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LETTER TO THE EDITOR

Inelastic scattering and the temperature dependence of thermoelectric power in quasi-2D systems

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Abstract. Recent calculations of the phonon-drag contribution S_g to the thermopower S of a 2DEG yield excellent agreement with experimental data for heterojunctions and MOSFETs. We review the effect on this agreement of uncertainty in the deformation potential E_1, inelasticity in the electron–phonon interaction, temperature dependence of the screening, non-degeneracy and the energy dependence of the electron relaxation time $\tau(\varepsilon)$. The uncertainty in E_1 amounts to about 50% which gives a much greater uncertainty in S_g. The energy dependence of $\tau(\varepsilon)$ has a marked effect on the predicted diffusion thermopower which constitutes 10–20% (or more) of the measured S which must be subtracted to yield 'experimental' values of S_g. It also affects the temperature dependence of S_g through a correction which can amount to 5(20)% or more in a heterojunction (Si MOSFET). Attention to these corrections, and others, in interpreting experimental thermopower data provides a useful way to refine the quantitative understanding of electron–phonon interactions in phonon absorption/emission experiments and supports the argument for a value of E_1 approaching 16 eV in GaAs/GaAlAs heterojunctions.

Cantrell and Butcher (1987a) provide a formula for calculating the low-temperature (T) phonon-drag contribution (S_g) to the thermoelectric power (S) in quasi-2D electron gases (2DEGs) found in heterojunctions and Si MOSFETs. Coupled electron and phonon Boltzmann equations are linearised and solved in the relaxation time approximation. The calculations of Cantrell and Butcher (1987b) show the method to be valuable in that the qualitative behaviour of S_g is described rather well. Most notably, the position of the peaks in the values of $-S_g/T^3$ (arising from coincidence of maxima in the phonon distribution factors and electron phonon scattering rate) compares very well with the measurements of Gallagher *et al* (1987) on Si MOSFETs. The large overestimate of $-S_g$-values (by a factor of about 40 in the MOSFET case and about 3 in a GaAs/GaAlAs heterojunction) are removed in the calculations of Smith and Butcher (1989) and Lyo (1988) by introducing screening and better descriptions of the electron confinement. Furthermore, Lyo introduces the piezo-electric mechanism of acoustic phonon scattering which is found to dominate over the deformation potential mechanism below about 1 K in the heterojunctions. These calculations appear to describe the measured thermopowers very well from a quantitative point of view. However, we emphasise here that there are several additional corrections making important contributions to S_g and some uncertainties in the parameter values which, when taken together, both improve and complicate the calculations and their comparison with experiment.

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In Cantrell and Butchers' formulae the product of state occupancy factors occurring in the transition rate is written

$$f(\varepsilon(\boldsymbol{k}))[1 - f(\varepsilon(\boldsymbol{k}) + \hbar\omega_Q)] = \frac{\hbar\omega_Q}{1 - \exp(-\hbar\omega_Q/k_B T)}\,\delta(\varepsilon(\boldsymbol{k}) - \varepsilon_F). \tag{1}$$

At very low temperatures the energy and momentum conservation conditions prevent all but the smallest wavevector phonons from contributing to S_g and the approximation of elastic scattering is expected to be valid. Arguing along these lines Lyo (1988) drops $\hbar\omega_Q$ from the energy conserving delta function $\delta(\varepsilon(\boldsymbol{k}+\boldsymbol{q}) - \varepsilon(\boldsymbol{k}) - \hbar\omega_Q)$ in the expression for the scattering rate and takes $\hbar\omega_Q \ll k_B T$, for the heterojunction case of Fletcher *et al* (1986) to simplify the prefactor of the delta function in (1). However, we find that, even at 10 K, $\hbar\omega_Q/k_B T$ at $2k_F$ is about 0.8 and the full form of (1) is needed to avoid making an underestimate of S_g of the order of 50%. The correction varies with temperature through the 'dominant wavevector' $\bar{q}$ which is determined by the variation of the drag effect over the phonon distribution and has a value of about $5k_B T/\hbar\nu_s$ (with ν_s an averaged speed of sound). Similarly we find $\hbar\omega_Q/\varepsilon_F \sim 0.1$ and by retaining $\hbar\omega_Q$ in the energy-conserving delta function we find an increase of about 10% in S_g.

