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Phonon-enhanced Landauer resistance

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Abstract. We present a perturbative method of calculating the temperature-dependent correction, ΔG, to the Landauer conductance which is due to the inelastic electron–phonon scattering. The limits of applicability of these methods as well as the critical interval of temperature (and other relevant parameters) on which the transition from the ballistic transport to the Boltzmann–Drude transport occurs are discussed.

1. Introduction

The classical Boltzmann–Drude conductivity, σ, is proportional to the average time, τ, that an electron travels without suffering any collisions. Up to a multiplicative constant of the order of unity,

$$\sigma \approx ne^2\tau/m^* \tag{1}$$

where n is the number of conduction electrons (per unit volume) and m^* is the effective mass. Consequently, even in the weak limit of the electron–phonon coupling constant, ζ, the perturbation theory cannot be employed directly for the calculation of conductivity. The first term in the expansion of σ in powers of ζ scales with ζ as ζ^{-2} and the calculation of σ typically requires solving of the Boltzmann equation.

There exist cases, however, where the expansion of σ in powers of ζ is possible. One such case is the transverse magnetoconductivity,

$$\sigma_{xx} \approx \frac{ne^2\tau/m^*}{1+(\omega_c\tau)^2} \tag{2}$$

where $\omega_c = eH/m^*c$ is the cyclotron frequency. When $\omega_c\tau \gg 1$, equation (2) can be expanded in powers of ζ^2 by making use of the perturbation theory applied, for example, to the Kubo formula (see for instance [1]). The classical formula (2) is valid for $\hbar\omega_c \ll k_BT$. In the quantum regime ($\hbar\omega_c \gg k_BT$), the transverse magnetoconductance, σ_{xx}, can also be legitimately expanded in powers of ζ^2 [1].

An analogous situation is found in the calculation of the AC conductivity in a high-frequency electric field. For

$$\omega\tau \gg 1 \tag{3}$$

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where ω is the frequency of field oscillations, the conductivity can be obtained by means of a perturbation expansion in powers of ζ^2. The expansion begins from a zeroth-order term of the form

$$\mathrm{Im}\,\sigma = \frac{ne^2}{m^*\omega}. \tag{4}$$

The next-order term in such an expansion is real. In the classical domain of frequencies, $\hbar\omega_c \ll k_B T$ (see for instance [2, 3, 4]), this term is

$$\mathrm{Re}\,\sigma \approx \frac{ne^2}{m^*\omega^2\tau} \tag{5}$$

where ω is the AC frequency. For

$$\omega\tau \gg 1 \tag{6}$$

equation (5) can be obtained from the perturbative expansion in powers of ζ^2. In the quantum regime ($\hbar\omega \gtrsim k_B T$) the expression (5) is replaced by a more complicated one. Nonetheless, such an expression is once again obtained from a perturbative expansion in powers of a small parameter proportional to ζ^2.

These examples show that the applicability of the perturbation theory depends on values assumed by the conductance, G, in the limit of $\zeta \to 0^+$. If G approaches infinity as $\zeta \to 0^+$, the perturbation theory cannot be directly applied. If, on the other hand, G remains finite as $\zeta \to 0^+$, there exists an interval of values of ζ where the perturbation theory is valid.

We use the perturbation theory for calculations of the variation in the Landauer conductance, ΔG, due to the interaction with phonons [5]. The results obtained by making use of such perturbative methods are then analysed in detail and the critical interval of the various parameter values required for the transition from the ballistic to the Boltzmann–Drude transport is estimated. We are not aware of any experimental work where the phonon contribution to the conductance of a nanostructure was systematically investigated. One of our purposes is to determine the best conditions (with regard to the temperature, chemical potential and dimensions of a nanostructure) for observation of such a contribution, which we pursue by working out a theory of the phonon-assisted part of current. In such a way we have obtained both the conditions for observation of quantum oscillations of the conductance in nanostructures and a ballistic transport as such (where the quantum oscillations are smeared out but nevertheless the transport cannot be considered as purely classical† because of the relatively small number of channels).

