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Phonon generation by current-carrying nanowires

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Abstract. Spectral and spatial distributions of phonons generated in a quantum wire by a transport current are investigated as a function of the voltage across the nanostructure and the gate voltage. We start with consideration of the simplest case of a uniform nanowire which connects two thermal reservoirs. Then the role of the leads is discussed. It is shown that both spectral and angular distributions of emitted phonons depend significantly on the bias voltage. Studies of phonon generation allows one to determine the electron-phonon coupling constant in ballistic devices.

Electron-phonon interaction leads to absorption and emission of phonons by the electrons in quantum wires. In the equilibrium there is a detailed balance between the emitted and absorbed phonons. However, out of equilibrium, the distributions of electrons penetrating into a biased quantum wire from the leads are characterized by different chemical potentials. Therefore the phonon emission prevails over the absorption. The generation rate of the phonons at a given frequency ω propagating along a given direction is a specific function of the bias voltage. Knowing this function one can determine electron-phonon coupling constant, get information about the device shape, etc.

As we will see, at a small bias voltage only the transitions within one mode of transverse motion are allowed, while at large voltages the interband transitions are also possible. Consequently the voltage dependence of the generation rate is a step-like function. The threshold voltages are directly related to the band gaps between the modes of transverse quantization, while the generation rates at the plateaus are related to the electron-phonon coupling constant inside the nanowire. It is important to note that in this way one can study electron-phonon interaction in nanowires.

The edges of the channel play a specific role. Namely, if the channel's shape is smooth enough, one can describe the situation in terms of a position-dependent band structure [1]. We will show that the phonons with a given frequency and propagation direction can be generated only near specific points where the local energy and quasimomentum conservation laws are met. Consequently, the phonons emitted from the edges bear information about the position-dependent band gaps between the modes of transverse quantization.

Uniform channel

In a *uniform* channel, the electron states are $\psi_{np}(\mathbf{r}) = L^{-1/2}\chi_n(\mathbf{r}_\perp)\exp(ipx/\hbar)$, where L is a normalization length close to the physical length of the wire, x is the longitudinal and $\mathbf{r}_\perp$ the transverse direction, p is the x-component of the electron quasimomentum, and $\chi_n(\mathbf{r}_\perp)$ is the wave function of transverse quantization, the energy being $\epsilon_n(p) = \epsilon_n^0 + p^2/2m$. Here m is the electron effective mass, and $\epsilon_n^0 \equiv \epsilon_n(p=0)$ is the

bottom of the n-th transverse band. The matrix element for phonon-induced transitions is $C_{nn'}(\mathbf{q}_\perp) = \langle\chi_{n'}|\exp(-i\mathbf{q}_\perp\mathbf{r}_\perp)|\chi_n\rangle$, where $\mathbf{q}$ is the phonon wave vector. For the phonon-electron collision operator one gets [2]

$$\left[\frac{\partial N_\mathbf{q}}{\partial t}\right]_{\text{coll}} = \frac{2}{\mathcal{A}}\sum_{nn'}\int d\xi_p\, W_\mathbf{q}\,|C_{nn'}(\mathbf{q}_\perp)|^2\,\left[f_{n,p+\hbar q_x}(1-f_{n'p})(N_\mathbf{q}+1)\right.$$
$$\left.-f_{n'p}(1-f_{n,p+\hbar q_x})N_\mathbf{q}\right]\,\delta[\epsilon_n(p+\hbar q_x)-\epsilon_{n'}(p)-\hbar\omega_\mathbf{q}]\,. \qquad (1)$$

Here $d\xi_p = dp/2\pi\hbar$, $\mathcal{A}$ is the cross section of the channel, while the factor 2 comes from the summation over electron spin (we assume all the transition probabilities to be spin-independent). The coupling coefficient W for the piezoelectric coupling is $W_\mathbf{q} = (\pi/\rho\omega_\mathbf{q})[4\pi e\beta_{q,lq}\nu_l/\epsilon_{qq}]^2$. Here e is the electron charge, $\beta_{i,ln}$ is the tensor of piezoelectric moduli (which is symmetric in the last two indices), ϵ_{il} is the tensor of dielectric susceptibility, and $\vec{\nu}$ is the polarization vector (that is the unit vector along the elastic displacement $\mathbf{u}$) of the phonon with the wave vector $\mathbf{q}$. The index q indicates the projection of a tensor on the $\mathbf{q}$ direction, while ρ is the mass density. For the deformation potential interaction we have $W = \pi\Lambda^2 q^2/\rho\omega_\mathbf{q}$, where Λ is the deformational potential constant for the phonon branch under consideration.

