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Quantized magneto-thermopower in tunnel-coupled ballistic channels: sign reversal and oscillations

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Abstract

The quantized electron-diffusion thermoelectric power S is studied for a general one-dimensional band structure in ballistic channels with applications to a single-quantum-well channel and tunnel-coupled double-quantum-well channels in a perpendicular magnetic field. We find a field-induced sign reversal of S and oscillations in double-well channels.

Transport properties of quasi-one-dimensional (1D) doped semiconductor structures are of current interest. An earliest form of 1D single-quantum-well wires (SQWRs) is the so-called quantum point contact illustrated in figure 1(a), where the channel length is very short, of the order of a fraction of a micrometre. Electrons pass through this wire (or channel) ballistically at low temperatures (T) under a DC bias. The conductance G is quantized and decreases in steps of $2e^2/h$ in a spin-degenerate system (assumed in this paper) when the channel width is reduced gradually [1]. Here, e is the absolute electronic charge and h is Planck's constant. Similar quantized G steps were observed in SQWRs as a function of a magnetic field B applied in the perpendicular (i.e., z) direction shown in figure 1(a) [2]. Recently, ballistic thermoelectric power (TEP) S was observed in SQWRs [3] and was also studied theoretically in zero B [3–5]. Previous studies of the TEP [3–5] are relevant to simple band structures with a single minimum for each sublevel. More complicated band structures with two minima and a maximum are generated in tunnel-coupled double-quantum-well wires (DQWRs) in the presence of a perpendicular B as shown in figure 1(b) [6, 7]. For simplicity, we assume that the wells are narrow and deep in the growth (z) direction, allowing only the ground-level occupation. However, channels may be wide in the x direction and allow multi-sublevel occupation. In this paper, we calculate the ballistic electron-diffusion TEP for a general 1D structure and apply the result to SQWRs and DQWRs in perpendicular B. We find that in ballistic DQWRs B causes a sign reversal of S and oscillations.

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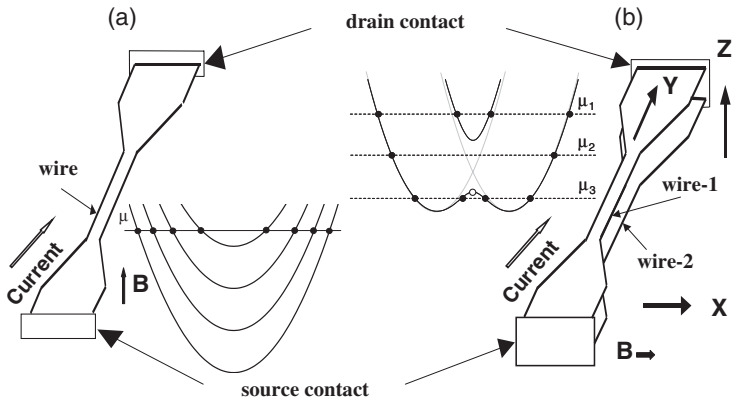

Figure 1. (a) A schematic diagram of a SQWR and the energy dispersion. A narrow channel is formed by applying a negative bias on the top split metallic gate, not shown. (b) A schematic diagram for DQWRs and the energy dispersion in a magnetic field. Electrons tunnel between the wires through the $Al_xGa_{1-x}As$ barrier in the z direction. Electrons behave like holes for the TEP at the hollow circle on the dispersion curve. A magnetic field B lies in the x direction for the DQWRs and in the z direction for the SQWR. Black dots denote the Fermi points.

