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LETTER TO THE EDITOR

Resonant optical phonon generation in nanowires

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Abstract. We investigate a new type of resonant behaviour in the 1D hot-electron ballistic transport in nanostructures. The resonances are manifested by sharp increases in the rate of optical phonon generation and are accompanied by sharp drops in the overall current. They occur whenever the separation between a pair of levels of transverse quantization is equal to the energy of an optical phonon, $\hbar\omega_o$, and a condition for generation of optical phonons $eV > \hbar\omega_o$ is met, where V is the voltage bias across the conductor. We calculate the rate of energy transfer from the electrons to phonons. The ratio between the decrease in electric current power and the rate of energy transfer from electrons to phonons appears to be linearly proportional to the voltage bias.

The effects of phonons on the 1D ballistic transport in nanostructures have been recently investigated theoretically in [1, 2, 3]. In the linear regime, Gurevich *et al* [1, 2] calculated an increase in resistance which is particularly pronounced near the threshold of propagation and is due solely to the acoustical phonons. In the nonlinear regime, Gurevich *et al* [3] predicted *electrophonon resonances* (EPR) [4] which are manifested by sharp increases in the rate of optical phonon generation and examined in detail the conditions for these resonances. In this paper we wish to closely examine the generation of optical phonons due to EPR.

The resonant condition is of the form [3]

$$\hbar\omega_o = \epsilon_m(0) - \epsilon_n(0). \tag{1}$$

Here ω_o is the frequency of the long-wavelength optical phonons whereas $\epsilon_m(0)$ is the threshold of propagation in the mth Q1D subband (channel). The physics of this phenomenon is associated with singularities which are peculiar to the 1D electron density of states. There exists a close resemblance between this resonant phenomenon and the magnetophonon resonance [5, 6, 7] since the same kind of singularity is also typical for a 3D electron spectrum in a magnetic field.

Particularly sharp resonances can be achieved only for sufficiently low temperatures. In addition, an overall condition for the generation of the optical phonons $eV > \hbar\omega_o$ has to be met along with equation (1) in order for the resonances to take place [8]. We will ignore the dispersion of optical phonons.

In the zeroth approximation the collisions with the lattice defects can be neglected and the electron transport may be considered as ballistic. In the linear response regime (see the review [9]), the conductance G is a steplike function of the Fermi level or the gate voltage, each step corresponding to the inclusion of a new mode of transverse quantization to the conduction process. For a 1D conductor the height of each step is equal to the quantum of conductance, according to the Landauer formula $G_0 = 2e^2/h$ [10]. We will consider here a uniform conductor. In the nonlinear regime a substantial deviation of current from the Ohmic value may be expected if the ratio eV/μ is not small—cf. [11]. The functional dependence of $J^{(0)}(V)$ may be rather peculiar, so that the differential conductance $g = \mathrm{d}J^{(0)}(V)/\mathrm{d}V$ appears to be an oscillating function of the potential difference V [2, 12]. The distribution function of electrons, $f^{(0)}(\epsilon)$, in the subband n is given by

$$f^{(0)}(\epsilon) = f^{(F)}(\epsilon \mp eV/2 - \mu)$$

where $f^{(F)}$ is the Fermi function while $\epsilon = \epsilon_n(0) + p^2/2m^*$, where p is the x-component of the electron quasimomentum, while m^* is the electron effective mass. The upper (lower) sign is for $p > 0$ ($p < 0$) and corresponds to electrons coming from the left (right) reservoir (cf. [9]).

The current $J^{(0)}$ is given by [2, 13]

$$J^{(0)} = \frac{e}{\pi\hbar} k_B T \sum_n \ln\left[\frac{1 + \exp(\mu_n^{(+)}/k_B T)}{1 + \exp(\mu_n^{(-)}/k_B T)}\right] \tag{2}$$

where $\mu_n^{(\pm)} = \mu \pm eV/2 - \epsilon_n(0)$. Here we assume that the average chemical potential μ is determined by the chemical potentials of the reservoirs with which the ballistic conductor is in contact. This equation describes half steps of the differential conductance in the basic units of G_0 predicted and observed in [11, 14, 15].

