

Reflection of electrons and phonon-assisted Landauer resistance

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(Received 28 November 1994)

A theory is developed for the combined effects of electron-phonon scattering and elastic reflection of electrons on electrical current through a nanostructure. We use a time-dependent quantum-linear-response theory, then take the limit of zero frequency. In addition we develop a parallel theory that is semiclassical. The results obtained by the two methods are the same. The effect of phonons on the current flow is small because in this effect final as well as initial electron states in the electron-phonon scattering must have nonzero transmission through the nanostructure.

I. INTRODUCTION

We have derived a theory for the combined effects of electron-phonon scattering and elastic reflection of electrons on the Landauer electrical conductance G that has maximum conductance $2e^2/h$ for each conductance channel.¹ See, for example, the steplike structures in G versus gate voltage in Fig. 1 that have step height $2e^2/h$. Conductance with the maximum value $2e^2/h$ in each

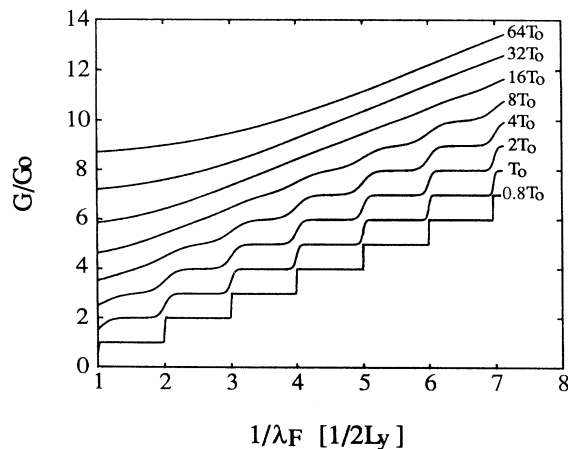


FIG. 1. Landauer conductance G of a model nanostructure with no electron-phonon scattering and in the absence of electron reflection in the few channels occupied in the nanostructure. $1/\lambda_F$ expresses a filling factor with n_y levels $1, 2, 3, \dots$ just beginning to be occupied when $1/\lambda_F$ just exceeds $1, 2, 3, \dots$ times $1/2L_y$. (The filling factor is changed, e.g., by changing a gate voltage.) The unit of temperature shown from 1 to 80 K on the eight curves is $T_0 = 1.25$ K. Each successive curve is displaced upward by an additional unit of conductance $G_0 = 2e^2/h$.

channel occurs only with the type of spatially localized transport electric field that occurs with current flow through nanostructures.² These are mesoscopic systems, which means with spatial extent along the current path that is much smaller than the inelastic scattering length l_{inel} .

In an earlier paper involving two of the present authors,³ a semiclassical theory was developed for the effects of electron-phonon scattering on G . The semiclassical method of Ref. 3 is limited to changes of G by small amounts $|\Delta G| \ll G$ and to nanostructures which are joined to macroscopically thick lead wires in a smooth or adiabatic manner.⁴ In that case the n th channel electron transmission probability is $T_n = 1$ for a few channels, N_{ch} in number, but $T_n = 0$ occurs for all other channels. (In a bulk-metal lead wire attached to a nanostructure the number of conductance channels $N_{\text{ch}}^{(0)}$ without the nanostructure interrupting the wire would be macroscopically large $N_{\text{ch}}^{(0)} > 10^{10}$.) Now we have extended the semiclassical theory to the case where elastic reflection of electrons occurs as well as phonon scattering, so that $T_n \leq 1$ rather than $T_n = 1$ among the N_{ch} channels where $T_n \neq 0$. Thus the effect of phonons on G has now been determined theoretically for the actual situation that occurs in a variety of nanostructures. We will present numerical results for a model nanostructure with constant cross section which has transverse dimensions small in comparison to the length of the nanostructure. Again the joining regions from lead wires to this structure are changing in cross-sectional area adiabatically slowly and smoothly as discussed by Glazman *et al.*,⁴ but we introduce a short potential barrier in the middle of the nanostructure which causes reflection $0 \leq T_N < 1$ in each of the N_{ch} channels. This model nanostructure is expected to simulate qualitatively an actual situation where, in general,

the nanostructure may not be smoothly or adiabatically joined to macroscopic lead wires.

We find the effect of phonons on the Landauer conductance to be small $|\Delta G| \ll G$ even at 80 K. The inelastic scattering time in ΔG is much larger than in a bulk electron system because the small N_{ch} restricts final as well as initial electron states in the electron-phonon scattering, i.e., $\Delta G \propto N_{\text{ch}}^2$ whereas $G \propto N_{\text{ch}}$. But the electron group velocity in nanostructures is very much smaller than in a bulk system.⁴ Thus the l_{inel} at a nanostructure is not strongly increased from l_{inel} for a bulk system. But the N_{ch}^2 factor in ΔG is important because without that, the condition $|\Delta G| \ll G$ at 80 K would not occur.

The effects of increasing temperature on quasiquantized Landauer conductance (at zero applied magnetic field) are still large: because nonzero Fermi occupation numbers for adjacent channels begin to overlap strongly at higher temperature at the steps in Fig. 1, the steps are smeared out and are gone when T is larger than 10 K, shown theoretically in the model nanostructure of Ref. 3 and widely observed experimentally.¹ But effects of phonons in limiting one-electron coherence effects in transport measurements are predicted here to be small, proportional to $|\Delta G| \ll G$, even up to 80 K. This suggests the possibility that some coherence effects in transport measurements may be observable even at liquid-air temperatures, e.g., Aharonov-Bohm interference patterns.¹ (One disappointing aspect of the many startling effects in mesoscopic physics has been the limitation to very low temperatures.) At this time that is only speculation because we have not yet developed a theory, e.g., for the magnetic Aharonov-Bohm effect at higher temperatures.

In the theory of Landauer conductances there has been continuing doubt in a wider community of theoreticians² about the derivation of G , but not the result, in heuristic or semiclassical methods. These methods, including our own in Ref. 3, require that the current-flow state of the system be characterized entirely by a quasichemical potential $\mu_i = eV_i$ for each lead wire, where V_i is an electrical voltage. In the Büttiker theory,⁵ great care was taken in defining a thermodynamic reservoir with chemical potential μ_i that is at some distance from the nanostructure. Moreover, equal care was taken in not specifying μ_i for any species of current carriers within or near the nanostructure itself.^{5,6} Proceeding well beyond the careful limitations specified by Büttiker in his heuristic theory, we have earlier in Ref. 3 taken quasichemical potentials *in the nanostructure itself* as characterized by $\mu_+ - \mu_- = e\Delta V$, as in Eqs. (16) and (18) below. (See the book by Shockley for a definition of quasichemical potentials and a discussion of chemical versus electrical potentials.⁷) The μ_{\pm} characterize forward-flowing (+) or backward-flowing (-) current carriers. ΔV is the electrical voltage drop, the line integral of electric field through the conductor. Ideally it is measured by a battery-based balanced potentiometer at room temperature wherein differences of the electrical potentials and the chemical potentials are known to be equal differences according to fundamental properties of a battery. But this known equality is not near or at the nanostructure.

In contrast to heuristic or semiclassical derivations of

G , quantum-mechanical transport theory must express current flow in terms of something that can be expressed in a Hamiltonian, a vector or scalar potential (or both) characterizing a transport electric field. We have extended an earlier quantum-response-theory derivation of G by one of the authors,² wherein no phonon scattering occurred, to include effects of both phonon scattering and elastic reflection on the Landauer conductance. It will be seen below that results of the quantum-linear-response theory are identical to those obtained in our semiclassical theory. But this and many other quantum-linear-response theories say nothing about chemical potentials of the current-flow state. In addition, however, in a separate publication one of the authors has used a gauge-invariant quantum-response theory, previously applied by Ambegoakar and Kadanoff to superconductors,⁹ to show that the relation $\mu_+ - \mu_- = e\Delta V$ required for the semiclassical theory does occur in the nanostructure itself.⁸ (As no current-flow state can arise in quantum mechanics without a time dependence in the Hamiltonian, even in the zero-frequency limit, the quantum theory is necessarily time dependent.) There are essential characteristics for current carriers leaving and approaching a nanostructure, at distances far from the nanostructure, in Büttiker's carefully defined thermodynamic reservoirs.⁵ In the quantum theory of Ref. 8, these characteristics as well as the e^2/h quantum of conductance are caused by quantum mechanics of the nanostructure itself. This may not be surprising: surely e^2/h must arise rather directly from the quantum mechanics and not depend critically on a careful thermodynamic definition for distant macroscopic bodies.