2. Theory

It is well known (see, for instance, the review [6]) that in the absence of scattering G is a step-like function of the Fermi level as shown in figure 1. Each step corresponds to the

† One must distinguish, in this respect, between the transverse and longitudinal degrees of freedom. In the case of a uniform wire, the electrons are confined in the transverse plane and are unconstrained in the longitudinal direction. The confinement in the transverse plane leads to the quantization, provided that the characteristic width of a wire is comparable to the Fermi wavelength. In the opposite case, where the wire width is large on a scale of the Fermi wavelength, namely, in the limit of $\mathcal{N} \gg 1$ which is equivalent to taking the Ehrenfest limit of $\hbar \to 0$ or $\lambda \to 0$ along the transverse directions, the motion in the transverse plane approaches its classical limit. It is in this sense and *only in this sense* that we refer to the conductance expressed by (14) as *classical*. The motion in the longitudinal direction is classical provided that the length of a wire is much larger than its width (and consequently, the Fermi wavelength) and particularly for the constant-cross-section wire that we consider here. Thus the actual value of $\mathcal{N}$ (dependent on the ratio of the wire width to the Fermi wavelength) in no way affects the nature of electron transport along the longitudinal direction, which is classical in the absence of any scattering.

inclusion of a new mode of transverse quantization to the conduction process. According to the Landauer formula, the height of each step is equal to the quantum of conductance $G_0 = 2e^2/h$ multiplied by a constant that has the physical meaning of a transmission probability.

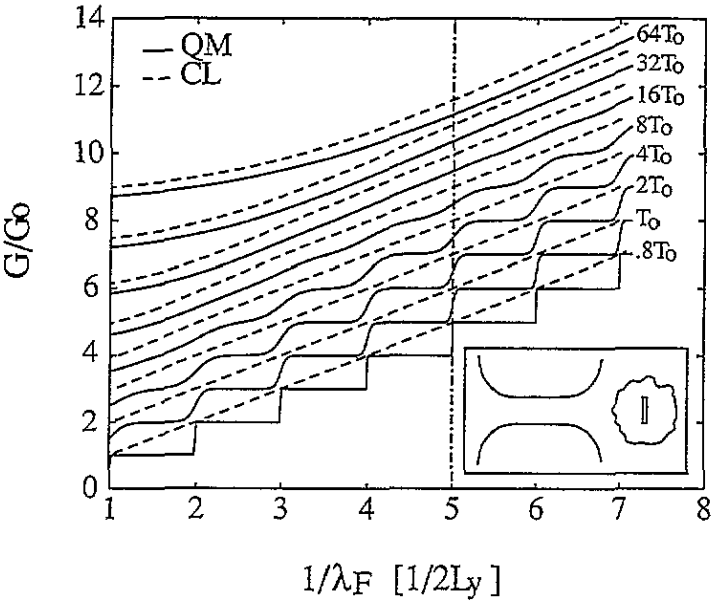

Figure 1. In the absence of dissipation, the Landauer conductance, G_{QM}, and its classical analogue, G_{CL}, are plotted as functions of λ_F^{-1} for various temperatures ($T_0 = 1.25$ K). These are computed from (13) and (14), respectively. Curves are vertically offset. The dashed–dotted vertical line marks $\lambda_F = 400$ Å which corresponds to $\epsilon_F = 14$ meV. Inset: a schematic and somewhat exaggerated representation of the QID structure being investigated.

With an onset of phonon scattering the electronic transport may still be regarded as ballistic (and be treated as such to zero order) provided that the change in the conductance, ΔG, due to the phonons is sufficiently small. In other words, only a small fraction of the total number of electrons suffer collisions with the phonons.

To apply a perturbative theory let us assume that the change of conductance is small. We consider here the simplest case of a uniform mesoscopic conductor of constant transverse cross section with respect to the x coordinate along the conductor. In such a case no redistribution of the electrostatic potential with the onset of the phonon scattering should be expected.

The distribution function of the electrons in the absence of the electron–phonon interaction is given by $f_n^{(0)}(p) = f^{(F)}(\epsilon \mp eV/2 - \mu)$ where $f^{(F)}$ is the Fermi function (see [6]). $\epsilon = \epsilon_n(p) = \epsilon_n(0) + p^2/2m^*$ is the electron energy, p is the x-component of the electron quasi-momentum, n is a subband index, and the upper (lower) sign is for $p > 0$ ($p < 0$).