Let us investigate the consequences of the energy and quasimomentum conservation $\epsilon_n(p+\hbar q_x) - \epsilon_{n'}(p) - \hbar\omega_\mathbf{q} = 0$. For the solution of this equation, $p_{nn'}$, one has

$$p_{nn'} = (m/\cos\theta)\,(s - \Delta_{nn'}/\hbar q) - (1/2)\hbar q\cos\theta\,, \qquad (2)$$

where $s = \omega/q$ is the sound velocity, θ is the angle between $\mathbf{q}$ and the x-axis, and $\Delta_{nn'} = \epsilon_n^0 - \epsilon_{n'}^0$. Consequently, the delta-function in Eq. (1) can be expressed as $(m/\hbar q|\cos\theta|)\,\delta(p-p_{nn'})$. Following Landauer-Büttiker-Imry (see e.g. [4]), we consider a semiconductor quantum channel connected to two reservoirs, each in independent equilibrium. Thus the equilibrium distribution functions are $f_n^{(0)}(p) = f^{(\mathrm{F})}[\epsilon_n(p) \pm eV/2 - \mu]$, where $f^{(\mathrm{F})}$ is the Fermi function.

Consider the transitions involving a phonon with a given x-component of the wave vector, $q_x > 0$. Such a phonon can be emitted by transition 1 from the state having positive initial momentum $p + \hbar q_x$ to the state with negative momentum p (see Fig. 1, left). As is usually accepted [4], the initial and final states are determined by the Fermi functions with chemical potentials $\mu^{(\pm)} = \mu \pm eV/2$ and the same temperature T. For $n = n'$, the solution $p_{nn'}$ of Eq. (2) is n-independent and equal to $p_1 = ms/\cos\theta - (1/2)\hbar q\cos\theta$. So the $n = n'$ part of the collision term for $T = 0$ (or, to be more specific, $\hbar\omega_\mathbf{q} \gg k_\mathrm{B}T$) can be rewritten as

$$\left[\frac{\partial N_\mathbf{q}}{\partial t}\right]_{\text{coll}} = \frac{mW_\mathbf{q}}{\pi\mathcal{A}\hbar^2 q|\cos\theta|}\sum_n |C_{nn}(\mathbf{q}_\perp)|^2\,\theta[\mu^{(+)} - \epsilon_n(k_1)]\,\theta[\epsilon_n(p_1) - \mu^{(-)}]\,. \qquad (3)$$

where $k_1 = p_1 + hq_x = ms/\cos\theta + \hbar q_x/2$. One can easily see that a *current-carrying channel can generate phonons*, the phonon generation being restricted to the frequencies $2ms^2/\hbar \le \omega_\mathbf{q} \le eV/\hbar$. In the right panel of Fig. 1 the angular dependence of the phonon emission rate is shown for different bias voltages. The typical rate is $\mathcal{R} = W_\mathbf{q}/2\pi\mathcal{A}\hbar s$. Assuming $4\pi\beta^2/\epsilon\rho s^2 = 4\times10^{-4}$, $s = 3\times10^5$ cm/s, ϵ=10, $\mathcal{A} = 10^{-12}$ cm^2, $q = 6ms/\hbar$, $m = 0.07m_0$, we get $\mathcal{R} \approx 5\times10^{11}$ s^{-1}. It is seen that the

