Exchange and electric fields enhanced spin thermoelectric performance of germanene nano-ribbon

Jun Zheng¹, Feng Chi² and Yong Guo³,⁴

¹ College of New Energy, Bohai University, Jinzhou 121013, People’s Republic of China
² School of Physical Science and Technology, Inner Mongolia University, Huhehaote 010023, People’s Republic of China
³ Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, People’s Republic of China
⁴ Collaborative Innovation Center of Quantum Matter, Beijing, People’s Republic of China

E-mail: junzheng@semi.ac.cn

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Abstract

The spin thermoelectric performance in a germanene nano-ribbon is studied by using the nonequilibrium Green’s function method. We demonstrate theoretically that the temperature bias ΔT can generate spin thermopower when an exchange field breaks the edge states of germanene leads. However, the spin thermoelectric efficiency is quite low with its maximum $ZT_s \approx 0.01$. When applying strong electric field in the central region, a relatively large spin-dependent band gap can be opened, and hence the spin figure of merit is predicted to be more than 100 times larger than the case without external field. The remarkably enhancement of $ZT_s$ (larger than one) comes from the suppression of the thermal conductance and the improvement of the spin Seebeck effect. These striking properties make ferromagnetic leads germanene nano-ribbon a promising pure spin thermoelectric nanogenerator.

Keywords: spin thermoelectric effect, germanene, exchange field, staggered potential

(Some figures may appear in colour only in the online journal)
promising for this purpose, when non-magnetic perturbations (e.g. defects or disorders) are introduced into the transport system, edge states are topologically protected against scattering while phonons are significantly scattered. Specifically, as the width of germanene decreases, transport of edge states remains unchanged but the lattice thermal conductance depresses [10]. These unusual properties make the germanene suitable for use in the high-performance thermal spintronic devices.

Recently, using ab initio numerical methods the silicene nano-ribbons with zigzag edges are investigated by Zberecki et al [11] They found that the local spin density of silicene reveals edge magnetism. Moreover, the Seebeck coefficient can be enhanced significantly when the Fermi level is in the energy gap. Subsequently, Zberecki et al [12] studied the thermoelectric effects in silicene with Al and P impurity atoms, and found that appropriately arranged impurities can lead to a net magnetic moment and the spin thermopower can be considerably enhanced by the impurities. Using first-principles techniques, Yang et al [13] investigated the thermoelectric properties in mixed silicon and germanium structures. They have considered the influence of different widths, and found that the charge figure of merit $ZT$ of germanium nano-ribbon can reach up to 2.5 with the width decreasing. In a very recent work, Xu et al [14] demonstrate theoretically that the size parameter can be tuned to enhance charge figure of merit $ZT$ to be significantly greater than 1.

We propose a high-efficiency thermospin device constructed by a top-gated germanene sandwiched between two ferromagnetic electrodes. As shown in figure 1(a), the temperatures of two germanene leads are individually held at $T + \Delta T/2$ and $T - \Delta T/2$, where $\Delta T$ is the temperature difference between two leads. The germanene sheet is taken on the xy-plane, and apply an electric field $E_z(x, y)$ perpendicular to the central germanium region. Due to the buckled structure (see figure 1(b)), a staggered sublattice potential $\lambda_s$ generated between germanium atoms at A sites and B sites. By approaching to the ferromagnetic materials [15], or by doping with ferromagnetic dopants [16], an uniform exchange field can be introduced without structurally disturbing the germanene leads. Since the energy band structures of the germanene can be externally controlled by applying electric field [17] and exchange field [18]. In this letter, we focus on how the spin Seebeck effect can be achieved and how the spin thermoelectric performance can be improved by modulating the local exchange field and staggered potential.

