Physica E 86 (2017) 154–157

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

Spin susceptibility of disordered gapped graphene systems

I. Grosu*, T.L. Biter

Department of Physics, "Babes-Bolyai" University, 400084 Cluj-Napoca, Romania

ARTICLE INFO

Keywords:
Gapped graphene
Disorder
Born approximation
T-matrix approximation
Spin susceptibility

ABSTRACT

We calculate the spin susceptibility for the case of gapped graphene systems in the presence of disorder. The average single-particle density of states in gapped graphene with disorder was calculated, using the Born and the *T*-matrix approximations. The temperature dependence of the static spin susceptibility was analyzed. The influence of the chemical potential position and disorder is also discussed.

1. Introduction

Graphene, a two-dimensional carbon atom based material, where carbon atoms are disposed on a hexagonal lattice, was synthesized about a decade ago [1]. This mono-layer material has unusual properties due to the Dirac-like band structure, where conduction and valence bands touch at six points at the edges of the honeycomb Brillouin zone [2,3], two of these being nonequivalent (named as K and K' points [4]). Around these points the quasiparticle excitations follow a linear Dirac-like energy dispersion responsible for many physical phenomena (see Refs. [4] and [5]). Despite of the graphene's outstanding physical properties, many electronic applications require the presence of an energy-gap between the bands. We have to mention that several experimental measurements indicate the presence of an energy-gap in the graphene quasiparticle spectrum [6–8]. Here the nature of the gap can be attributed to the effect of the substrate. Recently, magnetic measurements [9] revealed strong magnetism in fluorinated graphene. These materials exhibit a reversible magnetic response and a magnetic susceptibility that can be split into a temperature-independent term, a small Curie-like component, and a strong non-Curie spin susceptibility. The spin susceptibility reflects the low-dimensional nature of the spin system, and reveals the presence of an energy gap Δ. The gapped energy spectrum was considered in order to analyze the anomalous growth of thermoelectric power in graphene [10] (massive gapped spectrum), and the phenomenological massless gapped spectrum was introduced [11] to reconcile the gapped nature of the energy spectrum and the massless character of the particles in graphene, and to correctly explain several spectroscopic measurements [12]. On the other hand, the fabricated graphene samples are not pure. The presence of disorder can affect the properties of graphene, giving a finite lifetime of the electronic eigenstates. The lifetime damping rate gives a single-particle level broadening and changes the electronic density of states. Many of the physical properties will be modified through the changes of the electronic density of states. In the present paper we will calculate the density of states for a gapped system in the presence of disorder, and we will use the results in order to analyze, in a qualitative way, the temperature dependence of the static spin susceptibility, recently measured in graphene-based structures with lower fluorine contents [9]. The paper is organized as follows: In Section 2 we discuss the system's density of states, in a general form. In Section 3 we calculate the self-energies of a gapped system in the presence of disorder, working in the Born and in the *T*-matrix approximations. Using these results, in Section 4 we determined the static spin susceptibility and we analyze the influence of various parameters on its temperature dependence. In Section 5 we give the conclusions.

2. Density of states

The single-particle density of states is defined by [13] ($\hbar = 1$):

$$\rho(\varepsilon) = -\frac{g}{\pi}\sum_{\lambda}\int\frac{d^2k}{(2\pi)^2}\,ImG_{\lambda}(\vec{k},\varepsilon) \tag{1}$$

where: $g = g_s g_v = 4$ is the degeneracy factor for graphene, λ – the band index, and $G_{\lambda}(\vec{k},\varepsilon)$ – the retarded Green's function. The wavevector integration is taken over a circle of radius k_c. The retarded Green's function, expressed in terms of retarded self-energy $\Sigma_{\lambda}(\vec{k},\varepsilon)$, is given by:

$$G_{\lambda}(\vec{k},\varepsilon) = \frac{1}{\varepsilon - \varepsilon_{k,\lambda} - \Sigma_{\lambda}(\vec{k},\varepsilon) + i\delta} \tag{2}$$

Using Eq. (2), the single-particle density of states becomes:

* Corresponding author.