Adding weak electron–phonon interactions we have $f = f^{(0)} + \Delta f$ with Δf satisfying the equation $v\,\partial\Delta f/\partial x = I[f] + e(\partial\phi/\partial x)(\partial f^{(0)}/\partial p)$. The quantity $v = \partial\epsilon/\partial p$ is the electron velocity, ϕ is the electrostatic potential assumed to be independent of time, and $I[f]$ represents the electron–phonon collision term (see below). Here we assume that $L_x \gg \lambda$ (λ being the electron de Broglie wavelength) which permits us, within the semiclassical approximation, to treat f as a function of p and x. For $p > 0$ ($p < 0$) the

solution of the equation for $\Delta f(x)$ is

$$\Delta f(x) = \frac{1}{v}(x \pm L_x/2) I^{\gtrless}[f] + \frac{e}{v}\int \mathrm{d}x\, \frac{\partial \phi}{\partial x}\frac{\partial f^{(0)}}{\partial p}. \tag{7}$$

The zero of the coordinate system is assumed to be at the midpoint of the conductor of total length L_x, and we made use of the boundary condition $\Delta f = 0$, which is satisfied at $x = \pm L_x/2$.

The variation in the current, ΔJ, due to scattering is given by (compare with the classical case treated in [7])

$$\Delta J = 2e(x + L_x/2)\sum_n \int_0^\infty \frac{\mathrm{d}p}{2\pi\hbar} I^{>}[f_n(p)] + 2e(x - L_x/2)\sum_n \int_{-\infty}^0 \frac{\mathrm{d}p}{2\pi\hbar} I^{<}[f_n(p)]. \tag{8}$$

Here summation over all the phonon branches is implied. It is readily seen that, in accordance with the reasoning given above, $I[f]$, and therefore ΔJ, is proportional to the square of the electron–phonon coupling constant.

The collision term is given by

$$I^{\gtrless}[f_n(p)] = \sum_{n'} \int_{-\infty}^{\infty} \frac{\mathrm{d}p'}{2\pi\hbar}\Theta(\pm p') \int \frac{\mathrm{d}^d q_\perp}{(2\pi)^d} \left|\langle n'|\mathrm{e}^{\mathrm{i}q_\perp \cdot r_\perp}|n\rangle\right|^2 W_q (B^{(+)} + B^{(-)}) \tag{9}$$

$$B^{(\pm)} = [f'(1-f)\left(N_q + 1/2 \pm 1/2\right) - f(1-f')(N_q + 1/2 \mp 1/2)]\,\delta(\epsilon' - \epsilon \mp \hbar\omega_q)$$

where $\Theta(\cdot)$ is the step function, $\epsilon = \epsilon_n(p)$, $d = D - 1$ and D is the dimension of the system.

We consider only scattering by three-dimensional extended acoustic phonons (although the phonons localized within the nanostructure or near its interface with a bulk could have been easily included into the scheme). Then [9]

$$W_q = \frac{\pi Z^2 q^2}{\rho\omega_q} \tag{10}$$

where ρ is the mass density and Z is the deformation potential constant for the longitudinal phonons that has the physical significance of the coupling constant, ζ, introduced above.

The integrations in (9) are over the three components of the phonon wave vector. The two transverse wave vector components are indicated by $q_\perp$; the third integration is equivalent to the integration over the electron quasi-momentum, p', because of the conservation of quasi-momentum.

In the spirit of the method described above we insert the zeroth approximation ($f_n^{(0)}$) for the distribution function into (9). We assume that the phonons are in equilibrium and hence N is the Bose function. Detailed balance guarantees a vanishing collision term for the equilibrium distribution function and constant temperature and chemical potential. This means that the distribution functions, $f^{(0)}$, give a finite contribution in the collision term if and only if p and p' are of opposite sign, i.e. their chemical potentials are different. In other words, *only those phonons that can backscatter the electrons contribute.* It is readily seen that this condition imposes a certain lower limit for the magnitude of the phonon wave vectors. At low enough temperatures, $|\Delta G|$ must therefore increase exponentially with T.