2. Model and method

A generic buckled honeycomb germanene system is described by the four-band tight-binding model [19]

$$
H = -t \sum_{\langle ij \rangle, \sigma} e_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} e_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} + i \frac{\lambda_{so}}{3 \sqrt{3}} \sum_{\langle ij \rangle, \sigma} \sum_{\sigma' \sigma''} \nu_{ij} c_{i\sigma'}^\dagger \sigma_{ij \sigma''} c_{j\sigma''} + M \sum_{i \in \{L, R\}, \sigma} e_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma}
+ \lambda_v \sum_{i \in \{L, R\}, \sigma} \mu_i c_{i\sigma}^\dagger c_{i\sigma},
$$

where $i$ or $j$ is the index of the discrete honeycomb lattice site and $<ij>/<ij>$ run over all the nearest- or next-nearest-neighbor hopping sites. The spin index $\sigma = \uparrow, \downarrow$ corresponds with $\sigma = \pm 1$. The first term is the hopping term with the hopping energy $t$, $\nu_{ij}$ is the on-site energy, and in the absence of disorder, we set $\nu_i \equiv 0$ as the zero point of energy. The third term represents the effective spin–orbit coupling with strength $\lambda_{so}$. The fourth term represents the antiferromagnetic exchange magnetization with exchange field strength $M$. The $\lambda_v$ in last term is the staggered sublattice potential. Due to the buckled structure of germanene, the two sublattice planes are separated by a distance $2\sqrt{3}/3$ with $\ell^2 = 0.33 \, \AA$, as illustrated in figure 1(b). When applying an electric field $E_z(x, y)$, a staggered sublattice potential $\lambda_z = 2eE_z(x, y)$ can be generated between germanium atoms at A sites and B sites.

Using the Green’s function technique, the spin-dependent electric and heat currents in lead $\alpha$ can be expressed as the Landauer formula form [20, 21]

$$
\left( J^\alpha_x \frac{Q^\alpha}{Q} \right) = \frac{1}{h} \int \, dE \left[ e \left( E - E_{F_{\text{Val}}} \right) T_{\text{sc}} U_{\text{L}}(E) - f_{\text{B}}(E) \right],
$$

where $T_{\text{sc}} = \text{Tr} \left( U_{\text{L}}^0 G_{\text{sc}} U_{\text{L}}^0 G_{\text{sc}}^\dagger \right)$ is the electronic transmission coefficient with the linewidth function $\Gamma_{\text{sc}} = \text{Tr} \left( \Sigma_{\text{sc}}^{\text{ret}} - \Sigma_{\text{sc}}^{\text{in}} \right)$. The Green’s function $G_{\text{sc}}(E) = \left( G_{\text{sc}}(E) \right)^\dagger = \left[ E - \text{H}_{\text{sc}} - \Sigma_{\text{L}} - \Sigma_{\text{R}} \right]^{-1}$ where $\text{H}_{\text{sc}}$ is Hamiltonian matrix of the central region and $I$ is the unit matrix. $\Sigma_{\text{sc}}^{\text{ret}}$ is the retarded self-energy function of $\alpha$ lead. The self-energy function can be obtained from $\Sigma_{\text{sc}}^{\text{ret}} = \text{H}_{\text{sc}} \Sigma_{\text{L}}^{\text{ret}} \Sigma_{\text{R}}^{\text{ret}} \text{H}_{\text{sc}}$, where $\Sigma_{\text{L}}^{\text{ret}}$ is the coupling from central region to lead $\alpha$ and $\Sigma_{\text{R}}^{\text{ret}}$ is the surface retarded Green’s function of semi-infinite lead which can be calculated using transfer-matrix method [22, 23]. $f_{\text{B}}(E) = \left[ \frac{E - E_{F_{\text{B}}} + i\Gamma_{\text{B}}}{\sqrt{2}} \right]^\dagger$ is the Fermi-distribution function. As shown in figure 1, we set $T_L = T + \Delta T/2$ and $T_R = T - \Delta T/2$; $E_{F_{\text{L}}} = E_{F_{\text{R}}} + \Delta V_{\text{sc}}$, in which $\Delta V_{\text{sc}}$ is the spin bias induced by temperature difference $\Delta T$ across the device. After Taylor expansion of the Fermi–Dirac distribution function to the first order about $\Delta T$ and $\Delta V$, equation (2) can be written as

