Rate equations for the phonon peak in resonant-tunneling structures

Roger Lake, Gerhard Klimeck, M. P. Anantram, and Supriyo Datta
School of Electrical Engineering, Purdue University, West Lafayette, Indiana 47907
(Received 26 July 1993)

The ratio of the phonon peak current to the main peak current in double-barrier resonant-tunneling structures is significantly enhanced by barrier asymmetry. Previously, using the Keldysh formalism, we derived analytical expressions, valid in the zero-temperature, high-bias regime, which explained this effect. We now provide analytical expressions valid for finite temperature and bias obtained from (i) an intuitive derivation using a rate equation approach and (ii) a more general derivation using the Keldysh formalism. The results of the two different approaches are shown to be essentially identical for the experimental device parameters. The finite temperature expressions shed light on the effect of the Pauli exclusion factors in the contacts on the current. In particular, we show that in a transmission formulation, the transmission coefficients, $T(\varepsilon,\varepsilon')$, are themselves functions of the Fermi factors in the contacts.

The ratio of the phonon peak current to the main resonant peak current in double barrier resonant tunneling structures (DBRTS's) is enhanced by barrier asymmetry.[1] Recently, an asymmetric DBRTS displayed a phonon peak as large as the main peak.[1(d)] The fact that an off-resonant, inelastic channel carries as much current as the main resonant channel is surprising. In a recent paper,[2] using the Keldysh formalism, we derived simple analytical expressions for the phonon-peak current valid in the high-bias, zero-temperature limit which explained this effect. We now provide analytical expressions obtained from (i) an intuitive derivation using a rate equation approach valid for finite temperature and bias and (ii) a more general derivation using the Keldysh formalism valid for finite temperature and bias. The results of the two very different approaches are essentially identical for device parameters found in Ref. 1. By showing how and in what limits the Keldysh equations reduce to rate equations, we clarify both the limits in which the rate equation approach is valid and the physics contained in the Keldysh approach. The high-temperature limit of the current expression is shown to be the same as that obtained by replacing the electron-phonon interaction in the well with a weak coherent ac potential. The results are compared with those calculated from the scattering approach of Wingreen, Jacobsen, and Wilkins.[3–5] The finite temperature expressions shed light on the form of the transmission coefficient, $T(\varepsilon,\varepsilon')$, for a nonequilibrium, interacting system and the relationship between the transmission coefficient and the current.[4] In particular, Pauli-exclusion factors in the contacts arise naturally in the two derivations, and the transmission coefficients themselves are shown to be functions of the Fermi factors of the contacts.

We derive general analytical expressions for the current and occupation of the well using a tight-binding model of a weakly coupled central site with the electron-phonon interaction at the $j=0$ site. The Hamiltonian consists of six parts:

$$\begin{aligned}
H_E &= \sum_{j<0} \{ -t[c_j^\dagger c_{j-1} + c_{j-1}^\dagger c_j] + \varepsilon_E c_j^\dagger c_j \} , \\
H_C &= \sum_{j>0} \{ -t[c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j] + \varepsilon_C c_j^\dagger c_j \} , \\
H_W &= \varepsilon_0 c_W^\dagger c_W, \quad H_p = \hbar\omega_0 b^\dagger b , \qquad (1)\\
H_T &= -t_E[c_{-1}^\dagger c_W + c_W^\dagger c_{-1}] + -t_c[c_1^\dagger c_W + c_W^\dagger c_1] , \\
H_{ep} &= V c_W^\dagger c_W (b^\dagger + b) .
\end{aligned}$$

$H_{E(C)}$ is the Hamiltonian of the semi-infinite emitter (collector) regions on either side of the central site with site energies which are constant and differ between the two regions by the applied voltage. H_W and H_p are the Hamiltonians of the uncoupled central site and the phonon bath, respectively. H_T connects the central site to the emitter and collector leads. H_{ep} is the electron-phonon interaction at the central site. c_j is the electron annihilation operator at site j, and b is the phonon annihilation operator at the central site. The phonons are dispersionless with energy $\hbar\omega_0$. The dimensionless phonon coupling constant is $g \equiv V^2/(\hbar\omega_0)^2$.