Expanding the Fermi distribution functions in powers of the small parameter eV/k_BT, we arrive at the following result for the change in conductance due to collisions :

$$\Delta G_{\rm QM} = -\frac{4\pi\hbar^{d+1}G_0L_x}{k_{\rm B}T}\sum_{n'n}\int\frac{{\rm d}^dq_\perp\,{\rm d}p\,{\rm d}p'}{(2\pi\hbar)^{d+2}}\Theta(p)\Theta(-p')$$
$$\times N_qW_qf^{(\rm F)}(\epsilon)[1-f^{(\rm F)}(\epsilon')]M_{n,n'}\,\delta(\epsilon'-\epsilon-\hbar\omega_q) \tag{11}$$

where $M_{n,n'}(q_\perp) = \left|\langle n'|{\rm e}^{{\rm i}q_\perp\cdot r_\perp}|n\rangle\right|^2$. Here we wish to emphasize that the expansion in powers of the electron–phonon coupling constant can also be easily performed for a non-Ohmic case. We shall discuss a non-Ohmic conductance in nanostructures in a separate paper.

In order to restrict consideration to the first term of the expansion in the electron–phonon coupling constant squared, ζ^2, we require that the probability of the electron scattering within the nanostructure is much smaller than unity, or, in other words, that $|\Delta G|/G \ll 1$. We expect the perturbation theory to be applicable in this limit. This condition is satisfied for a wide range of parameters as can be seen in figures 2 and 3 where for a wire width, L_y, chosen to be 1000 Å, $|\Delta G|/G \ll 1$ for up to liquid nitrogen temperatures. In the remaining discussion this condition is explicitly assumed to be fulfilled.

To obtain the classical conductance change, $\Delta G_{\rm CL}$, we replace the sum over subbands n (n') in (11) by the integral over $p_\perp$ ($p'_\perp$), and the conservation of quasi-momentum is now restored. Then [8]

$$\Delta G_{\rm CL} = -\frac{2h\mathcal{V}G_0}{k_{\rm B}T}\int\frac{{\rm d}^Dp'\,{\rm d}^Dp}{(2\pi\hbar)^{2D}}\Theta(-p'_x)\Theta(p_x)$$
$$\times N_qW_qf^{(\rm F)}(\epsilon)[1-f^{(\rm F)}(\epsilon')]\,\delta(\epsilon'-\epsilon-\hbar\omega_q). \tag{12}$$

where $\mathcal{V}$ is the volume of the D-dimensional wire and $q = p' - p$. The quantum and the classical conductance are, respectively,

$$G_{\rm QM} = G_0\sum_n f^{(\rm F)}(\epsilon_n). \tag{13}$$

$$G_{\rm CL} = \frac{\mathcal{V}G_0}{\pi L_x}\int_0^\infty{\rm d}\epsilon\sqrt{\frac{2m^*\epsilon}{\hbar^2}}\left(-\frac{{\rm d}f^{(\rm F)}}{{\rm d}\epsilon}\right). \tag{14}$$

The classical conductance is independent of the length of a wire provided that boundary scattering is purely specular (or, in other words, that the conservation of all three components of the quasi-momentum holds), and is analogous to the 3D Sharvin's point contact conductance [10]. As can be seen from figure 1, at zero temperature $G_{\rm QM} = G_{\rm CL}$ provided that $\epsilon_{\rm F}$ is at the threshold of propagation in one of the subbands ($\mathcal{N} = k_{\rm F}L_y/\pi$ or $\epsilon_{\mathcal{N}}(0) = \epsilon_{\rm F}$). This follows directly from (14) and (13). Furthermore, with sufficient thermal smearing, in the limit where large number of channels participate in the conduction ($\mathcal{N} \gg 1$), we have $G_{\rm QM} \to G_{\rm CL}$.