In order to calculate the variation of the total current $\Delta J = J - J^{(0)}$ due to the electron–phonon interaction and to make use of the perturbative methods, $|\Delta J|/J^{(0)}$ was assumed small [1, 2, 3]. The total variation of the current, ΔJ, is a sum of currents carried by individual channels [1, 2]. The *channel currents* are made up of *partial currents* due to particular interchannel transitions. These are

$$\Delta J = \sum_n \Delta J_n \qquad \text{and} \qquad \Delta J_n = \sum_{n'} \Delta J_{nn'} \tag{3}$$

respectively. The partial currents are given by [3]

$$\Delta J_{nn'} = -2eL_x\left[1 - \exp\left(-eV/k_{\mathrm{B}}T\right)\right] \int \frac{\mathrm{d}^d q_\perp}{(2\pi)^d} \int_0^\infty \frac{\mathrm{d}p}{2\pi\hbar} \int_{-\infty}^0 \frac{\mathrm{d}p'}{2\pi\hbar}$$
$$\times C_{nn'} W_q \left(\mathcal{A}_{nn'}^{(-)} + \mathcal{A}_{nn'}^{(+)}\right) \delta(\epsilon' - \epsilon - \hbar\omega_q). \tag{4}$$

Here

$$\mathcal{A}^{(\pm)} = -\left[\tfrac{1}{2} \mp \tfrac{1}{2} - f^{(F)}\left(\epsilon' - \mu^{(\pm)}\right)\right]\left[\tfrac{1}{2} \pm \tfrac{1}{2} - f^{(F)}\left(\epsilon - \mu^{(\mp)}\right)\right]\left(\tfrac{1}{2} \pm \tfrac{1}{2} + N_q\right) \tag{5}$$

where $C_{nn'} = \left|\langle n'|\exp(\mathrm{i}q_\perp \cdot r_\perp)|n\rangle\right|^2$, $d = D - 1$, D is the dimension of the system, L_x is the total length of the conductor, N_q is the average phonon occupation number (which we assume to be the equilibrium Bose function) and $\langle r_\perp|n\rangle$ is the transverse part of the electron wavefunction. *The terms proportional to* $\mathcal{A}^{(+)}$ *and* $\mathcal{A}^{(-)}$ *describe the phonon emission and* absorption, respectively. This equation describes a contribution of a single phonon branch. As expected, ΔJ diminishes the total current.

We consider the scattering of electrons by the three-dimensional bulk polar optical phonons (although phonons confined within or near the nanostructure could be easily included in the scheme). Then [16]

$$W_q = \frac{4\pi^2 e^2 \omega_o}{q^2}\left(\varepsilon_\infty^{-1} - \varepsilon_0^{-1}\right) \tag{6}$$

where ε_∞ and ε_0 are the dielectric constants for infinite and zero frequencies, respectively.

In the same manner one can calculate the rate of energy transfer Q from electrons to the phonon system:

$$Q = \sum_q \hbar\omega_q \left[\frac{\partial N_q}{\partial t}\right]_{\text{coll}} = \frac{m^*\omega_o L_x}{2\pi h}\left[1 - \exp\left(-\frac{eV}{k_B T}\right)\right]^2 \sum_{nn'} \int \frac{d^2 q_\perp}{(2\pi)^2}$$
$$\times \int_0^\infty d\epsilon\, W_q C_{nn'} \frac{\Theta(\epsilon - R_{nn'})}{\sqrt{\epsilon(\epsilon - R_{nn'})}} f(\epsilon + \hbar\omega_o - \mu_n^{(+)})$$
$$\times \left[1 - f(\epsilon - \mu_n^{(-)})\right] f(\epsilon - \mu_n^{(+)}) \left[1 - f(\epsilon + \hbar\omega_o - \mu_n^{(-)})\right]. \tag{7}$$

From (4) and (7) it follows that

$$\frac{Q}{|\Delta J|\, V} = \frac{\hbar\omega_o}{eV}. \tag{8}$$

One can easily visualize this result in the following way: $|\Delta J|/e$ is the variation of the electron flux due to the electron–phonon scattering. The scattered electrons reverse their quasimomenta and thus no longer contribute to the total current (see [1, 2]). Since each electron that belongs to the blocked part of the flux emits just one phonon, one gets the following ratio:

$$Q = \hbar\omega_o |\Delta J|/e. \tag{9}$$

The ratio of Q to the power of total current is

$$\frac{Q}{JV} = \frac{Q}{(J^{(0)} - |\Delta J|)V} = \frac{\hbar\omega_o}{eV}\frac{|\Delta J|}{J^{(0)}}\left[1 - \frac{|\Delta J|}{J^{(0)}}\right]^{-1}; \tag{10}$$

the rate of energy loss to the optical phonons is particularly significant, as compared to the total power, if EPR takes place near the generation threshold of $eV = \hbar\omega_o$ (to within $k_B T$).

This situation is quite unlike the usual Landauer transport, where the electron–phonon (and the electron–electron) interactions are restricted to the contacts and hence all the heat is released in the contacts only. In our case some energy is transferred to the phonons and is released as heat in the vicinity of a nanowire. The rest of the heat is released in the reservoirs. These two mechanisms of heat release are physically quite different.