The quantum-response theory and the semiclassical theory will both be derived below. Following that, numerical results will be presented for a model nanostructure that incorporates both elastic reflection of electrons and electron-phonon scattering in several conductance channels.

II. QUANTUM-LINEAR-RESPONSE THEORY

The main result in the quantum-response theory of Ref. 2 was that whereas the Boltzmann-Drude transport theory descriptive for bulk metals was obtained for an effective transport electric field $\mathbf{E}(\mathbf{r}, t)$ that is characterized by a single wave vector \mathbf{q}_0 , with $\mathbf{q}_0 = 0$, the Landauer-Büttiker conductance G characterizing mesoscopic system⁵ is obtained only when $\mathbf{E}(\mathbf{r}, t)$ is localized in space to the region of the mesoscopic system itself—a continuous spectrum of \mathbf{q}_0 wave vectors. The theory of Ref. 2 included elastic scattering only. In the following we will first derive the conductance with only phonon scattering, for a transport field $E_x(q_{0x}, \omega_0)$ in the limit $\omega_0 \rightarrow 0$, with a continuous q_0 wave-vector spectrum representing an $\mathbf{E}(\mathbf{r}, t)$ that is localized in the current-flow x direction within a mesoscopic length L_E . For wave vector $q_0 \ll \pi L_E^{-1}$, the Fourier component $E_x(q_0, \omega_0)$ is equal to ΔV , the electrical voltage drop through the mesoscopic system. Following the derivation of the conductance $G + \Delta G$ with only phonon scattering, we will then determine $G + \Delta G$ with both elas-

tic and phonon scattering present.

The Hamiltonian for the system in the zero-current state is

$$\begin{aligned}
 H = & \sum_{n,k} \varepsilon_{nk} c_{nk}^\dagger c_{nk} + \sum_{\substack{n,k \\ n',k'}} V(nk, n'k') c_{n'k'}^\dagger c_{nk} \\
 & + \sum_q \hbar\omega_q (a_q^\dagger a_q + \frac{1}{2}) \\
 & + \sum_{\substack{n,k \\ q, n'}} g_{nn'q} c_{n'k+q_x}^\dagger c_{nk} (a_q^\dagger + a_q). \quad (1)
 \end{aligned}$$

The one-electron energy ε_{nk} is that of the basis function for a bulk metal or a two-dimensional electron system (2DES). There is a propagating-mode wave vector k in the current-flow x direction and one of the n -channel standing-wave states such as $\text{sink}_\perp \cdot \mathbf{r}_\perp$ from the \mathbf{k}_\perp spectrum. V is the k -wave and n -mode transform of an elastic scattering potential $V(\mathbf{r})$. The third and fourth terms of H are phonon and electron-phonon parts with $g_{nn'q}$ the n -mode transform of the usual electron-phonon coupling constant. The $T_n = 1$ Glazman *et al.* channel states⁴ or partially reflected channel states can be constructed for a nanostructure (with attached lead wires) as linear combinations of the nk basis states.

The quantum theory for linear current response to a time-dependent electric field in Ref. 2 used the Baym-Kadanoff formalism which derives Matsubara-Feynman response diagrams from the diagrams of the zero-current state. In contrast to the well-known impurity-averaging theory,¹⁰ the theory of Ref. 2 for elastic scattering only has no imaginary part in the one-electron energy. However, with inelastic phonon scattering instead of elastic scattering in the formalism of Ref. 2, there is an imaginary part in the one-electron energy. In this case the response diagram satisfies the diagram equation of Fig. (2). On each diagram the dashed lines on the right- and left-hand sides represent the transport electric field $E_x(x', t')$ and total current $I(x, t)$, respectively. The part between dashed lines including the two current-flow

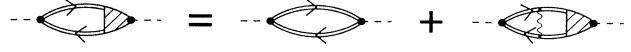


FIG. 2. Diagram integral equation for the phonon-renormalized current propagator \mathcal{D} , summing an infinite diagram series where noncrossing wiggly phonon lines occur 0, 1, 2, 3, . . . times. The double solid line is an electron line renormalized by phonon scattering, in the self-consistent approximation where only noncrossing phonon lines occur.

three-vertices is the current propagator \mathcal{D} from x', t' to x, t . (This is usually called a current-current correlation function.) We denote the Fourier transform of this by $\mathcal{D}_{n,n'}(q_0, \omega_0)$. The bare current three-vertex is $ev_{Fn\pm} = \pm ev_{Fn}$, electron charge times the Fermi group velocity. The full current three-vertex includes effects of the phonon scattering. In the Matsubara-Feynman diagram procedure of Ref. 2, the electron Green function (propagator for one Heisenberg field amplitude) is the retarded (R) or advanced (A) function

$$\mathcal{G}_{nk}^{R,A}(\omega) = \frac{1}{\omega - \varepsilon_{nk} - \Sigma_{nk}^{R,A}(\omega)}. \quad (2)$$

With $\omega \pm i\delta \rightarrow i\omega_v$, the Matsubara thermal frequency, \mathcal{G} is the thermal Green function. $\Sigma^{R,A}$ is the electron self-energy due to electron-phonon scattering. When the electron-phonon coupling is not too strong (not exactly the same condition as $|\Delta G| \ll G$), the electron self-energy can be easily derived with quantities such as $\text{Re}[\partial\Sigma(\omega)/\partial\omega]$ (real part) and $\text{Re}[\partial\Sigma(\omega)/\partial k]$ absorbed into a renormalized electron density of states $\rho_n(0)$ and renormalized Fermi velocity v_{Fn} , within the self-energy diagrams. There are factors $|g_{nn'q}|^2$ equal to $|g_q|^2 |\langle n | e^{iq \cdot r} | n' \rangle|^2$ and so on from the semiclassical theory of Ref. 3 that just change the usual self-energy from \mathbf{k} -wave to n -channel notation. [It can be shown that contributions from $\text{Re}\Sigma$ to v_{Fn} and $\rho_n(0)$ do not change the relation $\rho_n(0) = (hv_{Fn})^{-1}$ in the Landauer conductance.]

With real parts of Σ expressed in changes of E_F , $\rho_n(0)$, and v_{Fn} , the imaginary part of the self-energy is

$$\begin{aligned}
 \text{Im}\Sigma_{nk}^R(\omega + i\delta) &= - \sum_{n'} \int \frac{dk'}{2\pi} |\langle n' | e^{iq_1 \cdot r_\perp} | n \rangle|^2 W_q \delta_{q_x, k' - k} \\
 &\quad \times \{ [1 - f(\varepsilon_{n'k'}) + N_q] [\delta(\omega - \varepsilon_{n'k'} - \omega_q)] + [f(\varepsilon_{n'k'}) + N_q] [\delta(\omega - \varepsilon_{n'k'} + \omega_q)] \} \\
 &\equiv \sum_{n'} \text{Im}\Sigma_{nkn'k'}^R(\omega + i\delta). \quad (3)
 \end{aligned}$$

In $\text{Im}\Sigma$, the initial electron state in the electron-phonon scattering is on the energy shell, $\hbar\omega = \varepsilon_{nk}$, and $W_q = \pi Z^2 q^2 / \rho \omega_q$, where Z is the deformation potential and ρ the mass density. $f(\varepsilon_{nk})$ and N_q are Fermi and Bose distribution functions. This expression includes only ladder graph self-energy diagrams with noncrossing phonon lines and bare electron lines, which omits terms that are negligible when $v_{\text{sound}} |\text{Im}\Sigma| \ll v_F k_B T$.

