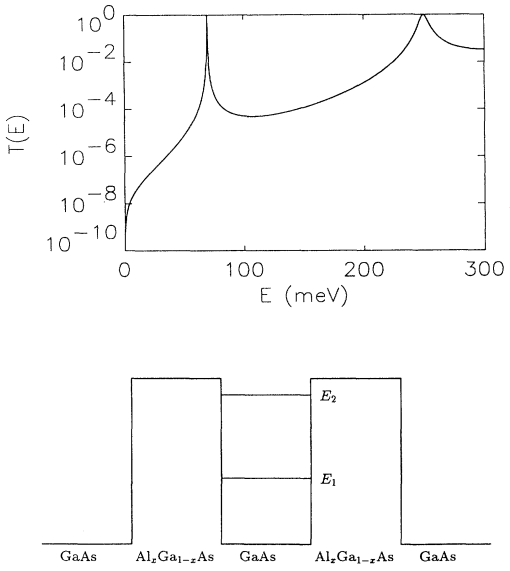

FIG. 1. A symmetric double barrier with $Al_xGa_{1-x}As$ barriers enclosing a GaAs well. The transmission spectrum corresponds to 50-Å barriers with 40% Al content, and a 60-Å well. There are two resonant levels, E_1 and E_2. The barrier height is 300 meV.

between the emitter contact Fermi level and the resonant level equals a LO phonon energy $\hbar\omega_0$.

The observation of phonon-assisted resonant tunneling has been followed by several theoretical papers over the last few years,[4–10] the scope of which has been to go beyond the phenomenological theories of earlier papers[11,12] and include the electron-phonon coupling on a microscopic level. Although the microscopic models involve some rather drastic simplifications, they have been quite successful in describing the experimental *I-V* curves; see, for example, Wingreen, Jacobsen, and Wilkins[5] or Rudberg.[9]

The motivation of the present work is twofold. First, we want to demonstrate how the electron–LO-phonon interaction is included in a simple tight-binding (TB) formalism, and how the recursive Green-function technique is applied in order to find the scattering amplitudes of the DBS in the presence of an inelastic-scattering process. Second, we shall be able to check the validity of one of the approximations in the model of Ref. 5. In that paper the elastic transmission coefficient $T_0(E)$ is modeled with a Lorentzian line shape, which is known to be a good approximation close to a resonant level. However, for representative DBS parameters, the energy width of a resonance in the elastic transmission coefficient is much smaller than the energy of a LO phonon.[13] Thus, the interaction couples resonant states to states far from resonance, and a Lorentzian $T_0(E)$ is no longer sufficient.

Our model is similar to the one applied in Ref. 5, but the recursive Green-function technique allows for a better approximation of the elastic transmission coefficient. We shall compare our results for the full transmission coefficient $T(E)$ with those of Ref. 5 and find that there are *no qualitative differences* between the two models. The *quantitative* effects depend upon the choice of parameters. For the DBS used in Ref. 3 our approach yields a 50% larger replica peak in $T(E)$ than does the model in Ref. 5.

Let us stress that we do not claim quantitative agreement between our model and existing experiments. The main object of this paper is to present an alternate approach to an already established model. One should note some of the limitations of this model. The transport is taken to be effectively one dimensional, which neglects the possibility of lateral momentum transfer due to the electron-phonon interaction. Further, the electrons are assumed to interact with LO phonons inside the double-barrier well only. This is based on the fact that resonantly tunneling electrons spend most of the tunneling time inside the well. However, there are barrier[14] and barrier-well interface[15] phonons with which the electrons also interact.[16] Before one compares with experiment, such effects should be taken into account.

We have organized the paper as follows. In the next section we briefly review the most important results from the elastic case before we include the LO-phonon term and the electron-phonon coupling in the Hamiltonian. Expressions for the transmission and reflection amplitudes are derived in Sec. III, and in Sec. IV we present our numerical results. Our conclusions are collected in Sec. V.

II. THE MODEL

We will study the transport properties of a double-barrier potential as shown in Fig. 2. Before we include phonons, let us repeat the major ingredients of the elastic model.[17]

