Physica B xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Physica B

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

Impurity effects in the magnetic oscillations on doped graphene with Zeeman splitting

F. Escudero[a], J.S. Ardenghi[b,*], Paula Jasen[b], A. Juan[b]

[a] Departamento de Física, Universidad Nacional del Sur, Av. Alem 1253, B8000CPB Bahía Blanca, Argentina
[b] Instituto de Física del Sur (IFISUR, UNS-CONICET), Av. Alem 1253, B8000CPB Bahía Blanca, Argentina

ARTICLE INFO

Keywords:
Graphene
Zeeman effect
Disorder
De Haas-van Alphen oscillations

ABSTRACT

The aim of this work is to describe the electronic and magnetic properties of graphene in a constant magnetic field, in the long wavelength approximation with random disorder. Taking into account the Zeeman effect, the electronic density of states for each spin is found and the de Haas van Alphen oscillations (dHvA) are found. The magnetic field is found to modulate the de Haas-van Alphen magnetization through the ratio of the Zeeman coupling and pseudospin-Landau coupling. In turn, the Pauli magnetization is studied showing that the Zeeman splitting and disorder introduces a dHvA oscillation period that depends on the magnetic field strength and generalizes the Onsager relation. In turn, a beat frequency appears that does not depend on B but increase linearly with the chemical potential. These results, which are different from those obtained in the standard nonrelativistic 2D electron gas, are attributed to its anomalous Landau level spectrum in graphene.

1. Introduction

Since its experimental isolation in 2004, graphene has become one of the most studied and promising material in solid state physics ([1–3]). Its interesting properties lie in his 2D hexagonal structure, made of two interpenetrating sublattices A and B that act as a pseudospin degrees of freedom [4]. With no impurities or defects, the conduction and valence bands touch at two inequivalent points at the corners of the Brillouin zone with the valence band full and the conduction band empty in the ground state [3]. Furthermore, in pristine graphene the density of states at the Fermi energy is zero, and thus the graphene is a semiconductor with zero band gap, or a semi-metal [5]. When a magnetic field is applied to graphene, discrete Landau levels are obtained [6] and these are not equidistant, as in classical electron gas. In turn, the large distance between the fundamental and first excited Landau levels allows the Quantum Hall effect to be observed in graphene at room temperatures ([7–9]). Moreover, the Landau levels create an oscillating behavior in the thermodynamics potentials. It is found that the magnetization oscillates as a function of the inverse magnetic field, the so called de Haas van Alphen effect (dHvA) ([10,11]). The different frequencies involved in the oscillations are related to the closed orbits that electrons perform on the Fermi surface [12] and is a powerful tool for mapping the electronic states at the Fermi energy [13]. It has been predicted in graphene that magnetization oscillates periodically in a sawtooth pattern, in agreement with the old Peierls prediction [14], although the basic aspects of the behavior of the magnetic oscillations for quasi-2D materials remains yet unclear [15]. In contrast to 2D conventional semiconductors, where the oscillating center of the magnetization M remains exactly at zero, in graphene the oscillating center has a positive value because the diamagnetic contribution is half reduced with that in the conventional semiconductor [16]. From an experimental point of view, carbon-based materials are more promising because the available samples already allows one to observe the Shubnikov-de Haas effect ([17,18]) and then may be easier to interpret the quantum oscillations in its transport properties. Because the dHvA signal in 2D systems are free of the k_z smearing, it should be easier to obtain much rich information about the electron processes. On the other side, it is well known that pristine graphene is ideal. Real world samples of graphene are essentially impure, as they always contain some amount of resonant impurities or ripples. Considering pristine graphene, these defects can break the pseudospin symmetries, depending on the matrix elements in the external potential [19]. The problem of scattering from subtitutional impurities in the presence of a magnetic field does not have yet a satifactory solution, although it is known that broadening of Landau levels in the electronic density of states is good approximation valid in weak magnetic fields [20]. This broadening has the technical advantage that if one consider first the dHvA oscillations with Dirac delta shaped Landau levels, the introduction of impurities implies to convolute the different quantities of interest with the appropriate distribution func-

* Corresponding author.
E-mail address: jsardenghi@gmail.com (J.S. Ardenghi).

http://dx.doi.org/10.1016/j.physb.2017.05.012
Received 12 March 2017; Received in revised form 3 May 2017; Accepted 7 May 2017

tions [14]. However, this is a simplification that is only valid if all the Landau levels have the same width. To obtain better theoretical approximations in this work the Born approximation will be used to compute the self-energies [21]. This work will be organized as follow: In section II, the magnetic Green function with diagonal on-site energies will be computed for graphene. In section III, single-site approximation will be applied and a system of coupled Soven equation will be found and solved. The discussion of the results is shown in section IV and the principal findings of this paper are highlighted in the conclusion. In Appendix the main theory used in the manuscript is explained.