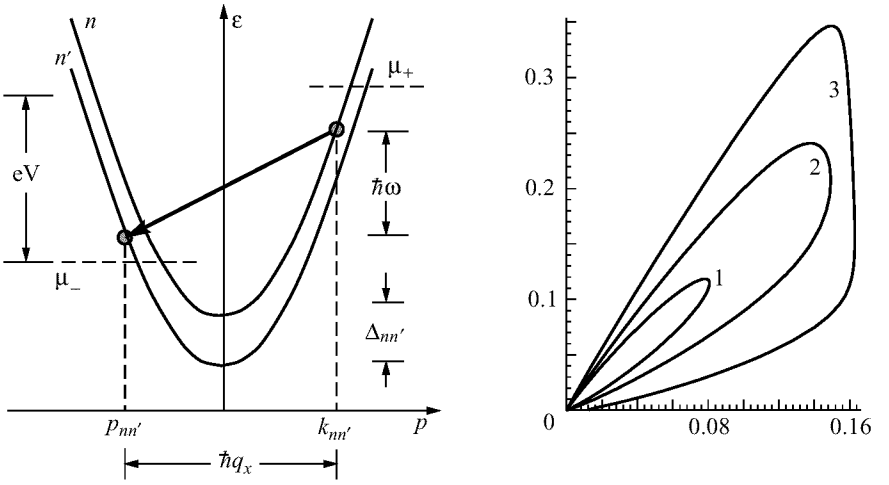

Fig 1. Left: Scheme of transitions. Right: Angular dependences of phonon generation rate near the threshold. eV/k_BT: 1 — 60, 2 — 65, 3 — 75.

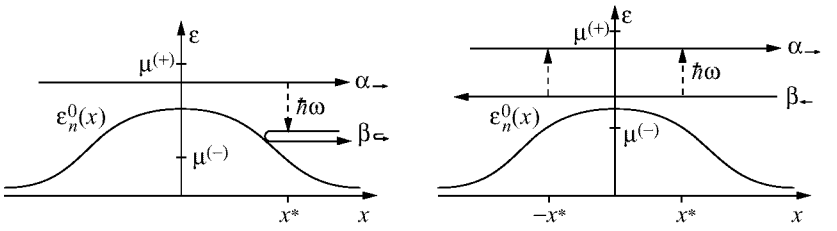

Fig 2. Left: Phonon emission in a nonuniform channel by a transition from a propagating to a reflected electron state. The transition is localized around the point x^*. Right: Phonon emission in a nonuniform channel by a transition between two oppositely directed propagating states. There are two transition points.

character of the angular dependence is changed at the threshold. The phonons can also be emitted by interband transitions. Qualitatively the angular dependences are similar to the case of intraband transitions, but the threshold values of voltage are shifted.

Nonuniform channel

Now consider an adiabatic *nonuniform* quantum channel with the width depending on coordinate x. The electron wave functions for such channels can be subdivided into two categories – the propagating states and the reflected states on each side. An important simplification is that at $qL \gg 1$ one can employ the *stationary phase approximation* for estimation of the transition probabilities. As a result, it is the *local* conservation laws at the stationary phase points x^* that enter transition probabilities. Let us again assume $T = 0$. Then the only possible phonon-generating processes are the ones shown in Fig. 2

For a transition of the kind in Fig. 2, right, there will in fact be *two* transition points,

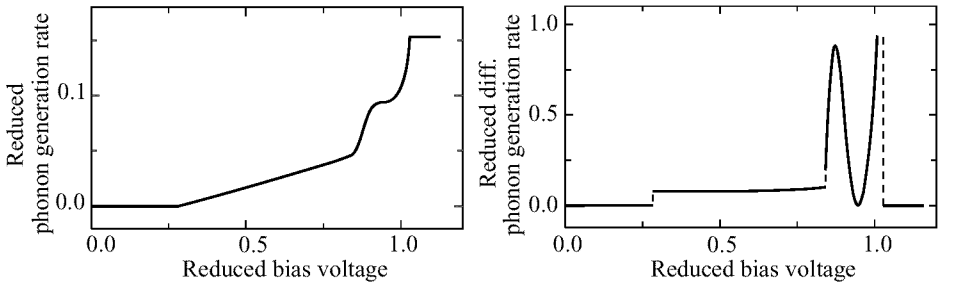

Fig 3. Dependence of the generation rate (left) and its voltage derivative (right) on bias voltage.

one on each side of the constriction The corresponding two parts of the transition amplitude give rise to the interference term $2\{1 + \sin[\varphi(x^*) - \varphi(-x^*)]\}$ where φ is the phase of the transition amplitude. Fig. 3 shows the dependence of the generation rate on the bias voltage that results from such a term for a set of typical parameters. As $eV = \mu^{(+)} - \mu^{(-)}$ increases, more and more phonon emitting transitions become possible, and so the rate increases.

In conclusion, we have calculated the rate of phonon generation by a current-carrying quantum channel. It is shown that the spectral and spatial distributions of emitted phonons bear information both on electron-phonon coupling in the vicinity of the device and on characteristics of the electron spectrum.

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