First, we derive the general expressions for the phonon-peak current and the occupation of the resonance using perturbation theory and rate equations. Then we show how the Keldysh approach leads to identical results. Transition rates between the leads and the resonant site are derived using elementary, time-independent perturbation theory, treating as the perturbation $H' = H_T + H_{ep}$. For weak electron-phonon coupling, the important inelastic channel occurs between the resonant energy E_r and the incident energy $E_i = E_r + \hbar\omega_0$ [see Fig. 1 and also Fig. 1(a) of Ref. 2]. Therefore, in the following derivation, we consider only the coupling between the resonant and incident energies and ignore higher energies such as $E_r + 2\hbar\omega_0$ and lower energies such as $E_r - \hbar\omega_0$. We treat the coupling of the central site to the leads to first order, so that the resulting expressions are valid for weakly coupled (large barrier) structures.

0163-1829/93/48(20)/15132(6)/$06.00 ©1993 The American Physical Society

We treat the coupling to the phonon bath to first order, so that the resulting general-temperature expressions are valid for $g \ll 1$. This is the case for the experimental structures in Ref. 1. In the nonequilibrium Green-function derivation, the corresponding assumptions are that $E_f \gg \Gamma^r$ and $(\hbar\omega_0)^2 \gg (\Gamma^i)^2/4$ which is the case for all of the experimental structures in Ref. 1. Superscripts r and i indicate that the quantity is to be evaluated at the resonant energy or the incident energy, respectively. E_f is the Fermi energy in the emitter and $\Gamma^{r(i)} = \Gamma_E^{r(i)} + \Gamma_C^{r(i)} + \Gamma_\phi^{r(i)}$ where Γ_ϕ is twice the imaginary part of the retarded self-energy due to the electron-phonon interaction and $\Gamma_{E(C)}/\hbar$ is the tunneling rate through the emitter (collector) barrier.

Consider our model system, Fig. 1. The state $|k_E\rangle$ is an eigenfunction of H_E and the states $|k_C^i\rangle$ and $|k_C^r\rangle$ are eigenfunctions of H_C; for example, the collector eigenstates satisfy $H_C|k_C\rangle = E|k_C\rangle$ where $E = \varepsilon_C - 2t\cos(k_C a)$ and

$$|k_C\rangle = \sqrt{2/N}\sum_{j=1}^{N-1}\sin(jk_C a)|j\rangle ,$$

where $k_C = n\pi/Na$ with $n \in \{1,2,\ldots,N-1\}$. The quantity a is the lattice spacing and $|j\rangle$ is the state localized at site j. The length of the contact regions is semi-infinite so that $N \to \infty$ and k is continuous. The dispersion relation for the emitter (collector) eigenstates is $E = \varepsilon_{E(C)} - 2t\cos(k_{E(C)}a)$. The state in the well, $|W\rangle$, is the unconnected localized state at $j=0$ with site energy ε_0. We define direct-product electron-phonon states $|k_E;N_p\rangle = |k_E\rangle \otimes |N_p\rangle$ where $|N_p\rangle$ satisfies $H_p|N_p\rangle = N_p\hbar\omega_0|N_p\rangle$.

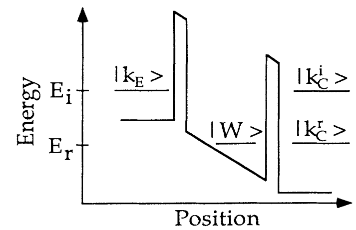

FIG. 1. Eigenstates of H_E, H_C, and H_W used in the perturbation calculations.

To calculate the total rate of transitions from $|k_E\rangle$ to $|W\rangle$ we consider the matrix elements between the initial states $|k_E;N_p\rangle$ and the final state $|W;N_p+1\rangle$.

$$R_{W,k_E} = \sum_{k_E}\frac{2\pi}{\hbar}\frac{|\langle W;N_p+1|H'|W;N_p\rangle\langle W;N_p|H'|k_E;N_p\rangle|^2}{[E(k_E)-\varepsilon_0]^2}\delta(E(k_E)-\varepsilon_0-\hbar\omega_0)$$
$$= \sum_{k_E}\frac{2\pi}{\hbar}\frac{2}{N}\sin^2(k_E a)t_E^2 g(N_B+1)\delta(E(k_E)-\varepsilon_0-\hbar\omega_0) = \frac{1}{\hbar}\Gamma_E^i g(N_B+1) , \quad (2)$$

where we have replaced N_p by its average value $\langle N_p\rangle = N_B(\hbar\omega_0)$ where N_B is the Bose-Einstein factor, and used the relations $\Gamma_E \equiv 2\sin(k_E a)t_E^2/t$ and $g \equiv V^2/(\hbar\omega_0)^2$. Note that Γ_E is simply t_E^2 times the spectral function at the $j=-1$ site. The rate from $|k_C^i\rangle$ to $|W\rangle$ is obtained by replacing Γ_E^i with Γ_C^i in (2).