A. The bare electron system

The conduction-band profile is modeled with a simple tight-binding lattice. The crystal is assumed to be perfectly translationally invariant in the lateral dimensions, so the transport may be taken as strictly one dimensional. The barrier layers are constructed by raising the local potential energy of the electron by an amount Δ corresponding to the conduction-band offset between barrier and contact material. The semiconductor heterostructure used in Ref. 3 consists of $Al_{0.4}Ga_{0.6}As$ barriers and GaAs in well and contacts. For such a system one has $\Delta \sim 300$ meV. The (trivial) parameter ε_0 determines the point of zero energy. In a simple nearest-neighbor TB model one has the dispersion relation

$$E(k)=\varepsilon_0+2u\cos(ka)\ . \tag{2.1}$$

Here u is the energy amplitude for transfering an electron from a site to one of its nearest neighbors. For simplicity we assume real "hopping" amplitudes u. The interatomic spacing is a. From (2.1) we find that the conduction band extends from $\varepsilon_0-|2u|$ to $\varepsilon_0+|2u|$. By choosing $\varepsilon_0=-2u$ and $u=-\hbar^2/2m^*a^2$, the model reproduces the effective-mass approximation with $E(k=0)=0$ in the limit of a very large bandwidth. For simplicity, and in order to compare our results directly with those of Ref. 5, we shall ignore the difference in effective mass in barrier and contact material, and use a constant value of u throughout.

As was shown in Ref. 17, we are able to treat an *arbitrary* potential profile of finite spatial extent, as long as the contact regions to the left and right of the profile have constant potential energy. Here we shall restrict ourselves to a *symmetric* DBS, where the two barriers both have width $N_b a$ and height Δ. The well width is $N_w a$. For this system the electron part of the Hamiltonian is

$$H_e=\sum_j[|j\rangle\varepsilon_j\langle j|+u(|j\rangle\langle j+1|+|j\rangle\langle j-1|)]\ , \tag{2.2}$$

with

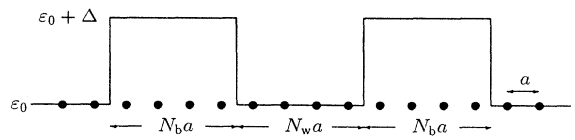

FIG. 2. A symmetric DBS in the tight-binding model. On the barrier atoms the potential energy is $\varepsilon_0+\Delta$, and in the well and the contacts it is ε_0. The barrier and well widths are $N_b a$ and $N_w a$, respectively, with a being the lattice constant.

$$\varepsilon_j = \begin{cases} \varepsilon_0+\Delta, & j\in[1,N_b] \text{ or } j\in[N_b+N_w+1,2N_b+N_w] \\ \varepsilon_0, & \text{otherwise} . \end{cases} \tag{2.3}$$

The atomiclike orbitals $|j\rangle$, centered at site j, are assumed to form a complete, $\sum_j |j\rangle\langle j|=1$, and orthonormal, $\langle i|j\rangle=\delta_{ij}$, set.

In Ref. 17 we derived expressions for the transmission and reflection amplitudes $t(k)$ and $r(k)$, respectively, in terms of the Green function, defined through

$$G(z)(z-H_e)\equiv 1 . \tag{2.4}$$

Here z is the energy variable, and $(z-H_e)$ should be understood as $\lim_{\eta\to 0^+}(z-H_e+i\eta)$, which means that $G(z)$ is the *retarded* Green function. In the present notation we have, for an electron coming in from $x=-\infty$ with $k>0$,

$$\begin{aligned} t(k) &= -2iu\sin(ka)e^{-i(2N_b+N_w+1)ka} \\ &\quad\times\langle 2N_b+N_w+1|G|0\rangle , \\ r(k) &= -2iu\sin(ka)\langle 0|G|0\rangle-1 . \end{aligned} \tag{2.5}$$

In addition to the scattering states there are also bound states above the upper edge of the conduction band, localized in the vicinity of the double-barrier potential. Such states were discussed extensively in Ref. 17. In the present paper we shall only be concerned with the asymptotic scattering states, since they are the ones that determine, e.g., the stationary current through the sample.

B. The bare phonon system

As mentioned in the Introduction, the dominant scattering process in polar semiconductors is due to coupling to LO phonons. We shall consider the simplest possible phonon Hamiltonian, namely that of a single LO-phonon mode, assumed to be dispersionless with a constant frequency ω_0. In reality there is always a weak dispersion $\omega(k)$, but the assumption of a so-called Einstein band of phonons seems to be a reasonable approximation.

In terms of a normal coordinate Q representing the displacements from the equilibrium positions of the atoms,[18] the Schrödinger equation for the phonons reads

$$H_p\phi_n(Q)=\epsilon_n\phi_n(Q) . \tag{2.6}$$

The phonon Hamiltonian is

$$H_p=-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial Q^2}+\tfrac{1}{2}M\omega_0^2Q^2 , \tag{2.7}$$

with eigenfunctions ϕ_n and corresponding energy eigenvalues $\epsilon_n=(n+\frac{1}{2})\hbar\omega_0$. Here M is the reduced mass of the oscillator, and n denotes the number of phonons in the mode.