The electron-diffusion TEP is the ratio of the heat current and the charge current of the electrons divided by T in the presence of a linear DC field. The ballistic heat ($Q^{(1)}$) and charge ($Q^{(0)}$) currents are given, for symmetric electronic structures, by

$$Q^{(\ell)} = 2(-e)^{1-\ell} \sum_{n,k} \frac{v_{nk}}{\mathcal{L}} (\varepsilon_{nk} - \bar{\mu})^{\ell} [\theta(-v_{nk}) f^{(0)}_{nk,\mathrm{R}} (1 - f^{(0)}_{nk,\mathrm{L}}) + \theta(v_{nk}) f^{(0)}_{nk,\mathrm{L}} (1 - f^{(0)}_{nk,\mathrm{R}})], \quad (1)$$

where $\ell = 0, 1$, $\mathcal{L}$ is the channel length, $\bar{\mu}$ is the chemical potential in the channel, and $\theta(x)$ is the unit step function. In equation (1), n is the sublevel index, k is the wavenumber, $v_{nk} = \partial\varepsilon_{nk}/\partial\hbar k$ is the velocity, and $f^{(0)}_{nk,\alpha}$ is the Fermi function for the 2D electron gas (2DEG) on the left- ($\alpha = \mathrm{L}$) and the right-hand ($\alpha = \mathrm{R}$) side, with the chemical potential μ_α. The physical meaning of equation (1) is self-evident. Equation (1) can be simplified, in view of $v_{n,-k} = -v_{nk}$, as

$$Q^{(\ell)} = \frac{2(-e)^{1-\ell}}{\pi} \sum_{n} \int_0^\infty |v_{nk}| (\varepsilon_{nk} - \bar{\mu})^{\ell} (f^{(0)}_{nk,\mathrm{L}} - f^{(0)}_{nk,\mathrm{R}})\, \mathrm{d}k. \quad (2)$$

Using $\mu_\mathrm{L} + eV = \mu_\mathrm{R} \equiv \mu$, $f^{(0)}_{nk,\mathrm{L}} - f^{(0)}_{nk,\mathrm{R}} = eV f^{(0)'}_{nk}$, and $\bar{\mu} \to \mu = \mu_\mathrm{L} = \mu_\mathrm{R}$ in the limit $V \to 0$, where V is the infinitesimal voltage difference between the left- and the right-hand 2DEGs, we find

$$Q^{(\ell)} = \frac{2eV(-e)^{1-\ell}}{\pi} \sum_{n} \left(\int_{\varepsilon_{n,k=0}}^{\varepsilon_{n,k_1}} + \int_{\varepsilon_{n,k_1}}^{\varepsilon_{n,k_2}} + \cdots + \int_{\varepsilon_{n,k^*}}^{\infty} \right) \mathrm{sgn}(v_{nk}) (\varepsilon_{nk} - \mu)^{\ell} f^{(0)'}_{nk}\, \mathrm{d}\varepsilon_{nk}, \quad (3)$$

where $f^{(0)'}_{nk}$ is the first derivative of the Fermi function $f^{(0)}_{n,k} = f^{(0)}(\varepsilon_{n,k})$ with respect to $\varepsilon_{n,k}$, and the lower limit equals the energy $\varepsilon_{n,k=0}$ at $k = 0$. In equation (3), the energy integration over the range $0 < k < \infty$ is chopped into the sum of the integrations between the successive extremum points ε_{n,k_m}, where $\varepsilon_{n,k}$ is a monotonic function of k and ε_{n,k^*} is the last extremum (minimum) point. Each integration can be carried out analytically for both $\ell = 0, 1$, yielding

$$S = \frac{Q^{(1)}}{T Q^{(0)}} = -\frac{k_\mathrm{B}}{eF} \sum_{n} \sum_{\gamma} C_{n,\gamma} \left[\beta(\varepsilon_{n,\gamma} - \mu) f^{(0)}(\varepsilon_{n,\gamma}) + \ln(\mathrm{e}^{\beta(\mu - \varepsilon_{n,\gamma})} + 1) \right], \quad (4)$$

where $\beta = 1/k_B T$ and

$$F = \sum_n \sum_\gamma C_{n,\gamma} f^{(0)}(\varepsilon_{n,\gamma}). \tag{5}$$

Here, γ-summation indicates summing over all the energy-extremum points on each curve n ($-\infty < k < \infty$). The quantity $\varepsilon_{n,\gamma}$ is the extremum energy. For a given curve n, $C_{n,\gamma} = 1$ for a local energy minimum point and $C_{n,\gamma} = -1$ for a local energy maximum point. The quantity F equals the number of pairs of the Fermi points at $T = 0$ and is related to G by $G = 2e^2 F/h$. The result in equation (4) is equivalent to the earlier result obtained for SQWRs with a single minimum point for each energy-dispersion curve [4]. It can also be obtained using an energy-dependent transmission-coefficient approach [4, 8, 9].

