RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 40, NUMBER 9 15 SEPTEMBER 1989-II

Magnetoquantum oscillations of the phonon-drag thermoelectric power in heterojunctions

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(Received 5 July 1989)

A theory is presented for the low-temperature phonon-drag thermopower S_{xx} in a semiconductor heterojunction in a strong magnetic field. Gigantic quantum oscillations (much larger than electron-diffusion contributions) are obtained. The temperature and field dependences of S_{xx} agree well with recent data. Localized states yield flat valleys for the $|S_{xx}|$ minima in agreement with the data.

Quantization of two-dimensional degenerate electron gases in high magnetic fields yields striking effects such as the integer and fractional quantum Hall effects (QHE's). In a high magnetic field, the thermoelectric power (TEP) S_{xx} equals the heat carried by the Hall current per unit charge and unit temperature. How the QHE is reflected in the TEP is an interesting question and the TEP has received increasing attention,[1-7] especially in heterostructures. To the author's knowledge, past theoretical studies have examined only the electron-diffusion TEP (EDTEP) and yielded approximately $-S_{xx}=60/p\,\mu$V/K at the maxima occurring at half-odd-integer values of the filling factor p.[6,7] Early data[1-4] in GaAs/Al_xGa_{1-x}As heterojunctions with mobilities of 0.5-50 m^2/V sec show $-S_{xx}\leq 60/p\,\mu$V/K and have been analyzed in terms of EDTEP. More recently, Fletcher *et al.*[5] reported S_{xx} data with peak values of 1-6 mV/K for samples with mobilities of 4.2-37.7 m^2/V sec. They found that surface polishing enhanced S_{xx} and suggested that the phonon-drag TEP (PDTEP) may be responsible for such large TEP.[5] Here we develop a theory of the PDTEP and resolve this unclear experimental situation. Our results give reasonable agreement with the data of Fletcher *et al.*[5] We find it essential to introduce localized states in the wings of the Landau levels (LL's) (as in the QHE) to reproduce the observed flat valleys in the $-S_{xx}$ minima.[5] A preliminary result of this work was reported earlier.[8]

The TEP S_{xx} is given from general thermodynamic relationships by[7]

$$S_{xx}=L_{\rm TE}^{yx}(\mathbf{H})/[\sigma_{yx}(\mathbf{H})T] \tag{1}$$

to the lowest order in $\gamma=(\omega\tau)^{-1}$ where $\omega=eH/m^*c$ and τ is the scattering time. The quantities e, H, m^*, and c denote the electronic charge, magnetic field, effective mass of the electron and the speed of light, respectively. The quantity $L_{\rm TE}^{yx}(\mathbf{H})$ is the heat current density (HCD) produced in the y direction by a unit electric field E in the x direction at uniform temperature and σ is the conductivity tensor. The electron HCD yields the EDTEP, while the phonon HCD (U_y) induced by the electron-phonon interaction (EPI) yields the PDTEP.

In the following we calculate U_y induced by $E\rightarrow 0$ in a magnetic field in the z (growth) direction. The electrons are in the ground sublevel and interact predominantly with the impurities. The phonons are scattered mainly by the boundaries. The relationship between the phonon and electron distribution functions $n_{\mathbf{q}s}$ and f_k is given by

$$\dot n_{\mathbf{q}s}+2\sum_{k,k'}[f_{k'}(1-f_k)(n_{\mathbf{q}s}+1)P^{+}_{k'\rightarrow k}(\mathbf{q},s)-f_k(1-f_{k'})n_{\mathbf{q}s}P^{-}_{k\rightarrow k'}(\mathbf{q},s)]\delta(\varepsilon_k+\hbar\omega_{\mathbf{q}s}-\varepsilon_{k'})=0\,, \tag{2}$$

