Thermoelectric current in tubular nanowires in transverse electric and magnetic fields

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Abstract. In the presence of a transverse magnetic field, the charge current in nanowires can flow from the hot to the cold reservoir, but also backwards. The sign change can be obtained by increasing the temperature bias or the magnetic field. This behavior occurs when the magnetic field is sufficiently strong. Here, we will investigate how the size of the anomalous backward-flowing current is affected by an electric field perpendicular to the nanowire. The interplay of the electric and magnetic field modifies the dispersion curves, which will show up in the transport properties. We will also investigate how the presence of impurities affects the anomalous current. The electric field affects backscattering due to impurities, and thus the thermoelectric current reversal. Preliminary results show that the current reversal can survive in the presence of impurities.

1. Introduction
A temperature gradient across a conducting material induces an energy gradient, which in turn results in particle transport. In an open circuit, where no net current flows, a voltage is then generated when two ends of a sample are maintained at different temperatures — this is the Seebeck effect and the linear voltage response is known as the thermopower. The hotter particles have larger average kinetic energy, and the net particle flow is therefore generally from the hot to the cold side. The thermopower and thermoelectric current can be positive or negative, depending on the type of charge carriers, i.e., electrons or holes.

In comparison to this macroscopic case, the thermopower at the nanoscale has special characteristics. For example, if the energy separation between the quantum states of the system is larger than the thermal energy, the thermopower may alternate between positive and negative values, depending on the position of the Fermi level relative to a resonant energy, which can be controlled with a gate voltage. These oscillations were predicted a long time ago [1], and subsequently experimentally observed in quantum dots [2, 3]. In these examples, the charge carriers are electrons and the sign change of the thermopower means that they travel from the cold side to the hot side, which may appear counterintuitive.

Observing negative thermopower at the nanoscale is difficult for two reasons: the currents are small (∼ pA [4]) and it is hard to maintain a large temperature difference across short distances [5]. However, cylindrical nanowires are well suited for observing negative thermopower since their length can reach µm and the currents are of the order of tens of nA [6]. Here, we focus on how an electric field affects the thermoelectric current.
2. Model and methodology

We model a cylindrical nanowire \([7, 8]\) as a two-dimensional sheet wrapped into a cylinder of radius \(R\). We choose the coordinate system such that magnetic field is along the \(x\)-axis, \(\mathbf{B} = (B, 0, 0)\), the vector potential being \(\mathbf{A} = (0, 0, By) = (0, 0, BR \sin \varphi)\). The electric field is also applied along the \(x\) axis, such that \(\mathbf{E} = (E_x, 0, 0)\). In this setup, the states are affected by a competition of the electric and magnetic fields. An electron traveling in the positive \(z\)-direction will tend to be pulled towards \(\varphi = -\pi/2\) by the Lorentz force and an electron traveling in the opposite direction will tend to be pulled to the opposite side of the cylinder, i.e., \(\varphi = \pi/2\) (see Fig. 1). The resulting states are known as snaking states \([9]\). The electric field tends to pull electrons toward \(\varphi = 0\), which will affect the number of electrons in the counterpropagating snaking states. As we will see later, this will affect the transport properties in the presence of impurities. The clean nanowire, i.e., in the absence of impurities, is translationally invariant along the \(z\) direction and the momentum operator \(p_z\) can be replaced by its eigenvalue \(\hbar k\). The Hamiltonian can be written as

\[
H(k) = \frac{\hbar^2}{2m_{\text{eff}}} R^2 \left[ -\frac{\partial^2}{\partial \varphi^2} + \left( Rk + \frac{eBR^2}{\hbar} \sin \varphi \right)^2 \right] + eE_x R \cos \varphi - \frac{g_{\text{eff}} \mu_B}{2} B \sigma. \tag{1}
\]

In this example, we consider material parameters for GaAs, i.e., the effective mass \(m_{\text{eff}} = 0.066 m_0\) and a \(g\)-factor \(g_{\text{eff}} = -0.44\), \(\mu_B\) being the Bohr magneton and \(\sigma = \pm Z\) being the spin label. For \(B = 0\) and \(E_x = 0\), the angular part of the Hamiltonian has eigenfunctions \(e^{i\varphi n}/\sqrt{2\pi}\), \(n \in \mathbb{Z}\), and the single-electron energy dispersions are ordinary parabolas as a function of \(k\). These eigenfunctions define a basis set, \(|nk\sigma\rangle\), which we use for \(B \neq 0\) to diagonalize numerically (1). The convergence is reached with \(|n| \leq 50\). It is convenient to introduce a length scale \(\ell_E = (\hbar^2 / (2meE_x))^{1/3}\) associated with the electric field strength \(E_x\). When \(\ell_E \gg R\), the effect of the electric field is small, but once \(\ell_E \lesssim R\), the electric field starts playing a role. Similar arguments hold for the magnetic length \(\ell_c = \sqrt{eB/\hbar}\), i.e., when \(\ell_c \lesssim R\), the magnetic field becomes important.

