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LETTER TO THE EDITOR

Thermoelectric power in the balance equation theory

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Abstract. The thermoelectric power of bulk semiconductors and quantum well structures is investigated for the first time using the balance equation transport theory extended to weakly non-uniform systems. In the linear transport limit the thermopower expressions obtained are independent of scattering and equivalent to the results derived from the Boltzmann equation with the relaxation time approximation. Effects of carrier heating (due to a current flow or due to an applied electric field in the crossed direction) are examined, showing that thermoelectric power is very sensitively dependent on the method of heating the electrons, and can change sign at low temperatures in the case of a strong electric field bias.

There has recently been an intensified interest in studies of the thermoelectric power and the thermoelectric figure of merit in different systems: mesoscopic quantum dots [1, 2], macroscopic thin quantum well structures [3], and bulk materials in the presence of carrier heating under a strong applied electric field [4]. Previous theoretical treatments of thermoelectric power in macroscopic systems are based on the Boltzmann equation [5, 6]. A recent investigation by Xing, Liu and Ting [4] by the non-equilibrium statistical operator method of Zubarev [7] yielded a different formula for thermoelectric power. The purpose of this letter is to point out that thermoelectric power can be conveniently analysed from the balance equation approach of Lei and Ting [8], and this has the advantage of easy inclusion of hot electron effects.

We consider electron transport under the influence of an electric field E and in the presence of a small lattice temperature gradient ∇T . The occurrence of the lattice temperature gradient makes the transport problem an inhomogeneous one. Since the temperature gradient is small we are dealing with a weakly non-uniform case. The Lei–Ting balance equation approach [8] for high-field electronic transport has been extended to weakly non-uniform systems [9], in which the carrier drift velocity v , the electron temperature T_e , the average relative electron energy u , the carrier density n and the chemical potential μ are all field quantities which are weakly dependent on the spatial coordinates, such that their spatial gradients are small. Retaining these small quantities to first order (neglecting all the second and higher orders of the spatial derivatives) we have the following hydrodynamic balance equations [9]:

$$\frac{\partial n}{\partial t} + \nabla \cdot (vn) = 0 \quad (1)$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}(\nabla \cdot \mathbf{v}) = -\frac{2}{3} \frac{\nabla u}{mn} + \frac{e\mathbf{E}}{m} + \frac{\mathbf{f}}{mn} \quad (2)$$

$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = -\frac{5}{3} u(\nabla \cdot \mathbf{v}) - w - \mathbf{v} \cdot \mathbf{f}. \quad (3)$$

Here \mathbf{f} , the frictional force (density), and w , the energy transfer rate (density), are functions of local quantities n , \mathbf{v} , T_e and T , having expressions exactly the same as in the uniform case [8, 9]. We consider electron transport in the presence of a small lattice temperature gradient along the x direction: $\nabla T = (\nabla_x T, 0, 0)$. There may be a small drift velocity (current flow) and a small electric field in the x direction in addition to the drift velocity (current) and the electric field along the y direction: $\mathbf{v} = (v_x, v_y, 0)$ and $\mathbf{E} = (E_x, E_y, 0)$. Here v_x and E_x are small, and the spatial variations of all the field quantities are assumed to be along the x direction only. We will treat the steady state transport and consider the particle number, force and energy balance equations to first order in the small quantities. For instance, the gradient operator $\nabla_x \equiv \partial/\partial x$ is a first-order small quantity and v_x is also a first-order small quantity, thus $\nabla_x v_x$ is a higher-order small quantity and can be neglected. With these factors in mind we obtain the following equations from the general balance equations (1)–(3):

$$0 = -\frac{2}{3mn} \nabla_x u + \frac{eE_x}{m} + \frac{f_x}{mn} \quad (4)$$

stating the force balance in the x direction,

$$0 = neE_y + f_y \quad (5)$$

stating the force balance in the y direction, and

$$w + v_y f_y = 0 \quad (6)$$

stating the energy balance. For small v_x , f_x is proportional to v_x , and

$$\rho = -\frac{f_x}{n^2 e^2 v_x} \quad (7)$$

is the resistivity in the x direction in the presence of drift velocity v_y in the y direction. Equation (4) can then be written as

