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Quantum-mechanical resonant tunneling in the presence of a boson field

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We solve exactly an approximate model for inelastic resonant tunneling in the presence of a boson field. The model is based on the many-body tunneling Hamiltonian formalism, which, in the appropriate limits, is shown to precisely reproduce the elastic resonant tunneling results of ordinary single-particle scattering theory. Bosons coupling with arbitrary strength to the resonant level broaden the energy dependence of the effective transmission probability. Applications to resonant tunneling in quasi-one-dimensional GaAs-$Al_xGa_{1-x}As$ heterostructures in the presence of LO phonons and to resonant tunneling in three-dimensional heterostructures in the presence of electromagnetic fields (laser beam or ac voltage) are discussed.

I. INTRODUCTION

An early triumph of quantum mechanics was the prediction that electrons may pass between two reservoirs through a classically forbidden region. Manifestations of *tunneling* through a barrier were soon observed experimentally, first in the context of field-induced ionizations of atoms. Later, tunneling developed into an important field also in solid-state physics, well elucidated in the extensive early review by Duke.[1] Today the old subject of tunneling is again in focus, partly due to the recent spectacular advances in semiconductor technology and electron tunneling microscopy.

We shall here be concerned with resonant tunneling. This is when the electron tunnels via a localized state in the barrier, whose energy matches (resonates with) energy levels in the reservoirs. The tunnel current is greatly enhanced when this resonant condition is met. This is why resonant tunneling is an important phenomenon in such diverse areas as scanning tunneling microscopy (STM) and the physics of transport in semiconductor heterostructures. In the former case the formidable spatial resolution of the STM has made it possible to probe tunneling from a metal surface to the sharp metal tip of the instrument via localized levels in a single adsorbed molecule. The tunnel current will show resonances as the applied tip-to-metal voltage is varied and the discrete energy levels in the absorbed molecule are scanned through. In particular STM has been used to study how the electronic energy level(s) interact with boson fields (rotational and vibrational "phonons"). We are referring to what has become known as inelastic electron tunneling spectroscopy.[2]

In the field of semiconductor heterostructures the peculiar transport properties brought about by resonant tunneling, as well as the possibility of controlling the energy of the resonant level by some gate voltage, has opened up potentially very fruitful device applications.[3(a)] By letting a potential switch the position of the localized level in and out of resonance the current can be turned "off" and "on" in a three-terminal resonant-tunneling (RT) device. This leads to potential applications both in terms of fast transistors and functional logical devices.[3(b)] As a two-terminal device a RT structure such as that in Fig. 1 has a region of negative differential resistance (NDR). This happens when the applied voltage is such that a further increase brings the localized level out of the resonance condition and hence diminishes the current. When the device is biased in the NDR region it is intrinsically unstable, and perhaps the main potential application of resonant tunneling in semiconductor heterostructures is to use the microwave radiation generated by the resulting current and voltage fluctuations.[4] Other possible applications for RT devices such as mixers and detectors are also due to the nonlinear current-voltage characteristics. Detection has been demonstrated at 2.5 THz (Ref. 5) and microwave generation at 18 GHz.[4] In order to develop these applications further it is important to understand resonant tunneling in the presence of electromagnetic fields (photons).

A common feature of the resonant-tunneling systems described above—all of considerable current interest—is that the tunneling electrons couple to a boson field. This field may be due to phonons or photons (the electromagnetic field of a laser beam to be detected or the oscillating ac voltage in a microwave generator, for instance). The coupling to the boson field leads to an exchange of energy

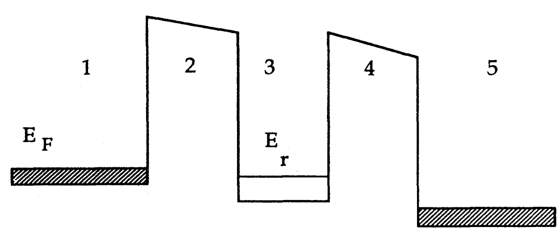

FIG. 1. A schematic resonant tunneling structure, where five regions (1–5) of different potential energy are indicated. The position of a resonant level in region 3 and bands of occupied electron states in regions 1 and 5 are shown.

between the electrons and the bosons and hence to *inelastic* resonant tunneling. Recently we[6] and others[7] have discussed the effect of inelastic scattering on resonant tunneling in semiconductor heterostructures. This effect obviously bears on the performance of RT devices, but is of general interest as well, for instance, in the context of interpreting data from inelastic electron tunneling spectroscopy.[8] Using a phenomenological model for the inelastic phonon scattering we conclude in Ref. 6 that inelastic scattering, which destroys the phase coherence, is an important effect that strongly reduces the probability for coherent tunneling of the Fabry-Pérot type. As a result, the tunneling will be mainly incoherent (sequential). However, in a model calculation we found that the tunneling current, which is related to the integrated tunneling probability, does not depend on which of the two mechanisms dominate as long as the resonant energy is well defined.

In the present paper we wish to go beyond the phenomenological description of the phonon scattering and consider an approximate microscopic model that is exactly solvable. We shall also extend the discussion to couplings with boson fields other than those of phonons. The main assumptions in the model are that the boson field couples only to the localized (resonant) state and that no momentum is transferred to it. The coupling strength may be arbitrarily large. We shall apply the results obtained to three cases of current interest where these assumptions are reasonable: (i) resonant tunneling in a quasi-one-dimensional semiconductor structure in the presence of LO phonons, (ii) resonant tunneling in a three-dimensional heterostructure in the presence of a laser beam or, (iii) an ac component in the applied voltage. The first case relates to the quasi-one-dimensional $GaAs/Al_{0.25}Ga_{0.75}As/GaAs/Al_{0.25}Ga_{0.75}As/GaAs$ structure recently studied by Reed *et al.*[9] The second and third cases correspond to the RT devices studied in Refs. 4 and 5.

Our strategy will be to map the problem onto the well-known problem of a localized electron (here an electron in a quantum well) interacting with independent bosons (phonons). This problem was solved almost 40 years ago[10] and the solution can be found in a textbook.[11] The same approach was recently applied by Glazman and Shekter[12] to the problem of inelastic resonant tunneling via a pointlike resonance center in an insulating barrier.

Although our discussion is more widely applicable, we find it instructive to refer to a specific resonant-tunneling structure. As in Ref. 6, our model structure consists of two barriers (regions 2 and 4) separating three regions of lower potential energy (regions 1, 3, and 5) as shown in Fig. 1. We have in mind a crude model for the conduction band in a $GaAs\text{-}Al_xGa_{1-x}As$ double-barrier heterostructure. The paper is organized as follows. In Sec. II we introduce the tunneling Hamiltonian formalism and discuss its applicability to a resonant-tunneling system. The model for coupling of the tunneling electron to a boson field is presented and solved under general conditions in Sec. III. In subsequent sections the implications for resonant tunneling in specific physical systems are discussed.

