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

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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 ZsT = 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 ZsT (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)

1. Introduction

In view of possible applications in spintronic devices, the recently invigorated field of spin caloritronics focuses on the interaction of spin with heat current [1]. A great stimulus for the field has been the discovery of the spin Seebeck effect [2], a spin analog of the usual Seebeck effect. This novel phenomenon offers a new way of controlling electron spin, and can be applied directly to make thermal spin generators for driving spintronic devices. In analogy to the charge Seebeck effect, the ability of thermoelectric materials to convert a temperature gradient into spin voltage or spin current can be measured by the spin figure of merit, which is defined as ZsT = SsT/(κs + κp) [3]. Improving the thermoelectric figure of merit is one of the greatest challenges in material science [4]. It has been theoretically predicted [5] and then experimentally confirmed [6, 7] that low-dimensional and nanostructured materials can have much larger values of ZsT than their bulk counterparts due to the quantum confinement effect and electronic interactions.

As a two-dimensional single atomic layer extracted from germanium, germanene sheet has been synthesized recently [8, 9]. Compared with graphene and silicene, germanene exhibits a sizable band gap at the Dirac point opened by the stronger spin–orbit coupling and higher buckling. To get a large quantity ZsT, higher spin thermopower Ss and conductance Gs, but lower thermal conductance κs + κp are required. The time-reversal symmetry protected edge states of germanene are quite...
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 \textit{ab initio} numerical methods the silicene nano-ribbons with zigzag edges are investigated by Zberecki \textit{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 \textit{et al} [12] studied the thermo-electric 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 \textit{et al} [13] investigated the thermo-electric properties in mixed silicon and germanium structures. They 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 \textit{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 \(E_x(x, y)\) perpendicular to the central germanene region. Due to the buckled structure (see figure 1(b)), a staggered sublattice potential \(\lambda_y\) 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 thermo-electric 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]

\[
H = -t \sum_{<ij>,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i} \epsilon_i c_{i\sigma}^\dagger c_{i\sigma} + \frac{\lambda_{so}}{3\sqrt{3}} \sum_{<ij>,\sigma} \epsilon_{ij} c_{i\sigma}^\dagger \sigma \sigma' c_{j\sigma'} + M \sum_{i \in (\text{L,R}),\sigma} c_{i\sigma}^\dagger c_{i\sigma} + \lambda_x \sum_{i \in (M\text{R})} \mu_i c_{i\sigma}^\dagger c_{i\sigma},
\]

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 \(\epsilon_i\) is the on-site energy, in the absence of disorder, we set \(\epsilon_i = E_0\) as the zero point of energy. The second 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 \(\lambda_y\) in last term is the staggered sublattice potential. Due to the buckled structure of germanene, the two sublattice planes are separated by a distance \(2\ell\) with \(\ell = 0.33\) Å, as illustrated in figure 1(b). When apply an electric field \(E_x(x, y)\), a staggered sublattice potential \(\lambda_y = 2\ell E_x(x, y)\) 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]

\[
\left( \frac{J^\alpha}{Q^\alpha} \right) = \frac{1}{\hbar} \int dE \left( -e - E + E_{\text{Ferm}} \right) T_{\text{ref}} U_{LL}(E) - f_{\text{ref}}(E),
\]

where \(T_{\text{ref}} = T[|\Sigma_{\text{ref}}|^2 G_{\text{ref}}(E)]\) is the electronic transmission coefficient with the linewidth function \(\Gamma_{\text{ref}} = i(\Sigma'_{\text{ref}} - \Sigma_{\text{ref}})\). The Green’s function \(G_{\text{ref}}(E) = [G_{\text{ref}}(E)]^\dagger = [E - H_0 - \Sigma_{\text{ref}} - \Sigma_{\text{ref}}]^{-1}\) where \(H_0\) is Hamiltonian matrix of the central region and \(i\) is the unit matrix. \(\Sigma'_{\text{ref}}\) is the retarded self-energy function of \(\alpha\) lead. The self-energy function can be obtained from \(\Sigma_{\text{ref}} = H_0 g_{\text{ref}} H_{\text{ref}}\), where \(H_{\text{ref}}\) is the coupling from central region to lead \(\alpha\) and \(g_{\text{ref}}\) is the surface retarded Green’s function of semi-infinite lead which can be calculated using transfer-matrix method [22, 23]. \(f_{\text{ref}}(E) = [\delta(E-E_{\text{Ferm}})] + 1\) is the Fermi-distribution function. As shown in figure 1, we set \(T_L = T + \Delta T/2\) and \(T_R = T - \Delta T/2\); \(E^R = E^R - \Delta V_r\) in which \(\Delta V_r\) 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