The wiggly line in the third response diagram of Fig. 2 is the phonon propagator renormalized by electron-phonon scattering, self-consistent with the noncrossing approximation. We can easily show by direct algebraic evaluation that in this third response diagram the phonon line, two electron-phonon three-vertices, the two electron lines to the right of the phonon lines, and the dressed current three-vertex are just together equal to

$-(2i/e)\text{Im}\Sigma_{nk''k''}\text{sgnk}''\mathcal{D}_{n''k''n''k'}$. (Summation over $n''k''$ is implied.) This equivalence is most easily seen by replacing the right-hand dressed three-vertices with the bare three-vertex $ev_{Fn'\pm}$, which algebraically yields $-(2i/e)\text{Im}\Sigma\mathcal{D}^{(0)}$, and then iterating the integral equation to infinite order. $\mathcal{D}^{(0)}$ is the current propagator with no phonon renormalization of the current three-vertex. The integral equation represented by the diagram equation of Fig. 2 is

tion to infinite order. $\mathcal{D}^{(0)}$ is the current propagator with no phonon renormalization of the current three-vertex. The integral equation represented by the diagram equation of Fig. 2 is

$$\mathcal{D}_{nk''k'}(\omega_0, q_0, \omega) = \mathcal{D}_{nk}^{(0)}(\omega_0, q_0, \omega)\delta_{n,n'}\delta_{k,k'} + \mathcal{D}_{nk}^{(0)}(\omega_0, q_0, \omega)(e^2v_{Fn})^{-1}[-2i\text{Im}\Sigma_{nk''k''}^R(\omega)\text{sgnk}\text{sgnk}'']\mathcal{D}_{n''k''n''k'}(\omega_0, q_0, \omega). \quad (4)$$

Summation over $n''k''$ is implied. $\mathcal{D}_{nk}^{(0)}(\omega_0, q_0, \omega)$ is defined by

$$\begin{aligned} \mathcal{D}_{n\pm}^{(0)}(q_0, \omega_0) &= \int d\omega \frac{\partial f(\omega)}{\partial \omega} \sum_{k \geq 0} e^2v_{Fn}^2 \mathcal{G}_{n,k \geq 0}^A \left[\omega - \frac{\omega_0}{2} \right] \mathcal{G}_{n,k \geq 0}^R \left[\omega + \frac{\omega_0}{2} \right] \\ &= \int d\omega \frac{\partial f(\omega)}{\partial \omega} e^2v_{Fn} [\omega_0 - v_{Fn\pm}q_0 - 2i\text{Im}\Sigma_{nk}^R(\omega)]^{-1} \\ &= \int d\omega \frac{\partial f(\omega)}{\partial \omega} \mathcal{D}_{n\pm}^{(0)}(q_0, \omega_0, \omega). \end{aligned} \quad (5)$$

In $\mathcal{G}^{A,R}$, the electron wave vector is $k - q_0/2$ for A and $k + q_0/2$ for R . $\mathcal{D}(\omega_0, q_0)$ is related to $\mathcal{D}(\omega_0, q_0, \omega)$ by an equation analogous to the last equality in Eq. (5).

The elements $\mathcal{D}_{nn'}$ of the full current propagator comprise a square matrix $\underline{\mathcal{D}}$ and we denote by \underline{K} the matrix of the elements $-2i(e^2v_{Fn})^{-1}\text{Im}\Sigma_{nn'}^R\text{sgnk}\text{sgnk}'$. The diagram equation of Fig. 2 becomes

$$\underline{\mathcal{D}} = \underline{\mathcal{D}}^{(0)} + \underline{\mathcal{D}}^{(0)}\underline{K}\underline{\mathcal{D}}. \quad (6)$$

Multiplying Eq. (6) on the left-hand side by $\underline{\mathcal{D}}^{(0)-1}$ and on the right-hand side $\underline{\mathcal{D}}^{-1}$,

$$\mathcal{D}_{nn'}^{-1} = \mathcal{D}_{n\pm}^{(0)-1}\delta_{n,n'} - K_{nn'}. \quad (7)$$

We define \mathcal{D}_n^{-1} as $\sum_{n'}\mathcal{D}_{nn'}^{-1}$ and K_n as $\sum_{n'}K_{nn'}$. Then

$$\mathcal{D}_{n\pm}^{-1} = \mathcal{D}_{n\pm}^{(0)-1} - K_n \quad (8)$$

$$\begin{aligned} &= (e^2v_{Fn})^{-1} \left[\omega_0 - q_0v_{Fn\pm} - \sum_{n'} 2i\text{Im}\Sigma_{nn'}^R(\omega)(1 - \text{sgnk}\text{sgnk}') \right] \\ &\equiv (e^2v_{Fn})^{-1} [\omega_0 - q_0v_{Fn\pm} + 2i\text{Im}\Sigma_n^{\text{tr}}(\omega)]. \end{aligned} \quad (9)$$

The quantity $2\text{Im}\Sigma_n^{\text{tr}}$ is \hbar times the inverse transport time, corresponding to the usual inverse transport time in bulk metals wherein the factor $1 - \cos\theta(\mathbf{k}, \mathbf{k}')$ occurs in a scattering integral. The approximation we have used is appropriate except right at the steps in Fig. 1, where $v_{Fn} \rightarrow 0$ and this approximation breaks down. We will comment on this later.

The full current propagator for the $E_x(q_0, \omega_0)$ component of the electric field including phonon scattering but no elastic scattering is

$$\begin{aligned} \sum_{n\pm} \mathcal{D}_{n\pm}(q_0, \omega_0, \omega) \\ = \sum_{n\pm} e^2v_{Fn} [\omega_0 - q_0v_{Fn\pm} + 2i\text{Im}\Sigma_n^{\text{tr}}(\omega)]^{-1}. \end{aligned} \quad (10)$$

Here the $\mathcal{D}_{n\pm}$ are the algebraic inverses of the $\mathcal{D}_{n\pm}^{-1}$ and are components of a diagonalized response matrix.

The current is obtained² by summing or integrating the

current propagator over the q_0 components and the electron energy ω , in the limit where the field frequency is $\omega_0 \rightarrow 0$. The q_0 component of \mathcal{D} is multiplied by $\exp[iq_0(x - x')]$ times $E(x')$. A factor \hbar deleted from $\hbar\omega_0$ and $\hbar q_0v_{Fn\pm}$ (in the usual convention) must be restored and there is a factor $i/2\pi$ as well. As with the elastic scattering case in Ref. 2, the full q_0 spectrum of the localized transport electric field for a mesoscopic system contributes a dominant real term to $I(x)$, here proportional to $\delta[\hbar\omega_0 - \hbar q_0v_{Fn\pm} - 2i\text{Im}\Sigma_n^{\text{tr}}(\omega)]$, and there is a (usually) negligible imaginary term from the principal part in the q_0 integration that is of order $\max(\omega_0 L_E / v_{Fn}, k_B T L_E / \hbar v_{Fn})$ compared to the real term. In the limit $\omega_0 \rightarrow 0$, the integration over the electron energy $\hbar\omega$ is weighted by a factor $\partial f(\omega) / \partial \omega$ as in Eq. (5).

With two spin states per channel, the current flow with only phonon scattering present is given in the limit $\omega_0 \rightarrow 0$ by

$$I(x) = \frac{-2e^2}{h} \sum_n \int_{\varepsilon_{n0}}^{+\infty} d\omega \frac{\partial f(\omega)}{\partial \omega} \int_{-\infty}^{+\infty} dx' \exp[-|x-x'|] 2 \operatorname{Im} \Sigma_n^{\text{tr}}(\omega) / \hbar v_{Fn} E_x(x'). \quad (11)$$

In Eq. (11), $\hbar\omega = \varepsilon_{nk}$ in each channel and so the lower limit on ω is ε_{nk} at $k=0$. This expression does not express current that is independent of x at zero frequency. This is because with no elastic scattering at all, i.e., with translational invariance in the x direction, the static $\omega_0 \rightarrow 0$ electric field localized to $-\frac{1}{2}L_E \leq x' \leq \frac{1}{2}L_E$ could not occur. We can still use Eq. (11) with no elastic scattering present in the theory for an actual physical case where all but a few of the macroscopically large number of channels $N_{\text{ch}}^{(0)}$ have zero electron transmission through the mesoscopic system. The remaining few channels must be for a smoothly entered mesoscopic system⁴ which has adiabatically changing $k_x(x)$ and transverse wave functions $\psi_n(\mathbf{r}_\perp, x)$ so that v_{Fn} becomes $v_{Fn}(x)$ and the transmission probability is $T_n = 1$. In this case $v_{Fn}(x \approx 0)$ is much smaller than $v_{Fn}(x \rightarrow \pm\infty)$ so that a localized $E_x(x')$ is consistent with $I(x) = I$ when $\omega_0 \rightarrow 0$. There must remain at large $|x'|$ a spatially constant part of $E_x(x')$ denoted by $E_0 \delta(q_0)$ that is added to the q_0 spectrum of the localized electric field.² Whereas the localized electric field at the mesoscopic system corresponds to a resistance on the kilohm scale over a very short distance, the field E_0 for a bulk metal corresponds to resistance of less than 1 Ω over macroscopic lengths of lead wire. The E_0 contribution to the voltage drop ΔV across the mesoscopic system is vanishingly small.

