Spin transport in graphene monolayer antiferromagnetic calculated using the Kubo formalism

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Abstract

We have employed the Dirac's massless quasi-particles together with the Kubo's formalism of the linear response to study the spin transport properties by electrons in the graphene monolayer. We have calculated the electric conductivity and verified the behavior of the AC and DC currents of this system, which is a relativistic electron plasma. Our results show a superconductor behavior for the electron transport with the AC conductivity tending to infinity in the limit $\omega \rightarrow 0$. This superconductor behavior for the electron transport in the graphene is similar to one recently obtained theoretically for the spin transport in the quantum frustrated Heisenberg antiferromagnet in the honeycomb lattice, verifying so a similarity between these two different kinds of transport what can generate futures applications in the modern electronic. Copyright © 2017 VBRI Press.

Keywords: Spin transport, graphene, monolayer, two-dimensional, honeycomb lattice, frustrated, antiferromagnet.

Introduction

Graphene is an allotropic form of carbon which is recently researched. It has semiconductor properties with low-lying excitations obeying the massless Dirac's equation [**1**]. The interplay between the antiferromagnetic and Kekule valence bond solid ordering in the zero energy levels of neutral monolayer and bilayer graphene has been studied in [**2**]. On the other hand, understanding of the dynamics of many interacting particles is a formidable task in physics. For electronic transport in the matter, the force of interactions can lead to a breakdown of Fermi liquid paradigm of the coherent quasi-particles scattering amplitude by the impurities of the lattice. In such situations, the complex microscopic dynamics can be coarse-grained to a hydrodynamics description of momentum, energy, and charge transport on long length and time scales [**3**, **4**].

The spin transport has received much attention in the actuality due its connection with the spintronics. In this field, the generation and detection of spin polarized currents have been studied extensively with the aim to use the spin degree of freedom to improve the electronic devices [**5**]. Within this filed, the spin transport in graphene has been theoretically studied in the literature using the Boltzmann's equation formalism [**6**, **7**]. In general, the graphene is an interesting material for spintronics, showing long spin relaxation lengths even at room temperature. For the future of spintronic devices, it is important to understand the behavior of the spins and the limitations for spin transport in structures where the dimensions are smaller than the spin relaxation length [**8**]. The electron spin lifetime in carbon materials is expected to be large because of the very abundance of the spinless nuclear isotopes 12C and the small size of spin orbit coupling. This leads to propose the graphene as an optimal material to store quantum information in the spin of the electrons confined. However, most of the experiments show that the spin lifetimes are in the range of nanoseconds, much shorter than expected from these considerations, which lies at the heart of the design of devices where graphene is used as a passive component to carry spin currents.

Above liquid helium temperatures, the electronic properties of graphene are intrinsic, being governed by thermal excitations only. This gives a way how close can one approach the Dirac point in graphene experimentally, where the Dirac point can be approached within 1 meV, a limit currently set by the remaining charge in homogeneity [**9**].

One standard formalism in the literature to study the transport (spin transport and electron transport) is the Kubo formalism of the linear response theory. This formalism has been employed to study the spin transport in magnetic materials [**10-18**]. Moreover, we have that the electron transport in zigzag graphene nanoribbons with upright standing carbon chains has been investigated using first-principles calculations. Being the calculated results showing a significant odd-even dependence [**19**].

From an experimental point of view, we also have an intense research about the spin transport by electrons in graphene and the quantum Hall effect for spins. [**19-23**]. The spin injection and transport in monolayer graphene can be investigated also using nonlocal magnetoresistance measurements (MR) [**24**].

The aim of this paper is to study the spin transport by electrons in graphene monolayer using the Dirac fermion formalism. The graphene consists in a fermionic system with a relativistic Dirac spectrum where the energy vanishes linearly at isolated points in the Brillouin zone. Dirac's fermions are provided by numerous new experimental realizations. These include d-wave superconductors and topological insulators [**25**].

This work is divided in the following way. In section 2, we discuss about the model, in section 3 we discuss about the Kubo's formalism of transport, in section 4 we discuss about the similarity between the electron conductivity of the graphene with the spin transport in quantum frustrated two-dimensional Heisenberg antiferromagnet in the hexagonal lattice and in the section 5 we present our conclusions and final remarks.