http://dx.doi.org/10.1016/j.physe.2016.09.010
Received 13 July 2016; Received in revised form 18 August 2016; Accepted 20 September 2016
Available online 21 September 2016

$$\rho(\varepsilon) = \frac{g}{\pi}\sum_{\lambda}\int\frac{d^2k}{(2\pi)^2}\frac{-Im\Sigma_\lambda(\vec{k},\varepsilon)}{[\varepsilon-\varepsilon_{k,\lambda}-Re\Sigma_\lambda(\vec{k},\varepsilon)]^2+[Im\Sigma_\lambda(\vec{k},\varepsilon)]^2} \tag{3}$$

In the following we will assume that the self-energy is $\vec{k}$ and λ independent, and we introduce the notations:

$$\Gamma(\varepsilon) = -Im\Sigma_\lambda(\vec{k},\varepsilon) \tag{4}$$

and:

$$\Omega(\varepsilon) = \varepsilon - Re\Sigma_\lambda(\vec{k},\varepsilon) \tag{5}$$

The dispersion law for graphene, in the presence of a gap Δ, is [6,7]:

$$\varepsilon_{k,\lambda} = \lambda\sqrt{v_F^2k^2+\Delta^2} \tag{6}$$

where $\lambda = \pm 1$, correspond to the conduction and valence bands, k - is the value of the wave vector, and v_F is the Fermi velocity of graphene. After performing the two dimensional wave vector integration, we obtain for the density of states:

$$\begin{aligned}\rho(\varepsilon) = \frac{g}{2\pi^2v_F^2}\Bigg\{&\frac{\Gamma(\varepsilon)}{2}\ln\frac{(\varepsilon_c^2+\Omega^2(\varepsilon)+\Gamma^2(\varepsilon)+\Delta^2)^2-4\Omega^2(\varepsilon)(\varepsilon_c^2+\Delta^2)}{(\Omega^2(\varepsilon)+\Gamma^2(\varepsilon)+\Delta^2)^2-4\Omega^2(\varepsilon)\Delta^2}\\ &+\Omega(\varepsilon)\Bigg[\arctan\left(\frac{\sqrt{\varepsilon_c^2+\Delta^2}-\Omega(\varepsilon)}{\Gamma(\varepsilon)}\right)\\ &-\arctan\left(\frac{\sqrt{\varepsilon_c^2+\Delta^2}+\Omega(\varepsilon)}{\Gamma(\varepsilon)}\right)+\arctan\left(\frac{\Delta+\Omega(\varepsilon)}{\Gamma(\varepsilon)}\right)\\ &-\arctan\left(\frac{\Delta-\Omega(\varepsilon)}{\Gamma(\varepsilon)}\right)\Bigg]\Bigg\}\end{aligned} \tag{7}$$

This result reduces to Eq. (16) from Ref. [14] when Δ tends to zero. Here: $\varepsilon_c = v_Fk_c$ is the energy cutoff. In the wide band limit, the above density of states can be approximated as:

$$\begin{aligned}\rho(\varepsilon) \simeq &\frac{4\Gamma(\varepsilon)}{\pi^2v_F^2}\left[\ln\left(\frac{\varepsilon_c}{\Gamma(\varepsilon)}\right)-\frac{1}{2}\ln\sqrt{\left(1+\frac{\Omega^2(\varepsilon)+\Delta^2}{\Gamma^2(\varepsilon)}\right)^2-\frac{4\Omega^2(\varepsilon)\Delta^2}{\Gamma^4(\varepsilon)}}\right]\\ &+\frac{2\Omega(\varepsilon)}{\pi v_F^2}\left[\frac{1}{2}-\frac{1}{\pi}\arctan\frac{\Gamma^2(\varepsilon)-\Omega^2(\varepsilon)+\Delta^2}{2\Omega(\varepsilon)\Gamma(\varepsilon)}\right]\end{aligned} \tag{8}$$

which is a result similar to the density of states obtained in Ref. [15] concerning impurity-induced quasiparticle transport in d-wave superconductors.

3. The self-energy

In the following we will consider the approximations to the self-energy, described below.