In Eq. (11), formally $\operatorname{Im} \Sigma_{nk_F}^{\text{tr}}(\omega)$ is exact. After the x' integration has been done, the approximation for $\operatorname{Im} \Sigma^{\text{tr}}$ in Eqs. (3)–(10) is made. For example, in a bulk degenerate semiconductor the effective transport field is homogeneous and the x' integration results in $E_x \hbar v_{Fn} / \operatorname{Im} \Sigma_{nk_F}^{\text{tr}}(\omega)$. Summing over a very large number of channels of a bulk system results in the standard expression for the conductivity $ne^2 \tau_{\text{tr}} / m$. Here $\tau_{\text{tr}}^{-1} = 2 \langle \operatorname{Im} \Sigma_{k_F}^{\text{tr}}(\omega) \rangle / \hbar$, where the angular brackets denote the thermal and Fermi-surface average. At this stage the approximation for $\operatorname{Im} \Sigma^{\text{tr}}$ in Eqs. (3)–(10) can be made and the result determines resistance or voltage drop to lowest order in $v_{\text{sound}} |\operatorname{Im} \Sigma| / v_F k_B T$. This is an excellent approximation in strongly degenerate semiconductors with, e.g., relative error less than 10^{-3} when $T = 77$ K for GaAs. We will comment later on the accuracy of this approximation in our determination of ΔG in nanostructures.

We now consider the combined effects of elastic and phonon scattering on the current response. In Ref. 2 the elastic scattering potential $V(\mathbf{r})$ in H of Eq. (1) was represented as an X on an electron line in the response diagram, representing $\mathcal{G}_{nk}(\omega) V(nk, n'k') \mathcal{G}_{n'k'}(\omega)$. The infinite sequence of such events sums as usual to an elastic scattering transition (not transmission) matrix $T_{nk'n'k'}(\omega)$ for transitions from state nk to state $n'k'$. (The transmission probability through the mesoscopic system in the n th channel is something different from that and denoted by T_n with only one subscript and no

energy argument.) For the localized $\mathbf{E}(\mathbf{r}, t)$ at a mesoscopic system, electron lines between two or more $T_{nk'n'k'}(\omega)$ are not distinguishable from an internal electron line within the infinite series summed by $T_{nk'n'k'}(\omega)$, so that a series of more than one T matrix collapses into the internal structure of one T matrix. Thus there can be only zero or one $T_{nk'n'k'}(\omega)$ on one upper or lower electron line on a response diagram in Fig. 2, in the absence of phonon scattering. [In contrast, an arbitrary number of $T_{nk'n'k'}(\omega)$ from one impurity can occur on one electron line in the response diagram of Ref. 2 for a bulk metal.] When we introduce phonon scattering, two distinct cases emerge. The first case is where pairs of electron-phonon three-vertices on one electron line are connected by a phonon line. When these connected pairs are between two X elastic scattering events, they constitute phonon renormalization of the energy-conserving and nk -conserving electron line between the two X events. Consistent with the noncrossing phonon-line approximation used above in Eq. (3), valid when $v_{\text{sound}} |\operatorname{Im} \Sigma| \ll v_F k_B T$, we restrict the renormalization again to noncrossing phonon lines. When there are phonon lines which connect two three-vertices that are on opposite sides of one X event, then this is renormalization of the elastic $V(\mathbf{r})$ scattering. We must self-consistently restrict to a nested set of noncrossing phonon lines at each X with each phonon line commencing on one side of X and finishing on the other side. Within $T_{nk'n'k'}(\omega)$ the internal k'' are summed over all states, so that effects of the renormalization are only of order $|\Sigma| / v_{Fn} k_{Fn}$, completely insignificant in almost every physical situation and the same order of magnitude or smaller than small terms that were dropped throughout Ref. 2.

The second case of phonon scattering added to elastic scattering is that an electron-phonon three-vertex is not connected to a three-vertex on the same electron arm (upper or lower) of a response diagram. Because no unconnected electron-phonon three-vertex can occur inside the elastic scattering $T_{nk'n'k'}(\omega)$, an electron line between two T matrices, which has one unconnected electron-phonon three-vertex on it, is distinguishable from internal electron lines of the T matrix. There is in this case no collapse of two T matrices into one. Including the full number of elastic and phonon scattering events means that in the diagram response equation of Fig. 2, every electron line may have zero or one $T_{nk'n'k'}(\omega)$ on it. For example, the third diagram in Fig. 2 with four electron lines is replaced by 16 diagrams to include every combination of zero or one T matrix on each of the four electron lines.

In the theoretical development of Ref. 2, it was shown that on each pair of upper and lower electron lines above and below each other on any response diagram, the four diagrams with zero, one, one, and two T matrices on this pair just result in the same electron pair with no T matrices, multiplied by the electron transmission probability

T_n through the mesoscopic system, given by

$$T_n = 1 - 2\pi^2 \sum_{n'', k_F''} \rho_{n''}(0) \rho_{n''}(0) |T_{nk_F n'' k_F''}(\omega)|^2 \times [1 - \cos\theta(k_F, k_F'')] . \quad (12)$$

T_n is not strongly dependent on ω near $\omega=0$ (except when there are special resonances near $\omega=0$) and we denote $T_n(\omega)$ near $\omega=0$ by T_n , which characterizes $T_n(\varepsilon_{nk_F})$.

Performing all the additions of T matrices to the response diagrams of Fig. 2 and then substituting T_n

$$I(x) = -\frac{2e^2}{h} \sum_n \int_{\varepsilon_{n0}}^{+\infty} d\omega \frac{\partial f(\omega)}{\partial \omega} T_n \int_{-\infty}^{+\infty} dx' \exp[-|x-x'| T_n 2 \text{Im} \Sigma_{nk_F n' k_F'}^{\text{tr}}(\omega) / \hbar v_{F_n}] E_x(x') . \quad (14)$$

Equation (14) replaces Eq. (11) above. Summation within the exponent over the repeated index n' is implicit.

The noteworthy feature of Eq. (14) is that effects of phonon scattering on the current through a mesoscopic system are scaled by the transmission probability only to second and higher powers, in contrast to the effect of elastic scattering alone which is first order in the transmission probability. The inelastic scattering time here can be much longer than for a bulk system. It should be noted that, even with $v_{F_n}(x)$ for $x \approx 0$ in the mesoscopic system much smaller than the $v_{F_n}(x = \pm \infty)$ in a bulk 2DES or bulk metal,⁴ the factor T_n in Eq. (14) means that in the mesoscopic system the inelastic scattering length $l_{\text{inel}}(x \approx 0) = \hbar v_{F_n}(x \approx 0) / \sum_n 2 \text{Im} \Sigma_{nn}^{\text{tr}} T_n$ is not too much smaller than the $l_{\text{inel}}(x = \pm \infty)$ of the bulk system or is even larger (except right at one of the steps in Fig. 1). That is because here T_n is zero for all but a few of the $N_{\text{ch}}^{(0)} > 10^{10}$ transmission channels that would occur at $x = \pm \infty$ in a bulk system. The electrons in $I(x)$ near $x=0$ traversing the mesoscopic system are affected by phonons in a rather large range $l_{\text{inel}}(x=0)$ that certainly will include some region of a bulk 2DES or bulk metal. In the Hamiltonian of Eq. (1), the phonon mode not specified in the third and fourth terms may in general include all the bulk-mode phonons as well as any localized phonon modes occurring at the mesoscopic system. Finally, it should be noted that for x very far from the mesoscopic system, so that x' for the localized electric field does not fall in the x' range from $x - l_{\text{inel}}(x)$ to $x + l_{\text{inel}}(x)$, the T_n all change and in fact there become $N_{\text{ch}}^{(0)} > 10^{10}$ channels with $T_n \neq 0$. [The theory for a homogeneous electric field $E_0 \delta(q_0)$ must be used for x far from the nanostructure, and in this case the x' integration in Eq. (14) becomes equal to l_{inel} .]