To calculate the reverse rate from $|W\rangle$ to $|k_E\rangle$ we consider the matrix elements between the initial state $|W;N_p\rangle$ and the final states $|k_E;N_p-1\rangle$.

$$R_{k_E,W} = \sum_{k_E}\frac{2\pi}{\hbar}\frac{|\langle k_E;N_p-1|H'|W;N_p-1\rangle\langle W;N_p-1|H'|W;N_p\rangle|^2}{[\varepsilon_0-E(k_E)]^2}\delta(E(k_E)-\varepsilon_0-\hbar\omega_0) = \frac{1}{\hbar}gN_B\Gamma_E^i , \quad (3)$$

where we have replaced N_p by its average value. Again, the rate from $|W\rangle$ to $|k_C^i\rangle$ is obtained by replacing Γ_E^i with Γ_C^i in (3).

To calculate the total rate from states $|k_C^r\rangle$ to $|W\rangle$, we need only first-order perturbation theory.

$$R_{W,k_c^r} = R_{k_c^r,W} = \sum_{k_c^r}\frac{2\pi}{\hbar}|\langle W;N_p|H'|k_C^r;N_p\rangle|^2\delta(E(k_C^r)-\varepsilon_0) = \frac{1}{\hbar}\Gamma_C^r . \quad (4)$$

The above rates will now be used in rate equations to obtain the inelastic component of the current and the occupation of the resonance at the phonon-peak bias.

To obtain the occupation of the resonance, we equate the in-scattering rate (multiplied by $\hbar$)

$$R_{\text{in}} = [f_E^i\Gamma_E^i g(N_B+1) + f_C^i\Gamma_C^i g(N_B+1) + f_C^r\Gamma_C^r](1-f^r) \quad (5a)$$

and the outscattering rate

$$R_{\text{out}} = f^r[\Gamma_E^i gN_B(1-f_E^i) + \Gamma_C^i gN_B(1-f_C^i) + \Gamma_C^r(1-f_C^r)] \quad (5b)$$

to and from the resonant state. Note that each rate calculated from perturbation theory is sandwiched between a factor of f for the initial state and $(1-f)$ for the final state. Setting $R_{\text{in}} = R_{\text{out}}$ and solving for f^r we obtain

$$f^r = \frac{\Gamma_C^r f_C^r + g(N_B+1)(\Gamma_E^i f_E^i + \Gamma_C^i f_C^i)}{\Gamma_C^r + gN_B[\Gamma_C^i(1-f_C^i)+\Gamma_E^i(1-f_E^i)] + g(N_B+1)[\Gamma_C^i f_C^i + \Gamma_E^i f_E^i]} . \tag{6}$$

The inelastic current is given by the transition rate from the emitter to the resonant state minus the reverse process,

$$I_{\rm in} = \frac{2e}{\hbar}[f_E^i \Gamma_E^i g(N_B+1)(1-f^r) - f^r g N_B \Gamma_E^i (1-f_E^i)] , \tag{7}$$

where we have multiplied by 2 for spin. Substituting (6) into (7) gives the general expression for the inelastic phonon-peak current

$$I = \frac{2e}{\hbar}\frac{f_E^i\Gamma_E^i g(N_B+1)\Gamma_C^r(1-f_C^r) - f_C^r\Gamma_C^r gN_B\Gamma_E^i(1-f_E^i)}{\Gamma_C^r + gN_B[\Gamma_C^i(1-f_C^i)+\Gamma_E^i(1-f_E^i)] + g(N_B+1)[\Gamma_C^i f_C^i + \Gamma_E^i f_E^i]} + \frac{2e}{\hbar}\frac{\Gamma_E^i g(N_B+1)\Gamma_C^i gN_B(f_E^i - f_C^i)}{\Gamma_C^r + gN_B[\Gamma_C^i(1-f_C^i)+\Gamma_E^i(1-f_E^i)] + g(N_B+1)[\Gamma_C^i f_C^i + \Gamma_E^i f_E^i]} . \tag{8}$$

The numerator of (8) has an intuitive form. The first term represents the current flowing from the emitter at the incident energy out to the collector at the resonant energy minus the reverse process. The second term which is second order in g represents electrons flowing in from the emitter at the incident energy, emitting a phonon and scattering down to the resonance, absorbing a (different) phonon and exiting through the collector back at the incident energy, minus the reverse process.