where $\dot n_{\mathbf{q}s}$ is the rate of creation of phonons of wave vector $\mathbf{q}$ and polarization s by all scattering channels other than the EPI and the first (second) term in the square brackets of (2) is a golden-rule expression of the one-phonon emission (absorption) rates through EPI. The factor of 2 in front of the second term on the left-hand side of (2) denotes the spin degeneracy. Spin splitting is ignored. The quantities $P^{\pm}_{k\rightarrow k'}(\mathbf{q},s)$ are quadratic in the EPI and contain the $\mathbf{q}$-conservation conditions. The quantity $k=(k_y,n=0,1,\ldots)$ denotes the electron quantum numbers in the asymmetric Landau gauge in the absence of interactions. We linearize the distribution functions in E:[9] $f_k=f_k^0-f_k^{0\prime}\delta\varepsilon_k$ and $n_{\mathbf{q}s}=n_{\mathbf{q}s}^0-n_{\mathbf{q}s}^{0\prime}\delta\hbar\omega_{\mathbf{q}s}$ where f_k^0 and $n_{\mathbf{q}s}^0$ are the Fermi and boson functions and the primes denote the first energy derivatives. The quantity $\delta\varepsilon_k$ is given by $\delta\varepsilon_k=-\hbar v_H(k_y+\lambda)$ in the limit $\gamma\ll 1$ with $v_H=cE/H$.[9] Here λ depends only on the energy and does not yield any contribution to the HCD. In a relaxation-time approximation $\dot n_{\mathbf{q}s}=(n_{\mathbf{q}s}^0-n_{\mathbf{q}s})/\tau_{\mathbf{q}s}^{\rm ph}$ the quantity $\delta\omega_{\mathbf{q}s}$ is linearly related to the quantities $\delta\varepsilon_k$ through (2) and is proportional to $q_y=k_y'-k_y$. Namely, the phonon distribution becomes shifted in the q_y direction, resulting in a HCD U_y obtained by summing $\hbar\omega_{\mathbf{q}s}\partial\omega_{\mathbf{q}s}/\partial q_y n_{\mathbf{q}s}$ over $\mathbf{q}s$. The sample volume is assumed to be unity and the Debye approximation is employed at low temperatures. Inserting $\sigma_{yx}=nec/H$ (n is the electron density) and $L_{\rm TE}^{yx}(\mathbf{H})=U_y/E$ in (1), we find

$$S_{xx}=-\frac{(k_B/e)}{p(k_BT)^2}\sum_{s\mathbf{q}}\tau_{\mathbf{q}s}^{\rm ph}\hbar\omega_{\mathbf{q}s}q_y\left[\frac{\partial}{\partial q_y}\hbar\omega_{\mathbf{q}s}\right]\times\sum_{n,n'}P_{n\rightarrow n'}(\mathbf{q},s)\equiv -S\,, \tag{3}$$

where the phonon scattering rate is dominated by $\tau_{\mathbf{q}s}^{\rm ph^{-1}}$ and

$$P_{n\to n'}(\mathbf{q},s)=\frac{2\pi}{\hbar}|V_{\mathbf{q}s}|^2\Delta_z(q_z)\Delta_{nn'}(q_\parallel)\int d\varepsilon\int d\varepsilon'\rho_n(\varepsilon)\rho_{n'}(\varepsilon')n^0_{\mathbf{q}s}f^0(\varepsilon)[1-f^0(\varepsilon')]\delta(\varepsilon+\hbar\omega_{\mathbf{q}s}-\varepsilon') . \quad (4)$$

Here the "q-conservation factors" read:[10,11]

$$\Delta_z(q_z)=[b^2/(b^2+q_z^2)]^3 , \quad (5a)$$

$$\Delta_{nn'}(q_\parallel)=\frac{n_<!}{n_>!}\chi^{n_>-n_<}\exp(-\chi)[L_{n_<}^{n_>-n_<}(\chi)]^2 , \quad (5b)$$

where $q_\parallel^2=q_x^2+q_y^2$, $\chi=(q_\parallel l_H)^2/2$, $l_H^2=\hbar c/(eH)$, $n_>$ ($n_<$) is the larger (lesser) of n and n', and $L_n^m(\chi)$ the associated Laguerre polynomial. In (5a), b is the parameter in the variational confinement wave function:[12] $b/k_F=[33e^2k_F/(64\kappa_s\varepsilon_F)]^{1/3}$. Here $\kappa_s=12.9$ is the bulk dielectric constant, k_F the Fermi wave number, and ε_F the Fermi energy at $H=0$.