II. TUNNELING HAMILTONIAN DESCRIPTION OF RESONANT TUNNELING

The tunneling Hamiltonian formalism has been successfully applied to describing tunneling between weakly coupled normal and superconducting metals.[1] Whether it can be applied to resonant tunneling in semiconductors, where the voltage drop over the tunnel structure is of the order of volts rather than millivolts, is not obvious.[11,13] We shall therefore first establish that we can rederive the usual expression of scattering theory for the resonant-tunneling current of free electrons in the absence of interactions. This is a generalization of the corresponding well-known result for a single barrier,[1] which in addition brings out the effects of possible relaxation phenomena among electrons in the resonant levels. These may occur in a system such as a three-dimensional $GaAs\text{-}Al_xGa_{1-x}As$ heterostructure where the electrons in the quantum well have degrees of freedom perpendicular to the tunneling direction.

Referring to our model system in Fig. 1, we now use the tunneling Hamiltonian formalism to separately describe the current, I_{13}, from the emitter (region 1) to the resonant level in the quantum well (region 3) and the current, I_{35}, from the quantum well to the collector (region 5). The actual tunneling current I_{15} is then obtained by demanding these two currents to be of equal magnitude.

We consider first the tunneling into the well. The proper Hamiltonian for this process is

$$H_T = H_1 + H_3 + H_{13} \ , \tag{1}$$

where H_1 describes the electrons in the emitter. Here, and in the rest of the paper we use a simple effective-mass approximation where the potential energy is one dimensional and the electron kinetic energy is the sum of parallel and perpendicular parts, corresponding to a decomposition of the wave vector $\mathbf{k}$ into a component k perpendicular to the heterostructure and a component $\mathbf{K}$ parallel to it, $\mathbf{k}=(k,\mathbf{K})$. Measuring energies from the bottom of the conduction band in the emitter, it follows that in our simple model system

$$\begin{aligned} H_1 &= \sum_{\mathbf{k}_1} E(\mathbf{k}_1) c^\dagger_{\mathbf{k}_1} c_{\mathbf{k}_1} \ , \\ E(\mathbf{k}) &= \frac{\hbar^2 k^2}{2m^*} + \frac{\hbar^2 \mathbf{K}^2}{2m^*} = E_z(k) + E_\parallel(\mathbf{K}) \ . \end{aligned} \tag{2}$$

The Hamiltonian H_3 describes the electrons in the quantum well. As the electrons are free to move in the parallel direction we find

$$\begin{aligned} H_3 &= \sum_{\mathbf{k}_3} E(\mathbf{k}_3) c^\dagger_{\mathbf{k}_3} c_{\mathbf{k}_3} \ , \\ E(\mathbf{k}_3) &= E_z(k_3) + E_\parallel(\mathbf{K}_3) = E_r + E_\parallel(\mathbf{K}_3) \ . \end{aligned} \tag{3}$$

Energies are again measured from the bottom of the band in the emitter. For simplicity we assume that there is only one resonant level E_r with respect to the motion perpendicular to the heterostructure. The intrinsic resonance energy E_r^0 is lowered by the applied voltage V. Assuming that, say, half of the total voltage drop occurs between the emitter and the well, the voltage dependence of the resonant level can be explicitly given as $E_r = E_r^0 - eV/2$. It goes without saying that in a complete treatment of the resonant-tunneling problem the position of the resonant energy level as well as the entire potential energy structure would have to be calculated self-consistently.

In the conventional discussion of single-barrier tunneling[1,11] the subsystem Hamiltonians H_1 and H_3 are considered to be strictly independent and commute term by term. Thermal equilibrium at different chemical potentials μ_1 and μ_3 are assumed to exist on each side of the barrier. The interaction comes from the tunneling part of the Hamiltonian H_{13}, where

$$H_{13} = \sum_{\mathbf{k}_1\mathbf{k}_3} (T_{\mathbf{k}_1\mathbf{k}_3} c^\dagger_{\mathbf{k}_1} c_{\mathbf{k}_3} + \text{H.c.}) \; . \tag{4}$$

The tunneling current through the barrier (region 2) is expressed as the rate of change of, say, the number of electrons N_1 in the emitter (region 1). This rate is found from the commutator of N_1 with the tunneling Hamiltonian,

$$\dot{N}_1 = \frac{i}{\hbar}[N_1, H_T] = \frac{i}{\hbar}[N_1, H_{13}], \quad N_1 = \sum_{\mathbf{k}_1} c^\dagger_{\mathbf{k}_1} c_{\mathbf{k}_1} \; . \tag{5}$$

The commutator is easily evaluated and one finds

$$\dot{N}_1 = \frac{i}{\hbar} \sum_{\mathbf{k}_1,\mathbf{k}_3} (T_{\mathbf{k}_1\mathbf{k}_3} c^\dagger_{\mathbf{k}_1} c_{\mathbf{k}_3} - \text{H.c.}) \; . \tag{6}$$

The current I_{13} from the emitter to the quantum well is defined as the average value of this operator, $I_{13} = -e\langle \dot{N}_1 \rangle$, and can be obtained by linear-response theory with the tunneling term H_{13} treated as the perturbation. We refer to Ref. 11 for details of the derivation. The result is that

$$I_{13} = \frac{2e}{\hbar} \sum_{\mathbf{k}_1,\mathbf{k}_3} |T_{\mathbf{k}_1\mathbf{k}_3}|^2 \times \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} A_3(\mathbf{k}_3,\varepsilon) A_1(\mathbf{k}_1, \varepsilon+\mu_1-\mu_3) \times [n_F(\varepsilon) - n_F(\varepsilon+\mu_1-\mu_3)] \; . \tag{7}$$

The current is here expressed in terms of the spectral functions in the emitter (region 1) and in the quantum well (region 3), respectively. A factor of 2 accounts for the spin summation and $n_F(\varepsilon) = [\exp(\varepsilon/k_B T)+1]^{-1}$ is the Fermi factor.