The derivation using the nonequilibrium Green-function formalism treats H_T exactly and H_{ep} in the self-consistent first Born approximation. The only difference in the results is that the central site energy is renormalized. The derivation of (6)–(8) begins with the general expressions for the emitter current per unit energy and the occupation of the central site derived in Ref. 2,

$$I_E = \frac{2e}{h}\frac{A}{\Gamma}\{\Gamma_E\Gamma_C(f_E - f_C) + \Gamma_E[f_E\hbar/\tau_n - (1-f_E)\hbar/\tau_p]\} , \tag{9a}$$

$$f = [\Gamma_E f_E + \Gamma_C f_C + \hbar/\tau_p]/\Gamma . \tag{9b}$$

All quantities in (9) are evaluated at the energy of interest. In (9), $A = \Gamma/[(E-\varepsilon_r)^2 + \Gamma^2/4]$ is the spectral function of the central site where

$$\varepsilon_r = \varepsilon_0 - \frac{t_E^2}{t}\cos(k_E a) - \frac{t_C^2}{t}\cos(k_C a) + \sigma^R$$

is the renormalized resonant energy, $\Gamma = \Gamma_C + \Gamma_E + \hbar/\tau_\phi$, and $\hbar/\tau_\phi = \hbar/\tau_n + \hbar/\tau_p$. The quantities $\hbar/\tau_\phi$, $\hbar/\tau_n$, and $\hbar/\tau_\phi$ are related to the self-energies by

$$\Sigma^<(i,0;E) = i\hbar/\tau_p(0;E)\delta_{i,0} ,$$

$$\Sigma^>(i,0;E) = -i\hbar/\tau_n(0;E)\delta_{i,0} ,$$

and

$$\Sigma^R(i,0;E) = [\sigma^R(0;E) - i\hbar/2\tau_\phi(0;E)]\delta_{i,0} .$$

The first term of (9a) is the coherent component of the current, and the second term is the inelastic component. Only energies E_r and E_i are considered when calculating the scattering rates $1/\tau_n$ and $1/\tau_p$:

$$\hbar/\tau_n^i = V^2(N_B+1)A^r(1-f^r) , \tag{10a}$$

$$\hbar/\tau_p^i = V^2 N_B A^r f^r , \tag{10b}$$

$$\hbar/\tau_n^r = V^2 N_B A^i(1-f^i) \simeq gN_B\Gamma^i(1-f^i) , \tag{11a}$$

$$\hbar/\tau_p^r = V^2(N_B+1)A^i f^i \simeq g(N_B+1)\Gamma^i f^i . \tag{11b}$$

The approximate relations in (11) are obtained from the following:

$$A^i/\Gamma^i \simeq 1/(E_i-\varepsilon_r)^2 \simeq 1/(\hbar\omega_0)^2 , \tag{12}$$

which is justified in the limits discussed after Eq. (1). Using the above expressions for the scattering rates (10a) and (10b) to evaluate the inelastic current per unit energy at the incident energy from (9a) gives

$$I_E^{\rm inelastic} = \frac{2e}{h}[f_E^i\Gamma_E^i g(N_B+1)A^r(1-f^r) - f^r A^r g N_B \Gamma_E^i(1-f_E^i)] , \tag{13}$$

where (12) is used to evaluate A^i/Γ^i. Since the spectral function is sharply peaked about the resonant energy, $E_r = E_i - \hbar\omega_0$, integrating over incident energies integrates out the spectral function of the resonance, A^r, resulting in a factor of 2π and Eq. (7).

