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Phonon-drag thermopower of a two-dimensional electron gas in a quantizing magnetic field

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A formula is developed which gives the phonon-drag thermopower S_g of a two-dimensional (2D) electron gas coupled to 3D acoustic phonons in a quantizing magnetic field. Evaluation of the formula with realistic parameter values for a GaAs-$Ga_xAl_{1-x}As$ heterojunction in a field of 15 T yields a maximum value of 16.4 $mV K^{-1}$ at 6 K in excellent agreement with experimental data [for sample 1 of Fletcher *et al.*, Phys. Rev. B **33**, 7122 (1986)].

Recently, very-low-temperature measurements of the thermopower S of a two-dimensional (2D) electron gas in a GaAs-$Ga_xAl_{1-x}As$ heterostructure have shown strong evidence of phonon-drag thermopower S_g in zero and nonzero magnetic fields.[1-4] In quantizing magnetic fields, the values of S_g are found to be a few $mV K^{-1}$ and are greater than the predicted values of diffusion thermopower S_d by 2 orders of magnitude.

Phonon-drag thermopower arises from momentum exchange between electrons and phonons as a result of electron-phonon interaction in the presence of either a temperature gradient ∇T or an electric field $\mathbf{E}$. There are correspondingly two approaches to the calculation of S_g: the Q approach and the Π approach by Herring.[5] In the Q approach, the nonequilibrium distribution of phonons is used to calculate the momentum transferred to the electrons, and thus S_g is calculated. In the Π approach, the electron distribution is calculated in the presence of $\mathbf{E}$ with $\nabla T=0$ and the phonons in their equilibrium distribution. Then, the nonequilibrium distribution of phonons resulting from momentum transfer is calculated. The perturbed distribution of phonons is used to calculate the energy flux which they carry and hence the phonon-drag contribution to the Peltier coefficient Π, which is equal to $TS_g(\mathbf{B})$ in consequence of the Kelvin relation.[5] Either approach should give the same result, but the Π approach is simpler as $\nabla T=0$.

In this Rapid Communication we calculate S_g using the Π approach and ignore the Zeeman splitting of the spin states. The electron system considered is a 2D electron gas in a GaAs-$Ga_xAl_{1-x}As$ heterojunction subjected to a quantizing magnetic field at very low temperatures. For zero magnetic field S_g is calculated (using the Q approach) by Cantrell and Butcher[6] and it accounts for the large thermopower observed in a 2D gas at liquid-helium temperatures. We model the 2D electron gas as follows. The electrons are assumed to be confined to a thin layer parallel to the xy plane by a potential well, which is a function of z. The thin layer of electrons is embedded in a block of semiconductors of size L_x, L_y, and L_z in the x, y, and z directions, respectively. The block is assumed to contain 3D phonons. We consider electron motion in the presence of a small electric field $\mathbf{E}$ along the x direction and a magnetic induction $\mathbf{B}$ along the z direction. Then the carriers drift along the y direction to produce a net electrical current in the y direction which causes a Peltier heat flux U_y in that direction.

The transport equations for $\nabla T=0$ are[7]

$$\mathbf{J}=\sigma\cdot\mathbf{E} \tag{1}$$

and

$$\mathbf{U}=\Pi\cdot\mathbf{J}\,, \tag{2}$$

where $\mathbf{J}$ and $\mathbf{U}$ are the 2D electrical and heat current densities, respectively, and σ is the 2D magnetoconductivity. For the situation described above,

$$\Pi_{yy}=\mathbf{U}_y/\mathbf{J}_y \tag{3}$$

and, using the Kelvin relation,

$$\mathbf{S}_{yy}=\Pi_{yy}/\mathbf{T}\,, \tag{4}$$

we have

$$\mathbf{S}_{yy}=\mathbf{T}^{-1}(\mathbf{U}_y/\mathbf{E})\rho_{xy}\,. \tag{5}$$

In writing Eq. (5), it is assumed that, for moderate disorder, $\rho_{xx}\ll\rho_{xy}$. Note that for the above situation there are only two independent coefficients: thermopower $\mathbf{S}_{xx}=\mathbf{S}_{yy}$ and the Nernst-Ettingshausan coefficient $\mathbf{S}_{yx}=-\mathbf{S}_{xy}$.