The model

The model of relativistic free-fermionic particles of the graphene in D = 1+1 dimension is described by the following Hamiltonian density **[26]**

$$H = J v_F \int d^2x \psi^{+}_{\alpha}(x) i\sigma_3^{\alpha\beta} \partial_x \psi_\beta(x), \tag{1}$$

where, $\psi_\alpha(x)$ with α=1,2 denote a two component Fermi field in D=1+1 and D=2+1 space dimensions and v_F is the Fermi's velocity. We have considered unities where $v_F = 1$ and $\hbar = 1$. The interaction term has the form up to the irrelevant additive constant

$$H = -2J\gamma \int d^2x(\bar{\psi}(x)\psi(x))^2, \tag{2}$$

which is the interaction term of the (1+1) dimensional Gross-Neveu-model.

Assuming that electrons in graphene are non-interacting, the standard band theory calculations on a honeycomb lattice in two spatial dimensions with nearest-neighbor hopping give two species of Dirac fermions with single-particle spectrum in the relativistic form [**3**].

$$\omega(\vec{k}) \approx v_F |\vec{k}| \tag{3}$$

where, in the massless (gapless) limit, the spectrum is linear, hence, time and space scale the same way T ~ L, as required by relativistic invariance **[26]**. There are local interactions such as $(\bar{\psi}\gamma\mu\psi)^2$ and $(\bar{\psi}\psi)$, where $\bar{\psi} = \psi^\dagger\gamma^0$. The action of the free Dirac's field is

$$S = \int d^2x \bar{\psi}_\alpha(x) i\gamma^\mu \partial_\mu \psi_\beta(x) \tag{4}$$

where, γ are the 4 × 4 Dirac's matrix.**1** is the unit 2 × 2 matrix, and σ are the components of Pauli's matrix where the Dirac γ-matrix, γ_0, γ_1 and γ_5 satisfy the algebra

$$\{\gamma_\mu, \gamma_\nu\} = 2g_{\mu\nu}, \quad \gamma_5 = i\gamma_0\gamma_1. \tag{5}$$

$g_{\mu\nu}$ is the Minkowski's metric tensor. In the theory of free massless Dirac's fermions there are a fixed point in the renormalization group **[26].**

Kubo formalism of transport

We use the low energy approach Dirac's fermion [**5**, **25**] to determine the regular part of the electron conductivity (AC conductivity) or continuum conductivity. An electron current appears if there is an electric field by the Ohm' Law $\mathbf{J} = \sigma\mathbf{E}$. In a similar way a spin current appears as a response of a magnetic field $\mathbf{J_S} = \sigma\nabla\mathbf{B}$, through the system, where it plays the role of a chemical potential for spins. If one connect a low dimensional magnet with two bulk ferromagnetic, they can act as reservoirs for spins [**21, 22**]. Then, one has a flow of spin current if there is a difference, $\Delta\mathbf{B}$, between the magnetic fields at the two ends of the sample. In the Kubo formalism [**8, 10, 27, 28**] the conductivity is given by:

$$\sigma(\omega) = \lim_{k\to 0} \frac{\langle K\rangle + \Lambda(\vec{k},\omega)}{i(\omega + i0^+)}, \tag{6}$$

Where, $\langle K\rangle$ is the kinetic energy and $\Lambda(\vec{q},\omega)$ is the current-current correlation function defined as

$$\Lambda(\vec{k},\omega) = \frac{i}{\hbar N}\int_0^\infty \langle J(\vec{k},t), J(-\vec{k},t)\rangle e^{-i\omega t} dt. \tag{7}$$

The current operator for graphene $J(\vec{k},t)$ is given by

$$\mathbf{J} = \bar{\psi}\gamma\mu\psi. \tag{8}$$

The real part of σ(ω), $\sigma'(\omega)$, can be written in a standard form as [**28**]

$$\sigma(\omega) = \sigma_0(\omega) + \sigma^{reg}(\omega), \tag{9}$$

where, $\sigma_0(\omega)$ is the DC contribution, given by $\sigma_0(\omega) = D_S\delta(\omega)$. D_S is the Drude's weight

$$D_S = \pi[\langle K\rangle + \Lambda'(\vec{k} = 0, \omega \to \vec{0})] \tag{10}$$

