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# Spin caloritronics in graphene

H.O. Frota, Angsula Ghosh *

*Department of Physics, Federal University of Amazonas, Av. Rodrigo Octavio 3000-Japiim, 69077-000 Manaus, AM, Brazil*

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ABSTRACT

Spin caloritronics, the combination of spintronics with thermoelectrics, based on spin and heat transport has attracted a great attention mainly in the development of low-power-consumption technology. In this work we study the thermoelectric properties of a quantum dot attached to two single layer graphene sheets as leads. The temperature difference on the two graphene leads induces a spin current which depends on the temperature and chemical potential. We demonstrate that the quantum dot behaves as a spin filter for selected values of the chemical potential and is able to filter electrons by their spin orientation. The spin thermopower has also been studied where the effects of the chemical potential, temperature and also the Coulomb repulsion due to the double occupancy of an energy level have been observed.



## 1. Introduction

The electron spin, the elementary nanomagnet, is a new paradigm for information processing. The growth of the information technology sector makes magnetism the main repository of information storage. Moreover, the dissipation of heat energy is one of the critical issues as we observe a decrease in the size of the electronic devices to nanoscale dimensions and an increase in the operating speed. Spintronics along with the thermoelectronics, generation of electric voltage in the presence of temperature difference, are studied in an emerging field called spin caloritronics. The spin-Seebeck effect is one of the core elements of spin caloritronics demonstrated recently in ferromagnetic metal (NiFe alloy), semiconductor (GaMnAs) and insulator ($LaY_2Fe_5O_{12}$) [1–3]. The temperature difference generates the spin-up and the spin-down current opening a possibility of conversion of heat into electricity and thus its applicability in low-power consumption devices. Moreover, spin-filters also offer a promising path to detect (read out) spin-single states. Spin filters in the form of magnetic semiconductors have been studied in recent years [4]. However, many recent proposals focus on spin-filtering in a two-dimensional electron gas as it allows easy integration with other devices such as electron spin entanglers [5]. Spin-dependent electron transport through a two-dimensional electron gas with giant Zeeman splitting has also been recently studied [6]. Moreover, quantum dots within a bi-dimensional electron gas have been shown to act as spin filters [7].

The fascinating electronic properties of graphene make it an excellent candidate for spintronic application [8–14]. The key attraction is the long spin lifetime due to the small spin–orbit coupling of carbon atoms and the absence of the nuclear spins for the main isotope. Moreover, the high electron velocity related to the linear dispersion relation increases its potential for spintronics. The spin diffusion distances in graphene exceed 100 μm and are much longer [15] than conventional metals and semiconductors. Thereby the devices in which the information is coded by pure spin currents are benefited. Several spintronic devices have been proposed. For example the “all spin logic” circuits are based on the transport and information coded by spin currents [16]. The transport of spin information with limited spin-losses (efficiency up to 75%) and the large electric signal due to spin-polarized currents have already been exhibited [15]. Hence, the identification of graphene as a pertinent medium for transport of spin information [17] over macroscopic distances with limited losses poses it as a potential candidate for further theoretical research. Studies involving interfaces with ferromagnetic materials or impurities [18,19], with large spin-orbit interactions [20–22] and structural tuning of magnetic properties deserve to be mentioned. Graphene nanoribbons are also notable for their application in spintronics devices such as spin-filter [23], spin valve [24,25], giant magnetoresistance devices [14,26], etc.

Recently, a high efficiency spin caloritronics device based on zigzag graphene nanoribbon, a heterojunction consisting of single-hydrogen-terminated ZGNR (ZGNR-H) and double-hydrogen terminated ZGNR ($ZGNR\text{-}H_2$) was proposed that predicted the properties of the spin current along with the spin-Seebeck effect [27]. Moreover, the thermally induced spin current in magnetized graphene nanoribbons

* Corresponding author.
*E-mail address:* angsula@ufam.edu.br (A. Ghosh).

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has also been explored [28]. In this work we calculate the spin current across the magnetic quantum dot (MQD) connected to two graphene leads which are in equilibrium with reservoirs kept at spin dependent chemical potentials $\mu_{\alpha,\sigma}$, where the lead $\alpha = L$, $R$ and $\sigma$ represents the spin. The spin currents are induced by $\Delta T$, the temperature difference between the left electrode ($T_L$) and the right electrode ($T_R$). The work proposes a device that acts as spin filter for specific values of the chemical potential. Spin filter devices can be used for initialization and read-out of spin quantum bits [29], thus serving as future applications in computer hardwares. The spin-Seebeck coefficient has also been considered for the MQD attached to graphene leads at different temperatures and various positions of the Fermi level compared to the energy level of the dot. The Seebeck coefficients of the spin-up and spin-down electrons have also been calculated for the above system.

