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Phonon-drag thermopower of a ballistic quantum wire

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The phonon-drag thermopower S^g of a quasi-one-dimensional ballistic quantum wire is calculated by using the Onsager relation to relate S^g to the phonon-drag contribution to $Q/\Delta V$, where Q is the heat flux produced by a small voltage difference ΔV across the wire. A general formula is derived for S^g and numerical results are presented for when two electronic subbands are involved. The dependence of S^g on the wire width exhibits peaks similar to those shown by the diffusion thermopower S^d. It is found, however, that the S^g maxima are up to 50–100 times larger than the corresponding ones for S^d when $T=1-10$ K. The dominance of S^g is apparent for all the values of the wire width and temperatures investigated. [S0163-1829(97)51040-X]

We calculate the phonon-drag thermopower S^g of a ballistic one-dimensional electron gas (1DEG). Previous authors have shown that the phonon-drag contribution to ballistic resistance is small[1] and others discuss acoustoelectric currents and conductivity produced by injecting phonon pulses.[2,3] Kozub and Rudin[4] consider S^g in a quantum point contact and they find a very different quantization picture than the one we predict here. The reason for this is that[4] the behavior of S^g is dominated by the electron-phonon interaction in the wide, tapering regions leading to the narrow gap in the middle of the contact, while here we consider a long 1DEG, and the behavior of S^g is dominated by the electron-phonon interaction *inside* the 1DEG.

The electronic structure we examine is a quasi-1DEG confined in a ballistic quantum wire (BQW) of width W. To model this structure, we consider a ballistic two-dimensional electron gas (2DEG) which is confined laterally by two parallel, straight, hard potential walls separated by a distance W. The wire is fed with electrons from reservoirs attached to the ends. We use a Cartesian coordinate system $Oxyz$ with Oxy in the plane of the 2DEG and Ox parallel to the axis of the wire. The hard wall potential in the y direction splits each 2D subband into several 1D subbands (channels). We assume that only the ground 2D subband is occupied. Then, the energy eigenvalues and electron wave functions for the 1D constriction in the effective-mass approximation are given by $E_{\alpha k}=E_\alpha+(\hbar^2k^2/2m^\star)$ and $\Psi_{\alpha k}(\mathbf{r})=(1/L_x)^{1/2}\exp(ikx)\phi_1(z)\theta_\alpha(y)$. Here, $E_\alpha=\hbar^2\alpha^2\pi^2/2m^\star W^2$ is the lowest energy of each 1D subband ($\alpha=1,2,3,\ldots$), k is the electron wave number associated with the electron motion along the x direction, $m^\star$ is the effective mass, $\mathbf{r}=(x,y,z)$, and L_x is the length of the quantum wire. The wave functions $\phi_1(z)$ and $\theta_\alpha(y)$ describe the electron confinement in the z and y direction: $\phi_1(z)$ is given by the Fang and Howard function[5] while $\theta_\alpha(y)$ is a sine function. In the case considered here the sum of all the transmission probabilities increases by unity each time a new channel propagates.

In these structures electrons exhibit strongly quantized behavior which is seen experimentally in the conductance G (Ref. 6) and diffusion thermopower S^d.[7,8] Electron transport in the quantum ballistic regime is described by the Landauer-Büttiker (L-B) approach.[9,10] Generalizations of the L-B formalism are given by Butcher[11] and by Sivan and Imry.[12] They relate the charge and heat fluxes in the wire to the chemical potential and temperature changes in the reservoirs.

The electronic system is embedded in a bath of 3D phonons. Above 0.5 K the phonon population is large enough to create enough electron-phonon scattering events to yield a measurable phonon-drag contribution to the thermopower. We consider temperatures $T\leqslant 10$ K, and ignore optical phonons and the effect of the interfaces on the acoustic phonons. The reservoirs have the same temperature T but the chemical potential in one of them is raised by $\Delta\mu$ so that a voltage difference $\Delta V=-\Delta\mu/|e|$ exists across the wire. Consequently, the electrons move towards the reservoir with the lower chemical potential and impart some of their momentum to the phonons through the electron-phonon interaction. Hence, a phonon heat flux Q is produced in the x direction. In standard notation we write[11,12]

$$Q=-M^g\Delta\mu/|e|. \tag{1}$$

We calculate Q and use Eq. (1) to obtain M^g. Then Onsager's relation, $M^g=-L^gT$ (Ref. 13) [where L^g is related to S^g by the equation $S^g=-L^g/G$ (Ref. 11)] yields