When L_E is not too long, we can expand the exponential in Eq. (14) as $1 - |x-x'|/l_{\text{inel}}(\omega) + \dots$. The first zeroth-order term in $1/l_{\text{inel}}(\omega)$, with the x' integral over $E(x')$ just the voltage drop ΔV , is the current corresponding to the Landauer conductance³

$$G = \frac{2e^2}{h} \sum_n T_n f(\varepsilon_{nk})_{k=0} . \quad (15)$$

where appropriate, we obtain the following equation for the current propagator that now replaces Eq. (4) above:

$$T_n \mathcal{D}_{nn'} = T_n \mathcal{D}_n^{(0)} \delta_{n,n'} + T_n \mathcal{D}_n^{(0)} [-2i(e^2 v_{F_n})^{-1} T_n \text{Im} \Sigma_{nn''}^R] \mathcal{D}_{n''n} . \quad (13)$$

(Here $\text{sgn} k \text{sgn} k''$ is implicit in Σ^R .)

By the same procedure that was used to obtain $I(x)$ for phonon scattering only in Eq. (11) above, we solve Eq. (13) and then obtain the current flow when both electron-phonon scattering and elastic electron reflection are present:

We can approximate $E_x(x')$ as constant in the range $-L_E/2 \leq x' \leq L_E/2$ and zero outside that range, so that $E = \Delta V / L_E$ within that range. In this case the term of order $l_{\text{inel}}^{-1}(\omega)$ in Eq. (14) and using Eq. (3) is exactly the same as ΔG in Eq. (34) below that which was obtained in the semiclassical method.

The quantum-linear-response theory expresses the current flow entirely in terms of its relation to the effective transport electric field, in the $\omega_0 \rightarrow 0$ limit of a time-dependent quantum mechanics arising from a time-dependent vector or scalar potential in a perturbation term H'_E that must be added to H of Eq. (1) above, in order to change from zero current to a current-flow state of the system.² In this, even in the $\omega_0 \rightarrow 0$ limit the time dependence is essential, without which no current-flow state can occur in quantum mechanics. In the single- q_0 response of a bulk metal in the $\omega_0 \rightarrow 0$ limit,¹¹ only current flow occurs if $\lim_{\omega_0 \rightarrow 0} (q_0 v_F / \omega_0) \ll 1$, whereas only density response occurs if $\lim_{\omega_0 \rightarrow 0} (q_0 v_F / \omega_0) \gg 1$.

What occurs in the Landauer conductance? In this case the dominant term in the response is proportional to $\delta(\omega_0 \mp q_0 v_{F_n})$ (neglecting phonons) and in the limit $\omega_0 \rightarrow 0$ both density and current response occur.² In the limit $\omega_0 \rightarrow 0$, the density response has infinite wavelength and is of different sign at $k_{F_n} > 0$ than at $k_{F_n} < 0$.⁸ This combined with $|q_0| v_{F_n} = \omega_0$ relating space and time means that within the quantum-mechanical mesoscopic system itself, the quasichemical potentials for positive-velocity and negative-velocity current carriers are not equilibrated with each other but are separated by electron charge times the electrical voltage drop across the system⁸ $\mu_+ - \mu_- = e \Delta V$. (This is not an arbitrary construction in Ref. 8, but a necessary result in the time-dependent quantum mechanics.) This condition is used for the semiclassical derivation of ΔG in the following section.

III. SEMICLASSICAL PERTURBATIVE METHOD

Let us assume that there is a partition at $x=0$, at the midpoint of the conductor of total length L_x . Let us denote by $f^>$ ($f^<$) the electron distribution function

unaffected by the phonons for $k > 0$ ($k < 0$). We have for $x < 0$

$$f_n^{(0)}(k) = f^{(F)}(\varepsilon_{nk} - eV/2 - \mu), \quad k > 0 \quad (16)$$

$$f_n^{(0)}(k) = |r_n(\varepsilon_{nk})|^2 f^{(F)}(\varepsilon_{nk} - eV/2 - \mu) + |t_n(\varepsilon_{nk})|^2 f^{(F)}(\varepsilon_{nk} + eV/2 - \mu), \quad k < 0. \quad (17)$$

Here $f_n^{(F)}(k)$ is the Fermi distribution function $f(\varepsilon_{nk})$ in Sec. II above. The energy ε_{nk} can be taken here as

$$\varepsilon_{nk} = \varepsilon_{n0} + \hbar^2 k^2 / 2m.$$

Here we will not take ε_{nk} relative to the Fermi level as was done in Sec. II. r_n and t_n are the reflection and transmission amplitudes, respectively. They satisfy the relation

$$|r_n|^2 + |t_n|^2 = R_n + T_n = 1,$$

where R_n and T_n are the reflection and transmission probabilities in the n th channel. As the scattering potential here depends only on x , there is no n -mode mixing. For $x < 0$

$$f_n^{(0)}(k) = f^{(F)}(\varepsilon_{nk} + eV/2 - \mu), \quad k < 0. \quad (18)$$

$$f_n^{(0)}(k) = |r_n(\varepsilon_{nk})|^2 f^{(F)}(\varepsilon_{nk} + eV/2 - \mu) + |t_n(\varepsilon_{nk})|^2 f^{(F)}(\varepsilon_{nk} - eV/2 - \mu), \quad k > 0. \quad (19)$$

The total current is given by

$$I = \frac{2e}{2\pi\hbar} \sum_n \left[\int_0^\infty F_{nk}^{(>)} v_{nk} dk + \int_{-\infty}^0 F_{nk}^{(<)} v_{nk} dk \right], \quad (20)$$

where $F^{(>)}$ and $F^{(<)}$ are the total electron distribution functions for $k > 0$ and $k < 0$, respectively, including the phonon contributions. Neglecting the latter, i.e., in the zeroth approximation in the electron-phonon coupling constant, and expanding in powers of $eV/k_B T$, using the $f_n^{(0)}(k)$ of Eqs. (16)–(19) results in the Landauer formula of Eq. (15) above.

Now we embark on calculation of the phonon-induced correction to the current ΔI . For this we need to calculate the corrections to the distribution functions $\Delta f^{(>)}$ and $\Delta f^{(<)}$. They should satisfy the following boundary conditions:

$$\begin{aligned} \Delta f_n^{>} |_{x=+0} &= |t_n(\varepsilon_{nk})|^2 \Delta f_n^{>} |_{x=-0} \\ &\quad + |r_n(\varepsilon_{nk})|^2 \Delta f_n^{<} |_{x=+0}, \\ \Delta f_n^{>} |_{x=-L_x/2} &= 0, \\ \Delta f_n^{<} |_{x=L_x/2} &= 0, \\ \Delta f_n^{<} |_{x=-0} &= |t_n(\varepsilon_{nk})|^2 \Delta f_n^{<} |_{x=+0} \\ &\quad + |r_n(\varepsilon_{nk})|^2 \Delta f_n^{>} |_{x=-0}. \end{aligned} \quad (21)$$

Now, to calculate Δf we will use the method of successive approximations in the electron-phonon coupling. Δf , being of the first approximation in the electron-phonon coupling constant squared, satisfies the equation

$$v \frac{\partial \Delta f}{\partial x} = M[f] + e \frac{\partial \phi}{\partial x} \frac{\partial f^{(0)}}{\partial \hbar k}, \quad (22)$$

where $M[f]$ is the electron-phonon collision term (see below) while $\phi(x)$ is the electrostatic potential assumed to be independent of time. The effect of the time dependence of $\phi(x, t)$, in the limit where the field frequency $\omega_0 \rightarrow 0$, has been included in the two different quasichemical potentials for $k > 0$ and $k < 0$, according to the derivation of $\mu_{>} - \mu_{<} = e\Delta V$ in Ref. 8. Since a time-independent $\phi(x)$ does not in itself cause any current flow, we can regard $\phi(x)$ as expressed in the x -dependent phase factor of each wave function as was derived in Ref. 8 for the linear-response limit, resulting in the two different quasi-Fermi levels for $k > 0$ and $k < 0$. $\phi(x)$ here must not contribute at all to Δf .

