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Quantized thermoelectric power and oscillating chemical potential in the ballistic transport regime

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Abstract. The thermoelectric power of a narrow constriction in a two-dimensional electron gas (2DEG) in $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ heterojunctions is theoretically investigated in the form of the transverse voltage by using an appropriate model for the recent experimental system. Our model gives not only the quantized thermoelectric power obtained theoretically and experimentally but also the oscillating chemical potentials in all the participating 2DEG regions. The temperature dependence of the transverse voltage is also studied focusing on the effect of the thermal broadening of the electron distribution functions.

1. Introduction

Recently there has been much interest in thermoelectric powers of 2DEG in $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ heterojunctions at low temperatures. It is well known that for the macroscopic system the phonon drag contribution to the thermoelectric power is dominant (Fletcher *et al* 1988, Ruf *et al* 1988, Lyo 1988, Okuyama and Tokuda 1990). For the ballistic electrons in a narrow constriction in the 2DEG, Streda (1989) has predicted the peak structure of the thermoelectric power S with quantized values of local maxima corresponding to the quantization of conductance (van Wees *et al* 1988, Wharam *et al* 1988). The peaks occur at the constriction widths where the number of the occupied 1D sub-bands in the constriction is changed by unity. The height of the peak is independent of temperature and is given by the electronic charge e , the Boltzmann constant k_B , and the number of the occupied sub-bands n (Streda 1989)

$$-S_n^{\max} = \frac{k_B}{|e|} \frac{\ln 2}{n + 1/2}. \quad (1)$$

A theory for thermoelectric power in more general multiterminal structures has also been worked out by Butcher (1990). Molenkamp *et al* (1990) have measured the thermoelectric power in the form of the 'transverse voltage' V_{trans} of the narrow 2DEG heated by a current I , using two different opposite point contacts as voltage probes (figure 1(a)). The temperature differences are produced between the central 2DEG region (C) and both the opposite 2DEG regions (L, R). The transverse voltage is caused by the difference between the thermoelectric powers of the two point contacts and exhibits the oscillations as the constriction width of one (say, the left one) of the point contacts is varied. The experimental data are well explained with Streda's theory and the prediction of the

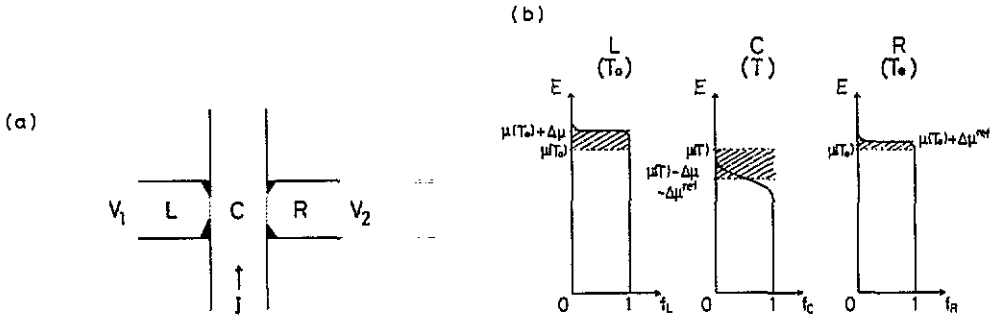


Figure 1. (a) Schematic representation of the experimental system used in the measurement by Molenkamp *et al* (1990). The point contact voltage probes are indicated in black. (b) The electron distribution functions in the left (L), central (C), and right (R) regions at the temperatures T_0 , T , and T_0 , respectively. $\Delta\mu$, $\Delta\mu^{net}$, and $-(\Delta\mu + \Delta\mu^{net})$ are the variations of the chemical potentials in the left, right, and central 2DEG regions, respectively.

quantized thermoelectric power has been confirmed experimentally. The model used in the analysis is, however, not appropriate for the understanding of the behaviour of the chemical potentials in the 2DEG regions.

In this paper we investigate theoretically the transverse voltage corresponding to the thermoelectric power in the ballistic transport regime focusing on the behaviour of the chemical potentials which necessarily modify the model of Molenkamp *et al* (1990). Moreover we study the temperature dependence of the transverse voltage over the wide temperature range.

2. Formalism

We write the electron distribution functions for the left, right, and central regions as f_L , f_R , and f_C , respectively. No net current draws through each constriction, which is the condition of a measurement of the thermoelectric power:

$$\int_0^\infty t_L(E)[f_L(E) - f_C(E)] dE = 0 \tag{2}$$

$$\int_0^\infty t_R(E)[f_R(E) - f_C(E)] dE = 0 \tag{3}$$

where $t_L(E)$ and $t_R(E)$ are the transmission probabilities summed over the 1D sub-bands that propagate through the left and right constrictions at energy E , respectively. The transmission probability for each sub-band is unity for the occupied sub-band and zero otherwise. Therefore