In general, there are contributions to $\mathbf{U}$ from both electrons and phonons. However, we are interested in calculating only the contribution due to phonons. To do so, we assume that 2D electrons interact with 3D phonons. At very low temperatures we may neglect all but acoustic phonons of energy $\hbar\omega_{\mathbf{q}s}$ and wave vector $\mathbf{q}=(\mathbf{q}_x,\mathbf{q}_y,\mathbf{q}_z)$ in the sth mode. The $\mathbf{U}$ is written as

$$\mathbf{U}=\mathbf{L}_z(2\pi)^{-3}\int d^3q\,\hbar\omega_{\mathbf{q}s}\mathbf{v}_{\mathbf{q}s}g_s(\mathbf{q})\,, \tag{6}$$

where $\mathbf{v}_{\mathbf{q}s}$ is the group velocity of the phonons,

$$g_s(\mathbf{q})=N_{\mathbf{q}s}-N^0_{\mathbf{q}s}\,, \tag{7}$$

in which $N_{\mathbf{q}s}$ is the phonon distribution function and $N^0_{\mathbf{q}s}$ is $N_{\mathbf{q}s}$ at thermal equilibrium, which is given by the Bose distribution at temperature T. We calculate $g_s(\mathbf{q})$ by

solving the steady-state Boltzmann equation for phonons:

$$(\partial N_{\mathbf{q}s}/\partial t)_{ep}+(\partial N_{\mathbf{q}s}/\partial t)_{\text{coll}}=0\,. \tag{8}$$

In Eq. (8), the first term is due to the electron-phonon interaction and the second term is due to other scattering processes such as phonon-phonon interactions and boundary scattering. Assuming that the latter interactions dominate, we write the second term in Eq. (8) in the relaxation-time approximation as

$$(\partial N_{\mathbf{q}s}/\partial t)_{\text{coll}}=-g_s(\mathbf{q})/\tau_s(\mathbf{q})\,, \tag{9}$$

where $\tau_s(\mathbf{q})$ is the phonon relaxation time. From Eqs. (8) and (9) we see that

$$g_s(\mathbf{q})=\tau_s(\mathbf{q})(\partial N_{\mathbf{q}s}/\partial t)_{ep}\,. \tag{10}$$

The rate of change of $N_{\mathbf{q}s}$ due to electron-phonon interaction is, in the Born approximation,

$$(\partial N_{\mathbf{q}s}/\partial t)_{ep}=\sum_{\alpha\alpha'}[P^{\text{em}}_{\mathbf{q}s}(\alpha'\rightarrow\alpha)f_{\alpha'}(1-f_\alpha) -P^{\text{ab}}_{\mathbf{q}s}(\alpha\rightarrow\alpha')f_\alpha(1-f_{\alpha'})]\,, \tag{11}$$

where $P^{\text{em}}_{\mathbf{q}s}(\alpha'\rightarrow\alpha)$ is the transition rate at which an electron goes from state α' to state α by emitting a phonon, $P^{\text{ab}}_{\mathbf{q}s}(\alpha\rightarrow\alpha')$ is the transition rate at which an electron goes from state α to state α' by absorbing a phonon, and f_α is the distribution function for electrons in state α.

The transition rates can be evaluated by using the one-electron wave function $\psi_\alpha(x,y,z)$ and eigenvalue $\mathbf{E}_\alpha$ for the 2D gas in crossed electric and magnetic fields. For an isotropic effective mass m^* we have, for electrons with charge $-e$ and cyclotron resonance frequency $\omega_c=eB/m^*$,

$$\psi_\alpha(x,y,z)=(L_y)^{-1/2}\exp(ik_y y)\Phi_m(z)\phi_n[x-x_0(k_y)]\,, \tag{12}$$