$$j_x = \frac{E_x}{\rho} - \frac{2}{3} \frac{\nabla_x u}{e\rho}. \quad (8)$$

Noticing that the local energy density of the relative electrons is given by

$$u = 2 \sum_k \varepsilon_k f[(\varepsilon_k - \mu)/T_e] \quad (9)$$

and the local number density n is related to the local chemical potential μ by

$$n = 2 \sum_k f[(\varepsilon_k - \mu)/T_e] \quad (10)$$

$f(x) = (e^x + 1)^{-1}$ is the Fermi function and $\varepsilon_k = k^2/2m$ for an isotropic parabolic band system), we can put equation (8) in the form

$$j_x = L^{11}(E_x - \nabla_x \mu/e) + L^{12}(-\nabla_x T_e) \quad (11)$$

where

$$L^{11} = 1/\rho \quad (12)$$

and

$$L^{12} = \frac{1}{e\rho} \left[\frac{5F_{\frac{3}{2}}(\zeta)}{3F_{\frac{1}{2}}(\zeta)} - \zeta \right] \quad (13)$$

with $\zeta = \mu/T_e$ and function $F_\nu(y)$ defined by

$$F_\nu(y) = \int_0^\infty \frac{x^\nu dx}{\exp(x-y) + 1}. \quad (14)$$

In the case where there is no current flow along the y direction, we have $T_e = T$ and $\nabla_x T_e = \nabla_x T$, and equation (11) becomes the well-known (weak) current transport equation [6] in the presence of temperature and chemical gradients. The thermoelectric power S is then [6]

$$S = L^{12}/L^{11} = \frac{1}{e} \left[\frac{5F_{\frac{3}{2}}(\zeta)}{3F_{\frac{1}{2}}(\zeta)} - \zeta \right]. \quad (15)$$

This is the same result as obtained from the Boltzmann equation for a one-parabolic-band material by assuming a constant relaxation time in [3]. If the relaxation time cannot be treated as a constant, Boltzmann theory predicts a thermoelectric power that may weakly depend on the scattering [6]. The thermoelectric power formula obtained in [4] using the non-equilibrium statistical operator method, which is different from that obtained with the Boltzmann-equation theory, also weakly depends on the scattering. The present balance equation theory, however, leads to a thermopower formula that is independent of scattering. This result is physically understandable: balance equation theory develops from the force balance of the system. In addition to contributing to the possible energy dissipation the only role the scattering plays is to induce a frictional force. Since thermoelectric power is defined under the open circuit (zero-current) condition [6], and the frictional force in the balance equation theory always vanishes when the drift velocity is zero, we should expect a thermoelectric power independent of scattering.

In the presence of a strong current flow in the y direction, electrons are heated. The electron temperature T_e is generally higher than the lattice temperature T . The gradient of the electron temperature $\nabla_x T_e$, however, depends not only on the gradient of the lattice temperature $\nabla_x T$, but also on the electron temperature itself and the method of controlling the electron heating. The thermoelectric power can be written as

$$S = \frac{1}{e} \left[\frac{5F_{\frac{3}{2}}(\zeta)}{3F_{\frac{1}{2}}(\zeta)} - \zeta \right] \frac{\delta T_e}{\delta T}. \quad (16)$$

$\delta T_e/\delta T$ stands for $\nabla_x T_e/\nabla_x T$ and should be calculated from balance equations (5) and (6) under the conditions pertinent to the experiment.