C. The electron-phonon interaction

As argued in the Introduction and in Ref. 19, we shall assume that the electrons interact with the LO phonons inside the well of the DBS only. The same assumption is also made in Ref. 5. As is usual, we take the electron-phonon coupling to be linear in the displacement coordinate Q. This corresponds to keeping the linear term only in an expansion of the electron-ion interaction.[20] Then one has

$$H_{ep}=\gamma\sum_{n,n'}\sum_{j\in\text{well}}|j,n\rangle Q_j\langle n',j| , \tag{2.8}$$

where Q_j is the displacement of the jth atom in the well. The strength of the interaction is given by the coupling constant γ. In what follows we let small letters m, n, and p denote phonon numbers, whereas other letters denote position in the TB lattice. Then the states $|j,n\rangle \equiv|j\rangle\phi_n(Q)$ represent our noninteracting electron-phonon system.

Our next approximation relies on the assumption that the electron-phonon interaction introduces no "mixing" between any two resonant levels in the well; i.e., we assume that the energy splitting between the resonances is large compared with the LO-phonon energy.[21] Then the energy of an electron, which was incident close to one resonance, is still far away from a nearby resonance after emission or absorption of a LO phonon. With this requirement fulfilled we may study the spectral properties of the DBS in the vicinity of one resonance without taking the others into account. In the TB model this means that the N_w atoms in the well may be mapped onto a *single site.* However, this must be accompanied by a renormalization of the coupling constant γ and the hopping amplitudes at the two barrier-well boundaries. Also, the potential energy in the well must be changed in order to reproduce the correct position of the resonant level. Thus, $\gamma\to\tilde{\gamma}<\gamma$, $u\to\tilde{u}$ with $|\tilde{u}|<|u|$ on the barrier-well boundaries, and $\varepsilon_0\to\varepsilon_w$ inside the well.

In the Appendix we show how to calculate ε_w and $\tilde{u}$ for the mapping of a well with N_w atoms onto a well consisting of a single site. In practice, however, if one wants to model, say, a particular $Al_xGa_{1-x}As$-GaAs DBS, one can first calculate the position and width of the lowest resonance in the effective-mass approximation. Subsequently, one chooses ε_w and $\tilde{u}$ such that the same position and width are also obtained in the single-site TB model.

Next we shall see how the localized electron-phonon interaction leads to a static displacement of the oscillator—the so-called polaron shift—accompanied by a gain in potential energy. We saw in Sec. II B that the eigenstates $\phi_n(Q)$ diagonalize the phonon Hamiltonian. However, inside the well of the DBS the phonons are described by a different set of states $\chi_n(Q)$, which diagonalize the Hamiltonian H_p+H_{ep}:

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial Q^2}+\tfrac{1}{2}M\omega_0^2Q^2+\tilde{\gamma}Q\right]\chi_n(Q)=\tilde{\epsilon}_n\chi_n(Q) . \tag{2.9}$$

Introducing a new coordinate $\tilde{Q}=Q+\tilde{\gamma}/M\omega_0^2$, one obtains

$$\tilde{H}_p\chi_n(Q)=(\tilde{\epsilon}_n+\tilde{\gamma}^2/2M\omega_0^2)\chi_n(Q) , \tag{2.10}$$

with $\tilde{H}_p=(-\hbar^2/2M)\partial^2/\partial\tilde{Q}^2+\frac{1}{2}M\omega_0^2\tilde{Q}^2$. From Sec. II B

$\tilde{H}_p$ has eigenfunctions $\phi_n(\tilde{Q})$ with eigenvalues $(n+\frac{1}{2})\hbar\omega_0$. Thus,

$$\chi_n(Q)=\phi_n(Q+\tilde{\gamma}/M\omega_0^2)\ ,$$
$$\tilde{\epsilon}_n=(n+\tfrac{1}{2})\hbar\omega_0-\tilde{\gamma}^2/2M\omega_0^2\ . \tag{2.11}$$

The equilibrium point of the oscillator is shifted by an amount

$$\Delta Q=-\tilde{\gamma}/M\omega_0^2\ , \tag{2.12}$$

and the relaxation energy due to this shift is

$$\Delta E=-\tilde{\gamma}^2/2M\omega_0^2\ . \tag{2.13}$$

An analogous derivation of (2.12) and (2.13) can be found in Ref. 20. Strictly speaking, (2.12) and (2.13) are only correct for a truly localized electron. However, they are good approximations for the DBS, especially in the opaque barrier limit, which covers most barriers of practical interest. The gain in energy is often expressed in terms of the LO phonon energy,

$$\Delta E=-g\hbar\omega_0\ , \tag{2.14}$$

which gives the relation between $\tilde{\gamma}$ and g,

$$\tilde{\gamma}=(2M\hbar\omega_0^3 g)^{1/2}\ . \tag{2.15}$$

The quantities ΔE and g are also referred to as the Franck-Condon energy and the Huang-Rhys factor, respectively.[22] In Ref. 5 the parameter g has been calculated for the case of interaction with a localized electron state. It is found that $g=2.02/L_0$ in the III-V compound GaAs, and $g=9.59/L_0$ in CdTe, which is a highly polar II-VI material. Here L_0 is the linear extent of the localized state in angstroms.