In principle the spectral functions in Eq. (7) could describe interacting electrons, as long as the interactions do not couple electrons in the different regions. This is, of course, the advantage of the formalism and will be used when we introduce the electron-boson interaction below. For the moment we stay with the free-electron system described by H_1 and H_3 of Eqs. (2) and (3). The corresponding spectral functions are[11]

$$A_1(\mathbf{k}_i,\varepsilon) = A_1^0(\mathbf{k}_i,\varepsilon) = 2\pi\delta(\varepsilon - E(\mathbf{k}_i) + \mu_i), \quad i = 1,3 \; . \tag{8}$$

The prescription for calculating the tunneling matrix element has been given by Bardeen.[14,1,11] It involves the wave functions $\Psi_{\mathbf{k}_1}$ in the emitter (calculated in the absence of well and collector) and the wave function $\Psi_{\mathbf{k}_3}$ in the well (calculated in the absence of emitter and collector),

$$T_{\mathbf{k}_1\mathbf{k}_3} = \frac{\hbar^2}{2m^*} \int_S (\Psi_{\mathbf{k}_3} \nabla \Psi^*_{\mathbf{k}_1} - \text{H.c.}) \cdot d\mathbf{S} \; . \tag{9}$$

The integral is taken over any surface in the barrier. The parallel momenta will be, and the total energy is assumed to be conserved in the tunneling process. One readily finds that for a free-electron model

$$|T_{\mathbf{k}_1\mathbf{k}_3}|^2 = \delta_{\mathbf{K}_1\mathbf{K}_3} \left[\frac{16 k_1 k_3 \kappa_2^2}{(k_1^2+\kappa_2^2)(k_3^2+\kappa_2^2)} \exp(-2\kappa_2 b_2) \right] \times \frac{\hbar^2}{4} v(k_1) v(k_3) \frac{1}{L} \frac{1}{d_{\text{eff}}} \; . \tag{10}$$

As usual $v(k) = \hbar k/m^*$, $\kappa_2 = [2m(U_2 - E_z)/\hbar^2]^{1/2}$, U_2 is the average height, and b_2 is the width of the barrier (region 2). (We approximate the potential in the barrier by its average in order to be able to give an explicit expression.)

We recognize the first factor of Eq. (10) as the transmission probability through the barrier (region 2) in the limit when the electron energy is well below the top of the barrier. We denote it by T_{13}. As for the rest of Eq. (10), we note two differences in comparison to the case of tunneling through a single-barrier structure:[1] (i) only one value of the perpendicular momentum k_3 is allowed, viz., the one that corresponds to the resonant condition, $E_z(k_1) = E_z(k_3) = E_r$ and (ii) the perpendicular part of the wave function $\Psi_{\mathbf{k}_3}$ is not a simple exponential. The corresponding normalization factor is therefore not $1/L$ but rather $1/d_{\text{eff}}$, the inverse effective width of the quantum well. The effective width differs from the physical width d because of the penetration of the wave function into the barriers (regions 2 and 4),

$$d_{\text{eff}} = d + \frac{1}{\kappa_2} + \frac{1}{\kappa_4} \; . \tag{11}$$

At this stage it is convenient to introduce the energy Γ_{13}. Later we will be able to relate it to the width of the resonant level and hence also to the escape rate $1/\tau$ from the quantum well through the left barrier to the emitter. We define it as

$$\Gamma_{13} = \frac{2\hbar}{\tau} = \frac{\hbar}{d_{\text{eff}}} v(k_3) T_{13} \; . \tag{12}$$

Note that we can interpret $v(k_3)/2d_{\text{eff}}$ as an attempt frequency and T_{13} as a probability for escaping through the left barrier.

We can now use Eq. (12) and the free-electron expressions Eq. (8) for the spectral functions to express the current I_{13} of Eq. (7) as

$$I_{13}=\frac{e}{L}\sum_{\mathbf{K}}\sum_{k_1} v(k_1)\Gamma_{13}\pi\delta(E_r-E_z(k_1))\times[n_F(E(\mathbf{k}_1)-\mu_1)-n_F(E(\mathbf{k}_1)-\mu_3)] . \tag{13}$$

An analogous expression gives the current through the second barrier. As current is conserved, the current out of the quantum well, I_{35}, must equal the current into it, I_{13}. By glancing at Eq. (13) for I_{13} we can immediately write down the expression for I_{35} as

$$I_{35}=\frac{e}{L}\sum_{\mathbf{K}}\sum_{k_5} v(k_5)\Gamma_{35}\pi\delta(E_r-E_z(k_5))\times[n_F(E(\mathbf{k}_5)-\mu_3)-n_F(E(\mathbf{k}_5)-\mu_5)] . \tag{14}$$

Equating the two currents leads to a constraint on the Fermi factor in the well, $n_F(E(\mathbf{k})-\mu_3)$. This point merits a small digression. In free-electron models such as we use here for the emitter and collector, the existence of a scattering mechanism is implicitly assumed in order to maintain thermal equilibrium. This unspecified scattering mechanism is, for instance, responsible for the energy relaxation of electrons elastically scattered into high kinetic energy states in the collector down to the chemical potential. If we insist that resonant tunneling occurs without any scattering in the barrier region there is no mechanism for obtaining thermal equilibrium in the quantum well. In this case there is no equilibrium Fermi distribution of electrons in the well and $n_F(E(\mathbf{k})-\mu_3)$ should be interpreted just as a *number* to be determined. This number, let us call it f_3, is readily obtained by adjusting the quantum-well occupancy in each $\mathbf{K}$ channel separately. Hence $f_3=f_3(\mathbf{K})$. After converting the sum over perpendicular momentum, k_1 (k_5) in Eq. (13) [Eq. (14)] to an integral over $E_z(k_1)$ [$E_z(k_5)$], one finds

$$f_3(\mathbf{K})=\frac{\Gamma_{13}n_F(E_r+E_{\parallel}(\mathbf{K})-\mu_1)+\Gamma_{35}n_F(E_r+E_{\parallel}(\mathbf{K})-\mu_5)}{\Gamma_{13}+\Gamma_{35}} . \tag{15}$$

Substituting this value in Eq. (13) and observing that the difference in chemical potential between the emitter and the collector is the applied voltage, one finds that the actual tunneling current I_{15} can be written as

$$I_{15}=\frac{e}{L}\sum_{\mathbf{K}}\sum_{k} v(k)T_{15}\times[n_F(E(\mathbf{k})-\mu)-n_F(E(\mathbf{k})-\mu+eV)] , \tag{16}$$

where

$$T_{15}=\tfrac{1}{2}T_{15}^{\mathrm{res}}\Gamma_{15}\pi\delta(E_r^0-\tfrac{1}{2}eV-E_z(k)) \tag{17}$$

and

$$T_{15}^{\mathrm{res}}=\frac{4T_{13}T_{35}}{(T_{13}+T_{35})^2},\quad \Gamma_{15}=\frac{\Gamma_{13}+\Gamma_{35}}{2} . \tag{18}$$

The sums in Eq. (16) are over the momenta in the emitter, $n_F(x)=[\exp(x/k_BT)+1]^{-1}$ is the Fermi factor and all energies are measured from the bottom of the band in the emitter.