The TEP is quantized at $T = 0$ K as $S = -(k_B/e) \ln 2/[G/(2e^2/h)]$ in general at the energy-extremum points $\mu = \varepsilon_{n,\gamma}$ in equation (4), where $G = (2e^2/h)(i + 1/2)$ with $i = 1, 2, \ldots$ as obtained earlier by Streda [4]. The peak heights of S and corresponding G values satisfy this relationship approximately even at nonzero temperatures in our numerical results to be displayed later.

In this paper, we study a SQWR and DQWRs illustrated in figure 1. We assume that, for both structures, the channel confinement is given by the parabolic potential energy $V(x) = m^* \omega_x^2 x^2/2$, where m^* is the effective mass. The eigenvalues are given for $B = 0$ by $\varepsilon_{nk} = (n + 1/2)\hbar\omega_x + \hbar^2 k^2/2m^*$ with $n = 0, 1, 2, \ldots$. The QW depth and widths for the z confinement are designated as V_0 and L_W, while the width of the centre barrier is given by L_B for DQWRs.

We first consider a SQWR illustrated in figure 1(a) with $B \| z$ perpendicular to the channel plane. The eigenvalues are given by $\varepsilon_{nk} = (n + 1/2)\hbar\Omega_x + \hbar^2 k^2/2m^{**}$, where $n = 0, 1, \ldots, \Omega_x = (\omega_x^2 + \omega_c^2)^{1/2}$, $\omega_c = eB/m^* c$, and $m^{**} = m^*/[1 - (\omega_c/\Omega_x)^2]$ [10]. The effective mass m^{**} becomes heavier as B increases, increasing the density of states. As a result, the sublevels n in figure 1(a) become depopulated successively for increasing B. Figure 2 shows G and S of a SQWR obtained from equation (4) for two temperatures as a function of B when several levels are occupied at $B = 0$. The parameter $\hbar\omega_x$ and the electron density n_{1D} are given in the inset. The result in figure 2(a) is independent of L_W and V_0 under the assumption that only the ground level is occupied in the z direction. The TEP is very small when μ lies away from the edges of the sublevels because the contributions to the heat current $Q^{(1)}$ in equation (3) from above μ ($\varepsilon_{nk} > \mu$) cancels those from below μ ($\varepsilon_{nk} < \mu$). This cancellation does not occur when μ is within the thermal energy $k_B T$ of the sublevel edges, yielding spikes for the TEP just before a level is depopulated at the knees of the quantum steps of G. These spikes broaden as T is raised. This behaviour is similar to the density dependence of the field-free TEP studied earlier [4].

For DQWRs, new interesting effects are obtained when B is in the x direction. The role of B is to displace the energy-dispersion parabolas of one QW relative to those of the other QWs in k space by $\delta k = d/\ell_c^2$, where d is the centre-to-centre distance of the QWs and $\ell_c = \sqrt{\hbar c/eB}$. The two parabolas in the QWs with the same n then anticross at the crossing point due to tunnelling, opening a gap Δ_{SAS} between the symmetric and antisymmetric states at $k = 0$ as shown in figure 1(b) for the ground level $n = 0$. In this case, the eigenvalue ε_{nk} and the magnitude of Δ_{SAS} (i.e., mixing of the wavefunctions in the two QWs) depend on the QW width L_W, barrier width L_B, and the barrier height V_0 and are calculated numerically [6, 11]. The parabolas move away from each other in the k-axis direction as $\delta k \propto B$ increases, pushing the gap through the chemical potential μ. The inset in figure 1(b) shows the relative positions of μ with respect to the gap for three different B values. This level splitting occurs for each n. The levels become depopulated as B increases.