The square of the EPI in (4) is given for longitudinal (l) and transverse (t) modes by

$$|V_{\mathbf{q}l}|^2=\frac{\hbar\omega_{\mathbf{q}l}}{2\varepsilon(q_\parallel)^2\rho c_l^2}\left[D^2+(eh_{14})^2\frac{A_l}{q^2}\right] , \quad (6a)$$

$$|V_{\mathbf{q}t}|^2=\frac{\hbar\omega_{\mathbf{q}t}}{2\varepsilon(q_\parallel)^2\rho c_t^2}(eh_{14})^2\frac{A_t}{q^2} . \quad (6b)$$

The first term in (6a) is the contribution from deformation potential (DP) scattering. The rest of the terms in (6) are the contributions from piezoelectric scattering which turns out to give larger contributions to S [cf. (3)] than DP scattering in the temperature range studied. In (6), the quantities ρ, c_s, D, and h_{14} are, respectively, the mass density, sound velocity, DP coefficient, and the piezoelectric constant. The anisotropy factors are given by[10] $A_l=9q_\parallel^4q_z^2/2q^6$ and $A_t=(8q_\parallel^2q_z^4+q_\parallel^6)/4q^6$. Finally, the static dielectric screening constant is given at low temperatures by[13]

$$\varepsilon(q_\parallel)=1+\frac{2\pi e^2}{\kappa_s q_\parallel}F(q_\parallel)\Delta_{NN}(q_\parallel)D(\mu) . \quad (7)$$

Here N is the quantum number of the LL where the chemical potential μ lies, $D(\mu)$ the density of states (DOS) per unit area, and $F(q_\parallel)$ the form factor

$$F(q_\parallel)=\left[8+9\frac{q_\parallel}{b}+3\left(\frac{q_\parallel}{b}\right)^2\right]\Bigg/\left[8\left(1+\frac{q_\parallel}{b}\right)^3\right] . \quad (8)$$

The spectral DOS at the nth LL is given by $\rho_n(\varepsilon)=\delta(\varepsilon-\varepsilon_n)$ [where $\varepsilon_n=(n+\frac{1}{2})\hbar\omega$] in the impurity-free limit. To consider the effect of the LL broadening properly, Eq. (2) should be replaced by the vertex equations of the phonon-drag "sausage diagrams" in Holstein's transport theory.[14] The final result is to replace $\rho_n(\varepsilon)$ by the imaginary part of the dressed electron Green's function of the nth LL slightly below the real axis divided by π:[14] $\rho_n(\varepsilon)=1/\pi\,\mathrm{Im}S_n(\varepsilon-i0)$. This quantity is proportional to the DOS for narrow LL's where the impurity-induced transfer of states between the LL's are small. To apply this result, we assume a Gaussian form for $\rho_n(\varepsilon)$ centered at ε_n with root-mean-square full width Γ.[15] Only the LL's adjacent to the Fermi level give contributions to S.

We now evaluate (3) and compare the result with the data from Ref. 5. The following parameters are used:[10] $m^*=0.07m_0$, $c_l=5.14\times10^5$ cm/sec, $c_t=3.04\times10^5$ cm/sec, $\rho=5.3$ g/cm^3, $h_{14}=1.2\times10^7$ V/cm, $D=-9.3$ eV, and the carrier density[5] $N=6.24\times10^{11}$ cm^{-2}. The TEP S is proportional to the phonon mean free path Λ ($=c_s\tau_{\mathbf{q}s}^{\mathrm{ph}}$). Λ is independent of the temperature and is determined by the boundary scattering at low temperatures.[5] Thermal conductivity measurement yields $\Lambda\approx2$ mm for the polished sample (BP4).[5] The width Γ is roughly given empirically[16] in the mobility range of interest ($\mu\approx18.6$ m^2/V sec) by $\Gamma\approx10\hbar\tau^{-1}=1$ meV. Wang *et al.*[17] found $\Gamma\approx2.5$ meV for $\mu=10$ m^2/V sec from specific-heat data. If Γ is scaled inversely with μ, the specific-heat data[17] would yield $\Gamma\approx1.34$ meV for $\mu=18.6$ m^2/V sec. We treat Λ and Γ as adjustable parameters; values chosen are comparable to the empirical values estimated above.