In the spirit of the method of successive approximations one should insert into the collision term the distribution function in the zeroth approximation, Eqs. (16)–(19). We observe that because of the identity $|r_n|^2 + |t_n|^2 = 1$, the function $1 - f(k)$ satisfies the same boundary relations given by Eqs. (18) and (19) as does $f(k)$. For the model considered in this section, the distribution functions of the zeroth approximation are coordinate-independent within the intervals $-L_x/2 < x < 0$ and $0 < x < L_x/2$. The solutions of the resulting differential equations with regard to the boundary conditions

$$\Delta f |_{x=\mp L_x/2} = 0 \quad (23)$$

are for $k > 0$, $x < 0$ and $k < 0$, $x > 0$ respectively,

$$\Delta f(x) = \left[x \pm \frac{L_x}{2} \right] \frac{1}{v} M[f^{(0)}] + \frac{e}{v} \int_{(\Gamma)} dx \frac{\partial \phi}{\partial x} \frac{\partial f^{(0)}}{\partial \hbar k}. \quad (24)$$

Here Γ is the electron trajectory.

The collision term reads (we omit the superscript 0 on the $f^{(0)}$ distribution functions)

$$M[f_n(k)] = \sum_{n'} \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \int \frac{d^d \mathbf{q}_\perp}{(2\pi)^d} |\langle n' | e^{iq_\perp \cdot r_\perp} | n \rangle|^2 W_q B, \quad (25)$$

where

$$B = [b^{(+)} \delta(\varepsilon_{n'k'} - \varepsilon_{nk} - \hbar\omega_q) + b^{(-)} \delta(\varepsilon_{n'k'} - \varepsilon_{nk} + \hbar\omega_q)], \quad (26)$$

with

$$b^{(\pm)} = [f'(1-f)(N_q + \frac{1}{2} \pm \frac{1}{2}) - f(1-f')(N_q + \frac{1}{2} \mp \frac{1}{2})]. \quad (27)$$

$d + 1$ is the dimension of the system.

For simplicity, only scattering by three-dimensional extended acoustic phonons will be considered where as before

$$W_q = \frac{\pi Z^2 q^2}{\rho \omega_q}. \quad (28)$$

We assume that the phonons are in equilibrium and therefore N_q is the Bose function.

We integrate in Eq. (26) over the three components of the phonon wave vector. \mathbf{q}_\perp indicates the two transverse wave-vector components. The third component is given by

$$q_x = \pm(k - k').$$

Therefore the integration is equivalent to the integration over the electron wave vector k' because of the conservation of quasimomentum.

We see that as in the case where the reflection coefficients for the electron waves vanish (see Ref. 3), detailed balance guarantees a vanishing collision term for the equilibrium distribution functions and constant temperature and chemical potential. This means that the electron distribution functions give a nonvanishing contribution in the collision term if and only if k and k' are of opposite sign so that their quasichemical potentials are different. One can trace in this way the origin of one factor $|t_n|^2$ in the expression for ΔG (see below). In other words, in this case too only those phonons contribute to ΔG that backscatter electrons.

Making use of the identities satisfied by the Fermi and Bose functions

$$1 - f(\epsilon_{nk} - \mu) = \exp\left[\frac{\epsilon_{nk} - \mu}{k_B T}\right] f(\epsilon_{nk} - \mu),$$

$$N_q + 1 = \exp(\hbar\omega_q/k_B T) N_q;$$

and taking into consideration conservation laws imposed by the δ functions, we get for $k > 0$ and $k' < 0$

$$b^{(+)} = -2 \sinh\left[\frac{eV}{2k_B T}\right] f^{(F)}(\epsilon_{nk} + eV/2 - \mu) \times f^{(F)}(\epsilon_{n'k'} - eV/2 - \mu) N_q \exp\left[\frac{\epsilon_{n'k'} - \mu}{k_B T}\right], \quad (29)$$

$$b^{(-)} = -2 \sinh\left[\frac{eV}{2k_B T}\right] f^{(F)}(\epsilon_{nk} - eV/2 - \mu) \times f^{(F)}(\epsilon_{n'k'} + eV/2 - \mu) N_q \exp\left[\frac{\epsilon_{n'k'} - \mu}{k_B T}\right], \quad (30)$$

whereas for $k' > 0$ and $k < 0$ we have the same expressions but with eV replaced by $-eV$.

One can check using properties of Fermi and Bose functions that the term linear in x in the equation for the current vanishes. Indeed the current, because of the charge conservation, should be coordinate independent. Then to calculate ΔI it is sufficient to consider its value at $x = 0$:

$$\Delta I = -\frac{2e}{2\pi\hbar} \sum_n \left[\int_0^\infty |t_{nk}(\epsilon)|^2 v_n \Delta f_n^>|_{x=0} dk + \int_{-\infty}^0 |t_n(\epsilon)|^2 v_n \Delta f_n^<|_{x=+0} dk \right]. \quad (31)$$

Now one can also trace the origin of the second factor $|t_n|^2$ in the equation for the current [see Eqs. (34) and (35) below].

Making use of Eqs. (29) and (30) we have

$$\Delta I = \frac{2eL_x}{(2\pi\hbar)^2} \sum_{nn'} \int_0^\infty dk \int_{-\infty}^0 dk' \int \frac{d^2\mathbf{q}_\perp}{(2\pi)^2} |\langle n' | e^{iq_1 \cdot r_1} | n \rangle|^2 |t_n(\epsilon_{nk})|^2 |t_{n'}(\epsilon_{n'k'})|^2 B, \quad (32)$$

where

$$B = [f(\epsilon_{nk} + eV/2)f(\epsilon_{n'k'} - eV/2) + f(\epsilon_{nk} - eV/2)f(\epsilon_{n'k'} + eV/2)] \times \sinh\left[\frac{eV}{2k_B T}\right] \left[\exp\left[\frac{\epsilon_{n'k'} - \mu}{k_B T}\right] \delta(\epsilon_{n'k'} - \epsilon_{nk} - \hbar\omega_q) + \exp\left[\frac{\epsilon_{nk} - \mu}{k_B T}\right] \delta(\epsilon_{n'k'} - \epsilon_{nk} + \hbar\omega_q) \right]. \quad (33)$$

This is still a non-Ohmic approximation for the current. The non-Ohmic equation is valid as far as the phonons can be considered to be in equilibrium or, in other words, N_q is the Bose function. To go to the Ohmic approximation one should expand Eq. (33) in powers of $eV/2k_B T$ retaining the first term. One gets it by replacing $\sinh(eV/2k_B T)$ with $eV/2k_B T$ and dropping $eV/2k_B T$ from the arguments of the Fermi functions. Further simplification can be reached by an interchange of the integration variables k and k' in the second term. As a result one gets the following equation for the change of the conductance ΔG due to the phonon scattering:

$$\Delta G = \frac{2hG_0L_x}{k_B T} \sum_{nn'} \int \frac{d^d\mathbf{q}_\perp}{(2\pi)^d} |\langle n' | e^{iq_1 \cdot r_1} | n \rangle|^2 C_{n'n}, \quad (34)$$

where

$$C_{n'n} = - \int_0^\infty \frac{dk}{2\pi} \int_{-\infty}^0 \frac{dk'}{2\pi} N_q W_q |t_n(\epsilon_{nk})|^2 |t_{n'}(\epsilon_{n'k'})|^2 \times f^{(F)}(\epsilon_{nk}) [1 - f^{(F)}(\epsilon_{n'k'})] \times \delta(\epsilon_{n'k'} - \epsilon_{nk} - \hbar\omega_q). \quad (35)$$

G_0 is the unit of conductance $2e^2/h$. Here we made use

of the following identities that are direct consequences of the time-reversal symmetry:

$$\begin{aligned} \omega_q &= \omega_{-q}, \\ |\langle n' | e^{iq_1 \cdot r_1} | n \rangle|^2 &= |\langle n' | e^{-iq_1 \cdot r_1} | n \rangle|^2. \end{aligned} \quad (36)$$

The result stating that one gets in the integrand of Eq. (35) the $|t_n(\varepsilon_{nk})|^2 |t_n'(\varepsilon_{n'k'})|^2$ factor is the same as the T_n and T_n' factors obtained in Sec. II by direct quantum-mechanical calculation, where $T_n(\omega = \varepsilon_{nk})$ (with ε_{nk} relative to the Fermi level) was taken as $T_n = T_n(0)$ for ω near zero. However, the formulations of the problems are much different.

