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Simple models of phonon-drag in 3D and quasi-2D

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Abstract. The simple 'metallic' formulae for the phonon drag thermoelectric power (S_g) of 3D free-electron systems appear to be in conflict with the model of Herring, by predicting different dependences of S_g upon electron density and temperature (T) at low T. We show that both approaches can be understood physically by considering the net phonon drift velocity. A simple quasi-2D expression for S_g is then obtained which predicts the underlying dependence upon T, phonon mean free path L, and electron surface density n, as LT^3/n which is the observed behaviour in heterojunctions and MOSFETs. This dependence is modified by the efficiency with which momentum is transferred between the electron and phonon systems. Boltzmann transport calculations confirm these conclusions and support the simple models by reproducing the simple formulae in appropriate limits.

1. Introduction

Phonon-drag in quasi-2D electron gases (2DEGs) is of current interest in phonon absorption and emission experiments on electrons confined in heterojunctions and MOSFETs (Karl *et al* 1988). Thermoelectric power (S) is of particular interest because it is a quantity which is very sensitive to the conduction mechanism, scattering, carrier type and anisotropy (Blatt 1968, Guenault 1971). In particular, it has become clear that the phonon-drag contribution (S_g) to S in heterojunctions and MOSFETs is dominant at temperatures around that of liquid helium (Fletcher *et al* 1988b, Ruf *et al* 1988) and is sensitive to the electron–phonon coupling mechanism, screening, phonon mean free path (L) and the coupling constants (Smith and Butcher 1989a, b). This dominance over the electron diffusion contribution (S_d) to S is significant because calculations of S_d in high magnetic fields ($\boldsymbol{B}$) predict accurate quantisation of the diagonal components of S_d (Girvin and Jonson 1982) which has not been observed. In practice, measured values of S are recorded which are two orders of magnitude larger than predicted and do not follow the expected trend (Fletcher *et al* 1986, 1988a, b, D'Iorio *et al* 1988, Ruf *et al* 1988). This is due to the presence of drag. Calculations of S_g in a magnetic field are now showing promise (Karyagin *et al* 1988, Kubakaddi and Butcher 1989) but even with $B = 0$ the integral formulae for S_g are difficult to interpret physically.

The calculation of S_g is complicated by the need to know the details of the non-equilibrium electron and phonon distribution functions. Calculations for heterojunctions and MOSFETs ()Smith and Butcher 1989a, b, Lyo 1988) based on the work of Cantrell and Butcher (1987) are now showing good agreement with experimental data (e.g. Fletcher *et al* 1986, Gallagher *et al* 1987). However, simple dependencies of S_g upon electron surface density (n) or temperature T, for example, are not readily apparent

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from the formulae. Attempts have been made to demonstrate such dependencies using simple formulae for S_g in 3D. Whilst inaccurate in detail these can be expected to provide insight into the expected behaviour. We show here that these formulae are of two types which give conflicting information. We put them on a firmer footing by showing that both can be derived for 3D from the Cantrell and Butcher formulae for quasi-2D by taking different limits and by defining relaxation times in specific ways. We are then able to show which model is appropriate under certain conditions and how the 3D formulae can be extended to the quasi-2D case of a heterojunction of MOSFET to predict the dependence of S_g upon n, T, and L. By using the idea of saturation of the phonon drift velocity (Herring 1954) a further model is obtained which is very similar to, and provides both of, the other simple results whose usefulness in different regimes then becomes apparent.