To illustrate, let us consider the low-temperature limit and ignore $N(\omega_o)$ as compared to unity. Then

$$\Delta J_n = -\frac{em^* L_x}{4\pi^2\hbar^2} \sum_m \int \frac{d^2 q_\perp}{(2\pi)^2} C_{nm} \int_0^\infty d\epsilon \frac{W_q \Theta(\epsilon - R_{nm})}{[\epsilon(\epsilon - R_{nm})]^{1/2}}$$
$$\times [1 - f^{(F)}(\epsilon - \mu_n^{(-)})] f^{(F)}(\epsilon + \hbar\omega_o - \mu_n^{(+)}) \tag{11}$$

where $R_{nm} = \epsilon_m(0) - \epsilon_n(0) - \hbar\omega_o$.

The singularities in (11) are due to the initial and final densities of states. As long as $R_{nm} \neq 0$ they are integrable and the integral in (11) is well behaved as a function of bias or gate voltages. However, when $R_{nm} \to 0$ or, equivalently, when the resonant condition equation (1) is met, the two singularities in equation (11), $1/\sqrt{\epsilon}$ and $1/\sqrt{\epsilon - R_{nm}}$, amount to a $1/\epsilon$ singularity which is no longer integrable (cf. [5]). A divergence of this type in the integral (11) leads to a significant increase in the resistance. There are no such singularities in the densities of states in the 2D and 3D cases, and for this reason, there are also no electrophonon resonances in our sense of the word in these cases either.

The integral (11) vanishes unless functions $f^{(F)}(\epsilon + \hbar\omega_o - \mu_n^{(+)})$ and $1 - f^{(F)}(\epsilon - \mu_n^{(-)})$ overlap. This amounts to the generation threshold condition $eV > \hbar\omega_0$ (to within $k_B T$) and is taken into account explicitly by the step function $\Theta(\cdot)$ in equation (11).

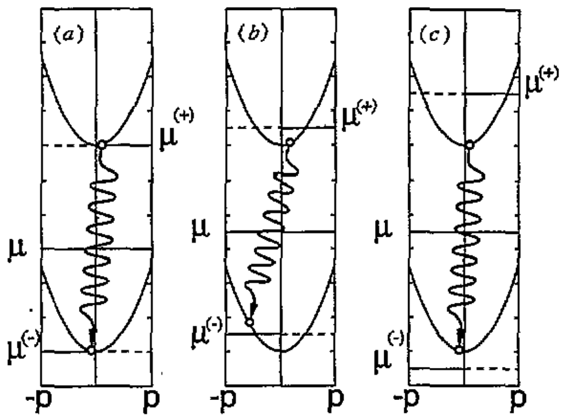

Figure 1. While the conditions for EPR are favourable in (a) and (c), no EPR is possible for (b).

Let us investigate the resonant behaviour of a partial current, say, ΔJ_{12}. In figure 1 we show schematically the transitions that correspond to ΔJ_{12}. If the position of the average Fermi level, μ, is exactly halfway between the bottoms of the subbands 1 and 2 and the applied voltage bias slightly exceeds the optical phonon energy the transition indicated by an arrow is allowed. Such a transition would correspond to the electrophonon resonance.

Indeed, in this case the right-hand part ($p > 0$) of band 2, near its bottom, is occupied by electrons whereas the left-hand part ($p < 0$) of band 1 is empty, hence backscattering of electrons by optical phonons from the bottom of band 2 to the bottom of band 1 is allowed. If, on the other hand, the position of the Fermi level is shifted by, say, $\Delta\mu$ upward from the midpoint between the bottoms of subbands of 1 and 2 (see figure 1(b)) then in general transitions between the subbands accompanied by optical phonon emission are still possible (as indicated by the arrow). However, they would not be resonant ones. Indeed, at $eV = \hbar\omega_o$ both the right-hand part of band 2 and the left-hand part of band 1 are occupied so that the resonant transitions are forbidden. In figure 1(c), however, the electrostatic potential exceeds the value of that shown in figure 1(b), to the extent that $\mu^{(-)} = \epsilon_1(0)$. The resonances are allowed once again although they take place at a higher voltage bias.

In figure 2 one can see a number of sharply sloping features; each of these corresponds to a dramatic increase in the generation of optical phonons which result in the current drop. Particularly sharp features are the manifestations of electrophonon resonances. The ones that are not so sharp correspond to a somewhat mismatched resonant condition, namely $\hbar\omega_o = \epsilon_m(0) - \epsilon_n(0) - \delta R$ (δR can be either positive and negative). Due to EPR, the efficiency of phonon generation can be significant, as is shown in figure 3.