$\sigma_0(\omega)$ represents the ballistic transport where we define ballistic transport as transport where the mean free path of the excitations is limited by the sample size. $\sigma^{reg}(\omega)$ is the continuum contribution to the conductivity or AC current. Therefore, when $D_S > 0$ we have an ideal conductor; $D_S=0$ and $\sigma^{reg}(\omega)>0$ means that the system is a conventional conductor and $D_S=0$ and $\sigma^{reg}(\omega) = 0$ means that the system is a insulator.

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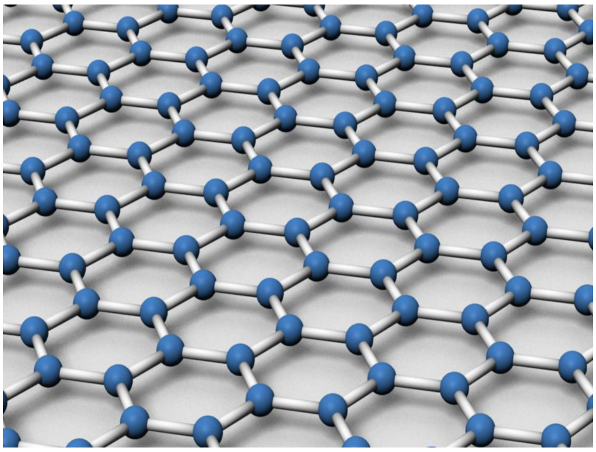

Fig. 1. A sheet of carbon atoms, graphene monolayer, with the carbon atoms in a honeycomb lattice.

Results

Discussion of the results

Using the Green's function method at finite temperature **[28]**, we obtain the Green's function for the model Eq. (1) as

$$\sigma^{reg}(\omega) = (g\mu_B)^2 \int_0^{\pi}\int_0^{\pi} \frac{d^2k}{(2\pi)^2}\frac{v_F^2}{\omega_k} f(\omega_k)\times$$

$$[1 - f(\omega_k)]\delta(\omega - 2\omega_k) \qquad (11)$$

where $f(\omega k) = 1/(e^{\beta\omega k} + 1)$ is the Fermi-Dirac distribution.

In **Fig.2**, we show the behavior of $\sigma^{reg}(\omega)$ with ω. We have getting a behavior of the *AC* conductivity tending to infinite when $\omega \to 0$, since the system is gapless. we have obtained therefore a superconductor electron transport for the electric current in the *DC* limit. We have found that this behavior is similar to one recently obtained for some quantum frustrated two-dimensional spin systems described by the two-dimensional Heisenberg antiferromagnet in the honeycomb lattice [**29**].

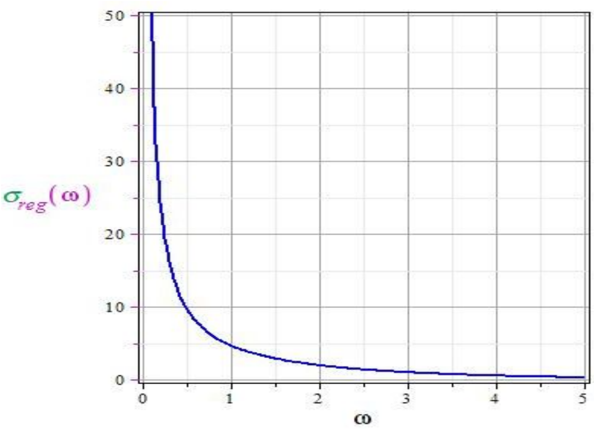

Fig. 2. Behavior of the AC conductivity for the value of T = 1.0J. Since the conductivity tends to infinity at $\omega \to 0$, we have an ideal conductor in DC limit.