The hydrodynamic balance equations (1)–(3) for weakly non-uniform cases are also valid in a two-dimensional system, if the prefactor $\frac{2}{3}$ in equation (2) is replaced by unity, and the prefactor $\frac{5}{3}$ in equation (3) is replaced by two. The thermoelectric power S for a two-dimensional system (e.g. a quantum well structure) is easily derived to be

$$S = \frac{1}{e} \left[\frac{2F_1(\zeta)}{F_0(\zeta)} - \zeta \right] \frac{\delta T_e}{\delta T} \quad (17)$$

in agreement with that given by [3].

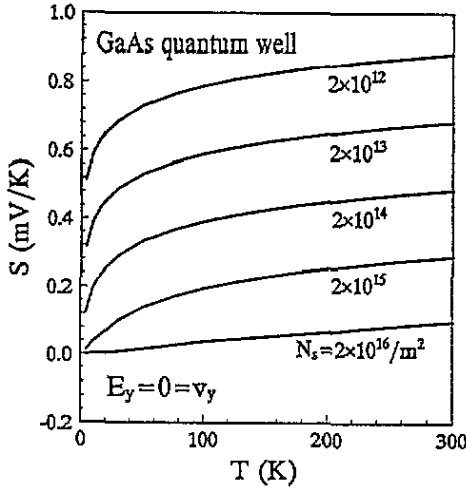


Figure 1. Thermoelectric power S of an n-type GaAs-based quantum well structure (10 nm thickness) at zero bias is shown as a function of lattice temperature T for different electron sheet densities N_s . The electron effective mass is taken to be $m = 0.07m_e$ (m_e is the free electron mass).

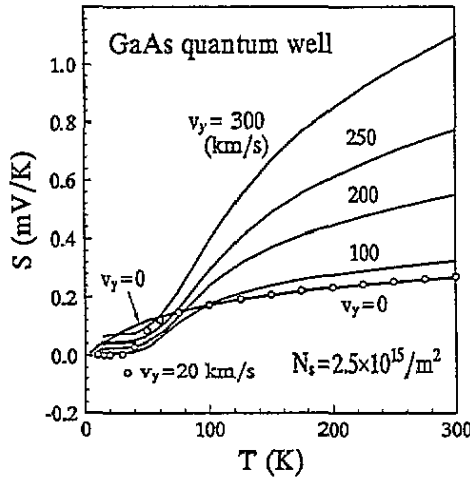


Figure 2. Thermoelectric power S under fixed-velocity bias condition is shown as a function of lattice temperature T for the same GaAs-based quantum well structure as described in figure 1 having electron sheet density $N_s = 2.5 \times 10^{15} \text{ m}^{-2}$ [2] for several different bias velocities $v_y = 0, 20, 100, 200, 250$ and 300 km s^{-1} .

To have an idea how the thermoelectric power depends on the carrier density, lattice temperature and the method of heating the electrons, we discuss an n-type GaAs-based thin (10 nm thickness along the z direction) quantum well structure. Electrons change band in the x - y plane, with a parabolic band having an effective mass $m = 0.07m_e$ (m_e is the free electron mass). Only the lowest subband occupation needs to be taken into account for the carrier density and temperature of interest. The thermoelectric power S as a function of

lattice temperature T , calculated from equation (17) for the case without a current flow in the y direction ($\delta T_e/\delta T = 1$), is shown in figure 1 for different carrier sheet densities N_s , ranging from $2 \times 10^{16} \text{ m}^{-2}$ to $2 \times 10^{12} \text{ m}^{-2}$.

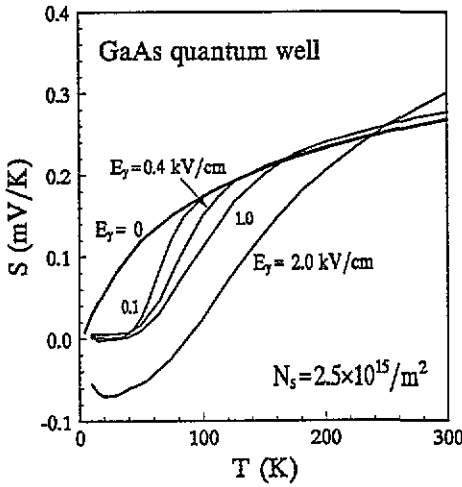


Figure 3. Thermoelectric power S under fixed-field bias condition is shown as a function of lattice temperature T for the same GaAs-based quantum well structure as described in figure 1 having electron sheet density $N_s = 2.5 \times 10^{15} \text{ m}^{-2}$ [2] for several different bias fields $E_y = 0, 0.1, 0.4, 1.0$ and 2.0 kV cm^{-1} .