A self-consistent calculation of f^r begins with (9b) written for the resonant and incident energies.

$$f^r = \frac{\Gamma_C^r f_C^r + g(N_B+1)\Gamma^i f^i}{\Gamma^r} , \tag{14}$$

$$f^i = \frac{\Gamma_E^i f_E^i + \Gamma_C^i f_C^i + V^2 N_B A^r f^r}{\Gamma^i} . \tag{15}$$

Substituting (15) into (14) and solving for f^r gives

$$f^r = \frac{\Gamma_C^r f_C^r + g(N_B+1)(\Gamma_E^i f_E^i + \Gamma_E^i f_E^i + \Gamma_C^i f_C^i)}{\Gamma^r - g(N_B+1)V^2 N_B A^r} . \tag{16}$$

The numerator is the same as in (6). We now evaluate the denominator by first evaluating Γ^r,

$$\Gamma^r = \Gamma_C^r + \hbar/\tau_n^r + \hbar/\tau_p^r = \Gamma_C^r + gN_B\Gamma^i(1-f^i) + g(N_B+1)\Gamma^i f^i . \tag{17}$$

Substituting the expression for f^i, Eq. (15), into (17), we find that the denominator of (16) is identical to the denominator of (6). Thus a self-consistent calculation of f^r from the Keldysh approach results in Eq. (6). The calculation of the current from the Keldysh approach resulted in (7) and substitution of (6) into (7) gives (8).

In both the rate equation and Keldysh approaches, we have, so far, ignored the coherent component of the off-resonant current. In the first approach, the rate of coherent transitions is obtained by considering the matrix element $\langle k_C|H'|W\rangle\langle W|H'|k_E\rangle$. Except for the renormalization of the central site energy, the current found is identical to that obtained from the Keldysh approach, Eq. (9a), after approximating A^i/Γ^i as $1/(E_i-\varepsilon_r)^2$.

The high-temperature limit $[N_B(\hbar\omega_0)=N_B(\hbar\omega_0)+1]$ of (8) is

$$I=\frac{2e}{\hbar}\frac{\Gamma_E^i g'\Gamma_C^r(f_E^i-f_C^r)}{\Gamma_C^r+g'[\Gamma_C^i+\Gamma_E^i]}+\frac{2e}{\hbar}\frac{\Gamma_E^i g'\Gamma_C^i g'(f_E^i-f_C^i)}{\Gamma_C^r+g'[\Gamma_C^i+\Gamma_E^i]}\ , \tag{18}$$

where $g'=gN_B(\hbar\omega_0)=g[N_B(\hbar\omega_0)+1]$. If we substitute a weak coherent ac potential $2U\cos(\omega_0 t)\delta_{j,0}$ for H_{ep} in the Hamiltonian (1) and, considering only the coupling between the incident and resonant energies, calculate the dc current as described in Ref. 6, we obtain Eq. (18) with $g'=U^2/(\hbar\omega_0)^2$.

Consider our expressions for the current, (7) and (8), in terms of transmission $T(\varepsilon,\varepsilon')$. First, we compare our results in the zero-temperature, high-bias limit to those obtained from the single particle transmission approach of Wingreen, Jacobsen, and Wilkins.[3] Then, the general current expression (8) is used to obtain transmission coefficients for the nonequilibrium, interacting system.

In the zero-temperature, high-bias limit, Eq. (7) for the current becomes

$$I=\frac{2e}{\hbar}g\Gamma_E^i(1-f^r)\ . \tag{19}$$

The single particle transmission coefficient calculated from scattering theory to first order in g consists of four contributions (see Fig. 9 of Ref. 3). At the phonon-peak bias for the typical thick barrier experimental structures, only the contribution from the emission of one real phonon is important. We refer to this as the real inelastic channel as opposed to the channels representing virtual processes. The transmission coefficient for this channel is (in the zero-temperature limit)

$$T(\varepsilon_f,\varepsilon)=\Gamma_E(\varepsilon)\Gamma_C(\varepsilon_f)V^2\delta(\varepsilon-\varepsilon_f-\hbar\omega_0)|G^R(\varepsilon)|^2\times|G^R(\varepsilon_f)|^2\ . \tag{20}$$