III. TRANSMISSION AND REFLECTION IN THE PRESENCE OF ELECTRON-PHONON COUPLING

In Sec. II A we had expressions for the transmission and reflection amplitude in the elastic case. When we allow the electrons to interact with phonons, the situation is slightly modified.

In Fig. 3 we have illustrated the physical situation. An electron is coming in from the left with energy E and scatters off the symmetric DBS. It may tunnel through or be reflected without emitting or absorbing any phonons. Alternatively, it may enter the well, emit or absorb one or more LO phonons, and eventually tunnel out through one of the barriers.

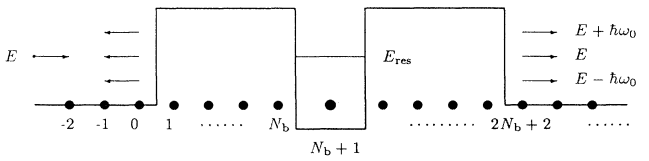

FIG. 3. Resonant tunneling through a symmetric DBS with coupling to LO phonons in the double-barrier well. The incoming electron, having energy E, may be transmitted or reflected with energy $E\pm p\hbar\omega_0$. Here p denotes the number of phonons absorbed or emitted in the well. The well is modeled with a single site. Thus, there is only one resonant level E_{res}. The conduction-band edge in the well has been shifted such that the resonant level corresponds to the lowest resonance in the original well consisting of N_w atoms.

If the initial and final numbers of phonons are n and m, respectively, we may write the incoming and outgoing states as

$$\Psi_{in}(j,Q)=e^{ik_n ja}\phi_n(Q),\quad j\le 0\ ; \tag{3.1}$$

and

$$\Psi_{out}(j,Q)=\begin{cases}\sum_m r_{mn}e^{-ik_m ja}\phi_m(Q), & j\le 0\\ \sum_m t_{mn}e^{ik_m ja}\phi_m(Q), & j>2N_b+N_w\ ,\end{cases} \tag{3.2}$$

respectively. Since the electron-phonon interaction is assumed to be localized to the double-barrier well, the asymptotic scattering states in (3.1) and (3.2) can be written as a product of a plane-wave electron part and a free-phonon part.

The electron must be transmitted or reflected,[23] so the transmission and reflection amplitudes must obey the sum rule

$$\sum_m(|t_{mn}|^2+|r_{mn}|^2)=1\ . \tag{3.3}$$

In (3.2) and (3.3) the sums run over all allowed values m of the final number of phonons. Since the final velocity v_m is, in general, different from the initial one v_n, the scattering amplitudes must be defined with an additional factor $(v_m/v_n)^{1/2}$ in order to conform to particle conservation. The result is

$$\begin{aligned}t_{mn}&=-2iu\sin(k_n a)\left[\frac{\sin(k_m a)}{\sin(k_n a)}\right]^{1/2}\\ &\quad\times e^{-i(2N_b+N_w+1)k_m a}\langle m,2N_b+2|G|0,n\rangle\ ,\\ r_{mn}&=[-2iu\sin(k_n a)\langle m,0|G|0,n\rangle-\delta_{mn}]\\ &\quad\times\left[\frac{\sin(k_m a)}{\sin(k_n a)}\right]^{1/2}\ .\end{aligned} \tag{3.4}$$

The elastic case, Eq. (2.5), is recovered by taking $k_m=k_n=k$ and suppressing the phonon number in the matrix elements.

We will eventually present numerical results for the transmission coefficient only. Therefore, we proceed by evaluating the matrix elements $\langle m,2N_b+2|G|0,n\rangle$ of the full Green function, corresponding to the total Hamiltonian

$$H=H_e+H_p+H_{ep}\ , \tag{3.5}$$

with

$$H_e=\sum_{j,n}|j,n\rangle\varepsilon_j\langle n,j|+u\sum_{j,n}{}'(|j,n\rangle\langle n,j+1| +|j,n\rangle\langle n,j-1|)$$
$$+\tilde{u}\sum_n(|N_b,n\rangle\langle n,N_b+1| +|N_b+2,n\rangle\langle n,N_b+1|+\text{c.c.}),$$
$$H_p=\sum_{j,n}|j,n\rangle(n+\tfrac{1}{2})\hbar\omega_0\langle n,j| , \tag{3.6}$$
$$H_{ep}=\sum_{n,m}|N_b+1,m\rangle\bar{\gamma}Q_{mn}\langle n,N_b+1| .$$