The phonon-drag effect of the larger wavevector phonons is therefore not negligible since the momentum cut-off condition occurs at above $2k_F$ where it is weighted by an increased phonon population. We find that, at above about 4 K, $\bar{q}$ is always above $2k_F$ for $n \leqslant 2 \times 10^{15}\ \mathrm{m}^{-2}$. The background T thus determines the importance of inelasticity through its influence on $\bar{q}$. This observation should be compared with the situation which arises in the ballistic phonon absorption experiment of Karl *et al* (1988) and other phonon absorption/emission experiments (such as those reported by Hensel *et al* (1983), Rothenfusser *et al* (1986) and Kent *et al* (1988)) in which there is no temperature gradient and hence no net phonon momentum flux, prior to phonons being injected. If we characterise the phonon momentum pulse in such experiments by a representative $\bar{q}$ it is clear that inelastic effects are much smaller if $\bar{q} \ll 2k_F$. Thus, the situation in these experiments is analogous to a phonon-drag thermopower measurement at very low $T \leqslant 1$ K. The observation of the dominance of piezo-electric phonon scattering in the phonon-drag imaging experiment of Karl *et al* (1988) using phonon frequencies of 120 GHz with $n_0 = 6 \times 10^{15}\ \mathrm{m}^{-2}$ is then to be expected because $\bar{q}/2k_F \simeq 4 \times 10^{-4}$. In thermopower measurements over the range 1–10 K $\bar{q}$ can be greater than $2k_F$ and then inelastic corrections are important. Furthermore, the change in the size of $\bar{q}/2k_F$ with T explains the observed fall in the temperature dependence of the thermopower. At very low T, $S_g(T)$ increases very quickly with the phonon population because $\bar{q} \ll 2k_F$ and the momentum conservation cut-off is unimportant. This is no longer the case at higher T and so the rate of increase of S_g is reduced.

In their calculations Cantrell and Butcher show that S_g is proportional to the phonon mean free path (L). Moreover, at the very low temperatures of interest, L is limited by boundary scattering and is taken as constant. Its size is then principally determined by the minimum specimen dimension (Fletcher *et al* 1988) which is typically less than 1 mm. To obtain a precise value the kinetic formula for the thermal conductivity κ has been used (see, for example, Fletcher *et al* 1986 and Ruf *et al* 1988) with the asymptotically exact expression for the low-temperature (harmonic) specific heat, to yield

$$L = (15\hbar^3/2\pi^2 k_B^4)(c^2\kappa/T^3) \tag{2}$$

where $1/c^3$ is the average inverse cube speed of sound for the three acoustic modes with c about $3\text{–}5 \times 10^3\ \mathrm{m\,s^{-1}}$. Thus L is obtained from measurements of κ which yield a

constant value when $\kappa \propto T^3$. Lyo obtains excellent agreement with the measurements of Fletcher *et al* (1986) 'without any adjustable parameters' by taking the value $L = 0.30$ mm obtained from the κ-measurement at 3 K. However, values of 0.2, 0.2, 0.1 and 0.07 mm can also be obtained for L from the same data at 2, 5, 7 and 10 K respectively. The T^3-dependence expected of κ in (1) is *not* followed by the data and the value of L is consequently very uncertain. A similar variation can be seen in the κ-data of Fletcher *et al* (1988) but Ruf *et al* (1988) find a better T^3-dependence and we find that a more consistent value of L ($\simeq 0.12$ mm) results. However, it remains uncertain whether a constant L can be taken in other cases.

A further uncertainty arises from the choice of the acoustic phonon deformation potential E_1 for a heterojunction the precise value of which is currently under some discussion (see, for example, Manion *et al* (1987) and references therein, Nolte *et al* (1987) and references therein). The values quoted range from 7 eV to as large as 16 eV. The accuracy of E_1-measurements is complicated by the degree to which the particular scattering mechanism can be isolated and by the validity of the interpretive theory (e.g., proper account should be taken of the confinement of electrons, screening and the presence of other scattering mechanisms). In Lyo's calculations the value $E_1 = 9.3$ eV is used. This is taken from the expeirments of Nolte *et al* (1987) in which E_1 is measured directly using transition metal defect levels as a reference. However another recent measurement (Manion *et al* 1987) suggests that the much larger value $E_1 = 16$ eV is appropriate. Uncertainty in E_1 is particularly important in the present context because deformation potential scattering provides the largest contribution to S_g for $T \geqslant 2$ K and because the square of E_1 enters S_g as a prefactor.