Equations (16)–(18) are precisely the weak-tunneling limit of the scattering-theory result, obtained by solving the Schrödinger equation in regions 1–5 of Fig. 1 and matching the wave function and its derivative (i.e., conserving the current) at the boundaries.[6] This result was also derived by Payne,[15] in a less-general, single-particle framework. In the scattering theory the above result obtains when the transmission probability through the whole structure, T_{15}, can be approximated by a delta function.[6] In fact, it can be approximated by precisely the delta function of Eq. (17) where Γ_{15} is the width of the (actual) resonant level and T_{15}^{res} is the transmission probability at resonance. This maximum transmission probability is unity if the barriers are equal, i.e., if the transmission probability through the left barrier, T_{13}, equals the transmission probability through the right barrier, T_{35}. Otherwise it is smaller than unity, which for the model of Fig. 1 will be the case for all finite applied voltages.

Before we conclude this discussion we shall elaborate somewhat on how scattering changes the expressions for the tunneling current. We have already noted that scattering events that couple electron states in different subsystems fall outside the validity of Eq. (7) with the tunneling matrix element given by the Bardeen relation Eq. (9). Taking them into account amounts to generalizing the tunneling matrix element to a vertex function.[1,11,14] Scattering within the subsystems can be described by the spectral functions A_i and we will have more to say about that below. Here we want to emphasize another effect of scattering, which is perhaps less obvious: If scattering is present in the quantum well the nonequilibrium distribution $f_3(\mathbf{K})$ of Eq. (15) will be changed *towards* an equilibrium distribution, $n_F[E_r+E_{\parallel}(\mathbf{K})-\mu_3]$. If the equilibrium distribution was reached, the chemical potential μ_3 would have to be such that the current in and out of the quantum well was the same. We have both electron-electron scattering and elastic and inelastic impurity and phonon scattering in mind. Perhaps this point is best illustrated by a simplified example. If the lattice temperature is zero we could envisage a situation where all states in the emitter below the Fermi level E_F were occupied and no state of corresponding energy was occupied in the collector (again referring to Fig. 1). Furthermore, we might take $\Gamma_{13}=\Gamma_{35}=\Gamma$, independent of energy. For the case with no scattering it then follows from Eq. (15) that $f_3(\mathbf{K})=0.5$ for all $\mathbf{k}$ with $0<E_{\parallel}(\mathbf{K})<(E_F-E_r)$. With elastic scattering present in the quantum well the equilibrium distribution in the same case would be $n_F(E_r+E_{\parallel}(\mathbf{K})-\mu_3)$ with $\mu_3=(E_F-E_r)/2$, i.e., $n_F=1$ for $0<E_{\parallel}(\mathbf{K})<(E_F-E_r)/2$ and $n_F=0$ for $E_{\parallel}(\mathbf{K})>(E_F-E_r)/2$ for the zero-temperature case.

One might ask under what circumstances the equilibrium distribution is reached. This is not straightforward to answer. Certainly the time scale for scattering would have to be compared to the time scale for resonant tunneling. However, the latter time scale is itself affected by the former.[6] In fact the two time scales seem to be the same and in general we therefore do not expect an equilibrium distribution to fully develop. To the extent that the tunneling matrix element $T_{\mathbf{k}_1\mathbf{k}_3}$ depends on the parallel energy $E_{\parallel}(\mathbf{K})$ in addition to the perpendicular energy $E_z(k)$, it matters how the electrons in the well are distributed in $\mathbf{K}$. Such a dependence may arise even in an effective-mass approximation, simply from a space-dependent effective mass.[16]

We have in this section demonstrated that the tunneling Hamiltonian formalism is applicable to resonant tunneling. The strength of the many-body tunneling Hamiltonian formalism is that it is suitable for including interactions. We shall now proceed to investigate how electron-boson interactions affect the tunneling current.

III. RESONANT TUNNELING IN THE PRESENCE OF A BOSON FIELD

In the previous section the tunneling current was expressed in terms of the electron spectral functions $A(\mathbf{k},\varepsilon)$ on each side of the tunnel barrier. This is useful as it allows us to describe interacting electrons as long as the interactions do not couple electron states on different sides of the barrier. We shall now discuss resonant tunneling in the presence of a boson field, i.e., inelastic tunneling, using the formalism introduced above.

Consider first the customary model Hamiltonian for electron-boson interactions,

$$H_{e-\mathrm{ph}}=\sum_{\mathbf{q}} M_{\mathbf{q}}\rho_{\mathbf{q}}(a_{\mathbf{q}}+a_{\mathbf{q}}^{\dagger})+\sum_{\mathbf{q}}\hbar\omega_{\mathbf{q}}a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}}\ ,\qquad \rho_{\mathbf{q}}=\sum_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}}^{\dagger}c_{\mathbf{k}}\ , \tag{19}$$

where ρ_q, here expressed in plane-wave representation, is the electron density operator. The interaction matrix element $M_{\mathbf{q}}$ will depend on the type of interaction we may want to consider, and will be discussed below.

To fully incorporate the interaction described by Eq. (19) would be intractable. As a first approximation we therefore neglect coupling of electrons in different regions (emitter, well, collector) by the bosons. As a second approximation we neglect the electron-boson interactions in the emitter and collector altogether. Hence in regions 1 and 5 or Fig. 1 we keep the free-electron form of the spectral functions $A(\mathbf{k},\varepsilon)$ as given in Eq. (8). Including the effect here would broaden the states in the emitter and collector by a small amount. This is not very important. The effect is larger on the (partly) localized states in the quantum well. We recall[11] that the renormalization of the electron energies depends on the electron dispersion and is largest for a localized electron (i.e., no dispersion, infinite effective mass). Hence we keep the electron-boson interaction in the quantum well only.

For a three-dimensional heterostructure the approximations outlined above do not lead to an exactly solvable model for a general case. The difficulty comes from the momentum transfer between bosons and electrons in the direction parallel to the heterostructure. Of course, the problem may be treated by approximate methods. Rather than doing so here, we shall discuss several cases where additional restrictions on the model are justified and enable us to find an exact solution. The first case is a (quasi-) one-dimensional semiconductor heterostructure.[9] Here, the resonant level is localized in all three dimensions, and momentum is not a good quantum number. With one resonant level only, the electron density operator should be written as

$$\rho_{\mathbf{q}}=\int d\mathbf{r}\,|\Psi_i(\mathbf{r})|^2\exp(i\mathbf{q}\cdot\mathbf{r})c_i^{\dagger}c_i\equiv f_i(\mathbf{q})c_i^{\dagger}c_i\ . \tag{20}$$

The form factor $f_i(\mathbf{q})$ in Eq. (20) carries the information that only bosons with wavelengths longer than the spatial extent of the resonant eigenstate, Ψ_i, couple to the resonant level.