\[
\left( J^\alpha \right) \left( Q^\alpha \right) = \left( \begin{array}{c} \frac{2e^2}{\hbar} K_{\text{ref}} + \frac{2e}{hT} K_{\text{ref}} \\ -\frac{2e}{hT} K_{\text{ref}} + 2 \frac{K_{\text{ref}}}{hT} \end{array} \right) \left( \Delta V_r \right). \Delta T \right)
\]

where \(K_{\text{ref}}(E_v, T) = \int dE \langle -\partial f\partial E\rangle(E - E_v)^r T_{\text{ref}}(E)\). Correspondingly, the spin-resolved conductance \(G_{\alpha}\), thermopower \(S_{\alpha}\), and electron thermal conductance \(\kappa_{\alpha}\) are respectively given by:

\[
G_{\alpha} = e^2 K_{\text{ref}}(E_v, T)/h, \quad S_{\alpha} = -K_{\text{ref}}(E_v, T)/[eT K_{\text{ref}}(E_v, T)], \quad \kappa_{\alpha} = \left[ K_{\text{ref}}(E_v, T) - K_{\text{ref}}(E_v, T)/K_{\text{ref}}(E_v, T) \right] / (hT).
\]

Finally, one can define the spin conductance \(G_{\alpha}\), spin spin thermopower \(S_{\alpha}\), and electron thermal conductance \(\kappa_{\alpha}\) of the forms \(G_{\alpha} = G_{\uparrow} - G_{\downarrow}\), \(S_{\alpha} = \{S_{\uparrow} - S_{\downarrow}\}, \quad \kappa_{\alpha} = \kappa_{\uparrow} + \kappa_{\downarrow}\), respectively. Once \(G_{\uparrow, \downarrow}\), \(S_{\uparrow, \downarrow}\), and \(\kappa_{\uparrow, \downarrow}\) are known, the spin figure of merit \(ZT = S_{\alpha}^2 G_{\alpha}/T\kappa_{\alpha}\) 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
transport system [14]. 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 $t_1 = 1.3$ 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 $T_{\sigma}$ have the perfect plateau structure, and obeys the electron–hole symmetry, $T_{\sigma} = T_{\overline{\sigma}}$, i.e. at the half-integer position, $g(n + 1/2)e^2/h$ with the degeneracy $g = 2$. Especially, $T_{\sigma}$ have a dip with $T_{\sigma} = 0$ 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 $X < k_x < \Gamma$ 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 1](image1.png)

**Figure 1.** Schematic plot of a germanene nano-ribbon with an exchange field on the leads and a metallic gate on the top of the central region. The temperatures of the left and right leads are individually $T_L = T_e + \Delta T/2$ and $T_R = T_e - \Delta T/2$.

![Figure 2](image2.png)

**Figure 2.** The band structure of ferromagnetic leads and non-ferromagnetic central region as a function of Fermi energy $E_F$ are shown in (a) and (b). (c) The transmission coefficient $T_{\sigma}$ versus $E_F$ for $M = 0.02t$. The system equilibrium temperature is fixed at 50 K.
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 $\Delta G = 2|\lambda_0 - \lambda_c|$. Within the bulk gap, there are two gapless edge states, corresponding to spin up ($\uparrow$) and down ($\downarrow$), respectively.

To facilitate discussion, the band indexes 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 $E_F > 0.6$, 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 $T_{\uparrow}(E_F) = 1$. Due to the presence of spin-resolved energy gaps, the spin-$\sigma$ 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 $T_{\uparrow\sigma}(E_F)$ in the other energy region can also be understood.

In figures 3(a) and (b), we plot the electric conductance $G$ and thermal conductance $\kappa_e$ versus Fermi energy at $k_B T = 50 K$.

At low temperatures where the Sommerfeld expansion is valid, $G_e$ and $\kappa_{e\sigma}$ can be simplified to $G_e = \frac{e^2}{h}T_{\uparrow\sigma}$ and $\kappa_{e\sigma} = \frac{e^2h}{2}\Sigma T_{\uparrow\sigma}$. The lineshape of spin-dependent electrical conductance (see, figure 3(a)) and thermal conductance (see, figure 3(b)) should resemble transmission coefficient $T_{\uparrow\sigma}$ (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, $G_{\uparrow}(\kappa_{\uparrow\downarrow})$ and $G_{\downarrow}(\kappa_{\uparrow\downarrow})$ become different from each other, giving rise to peaks and dips in the lineshape of $G_e = G_{\uparrow} - G_{\downarrow}$ and $\kappa_e = \kappa_{\uparrow\downarrow} + \kappa_{\uparrow\downarrow}$.