To compare calculations of S_g with measurements of $S = S_g + S_d$, the electron diffusion contribution S_d should be subtracted. This has been estimated (see, for example Nicholas (1985), Fletcher *et al* (1986), Lyo (1988)) by using the Mott formula:

$$S_d = -\tfrac{1}{3}(p+1)(\pi^2 k_B/e)(k_B T/\varepsilon_F) \tag{3}$$

where it is assumed that the energy dependence of the electron relaxation time $\tau(\varepsilon(\boldsymbol{k}))$ in the neighbourhood of ε_F is

$$\tau(\varepsilon(\boldsymbol{k})) = \tau_0 \varepsilon(\boldsymbol{k})^p. \tag{4}$$

For the heterojunction Lyo takes the value $p = 1$ proposed by Fletcher *et al* (1986) but, whilst the calculation of S_d through an explicit evaluation of $\tau(\varepsilon)$ by Kundu *et al* (1987) shows that this approximation is reasonable, these authors also suggest that a more refined calculation is necessary to describe S_d. Gallagher *et al* (1987) suggest a value of $p \sim -1$ for their Si MOSFET and when surface roughness scattering dominates, p can indeed be negative (Stern 1980). The value of S_d is important because, with $p = 1$, S_d constitutes 10–20% or more of the measured S. In practice the accuracy of (3) is limited both by (4) and because (3) assumes two-dimensionality, which is realised only approximately. Hence the accuracy with which the calculated S_g can be compared with experimental values of S should not be over emphasised because S_d is both significant and uncertain.

The form of (4) is important for a second reason involving the difference of $\tau(\boldsymbol{k})\boldsymbol{v}(\boldsymbol{k})$ for the electron states $\boldsymbol{k}$ and $\boldsymbol{k}+\boldsymbol{q}$ which enters into the S_g formula (where $\boldsymbol{v}(\boldsymbol{k})$ is the electron velocity in state $\boldsymbol{k}$). For an isotropic relaxation time $\tau(\boldsymbol{k})$ may be written as $\tau(\varepsilon(\boldsymbol{k}))$ and, using the conservation conditions, Cantrell and Butcher take

$$[\tau(\varepsilon_F + \hbar\omega_Q)\boldsymbol{v}(\boldsymbol{k}+\boldsymbol{q}) - \tau(\varepsilon_F)\boldsymbol{v}(\boldsymbol{k})] = -\hbar\boldsymbol{q}\tau(\varepsilon_F)/m \tag{5}$$

at ε_F, where $\hbar\omega_Q$ is the energy of a phonon with 3D wavevector $\boldsymbol{Q} = (\boldsymbol{q}, q_z)$. Equation (5)

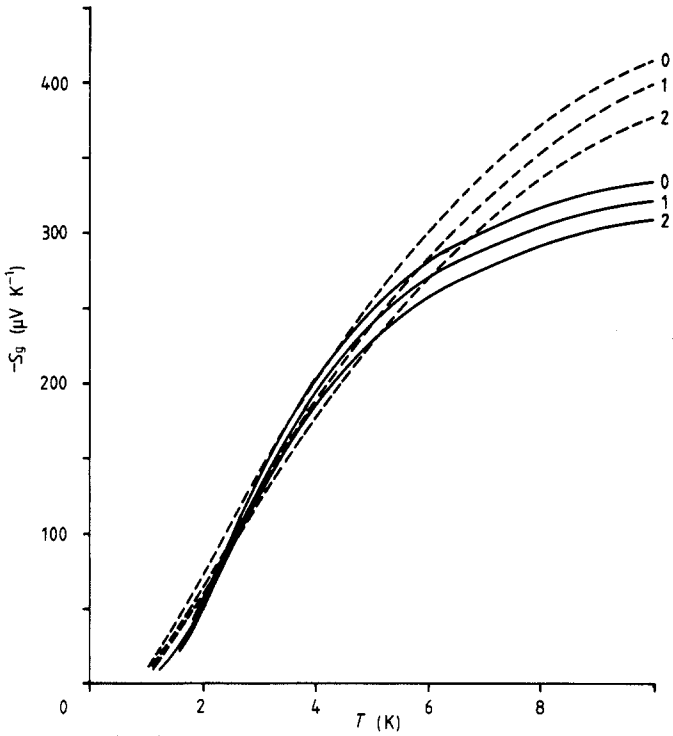

Figure 1. The effect of an energy-dependent relaxation time on the thermopower for the data of Ruf *et al* (1988). Full curves are calculated and broken curves experimental values (corrected for S_d), for $E_1 = 16$ eV. The numbers denote the value taken for p.