Another situation that can be described by an exactly solvable model in three dimensions concerns coupling to photons. Here, the momentum of the photons can be neglected, and only the zero-momentum component of the electron density operator enters and the density operator is diagonal in the parallel momenta, $\mathbf{K}$. In the long-wavelength limit, furthermore, the form factor corresponding to $f_i(\mathbf{q})$ in Eq. (20) is unity and one has

$$\rho_0=\sum_{\mathbf{K}} c_{\mathbf{K}}^{\dagger}c_{\mathbf{K}}\ . \tag{21}$$

In order to be able to discuss the general aspects of the different models alluded to above, we introduce a Hamiltonian for the quantum well, including the electron-boson interaction, of the form

$$H=\sum_{\mathbf{K}}\left[E(\mathbf{k})+\sum_{\mathbf{q}}M_{\mathbf{q}}(a_{\mathbf{q}}+a_{\mathbf{q}}^{\dagger})\right]c_{\mathbf{K}}^{\dagger}c_{\mathbf{K}}+\sum_{\mathbf{q}}\hbar\omega a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}}\ . \tag{22}$$

Here the electron energy is $E(\mathbf{k})=E_r+E_{\parallel}(\mathbf{K})$ and the phonon energy $\hbar\omega$ has no dispersion. The form of the matrix element, $M_{\mathbf{q}}$, will depend on the particular physical system and for the quasi-one-dimensional problem the summation over $\mathbf{K}$ drops out.

We shall now proceed to solve the resonant-tunneling problem with electron-boson coupling given by the Hamiltonian, Eq. (22), exactly. The Hamiltonian can be exactly diagonalized (see Ref. 11 for details). A canonical transformation,

$$\overline{H}=e^sHe^{-s},\quad s=\sum_{\mathbf{q}}\frac{M_{\mathbf{q}}}{\omega}(a_{\mathbf{q}}-a_{\mathbf{q}}^{\dagger})\sum_{\mathbf{K}}c_{\mathbf{K}}^{\dagger}c_{\mathbf{K}} \tag{23}$$

gives

$$\bar{H}=\sum_{\mathbf{q}}\hbar\omega a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}}+\sum_{\mathbf{K}}c_{\mathbf{K}}^{\dagger}c_{\mathbf{K}}[E(\mathbf{k})-\Delta],\quad \Delta=\sum_{\mathbf{q}}\frac{M_{\mathbf{q}}^{2}}{\hbar\omega}\ . \tag{24}$$

The spectral function $A_3(\mathbf{k}_3,\varepsilon)$ for electrons in the quantum well changes from the simple delta-function form $A_3^0(\mathbf{k}_3,\varepsilon)$ of Eq. (8) to a more complicated expression[11] involving a distribution of free-electron spectral functions,

$$A_3(\mathbf{k}_3,\varepsilon)=\sum_{n=-\infty}^{\infty}S_n A_3^0(\mathbf{k}_3,\varepsilon+\Delta-n\hbar\omega)\ , \tag{25}$$

where the peak labeled by n has a strength S_n given by

$$S_n=e^{-g(2N+1)}I_n(2g[N(N+1)]^{1/2})e^{n\beta\hbar\omega/2}\ . \tag{26}$$

In Eq. (26) I_n is a modified Bessel function, g is a dimensionless coupling strength, and N is the Bose factor,

$$g=\sum_{\mathbf{q}}\frac{M_{\mathbf{q}}^{2}}{(\hbar\omega)^2}\equiv\frac{\Delta}{\hbar\omega},\quad N=\frac{1}{\exp(\beta\hbar\omega)+1},\quad \beta=\frac{1}{k_BT}\ . \tag{27}$$

Before we return to discussing the particular physical systems briefly introduced earlier we shall comment on some general features of the spectral function, Eq. (25), which in the expression for the tunneling current will play the role of an effective transmission probability. As usual the spectral function $A(\mathbf{k},\varepsilon)$ is interpreted as the probability for an electron wave vector $\mathbf{k}$ to have energy ε. Here the spectral function describes coupled electron-phonon states where the index n corresponds to the number of bosons involved, negative (positive) n corresponding to absorption (emission) of bosons. In order to characterize the gross features of the spectral function we calculate its moments,

$$\langle\varepsilon^m\rangle=\int_{-\infty}^{\infty}\frac{de}{2\pi}\varepsilon^m A_3(\mathbf{k}_3,\varepsilon)\ . \tag{28}$$

By manipulating the modified Bessel functions as given by[17]

$$I_n(z)=\sum_{p=0}^{\infty}\frac{(z/2)^{2p+n}}{k!\Gamma(n+p+1)}\ , \tag{29}$$

where

$$\frac{1}{\Gamma(n+1)}=\frac{1}{n!}\quad\text{for } n=0,1,2,3,\ldots$$

and

$$\frac{1}{\Gamma(n+1)}=0\quad\text{for } n=-1,-2,-3,\ldots\ ,$$

we have calculated the three lowest moments. As appropriate for a probability function the zeroth moment is unity. The first moment, i.e., the average electron energy is found to be unaffected by the interactions, while the second moment of the spectral function, and hence the rms value of its width, depends on the strength of the interaction, g, as well as the temperature through the Bose factor N. We find

$$\langle\varepsilon^0\rangle=1,\quad\langle\varepsilon^1\rangle=E(\mathbf{k}_3)\ ,$$
$$(\langle\varepsilon^2\rangle-\langle\varepsilon\rangle^2)^{1/2}=\hbar\omega[g(2N+1)]^{1/2}\ . \tag{30}$$

There are three independent parameters in the model: temperature, boson frequency, and electron-boson coupling strength. The results for the three moments in Eq. (30) are independent of the parameter values, but the detailed shape of the spectral function is of course not. In particular the spacing, strength, and envelope of the peaks will vary. We shall now comment on how the spectral function, Eq. (26), depends on each of the parameters.