$$
\begin{pmatrix}
J_x
\frac{Q_s}{Q}
\end{pmatrix}
= \begin{pmatrix}
\frac{2e^2}{h} K_{\text{sc}} & \frac{2e}{hT} K_{\text{sc}}
\frac{2e}{hT} K_{\text{sc}} & \frac{2e}{hT} K_{\text{sc}}
\end{pmatrix}
\begin{pmatrix}
\Delta V_{\text{sc}}
\Delta T
\end{pmatrix},
$$

where $K_{\text{sc}}(E_{F_{\text{L}}}, T) = \int \, dE \left( -\frac{\partial f}{\partial \ln E} \right) (E - E_{F_{\text{L}}}) T_{\text{sc}}(E)$. Correspondingly, the spin-resolved conductance $G_{\text{sc}}$, thermopower $S_{\text{sc}}$, and electron thermal conductance $\kappa_{\text{sc}}$ are respectively given by:

$$
G_{\text{sc}} = \left( \kappa_{\text{sc}}(E_{F_{\text{L}}}, T) \right) / \hbar, \quad S_{\text{sc}} = -\kappa_{\text{sc}}(E_{F_{\text{L}}}, T) / \left( \hbar T K_{\text{sc}}(E_{F_{\text{L}}}, T) \right),
\quad \kappa_{\text{sc}} = \left[ K_{\text{sc}}(E_{F_{\text{L}}}, T) - K_{\text{sc}}(E_{F_{\text{R}}}, T) \right] / \left( \hbar T K_{\text{sc}}(E_{F_{\text{L}}}, T) \right).
$$

Finally, one can define the spin conductance $G_{\text{sc}}$, spin thermopower $S_s$, and electron thermal conductance $\kappa_s$ of the forms $G_{\text{sc}} = G_{\uparrow} - G_{\downarrow}$, $S_s = \left( S_\uparrow - S_\downarrow \right)$, $\kappa_s = \kappa_{\uparrow} + \kappa_{\downarrow}$, respectively. Once $G_{\text{sc}}$, $S_s$, and $\kappa_s$ are known, the spin figure of merit $ZT = S^2_s G/\kappa_s T$ can be calculated. For the topological insulators, the phonon thermal conductance can be significantly suppressed by reducing the system’s temperature and width or by introducing the non-magnetic perturbations (e.g. defects or disorders) into the
As the width and the temperature of germanene system is chosen to be relatively small, we neglected the phonon contribution to thermal conductance and restrict our discussion to the influence of electron.

### 3. Results and discussion

In the numerical calculations, we set the hopping energy $t$ as the energy unit, and fix $t = 1.3$ eV as in a real germanene sample [24]. The width of the sample is chosen as $N = 8$ in all calculations. In the experiment, a reasonable effective spin–orbit coupling value for germanene is about 43 meV [25], therefore we fix $\lambda_{so} = 0.03t$ throughout this paper.

We first consider the impact of exchange field (with strength $M = 0.02t$) on a perfect germanene nano-ribbon without staggered potential. The spin-resolved transmission function as well as the spin-polarized electronic bands calculated for two parallel ferromagnetic germanene leads, and non-ferromagnetic central region are presented in figure 2. As illustrated in figure 2(a), the spin-dependent transmission coefficient $T_{sa}$ have the perfect plateau structure, and obeys the electron–hole symmetry, $T_{sa}[−(EF − \sigma M)] = T_{sa}[(EF − \sigma M)]$. $T_{sa}$ exhibits the plateau structure with the plateau values at $1e^2/h$, $3e^2/h$, ..., i.e. at the half-integer position, $g(n + 1/2)e^2/h$ with the degeneracy $g = 2$. Especially, $T_{sa}$ have a dip with $T_{sa} = 0$ at $E_F = −\sigma M$.