2. Insight into S_g from simple models

To understand S_g it is helpful to consider the phenomenological transport equations for the EMF E' and heat flux $\boldsymbol{Q}$:

$$\boldsymbol{E}' = \rho \boldsymbol{J} + S\boldsymbol{\nabla} T \tag{1}$$

$$\boldsymbol{Q} = \Pi \boldsymbol{J} - \kappa \boldsymbol{\nabla} T \tag{2}$$

Considering cubic systems for simplicity, the quantities ρ (resistivity), S, Π (Peltier coefficient) and κ (thermal conductivity), become scalars. In what follows in this section it is supposed, for convenience, that all the vectors are parallel to the current density $\boldsymbol{J}$ and only their components in this direction are considered. We see that S is the EMF E' per unit temperature gradient when $J = 0$. We may imagine that a temperature difference ΔT initially gives rise to a flow of charge carriers which ceases when the internal electric field has built up to prevent further flow. One approach to calculating S_g is therefore to consider the balance between the thermoelectric force and the opposing emf acting on the carriers. An alternative to this 'balance approach' is the 'Π approach' (Herring 1954) in which Π is calculated in order to use the Onsager relation ($S = \Pi/T$) to obtain S. The quantity Π_g ($=S_gT$) is the contribution to Π arising from the energy flux of phonons dragged by an isothermal charge flux. The Π approach is conceptually easier because it involves a ratio of currents (heat to charge) rather than a balance of forces. Although either method can be used to obtain simple formulae for S_g the results appear to be in conflict, as described in what follows.

Herring (1954) obtains a simple formula from the Π approach. The phonon heat flux Q_g (say) in response to an isothermal current density J is written as

$$Q_g = v_s^2 P \tag{3}$$

where v_s is an averaged speed of sound and P is a net phonon momentum density which is assumed to follow:

$$P = P_0 e^{-t/\tau_p} \tag{4}$$

when disturbed from equilibrium, where τ_p is the phonon momentum relaxation time. On differentiating (4) with respect to t the net phonon force density is obtained. This is

the force arising from the dragging of phonons by the charge carriers and thus P is given by

$$P/\tau_p = f_{ep} N_v E e. \tag{5}$$

Here f_{ep} is the fraction of carrier momentum lost which is delivered to the phonons and $-N_v Ee$ is the force per unit volume acting on a gas of particles with charge $-e$ having volume density N_v. Using (5) in (3) and $-N_v e v_e$ for J, equation (2), with $\nabla T = 0$, gives

$$\Pi_g = -v_s^2 f_{ep} \tau_p E / v_e. \tag{6}$$

The result for S_g follows by writing the carrier drift velocity as $v_e = \mu E$, with μ the mobility, and writing the phonon mean free path L as $v_s \tau_p$. The result is

$$S_g = -f_{ep}(L v_s / \mu T). \tag{7}$$

Nicholas (1985) used such an equation to estimate S_g in a GaAs/GaAlAs heterojunction at liquid helium temperatures, although the quasi-two-dimensionality is not explicitly accounted for. At such low T, L is in the 'boundary scattering limit' and, since μ is independent of the carrier density N_v, the principal dependencies of S_g arise in this model from f_{ep}/T. However, unless f_{ep} is known, this result is difficult to interpret. If f_{ep} is assumed constant then S_g will be proportional to $1/T$ and independent of N_v. Experimentally, however, Gallagher *et al* (1987) find the dependence $S_g \propto 1/N_v$ for the Si MOSFET case and there is no sign of $1/T$ dependence in the data.

A different result is obtained from the balance approach which is normally used for metals (Blatt 1968). The phonon pressure G, say, is written in terms of the phonon (lattice) internal energy density $U(T)$ as

$$G = \tfrac{1}{3} U(T). \tag{8}$$

Differentiating with respect to displacement in the direction (x, say) of a temperature gradient, under the balance condition $J = 0$, the phonon force density is obtained. It is then supposed that some fraction f_{pe} of the force exerted by the phonons is exerted upon the carriers. Thus f_{pe} is the fraction of momentum lost by the phonons which is delivered to the carriers and, since $J = 0$, the carrier force balance condition is then

$$-N_v Ee = \tfrac{1}{3} f_{pe} C_v (\mathrm{d}T/\mathrm{d}x) \tag{9}$$

where the lattice specific heat C_v is taken as $\mathrm{d}U/\mathrm{d}T$. Comparing with (1) when $J = 0$, the result for S_g is (Blatt 1968)

$$S_g = -f_{pe} \tfrac{1}{3} (C_v / N_v e). \tag{10}$$

This is very similar to the result obtained by Guenault (1971). The low temperature T^3 dependence arising from C_v is modified only for f_{pe}.