Temperature. Temperature has two effects on the spectral function. One is through the Bose factor N, which multiplies the dimensionless coupling constant g. A larger temperature corresponds to a stronger effective coupling constant. The other effect comes through the factor $\exp(n\beta\hbar\omega/2)=[(N+1)/N]^{n/2}$ of Eq. (26). As the modified Bessel function $I_n(z)$ is even in the index n, only this exponential factor provides an asymmetry with respect to positive and negative values of n. This asymmetry is expected as we are talking about absorption and emission of bosons. Also as expected the asymmetry vanishes in the limit of infinite temperature ($\beta=0$). For zero temperature, on the other hand, all occupation factors are zero, $N=0$, only positive values of n contribute, and Eq. (26) for the peak strengths reduces to $S_n=\exp(-g)g^n/n!$.

Boson frequency. The boson frequency enters explicitly in the spectral function. It also appears in the dimensionless coupling constant g and the energy shift Δ. In the high-frequency limit, g and Δ both tend to zero. Hence the limiting value for the spectral function, which is the free-electron result, $A_3^0(\mathbf{k}_3,\varepsilon)$, is given by the $n=0$ term of Eq. (25). This is the familiar behavior of a harmonic oscillator driven at a frequency much higher than its resonance frequency; the oscillator cannot respond at all. In the opposite limit of vanishingly small frequency, the coupling constant g and the energy shift Δ both diverge. This implies contributions for large values of n. On the other hand, the energy positions of different terms in the sum over n are closely spaced. One can show[11] that the limiting form of the spectral function is a Gaussian, whose width is given by the rms value of Eq. (30).

For very low frequencies we have to reexamine the validity our analysis. In this case we would expect the correct result to be more like the free-electron value of the spectral function evaluated at an instantaneous value for a time-dependent electronic energy.[18,19] Instead, our formalism contains, as it were, a thermal averaging over all positions of this energy. This can be the correct result only for frequencies larger than the inverse resonant-tunneling time, so that the resonantly tunneling electron sees many periods of the boson field.

Electron-boson coupling strength. The strength of the interaction enters the coupling constant g and the energy shift Δ. For zero coupling strength we recover the free-electron result while for very strong coupling we again get a Gaussian distribution of peaks. In contrast to the zero-frequency limit discussed earlier, the distribution is not continuous in energy as the boson frequency may have any value.

Further comments on how the results of the model depend on the parameter values will be given below, where we apply our model to three specific physical systems.

IV. APPLICATIONS TO SPECIFIC PHYSICAL SYSTEMS

We shall in this section apply the above analysis to specific physical systems. We first consider resonant tunneling in a quasi-one-dimensional GaAs-$Al_xGa_{1-x}As$ heterostructure, still referring to Fig. 1. Recently Reed *et al.*[9] have observed resonances in the tunnel current through such a structure and attributed it to a discrete spectrum of resonant levels in the quantum well. We may apply our model to investigate the effect of coupling of one resonant level with LO phonons. Within a dispersionless Einstein model the following expression for the matrix element[11] applies:

$$M_{\mathbf{q}}^2=\frac{M^2}{\Omega q^2},\quad M^2=2\pi e^2\hbar\omega_{LO}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]. \qquad (31)$$

The structures used in the experiment were about 1 μm long and 1000–2500 Å in diameter.[9] From the point of view of the phonons they can be considered three dimensional. We assume that the phonon wave vectors are uniformly distributed in a sphere of radius $q_D=(6\pi^2)^{1/3}/a$, where a is the lattice spacing. The dimensionless coupling constant g and the energy shift Δ can be calculated from a modified version of Eq. (27) where we have to include the form factor $f_i(\mathbf{q})$ of Eq. (20). The form factor is approximated to give a cutoff at wave vectors correspond to the width of the quantum well, d, and to the width of conducting channel, L_c, respectively:

$$f_i(\mathbf{q})\approx\Theta(\pi/L_c-|q_x|)\Theta(\pi/L_c-|q_y|)\Theta(\pi/d-|q_z|)\,. \qquad (32)$$

Without the form factor and using parameters for GaAs (Ref. 20) a value of $g=1.3$ obtains. With the form factor and the values $d=50$ Å, $L_c=130$ Å suggested by the experiment[9] one finds a smaller value, $g=0.08$. As described above this comes about because phonons whose wave length is shorter than the spatial extent of the resonant state do not contribute to the coupling. Apparently the physical situation at hand corresponds to the weak-coupling limit of the electron-boson interaction. In Fig. 2 we plot the quantum-well spectral function $A_3(\mathbf{k}_3,\varepsilon)$. We emphasize again that this spectral functions plays the role of an effective transmission probability. Results for $g=0.16$ at $T=77$ and 300 K as well as for $g=1.3$ at 77 K are plotted. For the GaAs LO phonon energy of 36 meV, the Einstein temperature is 419 K. Hence temperatures of 77 and 0 K give essentially the same result. For the lower coupling strength we are clearly in the weak-coupling regime. From Eq. (26) one readily finds that the limiting behaviors of the relative strengths of successive peaks, S_n and S_{n+1}, are related as $S_{n+1}/S_n=g(N+1)/(n+1)\ll 1$ for positive n. The relation between the emission and absorption peaks of the same order is in the same limit given by $S_{-n}/S_n=[N/(N+1)]^n$. The spectral function is hence dominated by the no-phonon ($n=0$) contribution. At 300 K we see the one-phonon loss and gain contributions ($n=1$ and -1). The value $g=0.16$ was chosen rather than 0.08 to better illustrate the weak one-phonon peaks. For the larger coupling strength a number of peaks appear even at 77 K.

As a second application we consider resonant tunneling in a three-dimensional GaAs-$Al_xGa_{1-x}As$ heterostructure in the presence of a laser beam. In Sollner's experiment[5] the laser frequency v was 2.5 THz, while the intensity I of the beam was not specified. Already a low