## 2. The magnetic quantum dot model (MQD)

The present magnetic quantum-dot (MQD) model involves a magnetic quantum dot coupled to two single-layer graphene leads. The tight binding Hamiltonian of the electrons in graphene is deduced assuming the complicated energy structure of $sp^2$ bonded carbon atoms and can be obtained assuming the two sublattices with a nearest neighbor interaction. The Hamiltonian can be written in the momentum space utilizing the physics of the two bands in the honeycomb lattice. The Hamiltonian is thus given by

$$H = \sum_{\mathbf{k}\alpha\sigma} [\epsilon_{+\alpha}(\mathbf{k}) c^{\dagger}_{\mathbf{k}\alpha\sigma} c_{\mathbf{k}\alpha\sigma} + \epsilon_{-\alpha}(\mathbf{k}) d^{\dagger}_{\mathbf{k}\alpha\sigma} d_{\mathbf{k}\alpha\sigma}] + \epsilon_{f\sigma} c^{\dagger}_{f\sigma} c_{f\sigma} + \frac{1}{\sqrt{2}} \sum_{\mathbf{k}\alpha\sigma} V_{\alpha} [c^{\dagger}_{f\sigma} c_{\mathbf{k}\alpha\sigma} + c^{\dagger}_{f\sigma} d_{\mathbf{k}\alpha\sigma} + H.c], \quad (1)$$

where the operator $c_{\mathbf{k}\alpha\sigma}$ ($c^{\dagger}_{\mathbf{k}\alpha\sigma}$) and $d_{\mathbf{k}\alpha\sigma}$ ($d^{\dagger}_{\mathbf{k}\alpha\sigma}$) annihilate (create) states with spin $\sigma$ in lead $\alpha = L, R$ on the two sublattices of the graphene sheet. The energies on the two sub lattices are given by $\epsilon_{+\alpha}(\mathbf{k})$ and $\epsilon_{-\alpha}(\mathbf{k})$ with momentum $\mathbf{k}$. $c_{f\sigma}(c^{\dagger}_{f\sigma})$ is the annihilation (creation) operator of a MQD state with a spin $\sigma = \uparrow, \downarrow$. $n_{\sigma} = c^{\dagger}_{f\sigma} c_{f\sigma}$ is the occupation number operator of the MQD, $\epsilon_{f\sigma}$ is the energy of the MQD. The quantum dot is hybridized with the conduction bands with a strength $V_{\alpha}$. It is important to note that the dot level energy $\epsilon_{f\sigma}$ can be understood as the effective field that the electron experiences due to the presence of a Coulomb interaction, that leads to the magnetic non-magnetic transition. The splitting can thereby be understood from the Anderson model [30] where $\epsilon_{f\sigma} = \epsilon_f + U\langle n_{-\sigma}\rangle$, $U$ being the Coulomb interaction due to the double occupancy of the MQD. The Hamiltonian (1) is a good approximation for quantum dots with spin degeneracy that neither involves the spin–orbit interaction, nor a static magnetic field.

## 3. Transport quantities

The electric current of the electrons with spin $\sigma$ is given by [31]

$$I_{\sigma} = \frac{e}{\hbar} \int d\omega \, [f_{L\sigma} - f_{R\sigma}] T_{\sigma}(\omega) \quad (2)$$

where $e$ is the electronic charge, $\hbar$ is the reduced Planck constant and $f_{\alpha\sigma}$ is the Fermi Dirac distribution of the electrons with spin $\sigma$ in the lead $\alpha$. The transmission function of electrons with spin $\sigma$ is given by $T_{\sigma} = [V_L^2 V_R^2/(V_L^2 + V_R^2)] A_{f_{\sigma}}(\omega)$ where the impurity spectral function can be calculated from $A_{f_{\sigma}}(\omega) = -\frac{1}{\pi} \Im G^R_{f_{\sigma}}(\omega)$ and the retarded Green's function is the Fourier transform of the single particle Green's function:

$$G^R_{f_{\sigma}}(t) = -i\theta(t) \langle \{ f_{\sigma}(t), f^{\dagger}_{\sigma}(0) \} \rangle. \quad (3)$$

