Contents lists available at ScienceDirect

Physics Letters A







Anisotropic spin-dependent thermopower and current in ferromagnetic graphene junctions



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A R T I C L E I N F O

ABSTRACT

Article history: Received 15 July 2013 Received in revised form 6 October 2013 Accepted 23 October 2013 Available online 25 October 2013 Communicated by R. Wu

Keywords: Anisotropic spin thermopower Pure spin current Two-dimensional graphene

1. Introduction

Spin caloritronics, the combination of thermoelectrics and spintronics, focusing on heat and spin transport, has attracted much interest [1-13]. A notable recent discovery of spin caloritronics is the observation of spin Seebeck effect by Uchida et al. [1], which further inspires widely experimental and theoretical investigations. The spin Seebeck effect was observed in various materials ranging from the metallic ferromagnets Co₂MnSi [2] to the semiconducting ferromagnet (Ga,Mn)As [3], and even in the insulating magnets LaY₂Fe₅O₁₂ [4] and (Mn,Zn)Fe₂O₄ [8]. Jia and Berakdar [6] also theoretically investigated the anisotropic charge and spin thermopower across normal-metal/helical-multiferroic/ferromagnetic heterojunctions. However, the spin thermopower in these bulk samples is so weak that it may be overwhelmed by the accompanied charge thermopower of several orders larger. In addition, the temperature difference unavoidably generates also a regular voltage bias across the sample, which may preclude easy applicability in spintronic devices.

On the other hand the spin-dependent thermoelectric properties of graphene have also attracted a great attention [14–19]. Thermally driven spin-polarized currents through a magnetized zigzag graphene nanoribbon(ZGNR)-based device have been reported in Refs. [14–16]. Zeng et al. [17] found a very large multivalued and controllable thermal magnetoresistance and charge Seebeck effects in a spin valve which consists of ZGNR electrodes with different magnetic configurations. Cheng [18] investigated the

We study the spin-dependent thermoelectric transport through two-dimensional normal/ferromagnetic/ normal/ferromagnetic/normal graphene (NG/FG/NG/FG/NG) junctions. It is found that both charge and spin thermopowers depend on the FG's magnetization direction and exhibit an anisotropic behavior. Interestingly, the spin thermopower can be as large as the charge thermopower and even can exceed the latter in magnitude. Moreover, the pure spin thermopower and spin current emerge in this device. The results obtained here suggest a feasible way of enhancing thermospin effects and generating the pure spin current in two-dimensional graphene.

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spin thermopower and thermoconductance properties in a ferromagnetic zigzag edged graphene nanoribbon. The results indicate that two mechanisms, Klein tunneling and the band selective rule, are involved to determine the thermoelectric properties. However, the results obtained for such heterostructures were shown to be very sensitive to the device geometry, e.g., the device length and the disorder effects [14–16,18,20]. So, their use for realistic applications is not realized till now due to the extreme difficulty in the experimental implementation. In this view, besides better understanding the thermoelectric transport in graphene quantum structures, the investigation of the spin-dependent thermopower based on two-dimensional (2D) graphene is desirable for the development of such materials in spin caloritronics.

In this paper we study the spin-dependent thermoelectric transport through 2D normal/ferromagnetic/normal/ferromagnetic/ normal graphene (NG/FG/NG/FG/NG) junctions. Both charge and spin thermopowers depend on the magnetization direction of the right FG and become strongly anisotropic. The spin thermopower can be as large as the charge thermopower and even can exceed the latter in magnitude. Moreover, the pure spin thermopower and spin current can be obtained in this device.

2. Model and formulation

The device we consider here is a 2D NG/FG/NG/FG/NG junction with a temperature bias $\Delta T = T_L - T_R$, where T_L (T_R) is the temperature in the left (right) lead (Fig. 1(a)). The graphene is parallel to the *x*-*y* plane. The NG/FG (or FG/NG) interfaces locate at x = 0, *L*, 2*L*, and 3*L*, respectively, where the *x* axis is chosen to be perpendicular to the interface. The ferromagnetism in the FG regions can be induced by doping and defect or putting

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^{0375-9601/\$ -} see front matter © 2013 Elsevier B.V. All rights reserved. http://dx.doi.org/10.1016/j.physleta.2013.10.037



Fig. 1. (a) A schematic diagram of a 2D NG/FG/NG/FG/NG junction with a temperature bias. (b) Dispersion relation of the device in the parallel (antiparallel) magnetization configuration.