It is difficult to reconcile this 'metallic' result for S_g with the Herring formula (7) without knowledge of f_{ep} and f_{pe}. Some attempts have been made in this direction. Zavaritsky (1984), for example, uses a balance approach applied to the metallic conduction of quasi-2D electrons coupled to 3D phonons to obtain (10) with f_{pe} replaced by L/L_{pe} where L_{pe} is the phonon mean free path (longer than L) for phonon scattering of

electrons, alone. The factor L/L_{pe} can be obtained if f_{pe} is taken as the ratio of the phonon scattering rate due to scattering by electrons (τ_{pe}^{-1} say) to the total (τ_p^{-1}), i.e.

$$f_{pe} = \tau_p/\tau_{pe} = L/L_{pe} \tag{11}$$

which follows by multiplying both the τs, by v_s. Similarly f_{ep} can be written as

$$f_{ep} = \tau_e/\tau_{ep} \tag{12}$$

where τ_e is the total electron momentum relaxation time from all mechanisms and τ_{ep} is that due to scattering of electrons by phonons. Moreover, a further expression obtained by Herring is given by using (11) in (7), i.e.

$$S_g = (mv_s^2/eT)\tau_p/\tau_{ep} \tag{13}$$

where L is replaced by $v_s\tau_p$ and μ by $e\tau_e/m$. There still remains the problem, however, of calculating the relaxation ratios in such formulae before progress can be made.

When considering S_g in semiconductors Blatt (1968) describes another Π approach which can be applied more generally and the result, obtained more directly, is close to that from balance arguments but does not involve relaxation ratios. The phonon flux due to drag by an isothermal current density J is written as

$$Q_g = U(T)v_p. \tag{14}$$

This equation *defines* v_p as the net phonon drift velocity. since the low temperature limit is of interest here, it follows from the T dependence of C_v that

$$U(T) = \tfrac{1}{4}C_v T. \tag{15}$$

The 'drag thermopower follows by substituting these last results into (2), with ∇T zero, using $-N_v e v_e$ for J and hence

$$S_g = -\tfrac{1}{4}(C_v/N_v e)v_p/v_e. \tag{16}$$

This last expression is helpful since the variation of v_p with N_v is more readily understood than that of f_{ep} or f_{pe} arising in (7) and (10). These two expressions should give the same result for S_g when f_{ep} and f_{pe} are calculated in full since although (10) is regarded as a metallic formula, no mention has been made of the carrier statistics in either derivation. However, writing these fractions in full defeats the object of formulae derived from simple physical ideas. It is more helpful if f_{ep} and f_{pe} can be regarded as constants in particular limits, which must be different since one model predicts a T/N_v dependence and the other a $1/T$. The quantity v_p helps to shed light on this problem.

First consider the 'saturation effect', described by Herring (1954) in both approaches. In the Π approach there can be no net phonon flux (v_p) and Q_g are zero) when N_v is zero and therefore Q_g, and hence v_p, must initially increase with N_v. For low N_v it can therefore be supposed that $v_p \propto N_v$ and, from (16), it is then predicted that S_g should be initially independent of carrier density. By 'low' of course is meant in comparison to the phonon population. This limit therefore corresponds to assuming non-degenerate carrier statistics or a constant f_{ep} in (7). Suppose now that a phonon flux does exist and that N_v is increased further. Since there are more phonons with momenta parallel to the charge flow than against, collisions of carriers with phonons of opposite momenta become less frequent. The resistance offered by the lattice to the carrier flow is therefore reduced. Thus, the rate of transfer of carrier momentum to the phonons is less and there is less drag. Hence, the greater the phonon flux the more difficult it becomes to increase

it, i.e. the drag effect (and v_p) saturate at large N_v. The same conclusion is reached from the balance approach because, when N_v is sufficiently large, the phonon flux (which causes the drag) is reduced by electron scattering. Hence there is less flux to cause the drag, which becomes more difficult to increase. Thus, for some large N_v, v_p becomes independent of N_v and (16) predicts that $S_g \propto N_v^{-1}$. This is the metallic limit and corresponds to assuming a constant f_{pe} in (10).