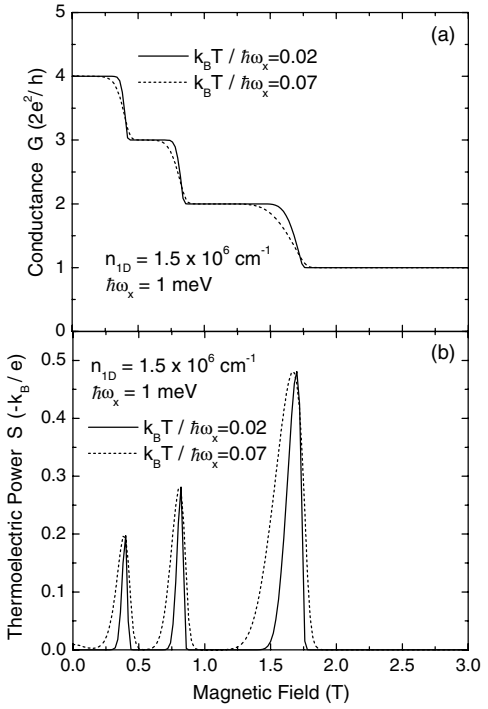

Figure 2. Ballistic (a) G and (b) S for two temperatures in SQWR with three levels occupied initially at $B = 0$. The parameters are defined in the text.

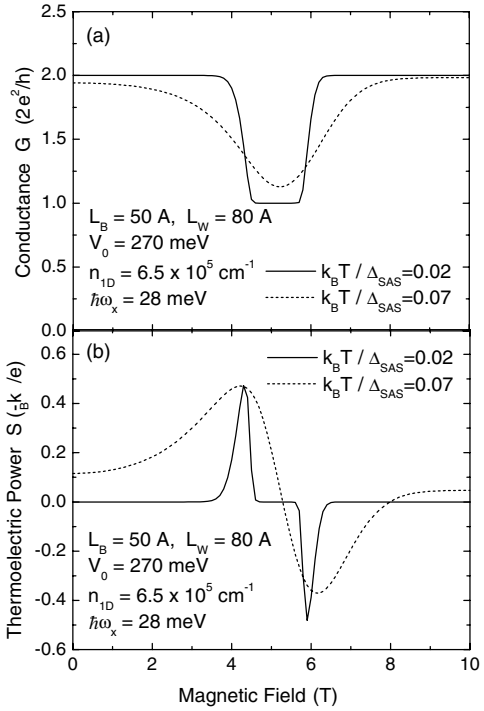

Figure 3. Ballistic (a) G and (b) S for two temperatures in DQWRs with only $n = 0$ occupied. The parameters are defined in the text.

Figure 3 shows S and G calculated from equation (4) for DQWRs at two temperatures for the case of large $\hbar\omega_x$ and low density where only the tunnel-split $n = 0$ doublet is occupied at $B = 0$ as indicated in figure 1(b). The structure parameters are given in the figure. The gap equals $\Delta_{\rm SAS} = 1.6$ meV for this structure and is insensitive to B. The conductance shows a minimum near $B = 5.1$ T and is V-shaped in striking contrast with the behaviour shown for a SQWR in figure 2(a). The conductance equals the number of pairs of Fermi points in units of $2e^2/h$, namely 2 for $\mu = \mu_1$, 1 for $\mu = \mu_2$, and 2 for $\mu = \mu_3$ in figure 1(b), where the horizontal dotted lines illustrate the fact that the anticrossing gap sweeps through μ as B increases, indicating the positions of the chemical potentials relative to the gap for three concomitant B values: $B_1 < B_2 < B_3$. The TEP shows a surprising feature: it changes sign near the G minimum just before it begins to rise again. At this point, μ crosses the local energy extremum (i.e., maximum) point marked by the hollow circle on the lower branch in figure 1(b), doubling the number of Fermi points and thus G. The dispersion is holelike (i.e., inverted) at this point, yielding a sign reversal for S.