The calculated S (solid curves) is compared with the data[5] (dashed curves) in Fig. 1 for $\Lambda=1.3$ mm and $\Gamma=1$ meV. The calculated temperature dependence of S (dashed curve) is compared with the data[5] (open circles) in Fig. 2 for the same parameters at a field $H=2.85$ T. The EDTEP is less than 2% of the data and is ignored. Major contributions to the TEP arise from one-phonon intra-LL scattering. The inter-LL contributions are small. We choose Γ to best fit the slope of the curve, which depends sensitively on Γ. For smaller values of Γ, S increases much more slowly, reaches a maximum, and decreases with increasing temperature as is shown by a dotted curve in Fig. 2 for $\Gamma=0.5$ meV and $\Lambda=1.3$ mm. This behavior follows from the fact that the maximum energies of the resonant phonons in the one-phonon processes are limited by Γ so that a classical (Dulong-Petit) regime is reached when the thermal energy becomes larger than the width. For a small Γ, the maximum of S occurs at a low temperature and is small. In this case, high-temperature

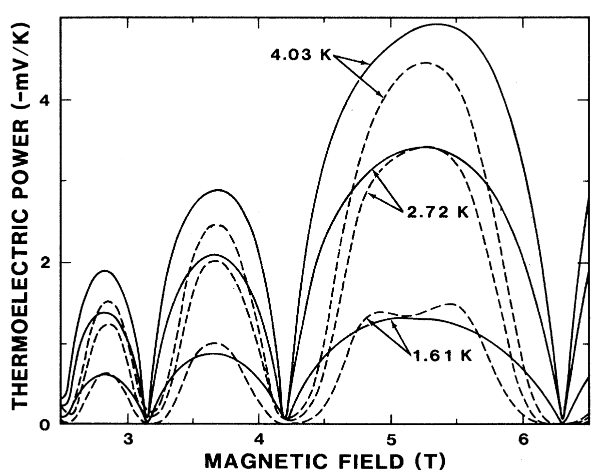

FIG. 1. Comparison of the calculated S (solid curves) with the data (Ref. 5) (dashed curves). No localized states are assumed. The parameters used are given in the text.

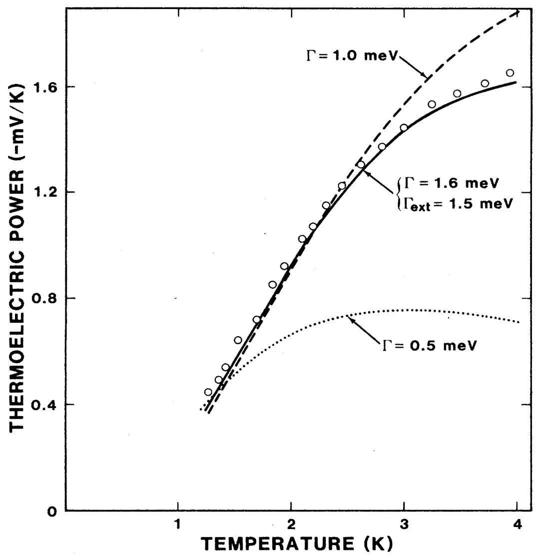

FIG. 2. The temperature dependence of the calculated S with (solid curve) and without (dashed, dotted curves) localized states at $H=2.85$ T. The parameters used are given in the text. The open circles denote the data (Ref. 5).