a magnetic insulator bar onto a graphene sheet [21,22]. The magnetization vector in the FG regions is $\vec{h}(\mathbf{r}) = h(\sin\theta, 0, \cos\theta)$ with h the magnitude of exchange field. The magnetization in the left FG is assumed along the z axis, i.e., $\theta = 0$; while that in the right FG orients along the $(\sin\theta, 0, \cos\theta)$ direction, which can be controlled by a weak external magnetic field. The Hamiltonian of such a structure simply reads [23]

$$\hat{H} = v_F \sigma_0 \otimes (\vec{\tau} \cdot \vec{p}) + (\vec{\sigma} \cdot \vec{h}(\mathbf{r})) \otimes \tau_0, \tag{1}$$

where $v_F \approx 10^6$ m/s is the Fermi velocity, $\vec{\tau} = (\tau_x, \tau_y)$ and $\vec{\sigma} = (\sigma_x, \sigma_y)$ are Pauli matrices in pseudospin and spin space, and σ_0 and τ_0 are unit matrices. Dispersion relation of the device in the NG and FG regions is illustrated in Fig. 1(b).

Consider a spin- σ ($\sigma = \uparrow, \downarrow$, or \pm) electron incident from the left lead on the NG/FG interface at an angle ϕ to the interface normal. The wave functions are given as follows. In the left and right leads $\Psi_L = \psi_{\sigma}^+ + r_{\uparrow\sigma}\psi_{\uparrow}^- + r_{\downarrow\sigma}\psi_{\downarrow}^-$, and $\Psi_R = t_{\uparrow\sigma}\psi_{\uparrow}^+ + t_{\downarrow\sigma}\psi_{\downarrow}^+$; In the middle NG region $\Psi_M = p\psi_{\uparrow}^+ + q\psi_{\downarrow}^+ + m\psi_{\uparrow}^- + n\psi_{\downarrow}^-$, ψ_{σ}^+ and ψ_{σ}^- are $\psi_{\uparrow}^{\delta} = (1, \delta e^{\delta i\phi}, 0, 0)^T e^{\delta i kx}$ and $\psi_{\uparrow}^{\delta} = (0, 0, 1, \delta e^{\delta i\phi})^T e^{\delta i kx}$, where the superscript T denotes transposition and $\delta = \pm 1$. In the left (right) FG region we have $\Psi_F = a_{L(R)}\psi_{F\uparrow}^+ + b_{L(R)}\psi_{F\downarrow}^+ + c_{L(R)}\psi_{F\uparrow}^- + d_{L(R)}\psi_{F\downarrow}^-$, where the wave functions are $\psi_{F\uparrow}^{\delta} = (\cos(\theta_1), \delta \cos(\theta_1) e^{i\delta\phi_{\uparrow}}, \sin(\theta_1), \delta \sin(\theta_1) e^{i\delta\phi_{\uparrow}})^T e^{i\delta k_{\uparrow}x}$ and $\psi_{F\downarrow}^{\sigma} = (-\sin(\theta_1), -\delta \sin(\theta_1) e^{i\delta\phi_{\downarrow}}, \cos(\theta_1), \delta \cos(\theta_1) e^{i\delta\phi_{\downarrow}})^T e^{i\delta k_{\downarrow}x}$ with $\theta_1 = 0$ ($\theta/2$) in the left (right) FG region. The wave vectors are $k = E \cos\phi/\hbar v_F$, $k_{\sigma} = \sqrt{(E + \sigma h)^2 - (\hbar v_F k_y)^2}/\hbar v_F$, and $k_y = E \sin\phi/\hbar v_F = (E + \sigma h) \sin\phi_{\sigma}/\hbar v_F$. By matching the wave functions at the NG/FG interfaces, we can obtain the reflection and transmission coefficients $r_{\uparrow\sigma}$ and $t_{\uparrow\sigma}$ ($t_{\downarrow\sigma}$ and $r_{\downarrow\sigma}$) in the spin-up (spin-down) channel. The current can be given as

$$I_{\sigma} = \frac{e}{h} \int dE N(E) \int d\phi \cos \phi T_{\sigma} \left[f_{L}(E) - f_{R}(E) \right]$$
(2)

with the transmission probability in the spin- σ channel $T_{\sigma} = |t_{\sigma\sigma}|^2 + |t_{\sigma\bar{\sigma}}|^2$, $N(E) = \frac{|E+V|W}{\hbar v_F}$ and W the width of the graphene sheet. $f_{L(R)}(E) = \{1 + \exp[(E - E_F)/k_B T_{L(R)}]\}^{-1}$ stands for the Fermi distribution function in the L(R) lead and E_F is the Fermi energy.