This behavior for the spin current in magnetic spin systems is a consequence of absence of gap in the excitation spectrum. Since the Dira's fermion model of the graphene does not present gap in the spectrum, thus we will not have electrons to form one electric current for all values of ω. In the same way happens in the frustrated antiferromagnet in the hexagonal (honeycomb) lattice. Moreover, if there is no scattering mechanism, it is expected that the conductivity to be divergent. The reason is that the spin-spin scattering is not treated properly in the mean field approach. In **Fig. 3** we show the Drude's weight behavior. Since we have obtained $D_S > 0$ for $T > 0$, we will have an ideal electron transport or a superconductor for $T > 0$. At $T = 0$, we have $D_S \to 0$ as showed in **Fig. 3** and $\sigma^{reg}(\omega) = 0$, Therefore, we must have an insulator behavior in this limit of T . The behavior of the Drude's weight $D_S(T) > 0$ is showed in the **Fig. 3**. Due the mean field approach used, we have that the results for small T are accurate however, for large T values, we must have only a qualitative description.

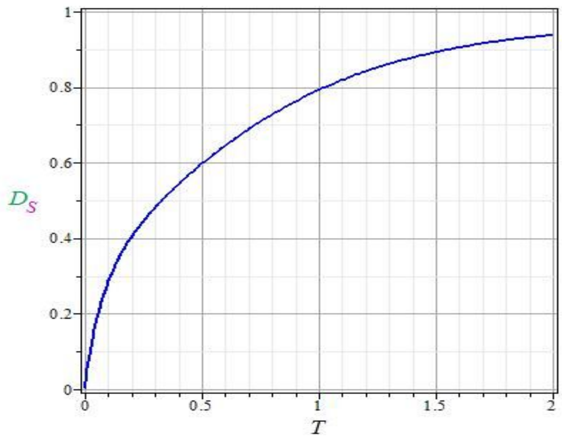

Fig. 3. Behavior of the Drude's weight, D_S (T), in function of T. Since we have D_S (T) > 0 for T > 0, hence we have a superconductor behavior for T > 0.

Relation with the spin transport in the quantum antiferromagnet in the honeycomb lattice

The model is defined as

$$H = J_1 \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y + R S_i^z S_j^z)$$
$$+ J_2 \sum_{\langle\langle i,j \rangle\rangle} (S_i^x S_j^x + S_i^y S_j^y + R S_i^z S_j^z) + D\sum_i (S_i^z)^2 \qquad (12)$$

We consider the integer spin, S = 1 [**30**].
The spin current operator:

$$\mathbf{J}_x = 2iJ_1 \sum_i (S_i^x S_{i+x}^y + S_i^y S_{i+x}^x) + 2iJ_2 \sum_i (S_i^x S_{i+\sqrt{3}x}^x + S_i^y S_{i+\sqrt{3}x}^y)$$

The spin current correlation function:

$$\Lambda_{xx}(\vec{k},\omega) = \frac{i}{\hbar N}\int_0^{\infty} \left\langle \mathbf{J}_x(\vec{k},t), \mathbf{J}_x(-\vec{k},0) \right\rangle e^{-i\omega t} dt$$

The Kubo formula :

$$\sigma_{xx}(\omega) = \lim_{\vec{k}\to 0} \frac{\langle K \rangle + \Lambda_{xx}(\vec{k},\omega)}{i(\omega + i0^+)} .$$

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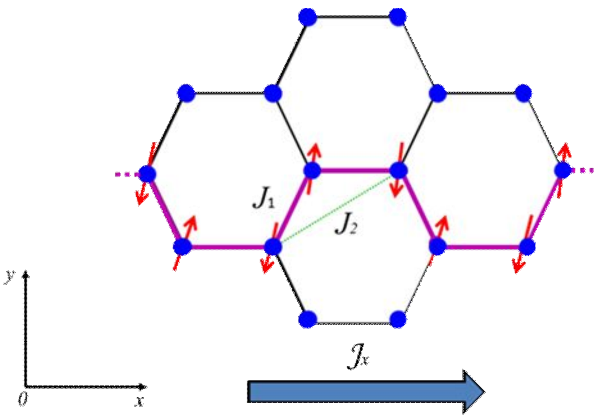

Fig. 4. The spin current in zig-zag in the two-dimensional antiferromagnet in the hexagonal lattice.