The primed sum in H_e means that the barrier-well boundary hopping elements are not included. Using results from Ref. 17 we have

$$\langle m,2N_b+2|G|0,n\rangle=\left[\prod_{j=2N_b+2}^{N_b+3}\Gamma_j^+(m)u\right]\Gamma_{N_b+2}^+(m)\tilde{u} \times\langle m,N_b+1|G|N_b+1,n\rangle \times\tilde{u}\Gamma_{N_b}^-(n)\left[\prod_{j=N_b-1}^{0}u\Gamma_j^-(n)\right] . \tag{3.7}$$

This expression comes about when using the Dyson equation $G=G^0+GH'G^0$ repeatedly. The Dyson equation expresses the Green function G of the total Hamiltonian H in terms of the perturbation $H'=H-H^0$ and the Green function G^0 of the unperturbed Hamiltonian H^0. In (3.7) $\Gamma_j^{\pm}(m)\equiv\langle m,j|G_{\pm}^0|j,m\rangle$ are "surface Green functions," i.e., diagonal elements of the Green function $G_{\pm}^0$ corresponding to the Hamiltonian $H_{\pm}^0=H-u(|j,m><m,j\mp1|+|j\mp1,m\rangle\langle m,j|)$. The Dyson equation yields recursion relations for $\Gamma_j^{\pm}$:

$$\Gamma_j^{\pm}(m)=[z-\varepsilon_j-(m+\tfrac{1}{2})\hbar\omega_0-u\Gamma_{j\pm1}^{\pm}(m)u]^{-1} . \tag{3.8}$$

Here z is the total energy variable, $\varepsilon_j=\varepsilon_0$ outside the barriers, and $\varepsilon_j=\varepsilon_0+\Delta$ inside the barriers. Clearly, $\Gamma_j^+(m)=\Gamma_{j+1}^+(m)$ for $j\geq2N_b+2$ and $\Gamma_j^-(m)=\Gamma_{j-1}^-(m)$ for $j\leq0$. This yields quadratic equations for $\Gamma_{2N_b+2}^+(m)$ and $\Gamma_0^-(m)$, and from (3.8) one readily calculates $\Gamma_{2N_b+1}^+,\ldots,\Gamma_{N_b+2}^+$ and $\Gamma_1^-,\ldots,\Gamma_{N_b}^-$.

Finally, we need to evaluate the matrix elements $\langle m,N_b+1|G|N_b+1,n\rangle$, which are diagonal in the electron coordinate but, in general, are off-diagonal in the phonon number. First, we need the matrix elements of the displacement, $Q_{mn}\equiv\langle m|Q|n\rangle$. This can be looked up in a quantum-mechanics textbook,[24] and the result is

$$Q_{mn}=\left[\frac{\hbar}{2M\omega_0}\right]^{1/2}(\sqrt{n+1}\,\delta_{m,n+1}+\sqrt{n}\,\delta_{m,n-1}) . \tag{3.9}$$

Now we can write down the desired matrix element of the Green function,

$$\langle m,N_b+1|G|N_b+1,n\rangle\equiv\langle m,N_b+1|(z-H)^{-1}|N_b+1,n\rangle =\langle m|\left[\sum_{n'}(|n'\rangle\{z-\varepsilon_w-(n'+\tfrac{1}{2})\hbar\omega_0-\tilde{u}^2[\Gamma_{N_b}^-(n')+\Gamma_{N_b+2}^+(n')]\}\langle n'| -[g(n'+1]^{1/2}\hbar\omega_0(|n'\rangle\langle n'+1|+|n'+1\rangle\langle n'|))\right]^{-1}|n\rangle , \tag{3.10}$$

where we have used (2.15). This can be viewed as the matrix element between two "sites" m and n in a semi-infinite chain extending from $n'=0$ to $n'=\infty$, with "position"-dependent potential energy $\varepsilon_{n'}=\varepsilon_w+(n'+\frac{1}{2})\hbar\omega_0+\tilde{u}^2[\Gamma_{N_b}^-(n')+\Gamma_{N_b+2}^+(n')]$ and hopping amplitudes $u_{n',n'+1}=[g(n'+1)]^{1/2}\hbar\omega_0$. Note that the potential energy $\varepsilon_{n'}$ is complex. Its imaginary part determines the energy width of the resonant level. Now we may apply the results of Ref. 17 again. The diagonal matrix element is

$$\langle n,N_b+1|G|N_b+1,n\rangle=\{z-\varepsilon_w-(n+\tfrac{1}{2})\hbar\omega_0-\tilde{u}^2[\Gamma_{N_b}^-(n)+\Gamma_{N_b+2}^+(n)]-g(\hbar\omega_0)^2[(n+1)\Sigma_{n+1}^++n\Sigma_{n-1}^-]\}^{-1} , \tag{3.11}$$

and the off-diagonal elements are

$$\langle m,N_b+1|G|N_b+1,n\rangle=\begin{cases}\displaystyle\prod_{n'=n+1}^{m}[\Sigma_{n'}^+(gn')^{1/2}\hbar\omega_0]\langle n,N_b+1|G|N_b+1,n\rangle, & m>n\\ \displaystyle\prod_{n'=m+1}^{n}[\Sigma_{n'}^+(gn')^{1/2}\hbar\omega_0]\langle m,N_b+1|G|N_b+1,m\rangle, & m<n .\end{cases} \tag{3.12}$$