The forward scattering of electrons by phonons to any channel in the first approximation of the perturbation theory does not change the overall current while the backscattering does and, in some cases of EPR, it could completely extinguish the current J_m thus almost altogether blocking the mth channel. With each additional increase in applied voltage bias new uppermost channels are populated, each adding a half integer of G_o to the overall differential conductance. For such a new uppermost channel m, if the partial current ΔJ_{nm} that flows from channel m to any n is large because it meets the resonance condition (1), then the total current J would not increase with increasing voltage bias as would be expected in the absence of EPR but actually it would decrease. Hence each resonant drop in the current can be attributed to the blockage of the uppermost current carrying channel that opens at the voltage bias which is associated with a dramatic increase in the rate of optical

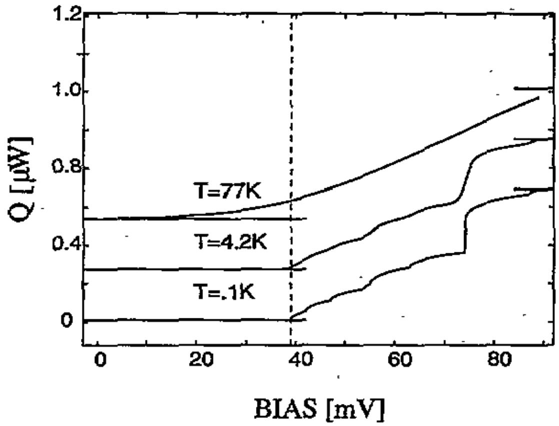

Figure 2. Energy transfer rate Q as a function of voltage bias V for $T = 0.1$, 4.2 and 77 K.

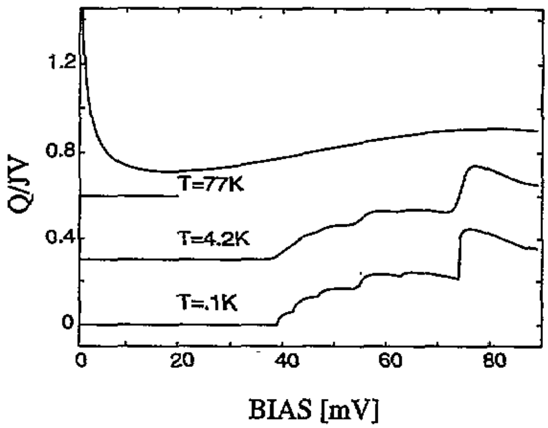

Figure 3. Ratio of energy transfer rate Q to JV as a function of voltage bias V for $T = 0.1$, 4.2 and 77 K.

phonon generation.

These sharp drops of the current can be compared with the Monte Carlo simulations in [17] (a Q1D wire) and the results in [18] (a Q2D semiconductor structure) where a different type of nonmonotonic dependence of the conductivity on the gate voltage related to the optical phonons has been found.

As explained above, to the first order in the electron–phonon scattering, the contributions from different phonon branches are additive. The acoustical phonons can also be generated in a strong electric field which would make the resonant pattern more complicated. However, due to a larger strength of the coupling with the optical phonons and their larger frequency and particularly to the existence of the limiting frequency ω_o one may expect that the acoustic phonon contribution would not mask the main features of the resonant behaviour predicted here.

In summary, we have calculated the rate of optical phonon generation accompanied by a negative change of current due to the electron–phonon scattering in nanowires connecting two thermal reservoirs with a large voltage bias. We have found pronounced resonant features in the heat release in the vicinity of the wire and also in the resistance as a function of the applied voltage bias. The resonances are a consequence of the confinement and of a special form of the DOS of electrons in the 1D case. The sharp resonances are absent from the 2, 3D cases for physical systems which are equivalent otherwise. As electrons undergo the transitions between the bottoms of the subbands, the resonant condition is met whenever the optical phonon energy is equal to the energy separation of the corresponding subbands. We have pointed out the apparent similarity between the magnetophonon and the electrophonon resonances. We have indicated that resonances of similar origin can be also due to the phonons confined within or near the nanowire. Finally, we find that at finite temperatures the voltage bias threshold required for the onset of EPR may be somewhat lower than the low-temperature threshold given by condition (1).

We believe that this effect can be of great experimental use when investigating various physical aspects of nanostructure systems. To name a few, one can investigate the character of the actual interactions between the electrons and optical phonons, or the details of the electron band structure and the actual positions of the levels of transverse quantization, or the spectrum of the confined phonons with a finite limiting frequency, or the role of nonequilibrium phonons in the transport phenomena. We also encourage experimentalists to think of a physical situation where a blockage of a single channel due to EPR may play a crucial role so that one can separate a one-channel contribution experimentally. Furthermore, it may be feasible to make use of this effect for the generation of optical phonons (and infrared radiation) in nanostructures. Finally, we stress the significance this effect may have on the practical application of the nanostructures.

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