$$t_L(E) = \sum_{n=1}^\infty \theta(E - E_n^L) \tag{4}$$

$$t_R(E) = \sum_{n=1}^\infty \theta(E - E_n^R) \tag{5}$$

where $\theta(E)$ is the step function, E_n^L and E_n^R are the bottoms of the n th sub-band energy for the left and right constrictions, respectively. We adopt the infinite square-well lateral confinement potential for the constrictions. The temperatures of the left and right regions are equal to the lattice temperature T_0 . We assume that a local electron temperature T ($> T_0$) is defined for the central region as a result of Joule heating. In response to the temperature difference the electrons can flow into the cold region from the hot region until enough charge has accumulated at the cold region to build up the electric field that cancels the flow. As a result the chemical potentials in both regions change. We model f_L , f_R and f_C by the following Fermi–Dirac distribution functions (figure 1(b)):

$$f_L(E) = [1 + \exp\{(E - \mu(T_0) - \Delta\mu)/k_B T_0\}]^{-1} \tag{6}$$

$$f_R(E) = [1 + \exp\{(E - \mu(T_0) - \Delta\mu^{ref})/k_B T_0\}]^{-1} \tag{7}$$

$$f_C(E) = [1 + \exp\{(E - \mu(T) + \Delta\mu + \Delta\mu^{ref})/k_B T\}]^{-1} \tag{8}$$

where $\Delta\mu$ and $\Delta\mu^{ref}$ are respectively the variations of the chemical potentials in the left and right regions due to the transfer of the electrons through the point contacts. The chemical potential at finite temperature is given by

$$\mu(T) = k_B T \ln[\exp(N_s \pi \hbar^2 / m^* k_B T) - 1] \tag{9}$$

where N_s is the electron concentration of the 2DEG, \hbar is the reduced Planck constant, and m^* is the effective mass of the electron in GaAs ($m^* = 0.067m_0$ and m_0 is the free-electron mass). To evaluate the variation of the chemical potential in the central region we have assumed that the total number of the electrons in the system is kept constant and the areas of the three regions are equal to each other. (The variations of chemical potentials in the three regions depend on the ratio of the areas but the transverse voltage and the thermoelectric power do not, because the ‘difference’ of the chemical potentials is uniquely determined by (2) and (3) regardless of the ratio of the areas.) As the chemical potential is nearly proportional to the electron concentration at low temperatures, it is deduced from this assumption that the variation of the chemical potential in the central region due to the transfer of the electrons is given by the sum of $\Delta\mu$ and $\Delta\mu^{ref}$. Here we have neglected the small difference between $\Delta\mu(T)$ ($\Delta\mu^{ref}(T)$) and $\Delta\mu(T_0)$ ($\Delta\mu^{ref}(T_0)$). The transverse voltage is then the difference between the voltages across each point contact

$$V_{trans} = V_2 - V_1 = (\Delta\mu - \Delta\mu^{ref})/|e|. \tag{10}$$

$\Delta\mu$ and $\Delta\mu^{ref}$ are obtained by calculating numerically (2)–(9). V_{trans} is related to the difference between the thermoelectric powers of two point contacts as follows

$$V_{trans} = (S_R - S_L)(T - T_0) \tag{11}$$

where S_L and S_R are the thermoelectric powers of the left and right constrictions, respectively

$$S_L = - \frac{2\Delta\mu + \Delta\mu^{ref}}{|e|(T - T_0)} \tag{12}$$

$$S_R = - \frac{\Delta\mu + 2\Delta\mu^{ref}}{|e|(T - T_0)}. \tag{13}$$

Before we proceed with a numerical calculation, we should mention the difference between the model of Molenkamp *et al* (1990) and ours. Molenkamp *et al* assumed that

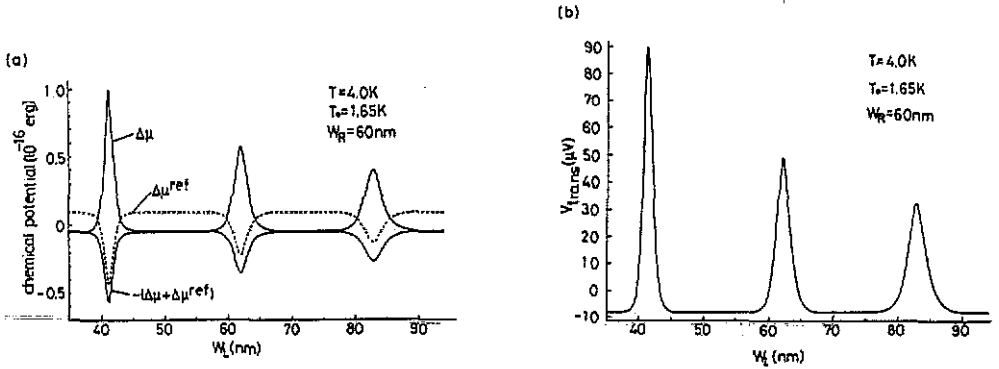


Figure 2. (a) The variations of the chemical potentials in the three regions versus the width W_L of the left constriction at $T = 4.0$ K, $T = 1.65$ K, and $W_R = 60$ nm. $\Delta\mu$, $\Delta\mu^{\text{ref}}$, and $-(\Delta\mu + \Delta\mu^{\text{ref}})$ are the variations of the chemical potentials in the left, right, and central regions, respectively. (b) The transverse voltage V_{trans} versus the width W_L of the left constriction at the same condition as (a).

the chemical potential in the central region is given by the Fermi energy E_F . In contrast, we take account of the variations of the chemical potentials in all the regions; which is as it should be.