In figures 2(a) and 3(a) we present numerical results for quasi-1D GaAs wires with $L_z = 100$ Å and $L_x = \mu$m (the x-axis being along the propagation direction, while the effective width of the channel is L_y) as functions of Fermi wavelength, $\lambda_{\rm F} \equiv h/\sqrt{2m^*\epsilon_{\rm F}}$ (for a fixed $L_y = 1000$ Å). In figures 2(b) and 3(b) the results are given as functions of the channel width L_y (with fixed $\epsilon_{\rm F} = 14$ meV corresponding to $\lambda_{\rm F} = 40$ nm). Variation of both L_y and $\lambda_{\rm F}$ can be accomplished experimentally by varying the gate voltage. One can see from figures 2 and 3 that this condition is fulfilled for a wide range of transverse wire dimensions and temperatures. For instance, for a wire with transverse dimensions 100×400 Å, this ratio is small up to liquid nitrogen temperatures. We wish to emphasize

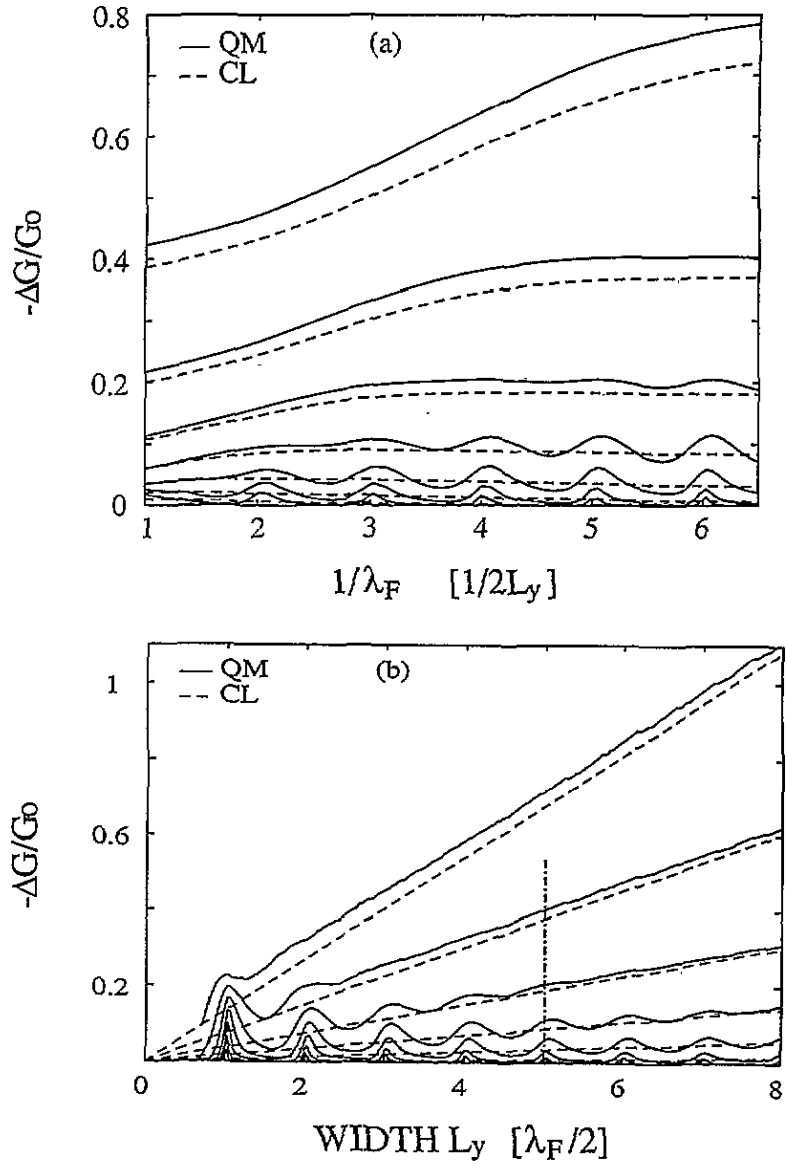

Figure 2. Both (a) $-\Delta G_{QM}(\lambda_F)$ (solid) and $-\Delta G_{CL}(\lambda_F)$ (dashed) (at $L_y = 1000$ Å) as well as (b) $-\Delta G_{QM}(L_y)$ (solid) and $-\Delta G_{CL}(L_y)$ (dashed) (at $\epsilon_F = 14$ meV) are computed from (11) and (12) for temperatures $T/T_0 = 1, 2, 4, 8, 16, 32, 64$ where $T_0 = 1.25$ K. The dashed–dotted vertical line marks $\lambda_F = 400$ Å which corresponds to $\epsilon_F = 14$ meV.

that at such high temperatures it is difficult to observe oscillations of the conductance but it is possible to observe both ballistic resistance and its enhancement by the phonons.