$$S^g=M^g/TG. \tag{2}$$

The calculation of Q for a ballistic 1DEG, which we outline here, follows a similar pattern to that described in more detail for a 2DEG in the quantum Hall regime.[14,15] In equilibrium a global chemical potential $\mu=E_F$ and temperature T characterize both reservoirs. Then, the occupation probability of the incident waves in channel α is given by the Fermi-Dirac function $f_0(E_{\alpha k})=\{\exp[(E_{\alpha k}-E_F)/k_BT]+1\}^{-1}$.[11,12] Phonons have the Bose-Einstein distribution: $N_0(\mathbf{q}s)=[\exp(\hbar\omega_{\mathbf{q}s}/k_BT)-1]^{-1}$ where $\hbar\omega_{\mathbf{q}s}$ is the energy of a phonon with wave vector $\mathbf{q}=(q_x,q_y,q_z)$ in mode s. When the chemical potential in the left-hand reservoir is raised by a small amount $\Delta\mu>0$, more electrons are injected into the BQW from the left while the number of electrons injected from the right remains the same. Hence the electron distribution function can be linearized as follows:[11]

$$f(E_{\alpha k})=\begin{cases} f_0(E_{\alpha k})+f_1(E_{\alpha k}), & k>0 \\ f_0(E_{\alpha k}), & k<0, \end{cases} \tag{3}$$

where $f_1(E_{\alpha k})$ is given by

$$f_1(E_{\alpha k})=-\Delta\mu\,\partial f_0(E_{\alpha k})/\partial E_{\alpha k}. \tag{4}$$

Eq. (3) shows that electrons acquire a net flux from the left to the right. The phonon heat flux produced in the x direction is

$$Q=\frac{L_x^{-1}V}{(2\pi)^3}\sum_s \int d\mathbf{q}\hbar\omega_{\mathbf{q}s}v_{px}N_1(\mathbf{q}s), \tag{5}$$

where V is the volume of the sample and v_{px} is the x component of the phonon group velocity. For isotropic phonons $v_{px}=v_s q_x/q$, where v_s is the sound velocity and q the magnitude of the phonon wave vector $\mathbf{q}$. Finally, $N_1(\mathbf{q}s)=N(\mathbf{q}s)-N_0(\mathbf{q}s)$ is the first-order perturbation of the equilibrium phonon distribution function $N_0(\mathbf{q}s)$, where $N(\mathbf{q}s)$ is the nonequilibrium phonon distribution function.

The phonon mean free path $l_p(\mathbf{q}s)$ is limited by lattice imperfections and crystal boundaries. We describe this scattering by a relaxation time $\tau_p(\mathbf{q}s)$ and use the steady-state Boltzmann's equation for phonons when $\Delta T=0$ to write[14,15]

$$\frac{N_1(\mathbf{q}s)}{\tau_p(\mathbf{q}s)}=2\sum_{\alpha k,\beta k'}\{f(E_{\beta k'})[1-f(E_{\alpha k})]P^e_{\mathbf{q}s}(\beta k',\alpha k) - f(E_{\alpha k})[1-f(E_{\beta k'})]P^a_{\mathbf{q}s}(\alpha k,\beta k')\}, \tag{6}$$

where the right-hand side of Eq. (6) is the rate of change of $N(\mathbf{q}s)$ due to electron-phonon scattering. $P^{a(e)}_{\mathbf{q}s}(\alpha k,\beta k')$ are the transition rates at which an electron in state αk is promoted to a state $\beta k'$ by absorbing (emitting) one phonon $\mathbf{q}s$. The factor 2 allows for the spin degeneracy.