3. Results and discussions

We calculate the transverse voltage V_{trans} as a function of the width W_L of the left constriction. In our calculation we take the following values: $N_s = 3.64 \times 10^{11} \text{ cm}^{-2}$ corresponding to $E_F = 13 \text{ meV}$, and the fixed width $W_R = 60 \text{ nm}$ for the right constriction. Under this condition the bottom of the third sub-band in the right constriction is located above the Fermi level. Here we take $T = 4.0 \text{ K}$ and $T_0 = 1.65 \text{ K}$. Figure 2(a) shows the variations of the chemical potentials of the three regions calculated using our model. Figure 2(b) shows the W_L -dependence of V_{trans} derived using (10). The result obtained using the model by Molenkamp *et al* (1990) is almost the same as that obtained above. Therefore, the agreement with the experimental data (Molenkamp *et al* 1990) is quite good. In figure 2(b) the highest peak corresponds to the beginning of the occupation of the second sub-band in the left constriction. A characteristic of our results is the oscillation of the chemical potentials. The chemical potentials in all the regions are oscillating corresponding to the peak positions of V_{trans} and the chemical potentials in the left and right regions oscillate out of phase while those in the right and central regions oscillate in phase keeping the difference between them almost constant. It is very interesting to observe experimentally these oscillations.

Now, we would like to clarify why the model of Molenkamp *et al* (1990) gives almost the same results on V_{trans} as ours regardless of the different formalism concerning the chemical potential. If we make the following approximations in our model

$$E_F = \mu(T) - \Delta\mu - \Delta\mu^{\text{ref}} \quad (14)$$

and

$$\mu(T) = \mu(T_0) \quad (15)$$

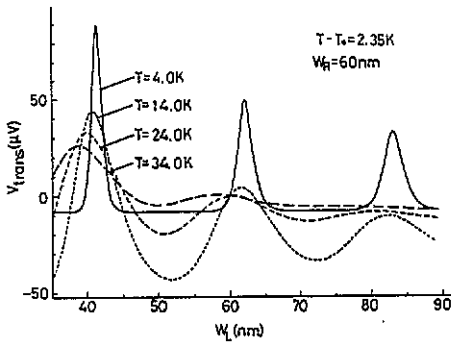


Figure 3. The transverse voltage V_{trans} versus the width W_L of the left constriction at $W_R = 60$ nm for four different pairs of T and T_0 .

our model reduces to the model of Molenkamp *et al.* Equation(15) holds fairly well provided that the difference $T - T_0$ is very small. As seen from our numerical results, the approximation by Molenkamp *et al* is quite good, because $\Delta\mu$ and $\Delta\mu^{ref}$ are found to be very small compared with $\mu(T)$. From our point of view, however, Molenkamp *et al* (1990) derived the variations of the chemical potentials in the left and right regions measured from the energy $\mu(T) - \Delta\mu - \Delta\mu^{ref}$. Therefore, the absolute variations of the chemical potentials cannot be dealt with in their model. The two models are almost equivalent for the estimates of the transverse voltage and the thermoelectric powers which depend on the difference of the chemical potentials. But our model can deal with the variations of the chemical potentials in three regions.

Next we consider the temperature dependence of V_{trans} in (10). Figure 3 shows V_{trans} at four different pairs of temperatures with the fixed temperature difference $T - T_0$. It is found that at low temperatures the amplitude of the oscillation follows the formula (Molenkamp *et al* 1990)

$$\Delta V_{trans}^n = \frac{k_B}{|e|} \frac{\ln 2}{n + 1/2} (T - T_0). \tag{16}$$

On the other hand, with increasing temperature, the amplitude decreases, the width of the peak structure becomes broad and the W_L giving the peak decreases slightly. These effects are due to the thermal broadening of the electron distribution functions. In this paper we have neglected all the scattering processes which become crucial at high temperatures. The ballisticity of electron transport must be lost in reality at high temperatures. Further studies taking account of the elastic and/or inelastic scattering processes are needed to gain a deeper understanding of the thermoelectric power at high temperatures.

In summary, we have investigated the thermoelectric power in the form of the transverse voltage in the ballistic transport regime, using an appropriate model for the recent experimental system. We have found that our model gives not only the quantized thermoelectric power but also the oscillating chemical potentials in all the participating 2DEG regions. We have also studied the effects of temperature on the oscillation of the transverse voltage by taking account of the thermal broadening of the electron distribution functions.

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