is exact when $\tau(\varepsilon(\boldsymbol{k}))$ is constant (and in the elastic case) and is a good approximation when $\tau(\varepsilon(\boldsymbol{k}))$ varies slowly near $\varepsilon(\boldsymbol{k}) = \varepsilon_F$ and $\hbar\omega_Q/\varepsilon_F \ll 1$. However, for the case of Fletcher *et al* (1986) $\hbar\omega_Q/\varepsilon_F \sim 0.1$ at $Q = 2k_F$ and hence, with $p \sim 1$, a correction to (5) may be necessary in heterojunctions. We have therefore investigated the effect of relaxing these conditions by using (4) to expand $\tau(\varepsilon_F + \hbar\omega_Q)$ about $\tau(\varepsilon_F)$ and obtain the correction factor:

$$\lambda(Q) = 1 + \tfrac{1}{2}p(\hbar\omega_Q/\varepsilon_F)[1 + (k_F/q)^2(\hbar\omega_Q/\varepsilon_F)] \tag{6}$$

which is to be applied to the right-hand side of (5). For $n = 2 \times 10^{15}$ m^{-2} we find a correction at $q = 2k_F$ and $q_z = 0$ of 5.5% when $p = 1$ and 11% when $p = 2$. Whilst small, this correction affects the temperature dependence of S_g because the value of $\bar{q}$, and consequently the mean value of ω_Q, increases with T. The corresponding corrections for a Si MOSFET of 23% ($p = 1$) and 46% ($p = 2$) are much larger because of the increased effective mass and valley degeneracy. However, the negative value of Gallagher *et al* (1987) gives a reduction rather than an increase in S_g. The form of $\tau(\varepsilon)$ is therefore doubly important since it can, in principle, through (3) and (6) change the sign of S_d and S_g.

In our current calculations for three recent heterojunction thermopower measurements (Fletcher *et al* 1986, Fletcher *et al* 1988 and Ruf *et al* 1988) we leave the value of the piezo-electric coupling constant h_{14} unchanged at 1.12 eV and avoid uncertainties in E_1 and L by obtaining fits to the data in the middle of the temperature range by varying

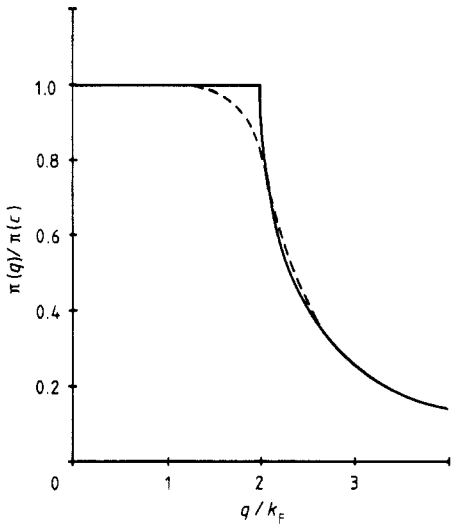

Figure 2. The effect of finite temperature upon the 2D polarisability in GaAs corresponding to $n = 1.78 \times 10^{15}\ m^{-2}$. The full curve is for the zero-temperature limit and the broken curve for $T = 10$ K.