In order to clarify the transport of the carriers, we present the band structures of the leads (see, figure 2(b)) and center region (see, figure 2(c)). Owing to the symmetry of bands, only the part of the moment $X < k_{xa} < \Gamma$ is shown. By applying an exchange field $M$ on the sample, the spin-up and spin-down bulk bands are split with the distance $2M$. Moreover, the corresponding pair of the gapless spin edge states is destroyed and a subgap is opened due to the
Figure 3. (a) The electrical conductance $G$, (b) thermal conductance $\kappa$, and (c) Seebeck coefficient $S$ as a function of Fermi energy $E_F$. (d) The spin figure of merit $ZsT$ versus $E_F$ for different values of exchange field $M$. The other parameters are the same as those of figure 2.

breaking of the local time reversal symmetry. Figure 2(b) clearly shows that the nanoribbon behaves like a ferromagnetic semiconductor with a spin-dependent energy gap in the vicinity around $E_F = -\sigma M$. For the non-ferromagnetic central region, we plot the typical band structure of a quasi-one dimensional ribbon in the topological nontrivial phase. As shown in figure 2(c), the bulk bands are gapped at Dirac points with magnitude $\Delta G = 2|\lambda_0 - \lambda_1|$. Within the bulk gap, there are two gapless edge states, corresponding to spin up (↑) and down (↓), respectively.

To facilitate discussion, the band indices are specified in figures 2(b) and (c). The +0-th and −0-th subbands in the band structures are nondegenerate, but other subbands are two-fold degenerated. According to the band-selective phenomenon [26], the electrons belong to the even (odd) parity subbands in the FM leads are transported only into the even (odd) parity subbands of the central region. Taking spin-up carriers for example, when $E_F > 0$, the +1-th subband and +0-th subband of the leads match that of the central region, hence the spin-up transmission coefficient is exactly 3. When $0.6 < E_F < 0$, only the +0-th subband is available, and $T_{\uparrow\uparrow}(E_F) = 1$. Due to the presence of spin-resolved energy gaps, the spin-σ channel is blocked for $E_F = -\sigma M$, where there is a dip in the transmission coefficient curve. By exactly the same reason, the nature of $T_{\sigma\sigma}(E_F)$ in the other energy region can also be understood.

In figures 3(a) and (b), we plot the electric conductance $G$ and thermal conductance $\kappa$, versus Fermi energy at $k_B T = 50 K$. At low temperatures where the Sommerfeld expansion is valid, $G_e$ and $\kappa_{\sigma\sigma}$ can be simplified to $G_e = c^2 T_{\sigma\sigma}$ and $\kappa_{\sigma\sigma} = 2\hbar T_{\sigma\sigma}$. The lineshape of spin-dependent electrical conductance (see, figure 3(a)) and thermal conductance (see, figure 3(b)) should resemble transmission coefficient $T_{\sigma\sigma}$ (see, figure 2(a)). However, it is worth noting that due to the influence of temperature (i.e. electrons are excited into the leads’ subgap), and due to the existence of scatter, $0 < G_e < 1$ in the energy rage of $[-\sigma 2M, 0]$. In the presence of exchange field, $G_\uparrow (\kappa_{\uparrow\uparrow})$ and $G_\downarrow (\kappa_{\downarrow\downarrow})$ become different from each other, giving rise to peaks and dips in the lineshape of $G_e = G_\uparrow - G_\downarrow$ and $\kappa_e = \kappa_{\uparrow\uparrow} + \kappa_{\downarrow\downarrow}$.