and

$$E_\alpha=E^0_\alpha+eEx_0(k_y) \tag{13a}$$

$$=E_m+(n+\tfrac{1}{2})\hbar\omega_c+eEx_0(k_y)\,, \tag{13b}$$

where α represents the set of quantum numbers (m, n, k_y) with m and n denoting non-negative integers. In Eqs. (13) we have dropped a term proportional to E^2. In Eqs. (12) and (13), k_y is a wave number in the y direction and $\Phi_m(z)$ is the normalized wave function of the mth electric subband with energy E_m. Finally, ϕ_n is the normalized wave function of a simple harmonic oscillator centered at

$$x_0(k_y)=-l^2(k_y+m^*E/\hbar B)\,, \tag{14}$$

where $l=(\hbar/eB)^{1/2}$ is the cyclotron radius. Note that the processes involved in Eq. (11) conserve momentum in the y direction: i.e., $k'_y=k_y+q_y$. Using Eqs. (7) and (10)–(14), we may solve for $g_s(\mathbf{q})$ to obtain

$$g_s(\mathbf{q})=[N^0(\hbar\omega^*_{\mathbf{q}s})-N^0(\hbar\omega_{\mathbf{q}s})]\frac{\Gamma_s(\mathbf{q})}{\Gamma_s(\mathbf{q})+\tau_s^{-1}(\mathbf{q})}\,, \tag{15}$$

where

$$\hbar\omega^*_{\mathbf{q}s}=\hbar\omega_{\mathbf{q}s}[1+(E/Bv_s)(q_y/q)]\,, \tag{16}$$

and

$$\Gamma_s(\mathbf{q})=(2\pi/\hbar)\sum_{\alpha\alpha'}|V_{\alpha'\alpha s}(\mathbf{q})|^2 \times(f_\alpha-f_{\alpha'})\delta(E_{\alpha'}-E_\alpha-\hbar\omega_{\mathbf{q}s})\,. \tag{17}$$

Here

$$|V_{\alpha'\alpha s}(\mathbf{q})|^2=|V_s(\mathbf{q})|^2\left|\int\psi_{\alpha'}(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}\psi_\alpha(\mathbf{r})d^3r\right|^2\,, \tag{18}$$

in which $\mathbf{r}=(x,y,z)$ and $|V_s(\mathbf{q})|^2$ represents the strength of electron-phonon interaction. To calculate $g_s(\mathbf{q})$ to first order in $\mathbf{E}$, we write

$$N^0(\hbar\omega^*_{\mathbf{q}s})-N^0(\hbar\omega_{\mathbf{q}s})=-\frac{E\hbar q_y}{B\beta(\hbar\omega_{\mathbf{q}s})^2}G(\beta\hbar\omega_{\mathbf{q}s}/2)\,, \tag{19}$$

in Eq. (15), where $\beta=(k_BT)^{-1}$ and $G(x)=(x/\sinh x)^2$. Then the f_α's in Eq. (17) may be replaced by their thermal equilibrium values given by the Fermi-Dirac distribution functions f^0_α, and E_α may be replaced by E^0_α [as defined in Eqs. (13a) and (13b)] both in f^0_α and in the Dirac δ function. From Eqs. (6), (15), and (19) we then have

$$\mathbf{U}=-\frac{L_zE}{8\pi^3B\beta}\int d^3q(\mathbf{q}/q^2)q_yG(\beta\hbar\omega_{\mathbf{q}s}/2) \times\frac{\Gamma_s(\mathbf{q})}{\Gamma_s(\mathbf{q})+\tau_s^{-1}(\mathbf{q})}\,, \tag{20}$$

which, using Eq. (5), gives a general expression for S_g.

The evaluation of $\Gamma_s(\mathbf{q})$ is simplified when all electrons are in the lowest Landau level ($n=n'=0$) and the lowest electric subband ($m=m'=0$). Replacing the Dirac δ function in Eq. (17) by a Lorentzian $\Delta_\mathbf{q}$ with width γ we obtain

$$\Gamma_s(\mathbf{q})=(L_xL_y/\hbar l^2)|V_s(\mathbf{q})|^2\exp(-\mathbf{q}_\parallel^2l^2/2)|F(q_z)|^2\Delta_\mathbf{q}\frac{\sinh(\beta\hbar\omega_{\mathbf{q}s}/2)}{\cosh(\beta/2)(E_0-E_F)\cosh(\beta/2)(E_0-E_F+\hbar\omega_{\mathbf{q}s})}\,, \tag{21}$$