In figure 3(c), we show the Seebeck coefficient $S_e$ as functions of Fermi energy $E_F$. According to $S_e = -K_{0\uparrow}(E_F, T)/(eTK_{0\uparrow}(E_F, T))$, 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 3. (a) The electrical conductance $G$, (b) thermal conductance $\kappa_e$, 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.
Figure 4. (a) The band structure of central region and electrical conductance $G$, (b) thermal conductance $k_{\sigma}$, and (c) Seebeck coefficient $S$ as a function of $E_F$ for $M = 0.02t$ and $\lambda_s = 0.04t$. (d) The spin figure of merit $Z_sT$ versus $E_F$ for different values of stagger potential $\lambda_s$. The other parameters are the same as those of figure 2.

Figure 3(d) depicts the spin figure of merit $Z_sT$ for different values of exchange magnetization $M$. As shown in figure 3(d), the positions of peaks can be changed by the exchange field, but the maximum magnitude of $Z_sT$ is unaffected by the strength of $M$. The higher peaks emerge close to the energy states, where the spin thermopower have large values. It is worth noting that only considers the effect of ferromagnetic electrodes, the $Z_sT$ values are quite small with its maximum value less than 0.015.

Next, we study the influences of the staggered potential $\lambda_s$ on the thermoelectric quantities. For the region of bulk gap, the transmission coefficients are sensitively depend on $\lambda_s$. As the dotted line shown in figure 4(a), a spin-dependent energy gap can be opened due to the inversion symmetry breaking induced by the staggered sublattice potential and the magnitude of the gap is $2\lambda_s$. As $2\lambda_s$ is much more greater than $k_B T$, the conductance channel with spin $\sigma$ carriers is blocked, therefore, spin $\sigma$ electric conductance and thermal conductance are suppressed in the vicinity of $E_F \in [-2\lambda_s, 0]$, which is depicted in figures 4(a) and (b).

The spin thermopower peak shown in figure 4(c) increases remarkably as compared to figure 3(c). This is because with the assistance of staggered potential $\lambda_s$, the damage of spin edge sates is strengthen, the transport of spin electrons is further suppressed. According to the definition of thermopower, in order to balance the thermal forces acting on the charge carriers, one has to add a larger bias for the lower electric conductance case, which in turn leads to a larger thermopower. Therefore, the enhancement of the buckled potential is accompanied by a concomitant increase in the maximum value of $S_s$.

In figure 4(d), we depicts the spin figure of merit $Z_sT$ for different values of staggered buckle potential $\lambda_s$. It should be pointed out that, in contrast to the zero staggered potential case where the maximum of $Z_sT$ originates mainly from the contribution of the spin thermopower $S_s$, the enhancement of $Z_sT$ 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 $E_s = 0.1 V \, A^{-1}$ experimentally [27]. In this condition $\lambda_s = 2E_F/\lambda_s \approx 0.04t$ can be obtained, the spin figure of merit $Z_sT$ 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 $Z_sT$ versus Fermi energy $E_F$ at fixed stagger potential $\lambda_s = 0.04t$ with different nanoribbon widths $N = 8, 16, 24, 32, 40$. As shown in figure 5, the spin figure of merit $Z_sT$ in the bulk gap decrease rapidly with increasing the width of germanene nanoribbon. The decrease of $Z_sT$ originates from the suppression of spin thermopower and the enhancement of electron thermal conductance. However, it should be pointed out that even the $Z_sT$ decays with the width, it still maintain orders of magnitude greater than the $Z_sT$ values found in the case of $\lambda_s = 0$.

4. Summary

In summary, we have studied the spin thermoelectric effects in a germanene coupled to ferromagnetic leads with stagger
values are favorable. The magnitude of spin figure of merit is less than 0.015 when only presence of exchange field $(\mathcal{M} \neq 0)$ 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 depressed thermal conductance. With increasing the staggered potential $\lambda_e$ 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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**References**

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![Figure 5](https://example.com/figure5.png)

Figure 5. The spin figure of merit $Z_T$ versus Fermi energy $E_F$ for different nanoribbon widths $N = 8, 16, 24, 32, 40$. The stagger potential is fixed at $\lambda_e = 0.04t$. The other parameters are the same as those of figure 2.