In figure 3(c), we show the Seebeck coefficient $S_e$ as functions of Fermi energy $E_F$. According to $S_e = -K_{\sigma\sigma}(E_F, T) / [e T (\sigma M, T)]$, spin-resolved Seebeck coefficient $S_e$ is an odd function of $E_F$, which means that contributions to $S_e$ from electrons and holes differ by a sign due to the electron-hole symmetry. Hence the Seebeck coefficient $S_e$ is negative (positive) for $E_F < -\sigma M$ ($E_F > -\sigma M$). $S_e$ peaks when Fermi energy crosses the discrete transverse channels where quantized transmission coefficient jumps from one step to another. As we discussed above, due to the existence of exchange field, the spin-up and spin-down electrons have different transmission coefficients, the Seebeck peaks of different spin orientations are separated in the energy space. It is interesting to note that, the spin-resolved thermopower $S_e$ vanishes, while $S_T$ remains finite, indicating that a pure spin-up or spin-down current can be obtained by a temperature gradient.
Figure 4. (a) The band structure of central region and electrical conductance $G$, (b) thermal conductance $\kappa_e$, and (c) Seebeck coefficient $S$ as a function of $E_F$ for $M = 0.02t$ and $\lambda_v = 0.04t$. (d) The spin figure of merit $ZsT$ versus $E_F$ for different values of stagger potential $\lambda_v$. The other parameters are the same as those of figure 2.

In figure 4(d), we depict the spin figure of merit $ZsT$ for different values of staggered buckle potential $\lambda_v$. It should be pointed out that, in contrast to the zero staggered potential case where the maximum of $ZsT$ originates mainly from the contribution of the spin thermopower $S$, the enhancement of $ZsT$ with regard to figure 4(d) comes from the combined action of the thermal conductance suppression and the spin thermopower enhancement. By using a STM probe, the local electric field could reach $E_l = 0.1 \text{ V} \text{ Å}^{-1}$ experimentally [27]. In this condition $\lambda_v = 2/E_F \approx 0.04t$ can be obtained, the spin figure of merit $ZsT$ is predicted to reach a maximum value of 1, which is two orders of magnitude larger than that achieved in figure 3(d).

Figure 5 shows the spin figure of merit $ZsT$ versus Fermi energy $E_F$ at fixed stagger potential $\lambda_v = 0.04t$ with different nanoribbon widths $N = 8, 16, 24, 32, 40$. As shown in figure 5, the spin figure of merit $ZsT$ in the bulk gap decrease rapidly with increasing the width of germanene nanoribbon. The decrease of $ZsT$ originates from the suppression of spin thermopower and the enhancement of electron thermal conductance. However, it should be pointed out that even the $ZsT$ decays with the width, it still maintain orders of magnitude greater than the $ZsT$ values found in the case of $\lambda_v = 0$.

4. Summary

In summary, we have studied the spin thermoelectric effects in a germanene coupled to ferromagnetic leads with stagger
potential. It is found that the thermoelectric efficiency is sensitively dependent on the exchange field and electric field. In the presence of exchange field ($M \neq 0$) on the leads of the sample, a spin-resolved subgap is opened due to the local time reversal symmetry breaking, so that the spin-dependent thermopower can be thermally generated when Fermi energy crosses the discrete transverse channels. However, the $Z_T$ values are quite small and are unaffected by different exchange field strength $M$. The maximum $Z_T$ is less than 0.015 when only the effect of ferromagnetic electrodes is considered.

In addition, we present a possibility of the optimization of thermoelectric properties by modulating the staggered potential $\lambda_s$ in terms of the enhanced thermopower, together with the depressed thermal conductance. With increasing the staggered potential of central region, the spin figure of merit can be increased by more than two orders of magnitude. Moreover, the pure spin-up (spin-down) Seebeck effect can be observed with relatively high $Z_T$ values. The magnitude of spin figure of merit can reach impressive values ($Z_T > 1$), which is favorable in the application of spin thermoelectric nanogenerator.

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