where $\mathbf{q}_\parallel=(q_x,q_y)$, E_F is the Fermi level, $E_0=\hbar\omega_c/2$,

$$|F(q_z)|^2=\left|\int\Phi^2(z)e^{iq_zz}dz\right|^2\,, \tag{22}$$

and

$$\Delta\mathbf{q}=\frac{(\gamma/\pi)}{(\hbar v_s\mathbf{q})^2+\gamma^2}\,, \tag{23}$$

with v_s denoting the velocity of sound for mode s. Assuming that the magnetoresistivity of the 2D gas is given by the classical formula

$$\rho_{xy}=B/n_se\,, \tag{24}$$

we find from Eq. (5) that S_g is

$$S_g = -\frac{k_B L_z}{4\pi^2 n_s e}\int_0^\infty q^2 dq \int_0^1 (1-\nu^2) G(\beta\hbar\omega_{qs}/2)\frac{\Gamma_s(\mathbf{q})}{\Gamma_s(\mathbf{q})+\tau_s^{-1}(\mathbf{q})}d\nu , \tag{25}$$

where n_s is the electron concentration per unit area, $\nu=\cos\theta$, and θ is the polar angle of $\mathbf{q}$. Note that the quantum-Hall effect is ignored in Eq. (24). It may be readily taken into account in more exact calculations.

To compare Eq. (25) with the experimental data of Fletcher *et al.*,[1] we evaluate the integral with the following simplifications. The electron-phonon interaction is assumed to be due to unscreened piezoelectric and deformation potentials. Explicit formulas for $|V_s(\mathbf{q})|^2$ are given in Ref. 8 for this case. The phonon scattering is supposed to be dominated by boundary scattering so that $\tau_s(\mathbf{q})=L/v_s$, where the phonon mean free path L and v_s are both independent of $\mathbf{q}$. Fang-Howard-Stern variational wave functions[9] are used to calculate $|F(q_z)|^2$ and the Fermi level is obtained by solving the equation

$$n_s = \int_0^\infty f^0(\epsilon)D(\epsilon)d\epsilon , \tag{26}$$

where

$$D(\epsilon) = (1/\pi l^2)(\gamma/\pi)/[(\epsilon-E_f)^2+\gamma^2] \tag{27}$$

is the density of states per unit area. We consider sample 1 of Fletcher *et al.*,[1] when $B=15$ T, and set $m^*/m_0=0.067$, $v_l=5.14\times10^5$ cm s^{-1}, $v_t=3.04\times10^5$ cm s^{-1}, the static dielectric constant $\kappa_s=12.9$, the mass density $\rho=5.3$ g cm^{-3}, and the piezoelectric constant $h_{14}=1.2\times10^7$ V cm^{-1}. For sample 1 Fletcher *et al.*[1] give $n_s=1.78\times10^{11}$ cm^{-2}, $L_z=0.036$ cm, and estimate $L=0.03$ cm.

The value of γ is estimated to 1.12 meV for sample 1 by using the self-consistent Born approximation for short-range scatterers[10] and then the measured value of the mobility: 2.26×10^5 cm^{2}V^{-1}s^{-1} at 4.2 K. However, by taking this value we find S_g values 2–3 times smaller than the experimental values. Moreover, the T dependence of S_g does not agree with the data. We have, therefore, varied γ to obtain better agreement between theory and experiment with regard to both the magnitude and temperature dependence of S_g. We find that $\gamma=0.4$ meV provides a good fit. This value, which is less than half that calculated above, is believed to indicate that long-range scattering mechanisms are important in GaAs-$Ga_xAl_{1-x}As$ heterostructures, which confirms the observations made by Obloh, Von Klitzing, and Ploog.[11]

We have used the deformation potential $E_1=11.5$ eV in the calculations, which is larger than the value of 7.0 eV accepted in bulk GaAs.[12] However, this value is reasonable in view of the fact that in GaAs-$Ga_xAl_{1-x}As$ heterostructures the observed low-T energy-loss rate is best fitted by $E_1=11.5$ and 16.0 eV for unscreened and screened electron-phonon interactions, respectively.[13] It can be noted that the study of the low-T energy-loss rate isolates the scattering of electrons by acoustic phonons from other scattering mechanisms. Moreover, the study of the other transport properties in these structures have established that $E_1\sim11$–16 eV.[14–16]