For small $\hbar\omega_x \ll \Delta_{\rm SAS}$ corresponding to wide channels, many levels are occupied in high-density DQWRs. In this case, G follows a V-shaped dependence on B as shown in figure 4 at two temperatures. A similar B dependence was observed earlier in DQWRs [12]. The inset illustrates the tunnel-split sublevels for this case at B near the G minimum. The B dependence of G can be explained in a similar way as in figure 3(a) by accounting for the Fermi points from all the levels n together with the B-dependent movement of μ with respect to the gap [7]. For SQWRs, G decreases stepwise monotonically as a function of B as in

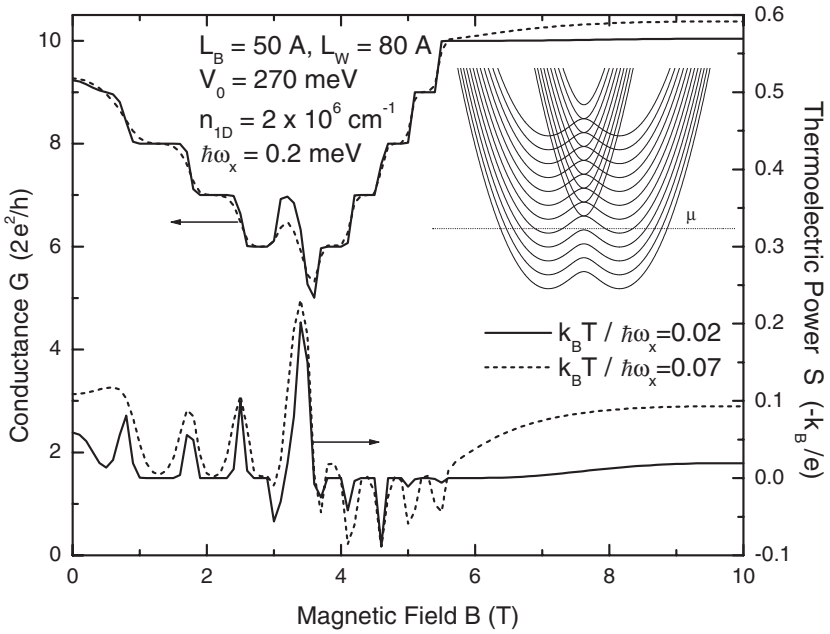

Figure 4. Ballistic G (left axis, upper curves) and S_d (right axis, lower curves) for two temperatures in DQWRs with many levels occupied. The parameters are defined in the text. The inset shows the tunnel-split energy dispersion at $B = 3.4$ T near the G minimum.

figure 2(a) and is not shown [2]. Ballistic S is also displayed for the DQWRs in figure 4 at two temperatures. Note that $-S$ shows positive peaks initially when μ crosses the bottoms of the upper branches successively for lower n values. It changes sign near the G minimum just before it begins to rise again. At this point, μ crosses the local energy maximum point at the top (at $k = 0$) of the lower branch, increasing the number of the Fermi points and thus G. For this point, the dispersion is holelike, yielding the sign reversal for S. From this point on, μ keeps crossing similar local energy maximum points belonging to lower n values, producing successive negative holelike peaks for $-S$. The $-S$ peak near the G minimum at 3.4 T is large because $-S$ is inversely proportional to G.

In summary, we have studied the electron-diffusion thermoelectric power for a general one-dimensional band structure in the ballistic regime. The result was applied to a single-quantum-well channel and tunnel-coupled double-quantum-well channels in a perpendicular magnetic field. In double-quantum-well channels, we showed a field-induced sign reversal and oscillations of the thermoelectric power.

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