Now reconsider (11) and (12) for f_{pe} and f_{ep} in the light of the insight arising from saturation. For large N_v, τ_p^{-1} will be dominated by scattering from electrons and f_{pe} will approach unity. This is the conclusion reached by Guenault (1971) and does indeed give $S_g \propto N_v^{-1}$. For low N_v, τ_{ep}^{-1} is independent of N_v as there is always an excess of phonons, i.e. the scattering environment of the carriers is not much altered by low electron densities. Since τ_e^{-1} is also independent of N_v the conclusion is that f_{ep} is constant at low N_v and hence, from (7), S_g is independent of N_v.

3. Extension to quasi-2D

In the quasi-2D case the phonon heat flux is parallel to the conducting layer, which forms a very small fraction (about 10^{-6}) of the specimen cross-section. Hence τ_{pe}^{-1} is a small fraction of τ_p^{-1} which is dominated by boundary scattering. Therefore, electron scattering is unlikely to reduce the phonon heat flux enough to cause v_p to saturate. For the same reason τ_{pe}^{-1} will be independent of N_v since there is always an abundance of phonons from the bulk which are unaffected by the carriers. Here f_{pe} in (12) can be usefully written as $\tau_{pe}^{-1} L/v_s$ and S_g becomes proportional to the phonon mean free path. The quantity τ_{pe}^{-1} is a measure of the phonon momentum transfer rate to electrons. This leads to enhancement of S_g when the dominant phonon wavevector exactly crosses the Fermi circle. The electron density in (16) or (10) is a (3D) volume density but in quasi-2D the (2D) surface density n is a more natural quantity. It is necessary then, to decide whether N_v should be replaced by n/δ (where δ is the channel width), to give the volume density of carriers in the channel, or by n/L_z (with L_z the specimen width in the confinement direction), to give the density with respect to the volume of the specimen. The answer from the Π approach must be n/L_z since in writing $\Pi = Q/J$ it has been assumed that Q is the *resultant* phonon heat flux, not merely that occurring within the channel, and J the charge flux through unit area of the *specimen*. Similarly, in the balance approach, multiplying both sides of (9) by the specimen volume (V) gives the balance of the *total* force on the charges. In quasi-2D the total charge $-N_v Ve$ on the left side is replaced by $-nAe$ (where $AL_z = V$) but on the right side f_{pe} is still the fraction of the total phonon momentum delivered to the electron gas. The low dimensionality of the conducting channel is thereby already accounted for. Hence dividing by V it is clear that n/L_z replaces N_v. All the dependence of S_g upon the confinement of the electrons to the channel therefore arises from the variation of τ_{pe}^{-1} with δ. Finally, the simple expression for S_g in quasi-2D is

$$S_g = \tfrac{1}{3}[C_v/(n/L_z)e](L/v_s)\tau_{pe}^{-1} \tag{17}$$

which in terms of simple dependencies predicts $S_g \propto LT^3/n$. This simple result is modified by the channel dependence, and some possible enhancement due to favoured phonon absorption, arising from τ_{pe}^{-1}. Furthermore, in quasi-2D the $1/n$ behaviour is not lost at low n since τ_{pe}^{-1} is already independent of n. At an extremely high density f_{pe}, and hence

the $1/n$ behaviour, might be affected, in principle, by saturation, but such densities may not be possible in practice.