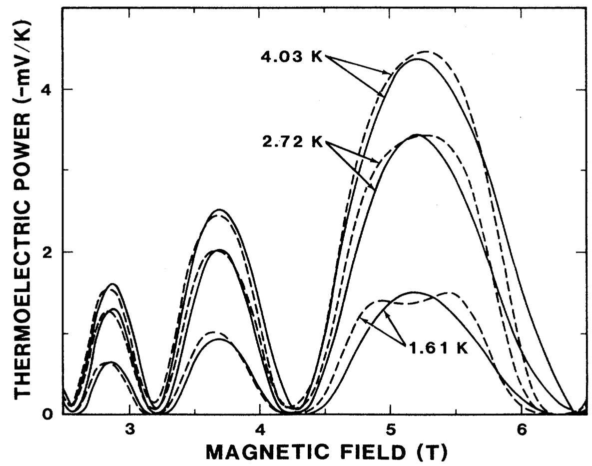

FIG. 3. Comparison of the calculated S (solid curves) with the data (Ref. 5) (dashed curves) for $\Gamma_{ext}=1.5$ and $\Gamma=1.6$ meV. Other parameters are given in the text.

RPA screening formula applies; two-phonon Raman processes are more efficient, yielding S comparable to EDTEP in the temperature range studied in Fig. 2.[18] After Γ is determined to fit the slope of the T vs S curve, the scaling factor Λ is then chosen to fit the magnitude.

The results in Fig. 1 show that the theory yields the right order of magnitudes for S. Also, double maxima are predicted for S at 1.61 K near 5.15 T consistent with the data. These double maxima grow considerably when Γ is decreased and begin to appear for other peaks. This is because S as well as the effect of screening is larger for a larger DOS at the Fermi level. When Γ (the DOS) is smaller (larger) than certain value, the screening effect becomes very large and creates minima of the TEP near the peak positions of the DOS by screening out the EPI.

An unsatisfactory aspect of the theoretical results in Fig. 1 is that the S-minima valleys are too steep compared to the data. The flat S-minima valleys of the data arise from the localized states (responsible for the QHE plateaus) lying between the mobility edges at the wings of the LL's. The TEP is expected to drop sharply at low temperatures when the Fermi level crosses the mobility edges into the localized regime. The width of the extended states (centered at ε_n) is denoted as Γ_{ext}. The extended states then have sharp edges in our model without the Gaussian tails. Therefore, to produce a temperature dependence similar to that of the dashed curve in Fig. 2, a value of Γ_{ext} larger than 1 meV is necessary. Also, S is expected to be larger for a larger ratio of Γ_{ext}/Γ. The calculated field dependences of S (solid curves) are compared with the data[5] (dashed curves) in Fig. 3 for $\Gamma=1.6$ meV, $\Gamma_{ext}=1.5$, and $\Lambda=2.5$ mm. The valleys are now flatter and the agreement is excellent. Finally, the calculated temperature dependence is displayed in Fig. 2 in a solid curve for the same parameters. The agreement with the data is again excellent. The value $\Lambda=2.5$ mm is close to the experimental estimate $\Lambda\approx 2$ mm.

In summary we presented a theory of the low-temperature phonon-drag magnetothermopower in a heterojunction. Large quantum oscillations are obtained. The temperature and field dependences agree reasonably well with recent data. The role of the localized states was discussed.

Note added in proof. The result in Eq. (3) can also be derived from the result of Puri[19] obtained for bulk semiconductors. The author thanks C. Herring for informing him of this work and of his earlier work[20] on phonon-drag effects. Recently, the author received an unpublished work by S. S. Kubakaddi, P. N. Butcher, and B. G. Mulimani who obtained a result similar to Eq. (3) by using a Lorentzian form for the spectral density. They study only the temperature dependence of S_{xx}.

The author thanks R. Fletcher for calling his attention to this problem, and D. E. Dahlberg and D. C. Tsui for valuable discussions. This work was supported by the U.S. Department of Energy under Contract No. DE-AC04-76DP00789.

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