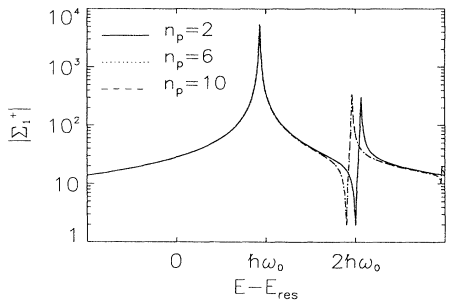

FIG. 4. Energy dependence of the "surface Green function" Σ_1^+ for different values of the maximum phonon number n_p (see the text). The curves for $n_p=6$ and 10 cannot be distinguished in the figure. Parameters correspond to the lowest resonant level in a GaAs-$Al_{0.4}Ga_{0.6}As$ structure with 50-Å well and barriers.

The "surface Green functions" $\Sigma_{n'}^{\pm}$ are diagonal elements of the Green function corresponding to the Hamiltonian

$$H-|N_b+1,n'\mp1\rangle\tilde{\gamma}Q_{n'\mp1,n'}\langle n',N_b+1| -|N_b+1,n'\rangle\tilde{\gamma}Q_{n',n'\mp1}\langle n'\mp1,N_b+1| .$$

They are determined by recursion relations analogous to those for Γ^+ and Γ^-,

$$\begin{aligned}(\Sigma_{n'}^+)^{-1}&=z-\varepsilon_w-(n'+\tfrac{1}{2})\hbar\omega_0 -\tilde{u}^2[\Gamma_{N_b}^-(n')+\Gamma_{N_b+2}^+(n')] -g(n'+1)(\hbar\omega_0)^2\Sigma_{n'+1}^+ ,\\ (\Sigma_{n'}^-)^{-1}&=z-\varepsilon_w-(n'+\tfrac{1}{2})\hbar\omega_0 -\tilde{u}^2[\Gamma_{N_b}^-(n')+\Gamma_{N_b+2}^+(n')] -gn'(\hbar\omega_0)^2\Sigma_{n'-1}^- ,\end{aligned} \tag{3.13}$$

now with initial conditions

$$\Sigma_{-1}^-=0 , \quad \Sigma_{\infty}^+=0 . \tag{3.14}$$

Clearly, we have to choose a maximum phonon number n_p such that $\Sigma_{n_p+1}^+=0$. This turns out to be a very good approximation even for modest values of n_p, since $\Sigma_{n'}^+\sim 1/n'$ for large values of n'. In Fig. 4 we have plotted $|\Sigma_1^+|$ versus energy for $n_p=2$, 6, and 10. As is seen, convergence is obtained already for $n_p=6$.

Now we have everything we need to calculate the transmission coefficient. We are mainly interested in the situation with no phonons present in the initial state, corresponding to zero temperature. Even at room temperature, the average phonon number is only $\langle n\rangle\simeq 0.3$ for LO phonons in GaAs. The $T=0$ case is also studied in Ref. 5, with which we shall compare our results in the next section.

IV. NUMERICAL RESULTS FOR THE TRANSMISSION COEFFICIENT

In this section we present numerical results for the transmission coefficient in the presence of electron-phonon interaction inside the well of the DBS. We have chosen parameters corresponding to the lowest resonance in an $Al_{0.4}Ga_{0.6}As$-GaAs system with well and barriers 50 Å wide. In Fig. 5 the *elastic* transmission coefficient of the tight-binding single-site model is compared with the Lorentzian line shape used in Ref. 5. We have also included the transmission coefficient when calculated within the effective-mass approximation. At the energy $E_{res}+\hbar\omega_0$ the TB model is much closer to the effective-mass result than is the Lorentzian. However, due to the single-site approximation, one will always have large deviations from the exact result when approaching the second resonance.

In Fig. 6 we have plotted the *total* transmission coefficient for the same parameters as in Fig. 5. The electron-phonon coupling strength is $g=0.036$, appropriate for a 50-Å GaAs well. In the inset we compare the first inelastic sideband, corresponding to resonant tunneling accompanied by emission of one LO phonon, in the TB model with the one in Ref. 5. The TB model yields an enhancement of the peak of about 50%.