The electron distribution functions appearing in Eq. (6) can be written in the linear form (3). Moreover, the transition rates $P^{a(e)}_{\mathbf{q}s}$ can be linearized: $P^{a(e)}_{\mathbf{q}s}=P^{a_0(e_0)}_{\mathbf{q}s}+P^{a_1(e_1)}_{\mathbf{q}s}$, where $P^{a_0(e_0)}_{\mathbf{q}s}$ corresponds to equilibrium and is proportional to $N_0(\mathbf{q}s)$ and $[N_0(\mathbf{q}s)+1]$, respectively, while the perturbations $P^{a_1(e_1)}_{\mathbf{q}s}$ are both proportional to $N_1(\mathbf{q}s)$. Using the detailed balance relation[15,16] and assuming weak electron-phonon coupling, we find that

$$N_1(\mathbf{q}s)=\frac{2\tau_p(\mathbf{q}s)}{k_BT}\sum_{\alpha k,\beta k'}\Gamma(\beta k',\alpha k)\left\{\frac{f_1(E_{\alpha k})}{\partial f_0(E_{\alpha k})/\partial E_{\alpha k}} - \frac{f_1(E_{\beta k'})}{\partial f_0(E_{\beta k'})/\partial E_{\beta k'}}\right\}, \tag{7}$$

where $\Gamma(\beta k',\alpha k)=f_0(E_{\alpha k})[1-f_0(E_{\beta k'})]P^{a_0}_{\mathbf{q}s}(\alpha k,\beta k')$ is the average equilibrium rate of absorption of phonons $\mathbf{q}s$ due to the electron transitions $\alpha k\rightarrow\beta k'$. The perturbation f_1 of the electron distribution function for the electrons injected from the left reservoir is given by Eq. (4), while for the electrons injected from the right, f_1 is zero. We see by inspection that only k and k' of opposite sign contribute to $N_1(\mathbf{q}s)$. Hence, Eq. (7) is written as

$$N_1(\mathbf{q}s)=-\frac{2\tau_p(\mathbf{q}s)}{k_BT}\Delta\mu\left\{\sum_{\alpha k>0}\sum_{\beta k'<0}\Gamma(\beta k',\alpha k) - \sum_{\alpha k<0}\sum_{\beta k'>0}\Gamma(\beta k',\alpha k)\right\}. \tag{8}$$

Substituting Eq. (8) into Eq. (5) and using Eqs. (1) and (2) we obtain the following formula:

$$S^g=\frac{L_x^{-1}V}{(2\pi)^3}\frac{2|e|}{k_BT^2}\frac{1}{G}\sum_s\int d\mathbf{q}\hbar\omega_{\mathbf{q}s}v_{px}\tau_p(\mathbf{q}s) \times\left\{\sum_{\alpha k>0}\sum_{\beta k'<0}f_0(E_{\alpha k})[1-f_0(E_{\beta k'})]P^{a_0}_{\mathbf{q}s}(\alpha k,\beta k') - \sum_{\alpha k<0}\sum_{\beta k'>0}f_0(E_{\alpha k})[1-f_0(E_{\beta k'})]P^{a_0}_{\mathbf{q}s}(\alpha k,\beta k')\right\}, \tag{9}$$

where we have substituted the explicit form for $\Gamma(\beta k',\alpha k)$. The conductance has the steplike form[8] $G=\frac{2e^2}{h}\Sigma_{\alpha=1}^{N_c}f_0(E_\alpha)$, where N_c is the number of occupied 1D subbands. At low temperatures phonon boundary scattering is dominant and $\tau_p(\mathbf{q}s)$ can be assumed to be independent of $\mathbf{q}s$.

It only remains for us to determine the transition rate $P^{a_0}_{\mathbf{q}s}(\alpha k,\beta k')$. By using the Golden Rule we have

$$P^{a_0}_{\mathbf{q}s}(\alpha k,\beta k')=\frac{\pi q^2\Xi^2(\mathbf{q}s)}{\rho V\omega_{\mathbf{q}s}}N_0(\mathbf{q}s)|Z_{11}|^2|Y_{\alpha\beta}|^2 \times\delta(E_{\beta k'}-E_{\alpha k}-\hbar\omega_{\mathbf{q}s})\,\delta_{k',k+q_x}. \tag{10}$$

Here, ρ is the density of the bulk material and $|Z_{11}|^2=|\int\phi_1^2(z)\exp(iq_z z)dz|^2$ is the q_z-conservation factor when only the ground 2D subband is populated. An analytical expression for $|Z_{11}|^2$ is given in Ref. 15. The q_y-conservation factor is defined as $|Y_{\alpha\beta}|^2=|\int_0^W\theta_\alpha(y)\exp(iq_y y)\theta_\beta(y)dy|^2$. Finally, $\Xi^2(\mathbf{q}s)$ is the ''effective'' acoustic potential describing the electron-phonon coupling. We confine our attention to GaAs/Al_xGa_{1-x}As structures. GaAs has a spherical conduction band and is polar: $\Xi^2(\mathbf{q}s)$ accounts for both deformation potential coupling and piezoelectric coupling. For the longitudinal acoustic branch and for each of the transverse branches we obtain[15] $\Xi^2(\mathbf{q}l)=\Xi_d^2+[(eh_{14})^2A_l/q^2]$ and $\Xi^2(\mathbf{q}t)=(eh_{14})^2A_t/q^2$, respectively. Here Ξ_d is the deformation potential constant associated with pure dilation,[16] h_{14} is the piezoelectric constant, and A_l, A_t are the anisotropy factors given by Price.[17]