Note that the Green functions appearing in (20) are different from the Green functions appearing in the Keldysh expressions. The Green functions in (20) are true single particle electron Green functions since they are defined as an ensemble average over the phonon states but as a matrix element of the electron vacuum [see Eq. (A10) of Ref. 3 and ensuing discussion]. In contrast, the Keldysh Green functions are ensemble averaged over both the electron and phonon states.[7,8] Integrating (20) over final energies gives

$$T(\varepsilon)=\Gamma_E(\varepsilon)\Gamma_C(\varepsilon-\hbar\omega_0)V^2|G^R(\varepsilon)|^2|G^R(\varepsilon-\hbar\omega_0)|^2\ . \tag{21}$$

Writing $|G^R(\varepsilon-\hbar\omega_0)|^2=A(\varepsilon-\hbar\omega_0)/\Gamma(\varepsilon-\hbar\omega_0)$ and assuming that A is sharply peaked about ε_r, we integrate (21) over incident energies to obtain the current

$$I=\frac{2e}{h}\int d\varepsilon\, T(\varepsilon)=\frac{2e}{\hbar}\frac{\Gamma_E(\varepsilon_i)\Gamma_C(\varepsilon_r)}{\Gamma(\varepsilon_r)}V^2|G^R(\varepsilon_i)|^2\ , \tag{22}$$

where $\varepsilon_i=\varepsilon_r+\hbar\omega_0$. Using the relation $|G^R(\varepsilon_i)|^2=A^i/\Gamma^i$ and Eq. (12), (22) becomes

$$I=\frac{2e}{\hbar}\frac{g\Gamma_E^i\Gamma_C^r}{\Gamma^r}\ . \tag{23}$$

Replacing Γ^r with the elastic resonance width ($\Gamma^r_{\text{elastic}}=\Gamma_C^r$ since $\Gamma_E^r=0$) gives

$$I=\frac{2e}{\hbar}g\Gamma_E^i\ . \tag{24}$$

Not surprisingly, the single particle result (24) matches our result (19) except for the Pauli-exclusion factor $(1-f^r)$. It is, therefore, independent of the collector barrier.

It is disconcerting to obtain an expression for the inelastic current which is independent of the collector barrier. Clearly, as the collector barrier becomes very large, the current must go to zero. To understand why this unphysical result is obtained, it is necessary to understand how the scattering problem is posed. Initially, at $t\rightarrow-\infty$, the device is prepared in the empty state and an electron is injected with energy ε_i towards the device from the left. Once the incident electron tunnels through the emitter barrier, it can always emit a phonon and scatter down to the resonant state since the resonant state is empty. At low temperature, phonon absorption can be neglected. Thus, for any finite size collector barrier, the electron that has scattered down to the resonant state will have leaked out into the collector as $t\rightarrow\infty$. Thus the transmission coefficient calculated from scattering theory for the low-temperature, real inelastic channel is indeed independent of the collector barrier. The error occurs not in calculating the transmission coefficient but in using the transmission coefficient to obtain a current. During the time that the electron dwells in the resonance, the next electron is prevented from entering. The attempt rate, $g\Gamma_E^i/\hbar$, must be multiplied by the probability of finding an empty state, $(1-f^r)$, to obtain the current. This is not taken into account in the single particle approach.

We note three things. First, a self-consistent first Born treatment of the electron-phonon interaction to calculate $G^R(\varepsilon_r)$ and thus a renormalized Γ^r leaves Γ^r essentially unchanged due to the single particle definition of the Green function. By contrast, in the Keldysh approach, the current expression can also be written as (23) with $\Gamma^r=\Gamma_C^r+\hbar/\tau_n^r+\hbar/\tau_p^r=\Gamma_C^r+g\Gamma^i f^i$ using (11) in the zero-temperature, high-bias limit ($N_B=0$). In this limit, from

(15), $f^i=\Gamma_E^i/\Gamma^i$ so that $\Gamma^r=\Gamma_C^r+g\Gamma_E^i$. Substituting this expression for Γ^r into (23) gives

$$I=\frac{2e}{\hbar}\frac{g\Gamma_E^i\Gamma_C^r}{g\Gamma_E^i+\Gamma_C^r} \; . \tag{25}$$