The electrostatic potential is assumed to be flat and to have infinite walls at the boundaries. As mentioned above, we consider here only extended phonons. The results are presented in the form of curves scaled in units corresponding to GaAs material constants and a particular sample size [11].

The changes in classical and quantum conductance as functions of Fermi wavelength λ_F

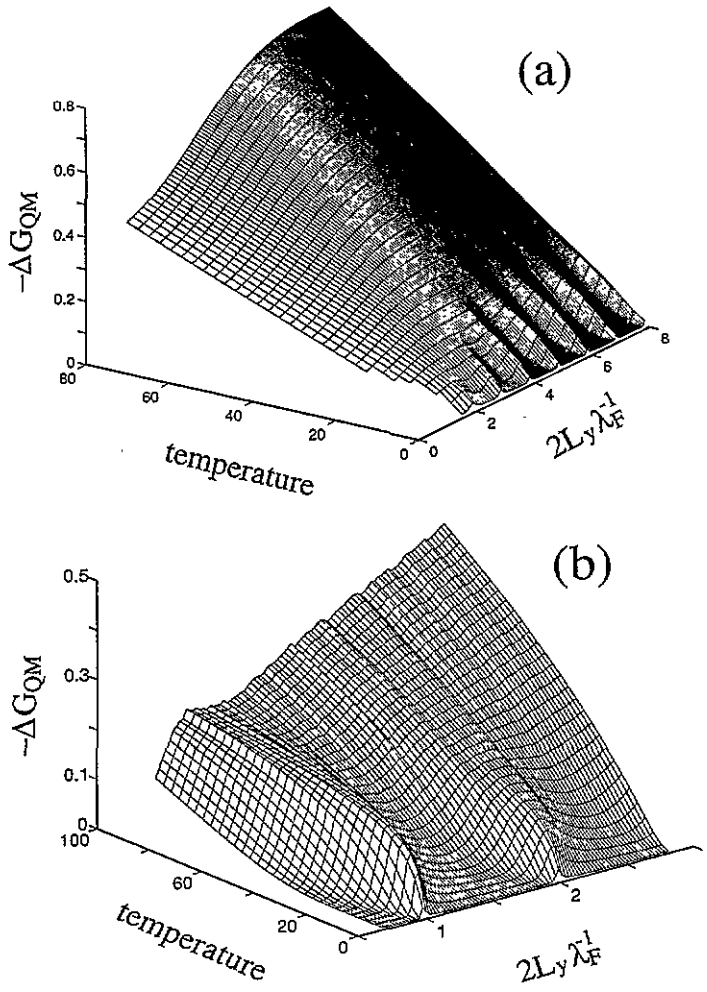

Figure 3. (a) $-\Delta G_{QM}(\lambda_F)$ is plotted as a function of temperature and λ_F^{-1} (for $L_y = 1000$ Å), and (b) $-\Delta G_{CL}(\lambda_F)$ is plotted as a function of temperature and L_y (for $\epsilon_F = 14$ meV).

are shown in figure 2(a). At sufficiently high temperatures ($k_BT > 1.5\epsilon_1(0)$) the oscillatory structure in ΔG, which is due to the size quantization, is smeared out (see figure 3(a)) and the classical and the quantum conductances become quite similar. For sufficiently large $\mathcal{N}$, one must have $k_BT \gg \epsilon_{\mathcal{N}}(0) - \epsilon_{\mathcal{N}-1}(0)$ with $\epsilon_{\mathcal{N}-1}(0) < \epsilon_F < \epsilon_{\mathcal{N}}(0)$ in order for ΔG_{QM} as expressed by (11) to approach its classical value. In the opposite case of a relatively large difference $\epsilon_{\mathcal{N}}(0) - \epsilon_{\mathcal{N}-1}(0)$, the $\mathcal{N} \gg 1$ limit fails to reconcile in full the quantum and the classical conductance changes which then differ not only by an oscillating part at low temperatures but also by a temperature-dependent factor at higher temperatures. For this reason, since the limit $\mathcal{N} \gg 1$ in our case is weakly enforced, the two conductances are not exactly equal even at higher temperatures as can be seen from figure 2(a). The saturation of ΔG_{QM} with λ_F is also temperature dependent. Since only half as many electron states can participate in the transport near the threshold of propagation of the lowest subband, the saturation value of ΔG_{QM} is almost twice that near the threshold of propagation. At lower temperatures ($k_BT < 1.5\epsilon_1(0)$), resonant behaviour of $\Delta G_{QM}(\lambda_F)$ begins to emerge.