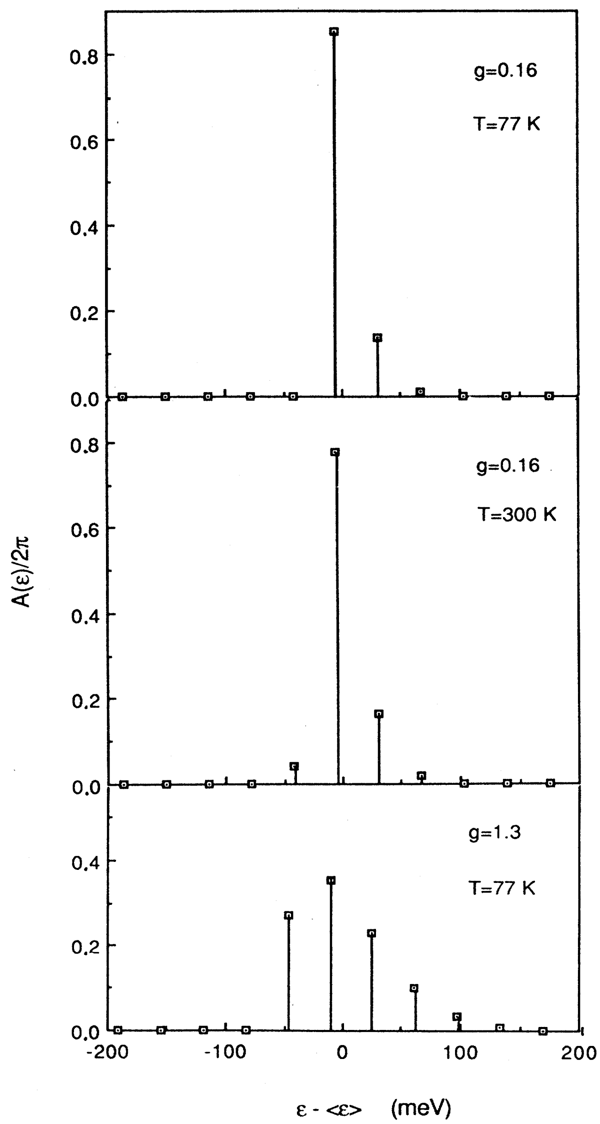

FIG. 2. Electron spectral function $A(\varepsilon)/2\pi$ for the coupled electron-phonon system in the quantum well of a quasi-one-dimensional GaAs-$Al_xGa_{1-x}As$ heterostructure as a function of energy ε. The height of the spikes gives the weight of the shifted free-electron values $A^0(\varepsilon+\Delta-n\hbar\omega)$ for different n, cf. Eq. (25). Results are shown for several values of the dimensionless coupling strength g and temperature T. The LO-phonon energy is taken to be 36 meV, corresponding to GaAs. For other parameters, see text.

intensity means, however, that the electromagnetic field can be treated classically. To see this we recall the relation between intensity and field strength $\mathcal{E}$, which in SI units is

$$I=\frac{1}{2}\left[\frac{\epsilon}{\mu}\right]^{1/2}|\mathcal{E}|^2 . \quad (33)$$

The energy content per unit volume, Ω, of the beam is I/c, where c is the velocity of light. This can be related to the photon energy and the number of photons N as

$$\frac{I}{c}=\frac{\hbar\omega}{\Omega}(N+\tfrac{1}{2}) . \quad (34)$$

Solving for N we find that for $I=10^8$ W/m^2, $\upsilon=2.5$ THz, $\mu=1$, and $\varepsilon=10.9$ (for GaAs) there are 2×10^6 photons in a volume of (100 Å)$\times$(1 mm^2). In other words, the electric field can be treated classically. In the Hamiltonian this corresponds to letting

$$(a+a^\dagger)\rightarrow 2\sqrt{N}\cos(\omega t),\quad M_q\rightarrow\frac{e\mathcal{E}d}{2\sqrt{N}} ,$$
$$N\rightarrow\infty\quad (T\rightarrow\infty,\beta\rightarrow 0) . \quad (35)$$

The Hamiltonian will now contain a term $W\cos(\omega t)$, where $W=e\mathcal{E}d$ is the amplitude of the potential energy modulation in the quantum well. Similar model systems have been studied earlier by numerical solution of a Schrödinger equation[19] and in the framework of classicial perturbation theory.[18] In our formalism we can simply read off the answer from the general result, Eq. (25). Using Eqs. (27) and (37) to make conversion

$$g(2N+1)\approx 2g\sqrt{N(N+1)}\approx 2gN\rightarrow\frac{1}{2}\left[\frac{W}{h\upsilon}\right]^2\equiv\bar{g} ,$$
$$\Delta=gh\upsilon\rightarrow 0 . \quad (36)$$

We find that the spectral function is a set of delta functions symmetric around the unperturbed electron energy. For $d=100$ Å, $\upsilon=2.5$ THz, and the electric field calculated from the beam intensity as above, the effective dimensionless coupling strength, $\bar{g}$ scales with the laser intensity as $\bar{g}=0.3(I/I_0)$, where $I_0=10^{12}$ W/m^2. We note that the chosen frequency corresponds to a photon energy of 10 meV. Many laser experiments are done with intensities of the order 10^8-10^9 W/m^2. For such intensities one is again clearly in the weak-coupling limit. We could easily imagine considerably more powerful laser beams, however. In Fig. 3 we plot the quantum-well spectral function for three values of the intensity, $I=1I_0$, $5I_0$, and $15I_0$. Our results are consistent with the numerical results of Ref. 19 for a double-barrier transmission coefficient in a related model. On the other hand the shape of the envelope of the peaks differs from what was found in Ref. 18, where essentially the same model as in Ref. 19 is studied. There the strength of the peaks depended on the ordinary Bessel function $J_n(z)$, which is an oscillating function of the index n, while or strengths depend on the modified Bessel function $J_n(z)$, which is a monotonic function of n.

A third and final application of our general discussion is to the case of an ac modulated voltage across a tunneling structure. Much of the previous discussion concerning the laser beam still holds, but the numbers will change. The amplitude of the voltage fluctuations, W, in a RT device used as a microwave generator[4] is of the order of 50 meV. For this amplitude the effective coupling strength $\bar{g}$ scales with frequency as $\bar{g}=74$ (1 THz/υ)^2. The photon energy scales as $h\upsilon=4.1$ [υ/(1 THz)] meV. For microwave frequencies we are clearly in the strong-coupling limit. As we remarked above, our analysis is really only valid for frequencies larger than the inverse tunneling time. Of course the tunneling time, and hence the lower frequency limit, is strongly dependent on the particular system we are considering. The tunneling time is strongly dependent on material and design of a heterostructure, but a typical value for a GaAs-Al_xGa_{1-x}As heterostructure is a picosecond. Hence we should only consider frequencies larger than 1 THz or so. In Fig. 4