The evaluation of the sums over k, k', and $\mathbf{q}$ follows the pattern described in Ref. 18. The explicit formula of S^g and results for one subband will be reported elsewhere. Here we concentrate on the more interesting case when two subbands are occupied. The values of the parameters used are standard ones for GaAs (Ref. 15) and l_p is taken to be 3 mm for all T. We calculate S^g for temperatures $0.3\ \mathrm{K}\leqslant T\leqslant 10\ \mathrm{K}$. The 2D

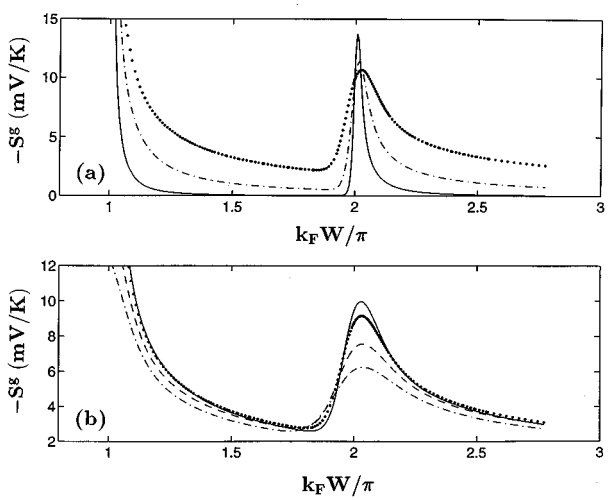

FIG. 1. $-S^g$ as a function of $k_F W/\pi$ calculated from Eq. (9) when two 1D subbands are occupied. (a) Results for 1 K (solid line), 2 K (chain line), and 4 K (dots). (b) Results for 5 K (solid line), 6 K (dots), 8 K (broken line), and 10 K (chain line).

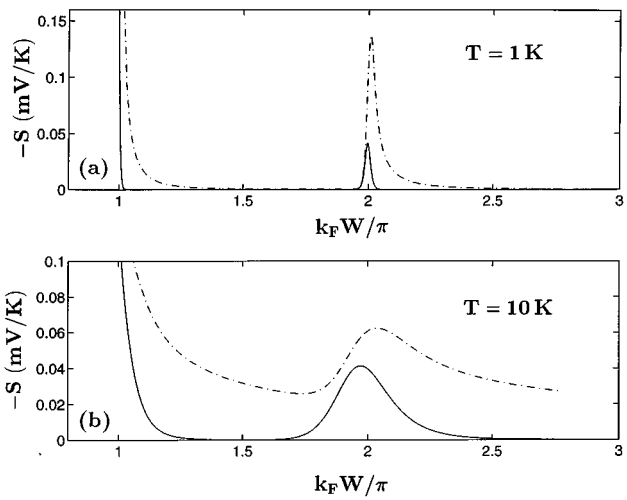

FIG. 2. Comparison of $-S^g$ and $-S^d$ for a ballistic 1DEG. The solid line is $-S^d$ (Ref. 8) and the chain line is $-0.01S^g$ at (a) $T=1$ K and (b) $T=10$ K.

electron density is fixed at $N_e=4.07\times10^{15}$ m^{-2}, which gives a Fermi level $E_F=14.56$ meV and a Fermi wave number $k_F=0.16$ nm^{-1}.