Equation (25) is equivalent to (19) as can be seen by substituting the zero-temperature, high-bias limit of (6) into (19). The renormalization factor $g\Gamma_E^i$ is due to the hole outscattering rate at the resonant energy $\hbar/\tau_p^r$ which is proportional to the electron density at the incident energy, $n(\varepsilon_i)=\langle c_w^\dagger c_w(\varepsilon_i)\rangle$ [see Eq. (11b)]. Since, in the scattering approach, brackets indicate a matrix element of the electron vacuum, this term is zero. Second, the exact expression derived by Wingreen, Jacobsen, and Wilkins [Eq. (32) of Ref. 4] is derived in the wideband limit for which $\Gamma^r=\Gamma_E^r+\Gamma_C^r$ where the tunneling rates Γ_E and Γ_C are independent of energy. Making this substitution into (23) matches their first-order result for the real inelastic channel,

$$I=\frac{2e}{\hbar}\frac{g\Gamma_E\Gamma_C}{\Gamma_E+\Gamma_C} \; . \tag{26}$$

In the limit of $\Gamma_C \gg \Gamma_E$, which is the limit considered in Ref. 3, all three expressions (24), (25), and (26) coincide. Finally, both the wideband limit and the scattering approach are only valid for the problem of the phonon peak in the limit $\Gamma_C \gg \Gamma_E$. The scattering approach does not account for the Pauli-exclusion factor which becomes important for $\Gamma_C \lesssim \Gamma_E$. The wideband limit allows reflection from the resonance to the emitter at the resonant energy. This is unphysical since at the phonon-peak bias, the resonance lies below the conduction band of the emitter. However, the reflection is insignificant for $\Gamma_C \gg \Gamma_E$ because any electron at the resonance escapes through the small collector barrier.

Now we attempt to write the first-order term of (8) in the form of either[4]

$$I=\frac{2e}{h}\int d\varepsilon\int d\varepsilon_f\{T_{C,E}(\varepsilon_f,\varepsilon)f_E(\varepsilon)[1-f_C(\varepsilon_f)] - T_{E,C}(\varepsilon_f,\varepsilon)f_C(\varepsilon)[1-f_E(\varepsilon_f)]\} \tag{27}$$

or

$$I=\frac{2e}{h}\int d\varepsilon\int d\varepsilon_f\{T_{C,E}(\varepsilon_f,\varepsilon)f_E(\varepsilon)-T_{E,C}(\varepsilon_f,\varepsilon)f_C(\varepsilon)\} \; . \tag{28}$$

To obtain (8) we integrated over incident energies to integrate out the spectral function of the resonance which resulted in a factor of 2π. Let us undo that integral and also multiply by an energy-conserving delta function $\delta(\varepsilon_i-\varepsilon_r-\hbar\omega_0)$. Then the first-order term of (8) can be written as

$$I=\frac{2e}{h}\int d\varepsilon_i\int d\varepsilon_r\{T_{C,E}(\varepsilon_r,\varepsilon_i)f_E(\varepsilon_i)[1-f_C(\varepsilon_r)] - T_{E,C}(\varepsilon_i,\varepsilon_r)f_C(\varepsilon_r)[1-f_E(\varepsilon_i)]\} \; , \tag{29}$$

where

$$T_{C,E}(\varepsilon_r,\varepsilon_i)=\Gamma_E(\varepsilon_i)g(N_B+1)\Gamma_C(\varepsilon_r) \times A(\varepsilon_r)\delta(\varepsilon_i-\varepsilon_r-\hbar\omega_0)/D(\varepsilon_i,\varepsilon_r) \; , \tag{30}$$

$$T_{E,C}(\varepsilon_i,\varepsilon_r)=\Gamma_C(\varepsilon_r)gN_B\Gamma_E(\varepsilon_i) \times A(\varepsilon_r)\delta(\varepsilon_i-\varepsilon_r-\hbar\omega_0)/D(\varepsilon_i,\varepsilon_r) \; , \tag{31}$$

and $D(\varepsilon_i,\varepsilon_r)$ is the denominator in (8) where the superscripts indicate the energy, ε_i or ε_r.