The charge current through the nanowire, driven by a temperature gradient, can be calculated using the Landauer formula

\[
I_c = \frac{e}{h} \int T(E) [f_R(E) - f_L(E)] \, dE, \tag{2}
\]

where \(f_{L/R}(E)\) are the Fermi functions for the left/right reservoir with chemical potentials \(\mu_{L/R}\) and temperatures \(T_{L/R}\). We consider a temperature bias, \(T_R > T_L\), beyond linear response, and no potential bias, \(\mu_L = \mu_R = \mu\).
Figure 2. The energy spectra for a cylindrical nanowire with $R = 30$ nm and $B = 4.0$ T. The spectrum for a weak electric field $\ell_E = 3.0R$ a) and strong magnetic field $\ell_E = 0.75R$ b). Degenerate cyclotron states at $k = 0$ in a) are split by the electric field as seen in b).

Realistic nanowires are never totally ballistic, but state-of-the-art nanowires are quasi-ballistic in the sense that transport measurements do show conductance steps [8, 10]. In order to model transport in the presence of impurities, we will introduce an impurity potential $V_{\text{imp}}(z, \varphi) = \sum_i W \delta(z - z_i) \delta(\varphi - \varphi_i)$, where $W$ is the impurity strength. We consider a fixed impurity configuration, i.e., no ensemble average. To some extent the results depend on the impurity configuration, as also seen in experiments. There, the conductance can show complicated, but reproducible behavior for a given nanowire, whereas the conductance for another nanowire will yield conductance whose structure (position of peaks, etc.) will be different [11], but reproducible as well. The transmission function in the case when impurities are included is obtained using the recursive Green’s function method [12, 6].

3. Results and discussion
In Fig. 2, a typical spectrum for the system is shown for $R = 30$ nm and magnetic field $B = 4.0$ T. A weak electric field $\ell_E = 3.0R$ in a) leaves the cyclotron and snaking states relatively unaffected but a stronger electric field, corresponding to $\ell_E = 0.75R$ in b), splits the states at $kR = 0$. Since the electric field is parallel to the magnetic field, the cyclotron states residing on the top and bottom of the nanowire get split by $E_x$, while the snaking states are mostly unchanged as the electrostatic potential is zero around $\varphi = \pm \pi/2$. The local magnetic field on the cylinder surface is determined by the orientation of the normal (which always points outwards) relative to the magnetic field (Fig. 1).

For given properties of the reservoirs ($\mu_{L,R}$ and $T_{L,R}$), the current is fully determined by the transmission function [12]. In the case of a ballistic wire, the transmission function can be found by simply counting the number of propagating modes. The important point here is that, due to the coexistence of cyclotron and snaking states the dispersion curve minima occur at non zero $kR$. Looking at the first energy band, one sees that, between the cyclotron maxima and snaking-state minima, there will be two propagating modes; when accounting for spin the transmission should be via $2 \times 2 = 4$ modes, which drops to $2 \times 1 = 2$ for energies above the cyclotron maximum at $kR = 0$. It is this drop in conductance, as a function of energy, that gives rise to the anomalous current [6]. The difference is Fermi functions is an odd function of energy around $\mu$, so placing $\mu$ where $T(E)$ drop, will lead to a negative (anomalous) current.

Figures 3 a) and 3 b) show the transmission function $T$ and the charge current $I_c$ versus temperature of the right contact, respectively, for $\ell_E = 3.0R$ (weak electric field) and for varying density of impurities, $n_i$. Analogous plots for a stronger electric field, $\ell_E = 0.75R$, are shown in Figures 3 c) and 3 d). The effect of the electric field is to split the cyclotron states at $k = 0$. The
Figure 3. For the weak electric field case $\ell_E = 3.0$, a) the transmission function $T$ and b) charge current $I_c$ are calculated for different impurity densities $n_i$. The anomalous current is clear and is in the range of 60 nA. In c) and d) the corresponding results for the strong electric field, $\ell_E = 0.75$, are shown. The lowest snaking states tend to get washed out more readily in the presence of a strong electric field.

cyclotron states that get lowered in energy are brought closer to the snaking states, making it easier to scatter from $k \rightarrow -k$. The impurities quickly reduce the anomalous structure in $T(E)$, eventually leading to full suppression at $n_i = 44$, see Fig. 3 d).

In conclusion, the applied electric field tends to suppress the snaking states, which in turn leads to a reduced anomalous current. The electric field also leads to increased effectiveness of electron backscattering from impurities. The electric field can thus be used to test the properties of the snaking states and the resulting current reversal.

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