4. Comparison with Boltzmann transport calculations for quasi-2D

It is interesting to ask how far the simple models agree with the Boltzmann transport result of Cantrell and Butcher (1987) to which the reader is now referred. Most convenient for this purpose is the 3D case which is obtained from their formula (39) by replacing $(\alpha, \boldsymbol{k})$ by $\boldsymbol{K}$, $(\beta, \boldsymbol{k}')$ by $\boldsymbol{K}'$, A by V and by performing a generalisation corresponding to that leading to their final result. The sum over $\boldsymbol{K}'$ can be dropped by replacing $\boldsymbol{K}'$ by $\boldsymbol{K} + \mathbf{Q}$, following the delta symbols in their expression for the scattering rate. Simplification is possible if $\tau_{\boldsymbol{K}}$ is assumed constant (τ_e) for all $\boldsymbol{K}$, which are 3D plane wave states. Hence $\boldsymbol{v}(\boldsymbol{K})$ is simply $\hbar\boldsymbol{K}/m$, the 3D conductivity is written $N_v e^2 \tau_e / m$ and $\boldsymbol{v}_p(\boldsymbol{Q})$ is taken as v_{sQ}/Q to give

$$S_g = \frac{2}{3N_v eVk_B T^2} \sum_{\boldsymbol{K},\boldsymbol{Q}} \frac{(\hbar\omega_{\boldsymbol{Q}})^2 \Gamma_{\boldsymbol{K}+\boldsymbol{Q},\boldsymbol{K}}}{F} \frac{dN^0_{\boldsymbol{Q}}}{d\hbar\omega_{\boldsymbol{Q}}}. \tag{18}$$

Writing C_v in the form

$$C_v = \frac{1}{V} \sum_{\boldsymbol{Q}} \hbar\omega_{\boldsymbol{Q}} \frac{dN^0_{\boldsymbol{Q}}}{dT} \tag{19}$$

S_g can be reduced to

$$S_g = -\tfrac{1}{3}(C_v/N_v e)\bar{\alpha} \tag{20}$$

when $\alpha(\boldsymbol{Q})$ is defined by

$$\alpha(\boldsymbol{Q}) = \tau^{-1}_{pe}(\boldsymbol{Q}) / (\tau^{-1}_{pe}(\boldsymbol{Q}) + \tau^{-1}_{pp}(\boldsymbol{Q})) \tag{21}$$

with the phonon scattering rate due to absorption and emission by electrons given by:

$$\tau^{-1}_{pe}(\boldsymbol{Q}) = \sum_{\boldsymbol{K}} 2\Gamma_{\boldsymbol{K}+\boldsymbol{Q},\boldsymbol{K}} \Big/ \left(-k_B T \frac{dN^0_{\boldsymbol{Q}}}{d\hbar\omega_{\boldsymbol{Q}}}\right) \tag{22}$$

and

$$\bar{\alpha} = \frac{1}{C_v V} \sum_{\boldsymbol{Q}} \hbar\omega_{\boldsymbol{Q}} \frac{dN^0_{\boldsymbol{Q}}}{dT} \alpha(\boldsymbol{Q}). \tag{23}$$

Thus the general quasi-2D S_g formula reproduces the 'metallic' formula when the relaxation time and average over $\boldsymbol{Q}$ are defined as above. The argument used here, however, is much stronger than those used to derive the simple formulae and, furthermore, the various τ make it possible to determine the conditions under which the Herring formula may also be valid.

By writing $\Gamma_{K+Q,K}$ out in full in equation (18) S_g can be written in the form

$$S_g = -\frac{2}{3}\frac{1}{N_v eTV}\sum_K f(K)(1-f(K+Q))\frac{\overline{\tau_{pK}}\overline{(\hbar\omega_Q)^2_K}}{\tau_{ep}(K)} \tag{24}$$