Utilizing the linear response assumption, i.e., $T_L \approx T_R = T$, the spin-dependent current can be rewritten as

$$I_{\sigma} = eL_{0\sigma} \Delta \mu_{\sigma} + \frac{e}{T} L_{1\sigma} \Delta T, \qquad (3)$$

where $\Delta \mu_{\sigma} = e \Delta V_{\sigma}$ is the difference in the chemical potentials of the two leads in the spin- σ channel, and $\Delta V_{\sigma} = (\Delta V_e + \frac{1}{2}\sigma \Delta V_s)$ with $\Delta V_e = [\frac{1}{2}(\mu_{R\uparrow} + \mu_{R\downarrow}) - \frac{1}{2}(\mu_{L\uparrow} + \mu_{L\downarrow})]/e$ the charge bias. As the transmission is spin dependent, the temperature gradient may lead to a spin accumulation in the leads, which generally results in a nonzero spin-voltage bias $\Delta V_s = (\delta \mu_R - \delta \mu_L)/e$, where $\delta \mu_i =$ $\delta \mu_{i\uparrow} - \delta \mu_{i\downarrow}$ (i = L, R) with $\delta \mu_{i\sigma}$ the electrochemical potential of the spin- σ channel in the *i* lead. The coefficients $L_{n\sigma}$ (n = 0, 1, 2) are defined as $L_{n\sigma} = \frac{1}{h} \int dE(E - E_F)^n N(E) \int d\phi T_{\sigma} \cos\phi[-\frac{\partial f(E)}{\partial E}]$, where f(E) is the Fermi–Dirac distribution function. Thus, one can introduce the spin-dependent thermopower S_{σ} by taking $I_{\sigma} = 0$ [6,24,25],

$$S_{\sigma} = \frac{\Delta V_{\sigma}}{\Delta T} = -\frac{1}{eT} \frac{L_{1\sigma}}{L_{0\sigma}}.$$
(4)

The charge thermopower S_c and the spin thermopower S_s are calculated as

$$S_c = \frac{1}{2}(S_{\uparrow} + S_{\downarrow}),\tag{5}$$

and

$$S_s = \frac{1}{2}(S_{\uparrow} - S_{\downarrow}). \tag{6}$$

3. Results and discussions

We perform numerical calculations for h = 5 meV, L = 500 nm and T = 10 K. In Fig. 2(a), the charge thermopower S_c and spin thermopower S_s are plotted as a function of the Fermi energy E_F . As shown in Fig. 2(a), S_c in both parallel $\theta = 0$ and antiparallel $\theta = \pi$ magnetization configurations vary rather sharply in the symmetry point $E_F = 0$, where S_c changes sign and reaches the maxima on one side of $E_F = 0$ and the minima on the other side. When E_F is far away from zero, $|S_c|$ decreases with E_F . However, in contrast to S_c , S_s strongly depends on the magnetization configuration. For the antiparallel magnetization configuration S_s is always zero (dash dot line in Fig. 2(a)). While for the parallel configuration S_s is an even function of E_F and can reach a minimum at $E_F = 0$, where S_c is zero, so we can obtain a pure spin thermopower. It should be pointed that S_s can be as large as S_c and even can exceed the latter in magnitude. This is very different from the results in Refs. [1-6], where S_s is so weak that it may be overwhelmed by the accompanied S_c of several orders larger.

In order to explain the underlying physics, we plot the spindependent thermopower S_{σ} in the parallel magnetization configuration as a function of E_F in Fig. 2(b). It is found that S_σ has the following symmetry $S_{\sigma}(E_F) = -S_{\bar{\sigma}}(-E_F)$. At $E_F = 0$, we obtains $S_{\uparrow}(0) = -S_{\downarrow}(0)$, so a pure spin thermopower but no charge counterpart can be generated. The behaviors of S_{σ} can be understood from the dispersion relation of the device we consider (Fig. 1(b)). For the parallel magnetization configuration, the dispersion relations for the spin-up and spin-down channels are symmetrical about $E_F = 0$. S_σ can be rewritten as $S_{\sigma} = -|S_{e\sigma}| + S_{h\sigma}$, where $-|S_{e\sigma}| (S_{h\sigma})$ is the contribution of electrons (holes) with energy near the Fermi energy to S_{σ} . Due to the symmetry of the dispersion relations we observe $|S_{e\sigma}(E_F)| =$ $S_{h\bar{\sigma}}(-E_F)$ and $|S_{e\bar{\sigma}}(-E_F)| = S_{h\sigma}(E_F)$, which leads to the relation $S_{\sigma}(E_F) = -S_{\bar{\sigma}}(-E_F)$. However, for the antiparallel configuration we can find the thermopower S_{σ} is spin-independent and S_s is zero. This can be understand as follows. For the antiparallel configuration, the transport of σ spin from left to right is equal to that for $\bar{\sigma}$ spin from right to left by the structure symmetry, so the transmission probabilities have the relation

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