IV. NUMERICAL RESULTS

For illustration of the combined effects of electron-phonon scattering and elastic reflection of electrons, we take a model quantum wire shown schematically in Fig. 3, with $L_E = L_x = 1 \mu\text{m}$, $L_y = 1000 \text{ \AA}$, and $L_z = 100 \text{ \AA}$. We take a capacitorlike transport electric field that is constant in x in the length L_E , zero for other x , and independent of y and z . The quantum wire is a square-well confining potential in L_y and L_z with infinite-potential walls. With small filling factor in the quantum wire, $N_{\text{ch}} \ll 100$, only the lowest n_z level in the L_z quantization is occupied. We vary the filling factor or Fermi level measured from that lowest n_z level so that n_y levels 1, 2, 3 are successively populated with increasing E_F . (This is analogous to changing a gate voltage.) It is most convenient to express this in terms of $\lambda_F = h\sqrt{2m^*E_F}$ so that at zero temperature the channel $n_y = 1, 2, 3, \dots$ is just occupied when $1/\lambda_F$ just exceeds 1, 2, 3, . . . in units of $1/2L_y$. The x current-flow direction is taken to have a quasicontinuous k spectrum. We take material parameters appropriate for GaAs: $m^* = 0.067m_e$ in an isotropic model, the velocity of sound is $v_s = 5.22 \times 10^5 \text{ cm/sec}$, the

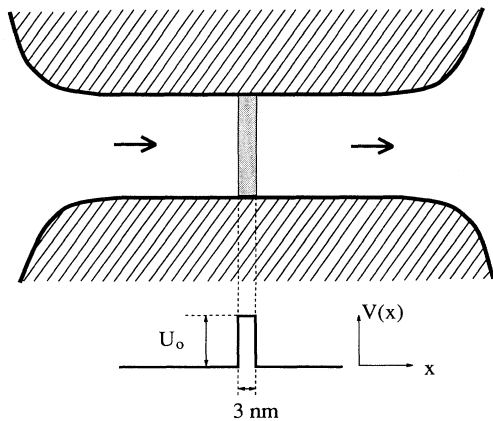


FIG. 3. Schematic diagram of the model nanostructure with a rectangular potential barrier of height U_0 at the midpoint on the current path.

acoustic mode deformation potential is $Z = 7.0 \text{ meV}$, and the mass density is $\rho = 5.36 \text{ g/cm}^3$. We include only model longitudinal acoustic phonons with isotropic and linear dispersion. Because l_{inel} is much larger than L_x , bulk-mode phonons are important for all nanostructures and particularly important for nanostructures that are defined by electrode voltages.

In an actual nanostructure the quantum wire may or may not be joined to macroscopic lead wires by regions that are widening adiabatically slowly on the length scale of λ_F . When the widening is not adiabatically slow, the few channels N_{ch} that are occupied in the wire will not have the $T_n = 1$ condition for adiabatic widening, but instead $T_n \leq 1$ will occur. To introduce nonzero reflection of electrons into a model nanostructure, we include in Fig. 3 a square potential barrier of height U_0 at the midpoint of the quantum wire, between $x = -a/2$ and $a/2$. U_0 is constant in y and z and so this barrier will not mix the channels. The transmission coefficient for this barrier is

$$\begin{aligned} T_n(\varepsilon_n) &= \frac{4\varepsilon_n(U_0 - \varepsilon_n)}{4\varepsilon_n(U_0 - \varepsilon_n) + U_0^2 \sinh^2 a \sqrt{2m(U_0 - \varepsilon_n)/\hbar^2}}, \\ & \quad 0 \leq \varepsilon_n \leq U_0 \\ &= \frac{4\varepsilon_n(\varepsilon_n - U_0)}{4\varepsilon_n(\varepsilon_n - U_0) + U_0^2 \sin^2 a \sqrt{2m(\varepsilon_n - U_0)/\hbar^2}}, \\ & \quad \varepsilon_n \geq U_0. \end{aligned} \quad (37)$$

Here $\varepsilon_n = \varepsilon_{nk_F} - \varepsilon_{n0}$ and as before, in Sec. III, we have in ε_{nk} taken the energy as quadratic in k . $T_n(\varepsilon_n = 0) = 0$ whereas $T_n(\varepsilon_n)$ approaches unity when ε_n becomes many times larger than U_0 . This general form will roughly characterize a wide variety of reflections in actual nanostructures. For the numerical results to follow we have in some cases taken $a = 30 \text{ \AA}$ and $U_0 = 14 \text{ meV}$ ($= \varepsilon_{n0}$ at $n = 5$) and in other cases we have taken $U_0 = 0$.

In Fig. 1 the Landauer conductance G of Eq. (15) is shown when there is no phonon scattering and no reflection of electrons $T_n = 1$ for $U_0 = 0$. The change here of the conductance from a staircase function of filling factor $1/\lambda_F$ when temperature is low $T \ll 10 \text{ K}$ to a smooth function when temperature is high $T \gg 10 \text{ K}$ occurs entirely because of temperature smearing of the Fermi occupation number $f(\varepsilon_{nk})$ in Eq. (15) above. In Fig. 4 we introduce phonon scattering according to Eqs. (34) and (35), but there is no electron reflection $U_0 = 0$ with $T_n = 1$ ($|t_n|^2 = 1$) in Eq. (35). The change in conduction ΔG in Fig. 4 due to phonon scattering is always an order of magnitude or more smaller than the Landauer conductance G in Fig. 1, even at temperatures as large as 80 K . [The peaks of ΔG near integer values of $1/\lambda_F$ would be decreased, not increased, if terms in $\text{Im}\Sigma$ of Eq. (3) were included beyond the noncrossing approximation.]

Figure 5 shows the change $\Delta G = -|\Delta G|$ from Landauer conductance G for this model nanostructure when there is both phonon scattering and electron reflection (for $U_0 = 14 \text{ meV}$). That is compared with ΔG for the case when there is only phonon scattering (for $U_0 = 0$).

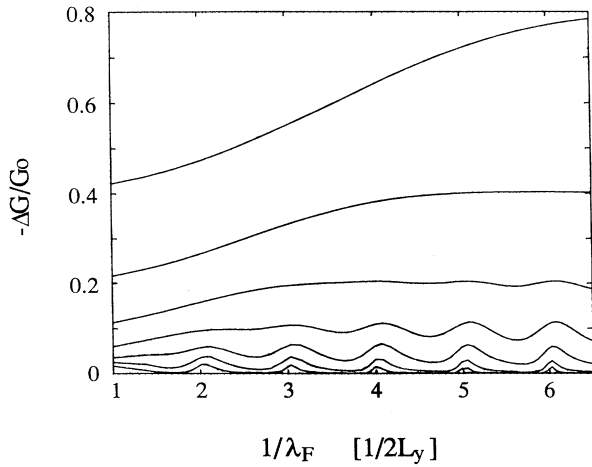


FIG. 4. Change of conductance ΔG of a model nanostructure due to electron-phonon scattering, with no electron reflection in the few channels occupied in the nanostructure. Each curve is at the temperature indicated on the corresponding curve in Fig. 1; e.g., the top curve is at temperature $64T_0 = 80$ K. The peaks centered near $1/\lambda_F = 2, 3, 4, \dots$ represent quasi-one-dimensional resonances in electron-phonon scattering for each just-occupied channel.