The Keldysh formalism appears to support Eq. (27) as the proper expression for the current. However, the transmission coefficients (30) and (31) are rather odd. The transmission coefficients themselves, in the denominator, $D(\varepsilon_i,\varepsilon_r)$, contain Fermi factors in the contacts. To understand why this occurs, consider the difference between the current expressions obtained from the Keldysh approach and the single particle scattering approach, Eqs. (19) and (24). In the Keldysh approach, the current is a function of the occupation of the states in the device (in this problem the device consists of a single state). The occupation of the device state is in turn a function of how electrons are injected at it from all of the different contacts at all energies, so that the occupation of the device state is a function of the Fermi factors in the contacts. Thus we should expect to find Fermi factors of the contacts appearing in the transmission coefficients (30) and (31). However, once we admit contact Fermi factors into the expressions for the transmission coefficients, it is no longer clear whether the factors of $(1-f)$ appearing in the current expression (29) should actually be considered as part of the transmission coefficients, $T_{E,C}$ and $T_{C,E}$. Depending on how the transmission coefficients are defined, the current can be cast in the form of either (27) or (28). To our knowledge, this is the first calculation of nonequilibrium, inelastic transmission coefficients $T(\varepsilon,\varepsilon')$ which goes beyond a single particle approach.[9,10] The view that emerges from the Keldysh formalism is not that of a scattering approach[11] but that of a complex set of quantum rate equations which balance and correlate the inscattering and outscattering of quasiparticles to and from each state in the device. Once balance is achieved, i.e., once the occupation of states is known, or, more generally, once $G^<(m,n;E)$ is known, where m and n represent states of the device, the current can be calculated.

In conclusion, analytical expressions valid for finite temperature and bias are derived from the phonon-peak current and occupation of the resonance using both the Keldysh approach and rate equations. The results are essentially identical for the device parameters found in Ref. 1. The high-temperature limit is equivalent to that obtained by replacing the electron-phonon interaction with a weak coherent ac potential. Transmission coefficients $T_{E,C}(\varepsilon,\varepsilon')$ and $T_{C,E}(\varepsilon,\varepsilon')$ for the interacting system are shown to contain within themselves Fermi factors of the contacts. Pauli-exclusion factors in the contacts arise naturally in the Keldysh and rate equation approaches.

One of us (R.L.) acknowledges useful communications with N. Wingreen and an informative comment of K. Hess. This material is based upon work supported by the Army Research Office (Contract No. 30369-PH-URI), the National Science Foundation (Grant No. ECS-9201446-01), and the Purdue Research Foundation.

---

[1](a) V. J. Goldman, D. C. Tsui, and J. E. Cunningham, Phys. Rev. B **36**, 7635 (1987); (b) A. Zaslavsky, V. J. Goldman, D. C. Tsui, and J. E. Cunningham, Appl. Phys. Lett. **53**, 1078 (1988); (c) E. S. Alves, L. Eaves, M. Henni, O. H. Hughes, M. L. Leadbeater, F. W. Sheard, and G. A. Toombs, Electron. Lett. **24**, 1190 (1988); (d) P. J. Turley, C. R. Wallis, S. W. Teitsworth, W. Li, and P. K. Bhattacharya, Phys. Rev. B **47**, 12 640 (1993).

[2]R. Lake, G. Klimeck, and S. Datta, Phys. Rev. B **47**, 6427 (1993).

[3]N. S. Wingreen, K. W. Jacobsen, and J. W. Wilkins, Phys. Rev. B **40**, 11 834 (1989).

[4]For further discussion, see F. Sols, Ann. Phys. **214**, 386 (1992).

[5]For a more recent use of this approach applied to resonant tunneling, see N. Zou and K. Chao, Phys. Rev. Lett. **69**, 3224 (1992).

[6]S. Datta and M. P. Anantram, Phys. Rev. B **45**, 13 761 (1992).

[7]L. V. Keldysh, Zh. Eksp. Teor. Fiz. **47**, 1515 (1964) [Sov. Phys. JETP **20**, 1018 (1965)].

[8]R. A. Craig, J. Math. Phys. **9**, 605 (1968).

[9]The integrand of the expression derived by Meir and Wingreen, Phys. Rev. Lett. **68**, 2512 (1992), Eq. (9), for the special case $\Gamma_E = \lambda \Gamma_C$ is not a transmission coefficient when inelastic processes are present. It contains no information about the energy distribution of the current flowing from the emitter to the device or from the device to the collector. It is simply a quantity which, when integrated over all energy, gives the total current.

[10]For equilibrium transmission coefficients for an interacting system see S. Datta, Phys. Rev. B **45**, 1347 (1992).

[11]R. Landauer, IBM J. Res. Dev. **32**, 306 (1988).