The 1D *current* through a DBS is essentially given as the energy integral of the transmission coefficient.[25] Then, if the Fermi energy in the emitter contact is smaller than a LO-phonon energy,[26] the magnitude of the replica peak or "shoulder" in the *I-V* curve will roughly be proportional to the area under the resonance peak in the inset of Fig. 6. Thus, without explicitly calculating the current, we expect the TB model to give a shoulder in the *I-V* curve about 50% higher than what was found in Ref. 5.

V. CONCLUDING REMARKS

We believe the model of Ref. 5 has convincingly shown that the transport process in the experiment of Goldman, Tsui, and Cunningham is resonant tunneling assisted by

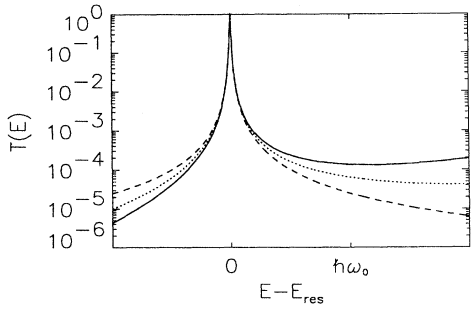

FIG. 5. The elastic transmission coefficient in the vicinity of the lowest resonant level in an $Al_{0.4}Ga_{0.6}As$-GaAs structure with 50-Å well and barriers. The solid curve is the effective mass result (however, not taking the material dependence of m^* into account), the dotted curve is calculated in the single-site tight-binding model, and the dashed curve is the Lorentzian line shape used in Ref. 5.

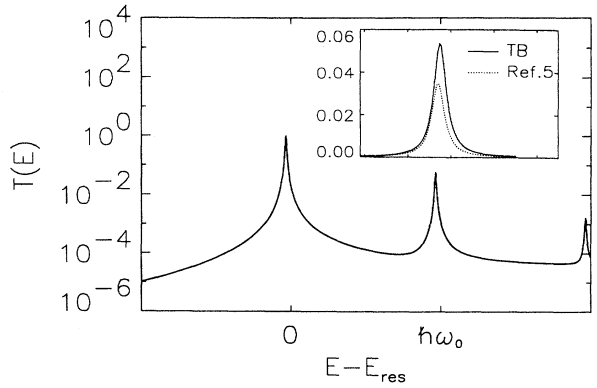

FIG. 6. The total transmission coefficient, including electron-phonon coupling in the double-barrier well. Barrier parameters are the same as in Fig. 5. The coupling constant is $g=0.036$. In a linear plot only the first inelastic sideband would be visible on the scale of the elastic peak. In the inset we compare the first inelastic sideband in the TB model (solid line) with the model in Ref. 5 (dotted line).

emission of a LO phonon. We have presented a tight-binding approach to the same physical model and find a total transmission coefficient with qualitatively the same features as were found in Ref. 5. However, a Lorentzian approximation of the *elastic* transmission coefficient is shown to underestimate the magnitude of the transmission peak corresponding to resonant tunneling via emission of a LO phonon.

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APPENDIX

In this appendix we shall study the mapping of a double-barrier well onto a single site. As argued in Sec. II C, we may consider tunneling through a single resonant level as long as the LO phonon energy is small compared with the splitting between the resonances.

Consider the electron Hamiltonian of a quantum well of depth Δ, consisting of N_w atoms,[27]

$$H_e^W=\sum_j[|j\rangle\varepsilon_j\langle j|+u(|j\rangle\langle j+1|+|j+1\rangle\langle j|)] . \tag{A1}$$

Here $\varepsilon_j=\varepsilon_0$ for $j\in[N_b+1,N_b+N_w]$, and $\varepsilon_j=\varepsilon_0+\Delta$ otherwise. Denote by $|\psi^{(l_0)}\rangle$ and E_{l_0} the lowest bound state and its energy, respectively. Thus,

$$H_e^W|\psi^{(l_0)}\rangle=E_{l_0}|\psi^{(l_0)}\rangle . \tag{A2}$$

The effective Hamiltonian for a single-site quantum well is

$$\begin{aligned}\tilde{H}_e=&\sum_{j\neq N_b+1}|j\rangle(\varepsilon_0+\Delta)\langle j|+|N_b+1\rangle\varepsilon_w\langle N_b+1|\\&+u\sum_{j\neq N_b,N_b+1}(|j\rangle\langle j+1|+|j+1\rangle\langle j|)\\&+\tilde{u}(|N_b\rangle\langle N_b+1|+|N_b+1\rangle\langle N_b|\\&+|N_b+1\rangle\langle N_b+2|+|N_b+2\rangle\langle N_b+1|) .\end{aligned} \tag{A3}$$

In order to model the lowest bound level of the original well, $\tilde{H}_e$ should reproduce the bound level position, i.e., $\tilde{H}_e|\tilde{\psi}\rangle=E_{l_0}|\tilde{\psi}\rangle$, and that part of the wave function that is located in the well, i.e., $\sum_{j=N_b+1}^{N_b+N_w}|\langle j|\psi^{(l_0)}\rangle|^2=|\langle N_b+1|\tilde{\psi}\rangle|^2$.