The Mean Field Schwinger boson formalism

In this formalism we choose the basis:

$$|x\rangle = \frac{i}{\sqrt{2}}\left(|1\rangle - |-1\rangle\right) \quad |y\rangle = \frac{i}{\sqrt{2}}\left(|1\rangle + |-1\rangle\right) \quad |z\rangle = -i|0\rangle$$

Where $|n\rangle$ are the eigenstates of S^Z

The spin operators are written via a set of three boson operators

$t\alpha, (\alpha = x, y, z)$

$$|x\rangle = t_x^{+}|v\rangle \qquad |y\rangle = t_y^{+}|v\rangle \qquad |z\rangle = t_z^{+}|v\rangle$$

where $|\, v\,\rangle$ is the vacuum state. We also have the constraint condition

$$t_x^{+}t_x + t_y^{+}t_y + t_z^{+}t_z = 1$$

We write the spin operators in terms of the bosons *t*

$$S^x = -i\left(t_y^{+}t_z + t_z^{+}t_y\right) \quad S^y = -i\left(t_z^{+}t_x + t_x^{+}t_z\right) \quad S^z = -i\left(t_x^{+}t_y + t_y^{+}t_x\right)$$

To study the disordered phases we introduce other two bosonic operators *u* and *d* with the constraint

$$u^{+}u + d^{+}d + t_z^{+}t_z = 1$$

$$S^{+} = \sqrt{2}\left(t_z^{+}d + u^{+}t_z\right) \quad S^{-} = \sqrt{2}\left(d^{+}t_z + t_z^{+}u\right) \quad S^{z} = u^{+}u + d^{+}d$$

The Schwinger's boson formalism is a mean field approximation that becomes accurate in the $N \to \infty$ limit.

We assume that the t_z bosons are condensed (Bose-Einstein Condensation):

$$\langle t_z \rangle = \langle t_z^{+} \rangle = t$$

In **Fig. 5**, we present the behavior of $\sigma^{reg}(\omega)$ with ω. Due to the hexagonal crystal lattice, we must have a spin current in zig-zag over the material as depicted in **Fig. 3**. Since the system is gapless we have obtained a behavior of the AC spin conductivity tending to infinity when $\omega \to 0$, that corresponds to the DC limit. Hence, we obtain a superconductor behavior for the spin transport in the DC limit. This behavior is similar to ones recently obtained for the two-dimensional ferroquadrupolar model [**31**] and for the triangular lattice, being a characteristics [**32**] of spin systems without gap in the excitation spectrum.

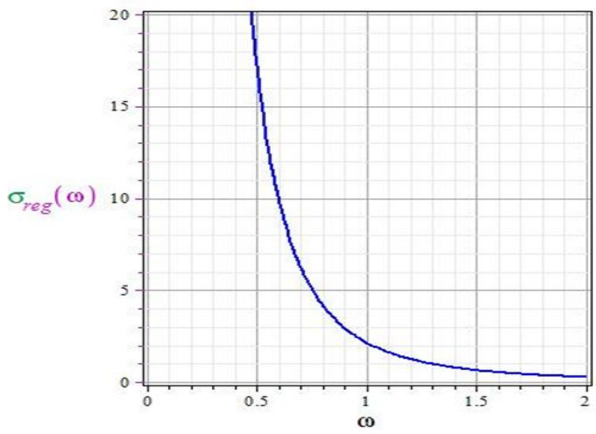

Fig. 5. The spin conductivity in the two-dimensional antiferromagnet in the hexagonal lattice.

Conclusion

In summary, we have verified a similarity between the transport properties at two different quantum models. The Dirac's fermion model of the graphene monolayer, which is a quantum paramagnet and the quantum two-dimensional antiferromagnet in the honeycomb lattice. We have obtained theoretically that the behavior of the electric conductivity of the graphene and the spin conductivity of the anisotropic two-dimensional frustrated Heisenberg antiferromagnet in the hexagonal lattice are the same. Experimental results for the spin transport in antiferromagnets in the hexagonal lattice can give a support to our theoretical results. In both cases, the AC conductivity t tends to infinite in the DC limit ($\omega \to 0$). However, more specific experimental results for the spin transport in quantum frustrated spin systems are necessary within this statement to support the claim.

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