In Fig. 1(a) we plot $-S^g$ against $k_F W/\pi$ for $T=1$ K (solid line), $T=2$ K (chain line), and $T=4$ K (dots). In Fig. 1(b) the solid line, the dots, and the broken and chain lines correspond to $T=5$, 6, 8, and 10 K, respectively. The bottoms of the first and second subband cross E_F at $k_F W/\pi=1$ (where $W=19.63$ nm) and $k_F W/\pi=2$ (where $W=39.27$ nm), respectively. As E_1 approaches E_F, $-S^g$ rises abruptly, especially at low temperatures because of the vanishing values of G for $E_1 \geqslant E_F$.[8] At $k_F W/\pi\sim2$ a peak occurs due to the contribution of the second subband. In contrast to the diffusion case[8] the height of the peak depends on temperature, and *decreases* from ~14 mV/K at $T=1$ K to ~6 mV/K at $T=10$ K. To understand this, we should mention that the q_y-conservation factors $|Y_{11}|^2$ and $|Y_{22}|^2$ are by definition functions of $q_y W$ (Ref. 18) and consequently, since $q_y\sim k_B T/\hbar v_s$, they depend on T. Now, for fixed $W=39.27$ nm these factors are decreasing functions of q_y (and consequently of T), for all the temperatures of interest to us, and they dominate the temperature dependence of S^g.[18]

Finally, in Fig. 2 we compare the diffusion thermopower $-S^d$ (Ref. 8) and $-S^g$ at 1 K [Fig. 2(a)] and 10 K [Fig. 2(b)]. $-S^d$ is given by the solid line and the theoretical estimations of $-S^g$ have been *divided by a factor of 100* (chain line). Both curves have a similar shape. The phonon-drag peak values at $k_F W/\pi=2$ are approximately two orders of magnitude larger than the corresponding diffusive ones.

The only arbitrary parameters involved in the calculation of S^g are N_e and l_p. However, the value of N_e used here is very close to what is measured experimentally in a number of one-dimensional electron systems.[6–8] The value of l_p at low T is determined by the spatial dimensions of the substrate and it is usually a few mm [see, for example, Ref. 19]. At higher temperatures l_p is expected to decrease with T and its exact temperature dependence can be calculated from thermal conductivity data for the substrate.[19] The pronounced dominance of S^g over S^d shown by Fig. 2 illustrates the importance of phonon drag in semiconducting materials. In 2DEG's S^g has also been found to be much larger than the S^d when $2<T<65$ K.[19]

The peak structure of $-S^g$ shown in Figs. 1 and 2 is the manifestation of a well-known singularity which is hidden in the right-hand side of Eq. (9) and is associated with the details of the 3D phonon coupling to 1D electrons inside the wire. To bring it out in a simple way we concentrate on one phonon mode, let $T\to0$, and neglect both intersubband scattering in Eq. (9) and $\hbar\omega_{\mathbf{q}}$ in the δ function in Eq. (10). Then, by carrying out the sums over k' and k we obtain

$$S^g \propto -\sum_{\alpha=1}^{N_c=2} \int d\mathbf{q}\,\delta\left(\frac{q_x^2}{4}+k_\alpha^2-k_F^2\right)|Y_{\alpha\alpha}|^2 q N_0(\mathbf{q})\Xi^2(\mathbf{q}), \tag{11}$$

where $k_\alpha=(2m^\star E_\alpha/\hbar^2)^{1/2}$. The new δ function which appears in Eq. (11) comes from the product of the electron occupation factors in Eq. (9). We see that it resonates when $q_x=2(k_F^2-k_\alpha^2)^{1/2}$, i.e., when q_x spans the electron dispersion curve for subband α at the Fermi level. In other words, we are concerned with a Kohn resonance.[20] By inspection of Eq. (11) we see that, for $q_y=q_z=0$, the integration over q_x results in a singularity of the form $(E_F-E_\alpha)^{-1/2}$ which explains the structure of the figures. At finite T the temperature smearing of the electron occupation factors prevents S^g from diverging when $E_F=E_\alpha$.

In the present analysis we have ignored screening. For GaAs, the screening of the 2DEG coupling to 3D phonons reduces S^g by a factor of 0.3–0.5.[21] Similar reductions are expected for a 1DEG. The incorporation of screening is not important at the moment because no experimental data for the phonon-drag regime are available. The Delft group[7,8] observed quantum oscillations in the thermopower in quantum point contacts. They heated the electrons without heating the

phonons by using current heating and did not expect any phonon-drag component. However, we have shown that the $-S^g$ maxima are $\sim 50-100$ times bigger than those of $-S^d$, and so a small rise of the phonon temperature could yield a significant phonon-drag contribution to the thermopower. Since S^g and S^d exhibit a similar structure as functions of $k_F W/\pi$, a calibration of the experimental data is needed to untangle the two contributions.

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