Assume that E_{l_0} and $|\psi^{(l_0)}\rangle$ have been found. Then we can determine the two unknowns ε_w and $\tilde{u}$. From the definition of the Green function, $G(z)=\sum_l(|\psi^{(l)}\rangle\langle\psi^{(l)}|)/(z-E_l)$, the simple poles in $G(z)$ give the discrete eigenenergies of the system. In particular, one has

$$\left.\frac{1}{\langle N_b+1|\tilde{G}(z)|N_b+1\rangle}\right|_{z=E_{l_0}}=0 . \tag{A4}$$

This gives an equation for ε_w:

$$E_{l_0}-\varepsilon_w-2\tilde{u}^2\Gamma_b(E_{l_0})=0 . \tag{A5}$$

Here Γ_b is the "surface Green function"[17] of the infinite barrier layers,

$$\Gamma_b(z)=\frac{1}{2u^2}\{z-\varepsilon_0-\Delta-[(z-\varepsilon_0-\Delta)^2-4u^2]^{1/2}\} . \tag{A6}$$

Also, from the definition of $G(z)$, one has

$$\begin{aligned}|\langle N_b+1|\tilde{\psi}\rangle|^2=&\lim_{z\to E_{l_0}}[(z-E_{l_0})\\&\times\langle N_b+1|\tilde{G}(z)|N_b+1\rangle]\\=&\frac{1}{1-2\tilde{u}^2\dfrac{\partial}{\partial z}\Gamma_b(z)|_{z=E_{l_0}}} ,\end{aligned} \tag{A7}$$

which determines $\tilde{u}$.

The procedure above yields a mapping of one of the resonances in a well of N_w atoms onto the resonance of a well consisting of a single atom. In practice, e.g., when modeling a particular experiment, one may instead *choose* ε_w and $\tilde{u}$ such that the desired position and width of the resonance is obtained in the single-site model. This method has been used in Sec. IV.

The mapping of the well onto a single site also requires that the electron–LO-phonon coupling constant be renormalized. We start by rewriting the interaction Hamiltonian (2.8) in terms of the energy eigenstates $|\psi^{(l)}\rangle$:

$$H_{ep}=\gamma\sum_j |j\rangle Q_j\langle j|$$

$$=\gamma\sum_j\sum_{l,l'} |\psi^{(l)}\rangle\langle\psi^{(l)}|j\rangle Q_j\langle j|\psi^{(l')}\rangle\langle\psi^{(l')}|$$

$$\simeq\gamma|\psi^{(l_0)}\rangle\sum_j|\langle\psi^{(l_0)}|j\rangle|^2 Q_j\langle\psi^{(l_0)}| \ . \tag{A8}$$

In the last step we again made the assumption that the level spacing in the well is so large compared with the phonon energy that we may consider one level only, $l=l_0$. The sum in (A8) is simply a product between two vectors $\mathbf{Q}=(Q_{N_b+1}\ldots Q_{N_b+N_w})$ and $\mathbf{V}=(|\psi^{(l_0)}_{N_b+1}|^2\ldots|\psi^{(l_0)}_{N_b+N_w}|^2)$ in the infinite-dimensional vector space spanned by the orbitals $|j\rangle$. Thus, we have

$$\sum_{j=N_b+1}^{N_b+N_w}|\psi_j^{(l_0)}|^2 Q_j=\alpha Q_V \ , \tag{A9}$$

where $\alpha=|\mathbf{V}|=(\sum_{j=N_b+1}^{N_b+N_w}|\psi_j^{(l_0)}|^4)^{1/2}$, and Q_V is the projection of $\mathbf{Q}$ along $\mathbf{V}$. In other words, the original well, consisting of N_w atoms and N_w oscillators, has been mapped onto a single electron state $|\psi^{(l_0)}\rangle$ and a single oscillator coordinate Q_V, and the electron-phonon coupling strength has been renormalized,

$$\tilde{\gamma}=\alpha\gamma<\gamma \ . \tag{A10}$$

From its definition above, one can see that α, and hence $\tilde{\gamma}$, scales with the inverse square root of the well width. This is consistent with Eq. (2.15), $\tilde{\gamma}\sim\sqrt{g}$, and the result in Ref. 5, $g\sim L_0^{-1}$, where L_0 is the linear extent of the electron wave function.

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[27]In a DBS the well is not completely isolated, but the coupling through the barriers is very weak, provided the barriers are high and/or wide.