(**a**). **Born approximation** In the Born approximation, and in the presence of a gap, the self-energy is given by the following expression:

$$\Sigma_B = \gamma_B\Sigma_0 \tag{9}$$

where:

$$\gamma_B = \frac{n_iU_0^2}{2v_F^2} \tag{10}$$

with n_i – the impurity density, and U_0 correspond to the Fourier transform of the impurity potential. The approximation $U(\vec{k}) = U_0$ is valid as long as the unscreened short-range disorder is considered, and the intervalley processes are neglected. The Σ_0 part is:

$$\Sigma_0 = 2v_F^2\int\frac{d^2k'}{(2\pi)^2}\sum_{\lambda'}G_{\lambda'}^{(0)}(\vec{k}',\varepsilon)F_{\lambda\lambda'}(\vec{k},\vec{k}') \tag{11}$$

Here $G_{\lambda'}^{(0)}(\vec{k}',\varepsilon)$ is the bare Green's function:

$$G_{\lambda'}^{(0)}(\vec{k}',\varepsilon) = \frac{1}{\varepsilon-\varepsilon_{k'\lambda'}+i\delta} \tag{12}$$

and $F_{\lambda\lambda'}(\vec{k},\vec{k}')$ is a function that describes the overlap between $|\psi_{k,\lambda}>$ and $|\psi_{k',\lambda'}>$ wave functions which are periodic with the lattice. Near the Dirac point:

$$F_{\lambda\lambda'}(\vec{k},\vec{k}') = \frac{1}{2}(1+\lambda\lambda'\cos\theta) \tag{13}$$

with λ and λ' – band indices, and θ – the angle between $\vec{k}$ and $\vec{k}'$. Considering elastic scattering, and neglecting the interband scattering, the self-energy in the Born approximation can be evaluated as:

$$\Sigma_B = -\frac{\gamma_B}{2}\left[\frac{\varepsilon}{\pi}\ln\left|\frac{\varepsilon_c^2}{\varepsilon^2-\Delta^2}-1\right|+i|\varepsilon|\right] \tag{14}$$

for energies $\varepsilon\in[-\sqrt{\varepsilon_c^2+\Delta^2},-\Delta]\cup[\Delta,\sqrt{\varepsilon_c^2+\Delta^2}]$ (due to the branch cuts of the logarithm function).

(**b**). **T-matrix approximation** In this case one has to consider the summation of the entire series of Feynman diagrams concerning scattering, using the bare Green's function. The impurity averaged T-matrix (self-energy), for a constant impurity potential, is:

$$\Sigma_T = \frac{\Sigma_B}{1-U_0\mathcal{G}} \tag{15}$$

with Σ_B given by Eq. (9). Here we introduced the notation:

$$U_0\mathcal{G} = U_0\int\frac{d^2k'}{(2\pi)^2}\sum_{\lambda'}G_{\lambda'}^{(0)}(\vec{k}',\varepsilon)F_{\lambda\lambda'}(\vec{k},\vec{k}') \equiv \frac{U_0}{2v_F^2}\Sigma_0 \tag{16}$$

The self-energy becomes:

$$\Sigma_T = \frac{\gamma_B\Sigma_0}{1-\frac{U_0}{2v_F^2}\Sigma_0} \tag{17}$$

In the presence of the gap, using Eqs. (14) and (9), we obtain:

$$\Sigma_T = Re\Sigma_T + i\,Im\Sigma_T \tag{18}$$

where:

$$Re\Sigma_T = \frac{\gamma_B}{N}\left\{Re\Sigma_0-\frac{U_0}{2v_F^2}([Re\Sigma_0]^2+[Im\Sigma_0]^2)\right\} \tag{19}$$

$$Im\Sigma_T = \frac{\gamma_B}{N}Im\Sigma_0 \tag{20}$$

with:

$$N = \left[1-\frac{U_0}{2v_F^2}Re\Sigma_0\right]^2+\left[\frac{U_0}{2v_F^2}Im\Sigma_0\right]^2 \tag{21}$$

($Re\Sigma_0$ and $Im\Sigma_0$ can be obtained immediately from Eq. (14)). We observe that both Σ_B and Σ_T depend only on energy, and are independent of k and λ.

4. The spin susceptibility

Using the densities of states, for the Born approximation and T-matrix approximation cases, the static spin susceptibility will be determined using the relation [16] ($k_B = 1$):

$$\chi = g_L^2\mu_B^2\int d\varepsilon\,\frac{\rho(\varepsilon)}{4\,T\cosh^2\left(\frac{\varepsilon-\mu}{2\,T}\right)} \tag{22}$$

Here g_L – is the Lande electron g-factor, μ_B – is the Bohr magneton, and μ – the chemical potential. For the disordered gapped system the energy integration range will be the interval determined in Sec.III (see also Ref.[17]).

For the Born approximation case, taking into account the appropriate density of states and self-energy, we plot in Fig. 1 the