The standard equation of motion yields

$$G^R_{f_{\sigma}}(\omega) = \frac{1}{\omega - \epsilon_{f\sigma} - \Gamma^R_{f_{\sigma}}(\omega)} \quad (4)$$

where $\Gamma^R_{f_{\sigma}}(\omega) = \sum_{\alpha} \Gamma^R_{f_{\sigma}\alpha}(\omega)$ while [33]

$$\Gamma^R_{f_{\sigma}\alpha}(\omega) = -V_{\alpha}^2 \frac{\omega}{D^2} \ln \left( \frac{|\omega^2 - D^2|}{\omega^2} \right) - iV_{\alpha}^2 \frac{\pi |\omega|}{D^2} \theta(D - |\omega|) \quad (5)$$

and $D$ is a high-energy cutoff of the graphene bandwidth, defined by ensuring the conservation of the total number of states in the Brillouin zone according to the Debye prescription and $\Delta = \pi V^2/D^2$ is the dimensionless hybridization. The real part of $\Gamma^R_{f_{\sigma}}(\omega)$ defines the quasiparticle residue of the impurity electrons while the imaginary part gives the broadening of the localized level due to hybridization. The formation of a magnetic moment is determined by the occupation of the two spin states at the impurity $n_{\sigma}$.

The self-energy $\Gamma_{\sigma}(\omega)$ takes into account the many body effects. The temperature difference between the leads is given by $\Delta T = T_R - T_L$. Hence the spin current mainly driven by the temperature difference of the two leads is given by $I_s = I_{\uparrow} - I_{\downarrow}$ and the spin polarization (SP) can be written as

$$\text{SP } (\%) = \frac{(I_{\uparrow} - I_{\downarrow})}{(I_{\uparrow} + I_{\downarrow})} \times 100. \quad (6)$$

The average chemical potentials in the leads are given by $\mu_{\alpha}$ and the spin dependent ones as $\mu_{\alpha\sigma}$. The electrical voltage is given by $eV = \mu_L - \mu_R$ and that of the spin voltage is $eV_s = (\mu_{L\uparrow} - \mu_{L\downarrow}) - (\mu_{R\uparrow} - \mu_{R\downarrow})$.

The spin Seebeck coefficient $S_s$ [32] is given by $S_s = S_{\uparrow} - S_{\downarrow}$ where $S_{\sigma}$ is given by

$$S_{\sigma} = \frac{1}{eT} \frac{\int d\omega \, \omega [-f'(\omega)] T_{\sigma}(\omega)}{\int d\omega \, [-f'(\omega)] T_{\sigma}(\omega)} \quad (7)$$

and the temperature $T = \frac{1}{2}(T_L + T_R)$ and $f(\omega)$ is the Fermi distribution function.

## 4. Results and discussion

The thermoelectric effect is one of the most useful properties for spintronics where the spin degrees of freedom plays a fundamental role. In this work, we present the behavior of the spin current and the electrical current of the spin-up and the spin-down electrons in the presence of a magnetic-quantum dot along with the graphene leads maintained at temperatures $T_{\alpha}$. The right lead is always at a higher temperature than the left lead. Moreover, the temperature dependence and the chemical potential dependence of the spin-Seebeck coefficient, one of the core elements of spin caloritronics, are also presented. We choose both the cases where the impurity is below ($\epsilon_f < 0$) and also above ($\epsilon_f > 0$) the Dirac point [33] as the magnetic boundary is not symmetric between the above cases. The high-energy cutoff is of the order of the bandwidth ($D = 7$ eV). We assume that $|\mu| \ll D$, where band effects related to the exact definition of the cutoff are not important. We also consider the hybridization parameter to be independent of the leads, $V_L = V_R = V$. The average chemical potential in the leads $\mu_{\alpha} = (\mu_{L\uparrow} + \mu_{L\downarrow})/2 = \mu \pm \delta$ where $\delta$ is a very small number. Hence we observe a very small electrical voltage $eV = \mu_R - \mu_L$ applied between the two leads. However, the spin voltage $eV_s = (\mu_{L\uparrow} - \mu_{L\downarrow}) - (\mu_{R\uparrow} - \mu_{R\downarrow})$ is zero in all the cases. The spin current is thus driven by the temperature difference of the two leads. All the parameters are in terms of the hybridization parameter $V$. The currents $I_{\sigma}$ and $I_s$ plotted in the figures below are all in the form $I_{\sigma}/I_0$ and $I_s/I_0$ respectively, where $I_0 = e/h$. The Seebeck coefficient is in terms of the electronic charge $e$.

In Fig. 1 we present the chemical potential dependencies of the thermal spin currents $I_s$ for $U = 0.25$ (solid line), 0.26 (dashed line)