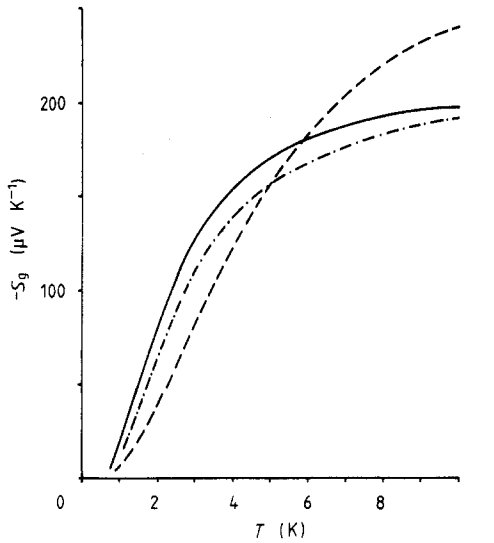

Figure 3. The resultant effect of all the corrections considered for the data of Fletcher *et al* (1986); the broken curve gives the experimental results with $S_d(p = 1)$ subtracted, the chain curve is the calculated result with all corrections included and the full curve is the elastic result with $E_1 = 9.3$ eV and $L = 0.30$ mm.

L for the different choices of E_1. We illustrate our results for the data of Ruf *et al* (1988) in figure 1 for $p = 0$, 1 and 2. The remaining data are taken from Lyo (1988). In this way we find $E_1 = 16$ eV to be the most favoured value because, when $p = 1(2)$, the fit value $L = 0.14(0.13)$ mm arises, which is much closer to the value of 0.12 mm determined from $\kappa(T)$ than that obtained when $E_1 = 9.3$ eV which is 0.35 mm. For the data of Fletcher *et al* (1986) $E_1 = 9.3$ eV gives $L = 0.28$ mm. This is very close to the value $L = 0.30$ mm used by Lyo (1988). Taking $E_1 = 16.0$ eV gives $L = 0.10$ mm which although much smaller, remains within the range already discussed. For the aforementioned reasons, though, we do not attach much physical significance to the value of L that fits S-data for which $\kappa \propto T^3$ is not followed. We find that the case of Fletcher *et al* (1988) is similar. Nevertheless, our calculations suggest that E_1 is at the high end of the range 7–16 eV in a GaAs/GaAlAs heterojunction. The Si MOSFET case is more certain (Gallagher *et al* 1988, Smith and Butcher 1989) but more complicated because the different acoustic modes couple differently to the electrons.

Figure 1 shows very clearly that the energy dependence of the electron momentum relaxation time $\tau(\varepsilon(\boldsymbol{k}))$ affects both the calculated value of S_g and the measured value with which it is compared. The energy dependence of τ increases the T-dependence of the calculated drag thermopower as the dependence upon $\hbar\omega_Q/\varepsilon_F$ of the correction $\lambda(\boldsymbol{Q}) - 1$, calculated from (6), is linear and its average value increases with $\bar{q}$ (and hence T) because inelasticity increases the drag effect of large wavevector phonons. The effect upon S_g of taking $p = 2$ is about 10% but the effect on S_d and hence S can be larger as is seen in the corrected experimental values given in the figure. We conclude that: (i) the energy dependence of $\tau(\varepsilon(\boldsymbol{k}))$ is important for both S_d and S_g, (ii) S_d is not negligible and (iii) a small increase in the T-dependence of S_g results from the increased inelasticity introduced because $\hbar\omega_Q/\varepsilon_F$ is not negligible. These conclusions warrant a more accurate calculation than that performed here using (3) and (4).

In addition to the aforementioned corrections which have been used in the calculations for figure 1, we also need to consider corrections which are necessary because the electron distribution function is not completely degenerate. The non-degeneracy affects both the polarisability and (1). The polarisability $\pi_0(q)$ has been recalculated in the manner of Maldague (1978) to give $\pi(q)$ which allows for T-dependence in the screening. Representative values are illustrated in figure 2. The effect clearly increases with $k_B T/\varepsilon_F$ but, even though $\pi(q)/\pi_0(q)$ is 0.8 at $2k_F$, the net effect on S_g, even at the lowest n_0 (and ε_F) and highest T (10 K) is an increase of only 3%. This shows further the importance of the range of q-vectors contributing to S_g even at 10 K. Retaining the explicit form of the Fermi function for the heterojunction in (1) we find a decrease in $S_g(T)$ of 5–8%. The outcome of all the corrections we have made is an overall change smaller than individual competing changes and is illustrated in figure 3. The uncertainty in E_1, $L(T)$, $\tau(\varepsilon)$ at ε_F and S_d prevents an accurate comparison with experiment although a relatively large value of E_1 is supported. Detailed calculation of $\tau(\varepsilon)$ and S_g for quasi-2DEGs should resolve the present difficulties.

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