In order to see the hot electron effect on thermoelectric power we examine two kinds of bias situation: (a) a fixed current flowing along the y direction (fixed velocity bias), or (b) applying a fixed electric field along the y direction (fixed field bias). The electron temperature T_e and $\delta T_e/\delta T$ are calculated from equations (5) and (6) under the appropriate bias condition. The carrier sheet density is assumed to be $N_s = 2.5 \times 10^{15} \text{ m}^{-2}$, which is high enough for the balance equation theory to apply. Scatterings by the remote (located at a distance 18 nm from the well centre) and background impurities, acoustic phonons (deformation potential and piezoelectric couplings with electrons), and polar optical phonons (Fröhlich coupling with electrons) are included. Full dynamic electron–electron screening is considered within the random phase approximation. The material and the electron–phonon coupling parameters used here are the same as those used in [10], and the impurity scattering strength is such that the low-temperature linear mobility is equal to $1.0 \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1}$. The thermoelectric power as a function of lattice temperature T , obtained under fixed velocity bias conditions, is plotted in figure 2 for different bias velocities $v_y = 0, 20, 100, 200, 250$ and 300 km s^{-1} . Figure 3 shows the thermoelectric power as a function of lattice temperature T for the same system but under fixed field bias conditions at several different bias fields $E_y = 0, 0.1, 0.4, 1.0$ and 2.0 kV cm^{-1} . Unlike in the zero-bias case where the thermopower S is determined only by the temperature, under hot carrier conditions S depends not only on the electron temperature T_e , but also on the factor $\delta T_e/\delta T$, which varies dramatically with the bias conditions. In the case of fixed velocity bias, $(\delta T_e/\delta T)_{v_y}$ is always positive, and so is the thermopower S , as shown in figure 2. In the case of fixed field, however, we find that under high bias fields ($E_y > 1 \text{ kV cm}^{-1}$) $(\delta T_e/\delta T)_{E_y}$, and thus S , can be negative within a small low-temperature range. For instance, at bias $E_y = 2.0 \text{ kV cm}^{-1}$ thermopower S become negative at temperature $T < 85 \text{ K}$. This finding is, to certain extent, in agreement with that reported in [4].

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References

- [1] Beenakker C W J and Staring A A M 1992 *Phys. Rev. B* **46** 9667
- [2] Molenkamp L W, Staring A A M, Alphenaar B W and van Houten H 1993 *Proc. 8th Int. Conf. on Hot Carriers in Semiconductors, (Oxford, 1993)*
- [3] Hicks L D and Dresselhaus M S 1993 *Phys. Rev. B* **47** 12 727
- [4] Xing D Y, Liu M and Ting C S preprint
- [5] Conwell E M and Zucker J 1964 *J. Appl. Phys.* **36** 2192
- [6] Ashcroft N W and Mermin N D 1976 *Solid State Physics* (New York: Holt, Rinehart and Winston) ch 13
- [7] Zubarev D N 1974 *Nonequilibrium Statistical Thermodynamics* (New York: Consultants Bureau)
- [8] Lei X L and Ting C S 1984 *Phys. Rev. B* **30** 4809; *Phys. Rev. B* 1985 **32** 1112
- [9] Lei X L, Cai J and Xie L M 1988 *Phys. Rev. B* **38** 1529
- [10] Lei X L, Birman J L and Ting C S 1985 *J. Appl. Phys.* **58** 2270