One observes periodic oscillations in λ_F^{-1} with a period of $0.5L_y^{-1}$ where $\mathrm{Int}(2L_y/\lambda_F)$ is the number of propagating channels at zero temperature. The variation in conductance has a maximum near the opening of each new quantum channel. At even lower temperatures ($k_BT \prec 0.2\epsilon_1(0)$), the back-scattering current is almost exclusively carried by the uppermost propagating channels.

The behaviour of ΔG_{QM} as a function of L_y is shown in figures 2(b) and 3(b). At low temperatures, the resonant structure in ΔG_{QM} is again evident. The oscillations in L_y have a period of $\lambda_F/2$ and persist until L_y is sufficiently large so that ΔG_{QM} approaches its linear classical limit. (At temperatures of the order of a millikelvin, one should expect to observe these oscillations for wires as wide as a micron.) At high temperatures, ΔG_{QM} is linear at low values of L_y, and the oscillations are almost altogether absent (see figure 3(b)).

The reason that ΔG_{QM} approaches its classical limit in figure 2(b) and not in figure 2(a) is related to the energy subband structure that is specific to our choice of an infinite-square-well bounding potential. As L_y increases at constant temperature and ϵ_F, both the number of propagating subbands and the thermal smearing increase, which guarantees that ΔG_{QM} approaches its classical limit. In contrast, as $1/\lambda_F$ increases, keeping temperature and L_y constant, only the number of propagating subbands increases, while the thermal smearing condition begins to break down since $\epsilon_N(0) - \epsilon_{N-1}(0) \ll k_BT$ is no longer met at higher ϵ_F and N. Even at higher temperatures, the oscillations in ΔG_{QM} begin to appear at sufficiently high ϵ_F as ΔG_{QM} diverges away from its classical limit. ΔG_{QM} and ΔG_{CL} in figure 2(a) are not equal precisely for this reason; however, these conductances are identical for large L_y except at very low temperatures.

3. Conclusion

We have worked out a perturbative method to treat the phonon-assisted part of the ballistic resistance. We believe that the approach developed should be applicable to a number of mesoscopic problems. The limits of applicability of such an approach have been discussed. As an illustration, a particularly simple nanostructure consisting of a uniform mesoscopic wire connecting two thermal reservoirs is investigated. By performing a perturbation expansion, we have calculated a negative change of conductance in such a wire due to the interaction between electrons and acoustic phonons in the linear response regime. The dependence of this conductance on temperature, wire width and Fermi level was determined. The oscillations of the change in conductance ΔG_{QM} with wire width and Fermi wavelength have been found. These oscillations, along with the usual thermal broadening associated with the equilibrium thermal distribution of electrons, fully determine the broadening of the conduction steps due to increasing temperature.

Until now, to the best of our knowledge, no experimental attempts to resolve phonon-assisted contributions to the conductance of a nanostructure leading to such a broadening have been made. We hope that our results will change the situation and will motivate experimental work that would attempt to confirm our predictions. Experimental investigation of the phonon-controlled contribution to the conductance can provide valuable information about the electron–phonon interaction within a nanostructure and can help single out the type of phonon that is mainly responsible for the electron scattering under given conditions (temperature, chemical potential, width of the channel, etc). These experiments can also help answer the following important question: under which applied voltage and with what accuracy can the distribution of the phonons be considered an equilibrium one? Although the oscillations in ΔG_{QM} disappear with increasing temperature, ΔG_{QM} does not approach its classical limit, ΔG_{CL}, since only a small number of channels participate in the conduction

process. At low temperatures, as is evident from figure 2, the classical limit greatly differs from ΔG_{QM}, except in the case of extremely wide wires. In this sense, no true classical transport should be expected in mesoscopic wires. Finally, a critical range of temperatures at which the electron–phonon interaction in nanostructures may begin to have a pronounced effect on the conductance is determined.

Acknowledgments

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