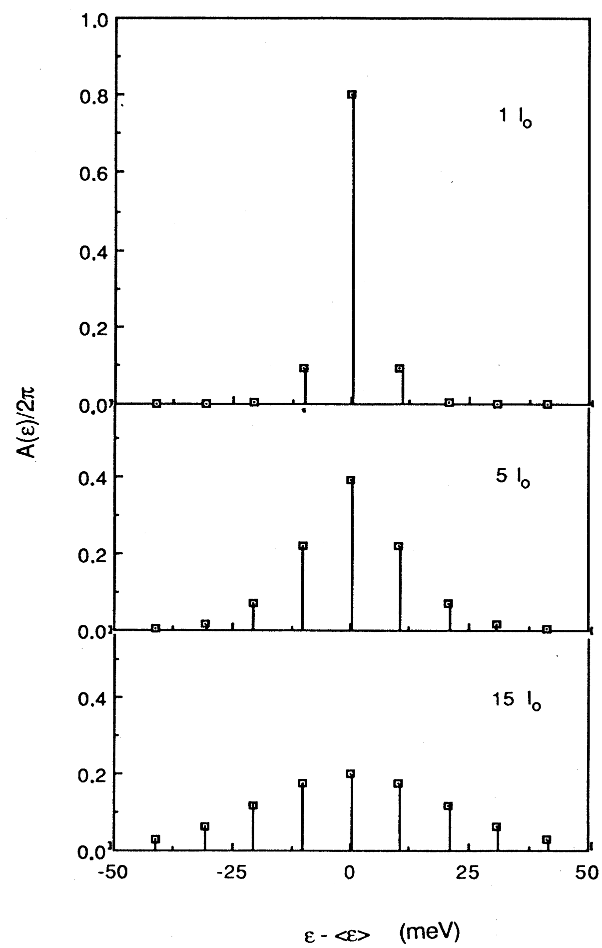

FIG. 3. Electron spectral function $A(\varepsilon)/2\pi$ for the coupled electron-photon system in the quantum well of a three-dimensional GaAs-Al_xGa_{1-x}As heterostructure as a function of energy ε. Results are shown for different intensities of a laser beam that interacts with system. The intensity is given in units of $I_0=10^8$ W/cm^2. The frequency of the laser beam is 2.5 THz. For other parameters see text.

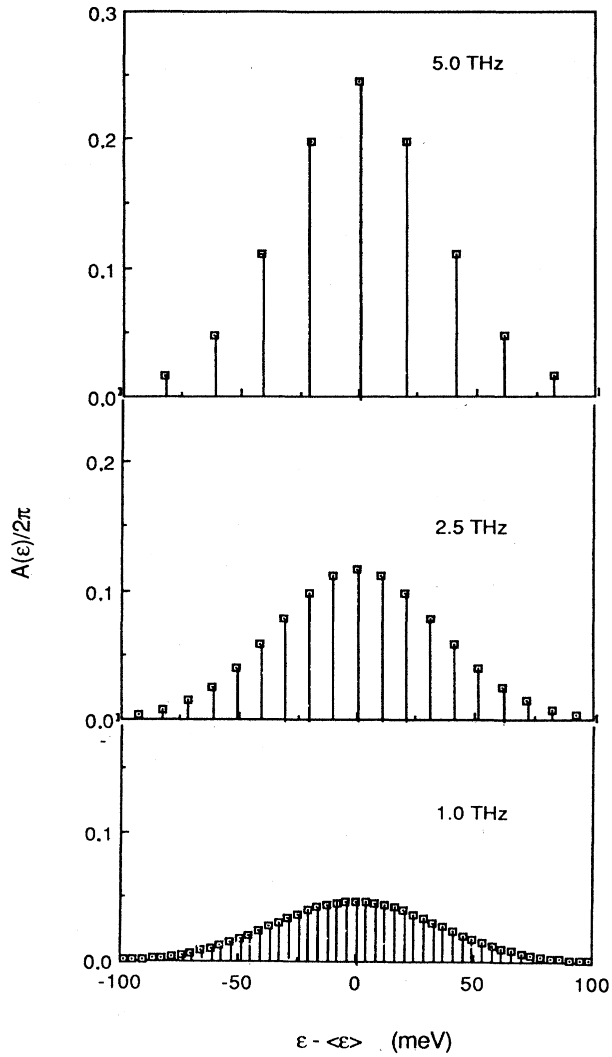

FIG. 4. Electron spectral function $A(\varepsilon)/2\pi$ for the coupled electron-photon system in the quantum well of a three-dimensional GaAs-$Al_xGa_{1-x}As$ heterostructure as a function of energy ε. Results are shown for different frequencies of a modulating ac voltage over the quantum well. The amplitude of the modulation is 50 meV. For other parameters, see text.

we plot the quantum-well spectral function for $v = 1, 2.5$, and 5 THz. The width of the Gaussian is from Eqs. (30) and (36) always $W/\sqrt{2}$. What varies is the density and strength of the peaks. Finally, we add that in a model that includes, say, an additional elastic scattering mechanism, the free-electron delta-function form of the spectral function, $A_3^0(\mathbf{k}_3,\varepsilon)$, in Eq. (25) is anticipated to acquire a finite width.

V. CONCLUSIONS

We have in the preceding section exactly solved an approximate model for inelastic resonant tunneling. The model is applicable when there is no momentum transfer between the tunneling electron and the boson field. The key quantity that plays the role of an effective transmission probability and hence controls the tunneling current is the spectral function for electrons in the resonant level. The initially sharp level broadens into a set of distinct peaks in the presence of a boson field. As the strength of the electron-boson coupling increases the envelope of the peaks tend to a Gaussian, while the separation between peaks increases with the boson frequency. Several physical situations, where the model might be applicable, have been discussed. Our intention has not been to furnish a detailed solution in any of these cases, but rather to point to some general features of the solution. Certainly, corrections due to the existence of several resonant levels and to a self-consistent treatment of the charge distribution may be important. Nevertheless it is interesting to consider the consequences of our model for the current voltage characteristics of a RT structure, such as that of Fig. 1. The analysis of Eq. (16) which gives the tunnel current, is greatly simplified by the observation that for parameters corresponding to a typical experiment all factors of the integrand except the transmission probability T_{15} vary slowly around the resonance energy. They vary on the scale of the chemical potential in the emitter. The effective transmission probability will in our theory be proportional to the spectral function $A_3(\mathbf{k}_3,\varepsilon)$. Without electron-phonon interaction this is a delta function, and the full weight of the spectral function contributes to the current if the delta function falls with the emitter band. It is well known this leads to an essentially linearly increasing tunnel current for applied potentials in the interval $2(E_r - E_F) < eV < 2E_r$. For larger applied voltages the resonant level drops below the bottom of the emitter band and the current is drastically reduced. This is the region of negative differential resistance, which is of great interest for device applications. The effect of the electron-boson interaction is to broaden the spectral function. This broadening was described phenomenologically in Ref. 6 by a Lorentzian with a width related to the inelastic mean free path. In this paper we have calculated the broadening microscopically. The picture in Ref. 6 that the tunnel current is affected only when the width of the transmission probability or spectral function is of the order the Fermi energy in the emitter is confirmed. The energy scale of the broadening of the spectral function in our theory is set by the boson energy, the temperature, and a dimensionless coupling constant. We feel that the theory provides a framework for more detailed calculations relating to the performance of various resonant-tunneling structures. These we hope to do in the future.

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