With the above parameters we find excellent agreement between calculated values and experimental values of S_g. It can be seen from Fig. 1 that both piezoelectric and deformation-potential scattering are important in the temperature range of interest. Piezoelectric scattering dominates over deformation-potential scattering for T below 3–4 K. The small departures between calculated and experimental values at high T may be due to our neglect of phonon-phonon interactions in calculating the $\tau_s(\mathbf{q})$. At higher T, phonon-phonon interactions are expected to decrease $\tau_s(\mathbf{q})$. We suggest that this is the reason why the experimental points fall below theoretical curve (3) at the highest temperatures considered. Finally, we note that for the parameter values considered, $\Gamma_s(\mathbf{q})\ll\tau_s^{-1}(\mathbf{q})$ in Eq. (25) so that S_g is proportional to L, as is found experimentally.[2,3]

There are a number of corrections to be considered in a more refined calculation. S_g calculations with $B=0$ show that the screening of the electron-phonon interactions is important[8,17] and reduces S_g by almost 50% in GaAs-$Ga_xAl_{1-x}As$ structures.[8,18] If we take $E_1=16.0$ eV and scale by 65%, for example to account for the screening, the calculations are again in agreement with the experimental results. We should also substract a small term from the measured S to allow for diffusion thermopower S_d before comparing the measurements with calculated values of S_g. For an unbroadened Landau level, the maximum value of S_d is[1]

$$S_d = -(k_B/e)\ln 2/(n+\tfrac{1}{2}) , \tag{28}$$

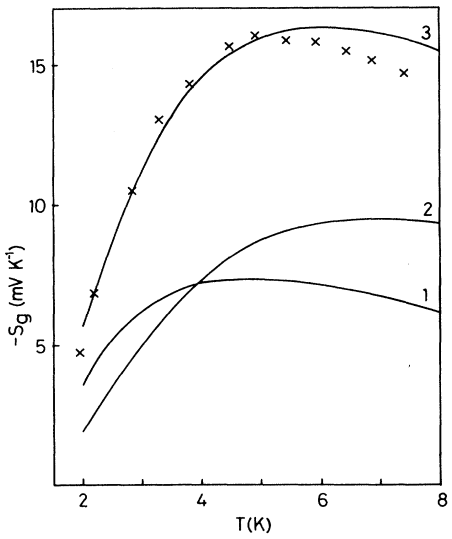

FIG. 1. Comparison of the calculated temperature dependence of S_g (curves 1–3) with experimental data (points) for a GaAs-$Ga_xAl_{1-x}As$ heterojunction at a magnetic flux density of 15 T. (1) Piezoelectric scattering alone, (2) deformation-potential scattering alone, (3) piezoelectric and deformation-potential scattering combined. Parameter values are given in the text.

which gives 120 $\mu V K^{-1}$ for Landau-level index $n=0$. This value is smaller than the experimental data by 2–3 orders of magnitude. Moreover, calculations made with a broadened Landau level further reduce S_d by 30–50%.[19] Finally, it is important to notice that the magnitude and behavior of S_g, when B is large, are determined by the strength of the electron-phonon interaction and the position of E_F with respect to Landau level. E_F is strongly influenced by γ, which we have assumed to be constant. In reality, it depends on the scatterers, the magnetic field, and the temperature.

To summarize, we have given for the first time a simple theory of phonon-drag thermopower for a 2D electron gas in a magnetic field coupled to 3D phonons. There is excellent agreement between the theory and experimental data for GaAs-$Ga_xAl_{1-x}As$ heterojunctions at liquid-helium temperatures. In the quantum limit the theory requires a number of small corrections which will be discussed in a more extensive paper dealing with the dependence of S_g on B, which has been set equal to 15 T here so as to put the system in the quantum limit. As B is decreased, successive Landau subbands are populated and the resulting oscillations of S_g which have been observed are contained in the general formulas of Eqs. (25), (17), and (18).

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