The strong reduction in $|\Delta G|$ by electron reflection arises from the quadratic dependence of ΔG on the transmission probability T_n . This contrasts with much smaller linear-in- T_n reductions of G in Fig. 1 that would occur if T_n were changed from unity to $T_n(\varepsilon_n) \leq 1$ when U_0 changes from 0 to 14 meV. However, the transmission

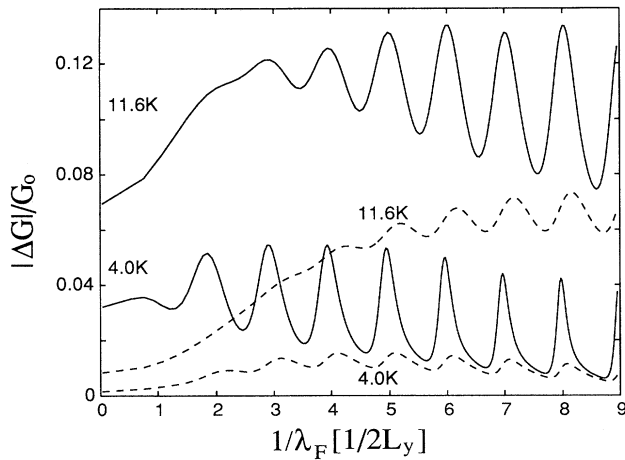


FIG. 5. Comparison of the change to conductance ΔG due to electron-phonon scattering when electron reflectance occurs and does not occur. The dashed lines represent the case of nonzero reflectances when the height of the potential barrier is $U_0 = 14$ meV, whereas the solid lines represent the case of zero reflectance when $U_0 = 0$. The sharp peaks are centered very near to where $T_n(\varepsilon_n) = 0$ when $U_0 \neq 0$ so that suppression of the peak structure is a stronger effect than the overall reduction of $|\Delta G|$.

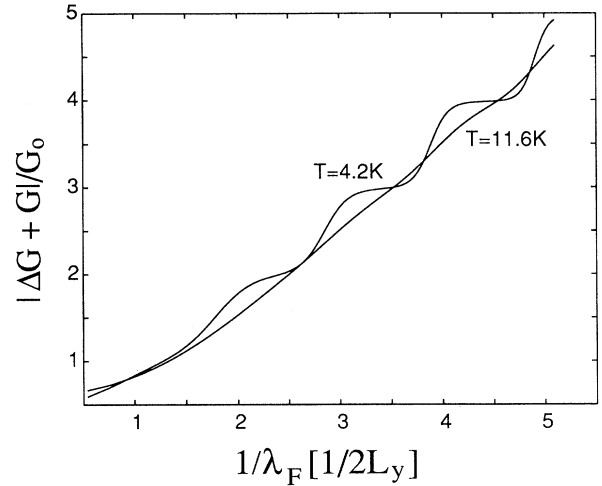


FIG. 6. The sum $G + \Delta G$: the Landauer conductance G plus the change of conductance $\Delta G < 0$ due to electron-phonon scattering. Here $U_0 = 0$ so that no electron reflection occurs, which is the case where the ratio $|\Delta G|/G$ is largest.

probability $T_n(\varepsilon_n) \rightarrow 0$ when $\varepsilon_n \rightarrow 0$ in Eq. (37) would also mean strong smearing of the staircase form of G in Fig. 1 even when $T \ll 10$ K. Sharp steps in G are expected and observed only when there are adiabatically slowly widening regions between a nanostructure and a lead wire.^{1,4}

For completeness, we show in Fig. 6 the sum $G + \Delta G < G$ when there is phonon scattering but no electron reflection ($U_0 = 0$). Even at high temperatures, G in Fig. 6 is not much changed from the Landauer conductance G of Fig. 1 when there is no electron-phonon scattering $|\Delta G| \ll G$ at all temperatures and all filling factors $1/\lambda_F$. The smallness of $\Delta G \propto T_n^2$ in comparison to $G \propto T_n$ is much more pronounced when there is electron reflection $T_n \leq 1$ replacing $T_n = 1$ for the few channels that are filled. (Of course, even when there is no reflection in the few N_{ch} channels occupied in the nanostructure, the effect of the second T_n factor in ΔG is still a strong effect because T_n is zero for all but a few of the $N_{\text{ch}}^{(0)} > 10^{10}$ channels that would occur in a bulk-metal lead wire.)

V. SUMMARY AND DISCUSSION

We have developed a theory for the combined effects of electron-phonon scattering and electron reflection on the electrical conductance of a nanostructure. We have done this by the quantum Baym-Kadanoff linear-response theory.² This formalism is the same as the Kubo linear-response theory except that it is manifestly gauge invariant and conserving, producing exactly the Feynman diagrams for the time-dependent linear response that must be used corresponding to any quantum-mechanical zero-current state of the system. This quantum-response theory expresses the current flow through the system as a linear function of a voltage drop ΔV that is the line integral of the transport electric field through the nano-

structure. But all such quantum-linear-response theories say nothing at all about any chemical potential in the current-flow state of the system. One of the authors has shown in a separate paper⁸ that, within the nanostructure itself, the quantum mechanics of the current-flow state mean that quasicheical potentials⁷ for current carriers with positive and negative group velocities satisfy the relation $\mu_+ - \mu_- = e\Delta V$, where ΔV is again the line integral of the transport electric field. (This occurs because acceleration of current by the electric field for one sign of velocity means increased kinetic energy for that current species. But current carriers with opposite velocity suffer deceleration and reduction of kinetic energy.) Using the condition $\mu_+ - \mu_- = e\Delta V$, we have then determined the combined effects of electron-phonon scattering and electron reflection on the conductance in a semiclassical theory using rate equations based on this condition. The results are the same as those that were obtained in the Baym-Kadanoff formalism.² Thus there are two equivalent formalisms using (a) a time-dependent transport electric field with $\omega_0 \rightarrow 0$ in a quantum-linear-response theory and (b) a semiclassical theory using quasicheical potentials $\mu_+ - \mu_- = e\Delta V$ for $\omega_0 \rightarrow 0$ in the nanostructure itself that were also derived in a quantum theory.⁸ In theory (a), linearization means that the electric field occurs explicitly but a field-induced change of the electron Fermi level does not occur. In theory (b) linearization means exactly the opposite—once the effect of electric field with line integral $e\Delta V$ has been explicitly expressed in changed Fermi energies $\mu_0 \rightarrow \mu_+$ and $\mu_0 \rightarrow \mu_-$ with $\mu_+ - \mu_- = e\Delta V$, no other effect of electric field enters the linear response. The equivalence of the two theoretical formalisms, including when electron-phonon scattering and electron reflection are both present, is shown in the results here.

The effects of phonon scattering on the electrical conductance of a nanostructure are shown here to be small even at temperatures as high as 80 K. This indicates that electron coherence effects may persist to temperature $T \gg 10$ K. Further theoretical study is required on the coherence effect itself, on, e.g., the Aharonov-Bohm interference effect in electrical conductance when $T \gg 10$ K. The smallness of phonon effects in the electrical conductance of a nanostructure at temperatures as high as 80 K occurs because final as well as initial electron states in the electron-phonon scattering must have nonzero transmission through the nanostructure. The same effect, that change of the current flow due to electron-phonon scattering is proportional to the square of one-electron transmission probability, is found as well in theory of tunnel junctions¹² and has been found before as well in theory of nanostructures.¹³

The conductance determined in this study, of order $(k\Omega)^{-1}$, is the ratio of current flow to electrical voltage drop, where the latter is equal to the line integral through the mesoscopic system of the transport electric field. As discussed by Shockley,⁷ in lead-wire experiments the measured potential difference is a difference of chemical potentials. The electrical voltage drop occurs at the nanostructure.⁸ But the measured difference of chemical potentials is equal to the full electrical voltage drop only when those two chemical potentials are both at distances from the mesoscopic system which are large compared to the inelastic scattering length.^{8,14}

ACKNOWLEDGMENT

We greatly appreciate a NATO linkage grant that facilitated our collaboration on the physics discussed in this paper.

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