Here, an averaged total phonon scattering relaxation time $\overline{\tau_{pK}}$ has been defined by

$$\overline{\tau_{pK}} = \sum_Q (\hbar\omega_Q)^2 P^{a0}(K, K+Q)\tau_p(Q) \Big/ \sum_Q (\hbar\omega_Q)^2 P^{a0}(k, K+Q) \tag{25}$$

where

$$\tau_p^{-1}(Q) = \tau_{pp}^{-1}(Q) + \tau_{pe}^{-1}(Q) \tag{26}$$

and is the total phonon scattering rate given by $F/(-\mathrm{d}N_Q^0/\mathrm{d}\hbar\omega_Q)$ and

$$\overline{(\hbar\omega_Q)^2_K} = \tau_{ep}^{a}(K)\sum_Q (\hbar\omega_Q)^2 P^{a0}(K, K+Q) \tag{27}$$

in which:

$$\frac{1}{\tau_{ep}^{a}(K)} = \sum_Q P^{a0}(K, K+Q), \tag{28}$$

and is the total electron scattering rate in state K by phonon absorption. For both the non-degenerate and degenerate limits this allows S_g to be written in a form similar to the Herring formula (13) providing the average over Q, at given K, and the scattering times in (30), can be replaced by constant average values and moved to in front of the summation, i.e.

$$S_g = -\frac{2}{3}\frac{1}{N_v eTV}\frac{\tau_p}{2\tau_{ep}}\overline{(\hbar\omega_Q)^2_K}\sum_K f(K)(1-f(K+Q)). \tag{29}$$

where

$$\tau_{ep}^{(e)-1} + \tau_{ep}^{(a)-1} = \tau_{ep}^{-1} \simeq 2\tau_{ep}^{(a)-1} \tag{30}$$

is assumed. For the non-degenerate limit it is assumed that $\overline{(\hbar\omega_Q)^2_K} \simeq 2mv_s^2 k_B T$. Then, since $f(K) \ll 1$, $f(K+Q)$ can be dropped and

$$S_{g(\text{non-deg})} \simeq -\tfrac{1}{3}(mv_s^2/eT)\overline{\tau_p}/\overline{\tau_{ep}}. \tag{31}$$

For the degenerate case $\overline{(\hbar\omega_Q)^2_K} \simeq 2mv_s^2\varepsilon_f$. Assuming elastic scattering, whereby $\varepsilon(K') = \varepsilon(K)$, and using

$$\frac{1}{V}\sum_K f(K)(1-f(K)) = \tfrac{1}{2}k_B T\,\mathrm{d}N_v/\mathrm{d}\varepsilon_f \tag{32}$$

and taking $N_v \propto \varepsilon_f^{3/2}$, the result for S_g reduces to

$$S_{g(\text{deg})} \simeq -\tfrac{1}{2}(mv_s^2/eT)\overline{\tau_p}/\overline{\tau_{ep}}. \tag{33}$$

Hence the more general formula reproduces the expected results, when the averaged τ-values are appropriately defined. Both the metallic formula (10) and Herring formula (13) are obtained approximately, although the latter is valid for the non-degenerate limit, or the degenerate limit when the scattering is elastic. The difference between (31)

and (33) in terms of trivial numerical constants is of no significance in view of the approximate averaging used in their derivation.

5. Conclusions

It is now clear that the simple Herring and metallic S_g formulae are not in conflict but are most helpful in different limits: the metallic formula for degenerate electron statistics and the Herring formula for the non-degenerate case. Both models provide insight into phonon-drag and can be understood physically in terms of the net phonon energy drift velocity v_p. These conclusions are confirmed by the Boltzmann transport formalism of Cantrell and Butcher applied to 3D electronic conduction. In quasi-2D the dependence expected of S_g is as LT^3/n but this has been shown to be naive and is modified by the behaviour of τ_{pe}^{-1}. This factor is responsible for the interesting structure which has been noted in plots of $-S_g/T^3$ against T. More simplistically the T^3 dependence allows S to be written as:

$$S = S_d + S_g = aT + bT^3 \tag{34}$$

at low T. Hence, at very low T, S_d (which is linear in T) will most likely dominate but at higher T, depending on the values of a and b, it will be S_g which dominates. At higher T still, L will no longer be limited by boundary scattering and will fail. Then S_g will also be reduced and S_d may again dominate. This dominance changeover $S_d \rightarrow S_g \rightarrow S_d$ is apparently that which is observed in the results of Ruf *et al* (1988).

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