2. Single-site approximation

For a self-contained lecture of this paper, the self-consistent Born approximation will be explained in this section in order to obtain the generalization to the results obtained in [22], Eq. (68) to Eq. (72). The Hamiltonian in the two inequivalent corners of the Brillouin zone in the long wavelength approximation reads

$$H = v_F \begin{pmatrix} 0 & \pi_x - i\pi_y & 0 & 0 \\ \pi_x + i\pi_y & 0 & 0 & 0 \\ 0 & 0 & 0 & \pi_x + i\pi_y \\ 0 & 0 & \pi_x - i\pi_y & 0 \end{pmatrix} \tag{1}$$

where $\pi_i = p_i - eA_i$, being A_i the vector potential. This approximation holds for $E < E_C$ where $E_C = v_F k_C \sim t \sim 2.7\, eV$ (see [22] above eq. (24)). By considering that $\mathbf{A} = (-By, 0, 0)$ and by writing the wave function as $\psi = e^{ikx}\phi(y)$, then p_x transform as $p_x \to \hbar k$. By making the following transformation $y = \frac{\hbar}{\sqrt{eB}}\overline{y} + \frac{\hbar k_x}{eB} = l_B\overline{y} + kl_B^2$, the last Hamiltonian can be written as

$$H_0 = v_F\sqrt{2eB\hbar}\begin{pmatrix} 0 & a^\dagger & 0 & 0 \\ a & 0 & 0 & 0 \\ 0 & 0 & 0 & a \\ 0 & 0 & a^\dagger & 0 \end{pmatrix} \tag{2}$$

where $a = \frac{1}{\sqrt{2}}(\overline{y} + \partial_{\overline{y}})$ and $a^\dagger = \frac{1}{\sqrt{2}}(\overline{y} - \partial_{\overline{y}})$. This Hamiltonian can be written in terms of two copies of identical valley Hamiltonians

$$H_0 = \hbar\omega_L(\sigma_+ a^\dagger + \sigma_- a) \otimes \hbar\omega_L(\sigma_- a^\dagger + \sigma_+ a) \tag{3}$$

where $\sigma_\pm = \sigma_x \pm i\sigma_y$ acts on the sublattice basis and where $\omega_L = v_F\sqrt{\frac{eB}{2\hbar}}$ is the cyclotron frequency. The tensor product is introduced to denote the valley subspaces. In order to simplify the problem, we can consider only the K valley. Because the magnetic field can interact with the spin of electrons, then we can add the Zeeman Hamiltonian by adding the spin space. Then, the Hamiltonian will be a 2×2 block diagonal matrix, where the first block is for spin up and the second block for spin down, both for the same K valley.[1] The wave function can be written as

$$|\psi_{k,n}\rangle = \begin{pmatrix} c_1|k, n\rangle \\ c_2|k, n-1\rangle(1-\delta_{n,0}) \\ c_3|k, n\rangle \\ c_4|k, n-1\rangle(1-\delta_{n,0}) \end{pmatrix} \tag{4}$$

where the coordinate representation of $|k, n\rangle$ is $\langle r|k, n\rangle = e^{ikx}\phi_{n,k}(\overline{y})$, where $\phi_{n,k}(\overline{y})$ is the wave function of the harmonic oscillator.[2]

$$\phi_{n,k}(\overline{y}) = \frac{\pi^{-1/4}}{\sqrt{2^n n!}} e^{-\frac{1}{2}\overline{y}^2} H_{n,k}(\overline{y}) \tag{5}$$

and where $H_{n,k}(\overline{y})$ are the Hermite polynomials. After straightforward manipulations, the eigen problem reduces to

$$\begin{pmatrix} -\hbar\omega_z & \hbar\omega_L\sqrt{n} & 0 & 0 \\ \hbar\omega_L\sqrt{n} & -\hbar\omega_z & 0 & 0 \\ 0 & 0 & \hbar\omega_z & \hbar\omega_L\sqrt{n} \\ 0 & 0 & \hbar\omega_L\sqrt{n} & \hbar\omega_z \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = E\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} \tag{6}$$

Then, the eigenvalues can be written as

$$\epsilon_n^{(\alpha,s)} = -s\hbar\omega_Z + \alpha\hbar\omega_L\sqrt{n} \tag{7}$$

where $\alpha = +1(-1)$ for the conduction (valence band), $s = +1(-1)$ for the spin up (spin down). The eigenfunctions read

$$|\psi_{k,n,s,\alpha}\rangle = \frac{1}{\sqrt{(2-\delta_{n,0})L}}\begin{pmatrix} \frac{\alpha}{2}(1+s)|k, n\rangle \\ -\frac{1}{2}(1+s)|k, n-1\rangle(1-\delta_{n,0}) \\ \frac{\alpha}{2}(s-1)|k, n\rangle \\ \frac{1}{2}(s-1)|k, n-1\rangle(1-\delta_{n,0}) \end{pmatrix} \tag{8}$$

where $L^2 = A$, where A is the area of the graphene sheet. In the basis that diagonalize the Hamiltonian, the Green function reads

$$G_0 = \sum_{\alpha=\pm 1, s=\pm 1}\sum_{k,n}\frac{1}{z - \epsilon_n^{(\alpha,s)}}|\psi_{k,n,s,\alpha}\rangle\langle\psi_{k,n,s,\alpha}| \tag{9}$$

where z is a complex number that can be written as $z = E + is$, where E is the energy and s is some real and positive number. At this point we can include disorder as random impurities in our model in the most simple way in order to gain a physical understanding of its effects. By considering an impurity potential in the coordinate representation (see Eq. (59) of [22]) $V(r) = V_0\sum_N^{i=1}\delta(r - R_i)I$, where R_i are the random positions of the impurities and I is the identity matrix, it can be shown that when configurational averaging is applied over the random positions of the impurities, the system restore translation invariance and the configurational averaged Green function $\langle G\rangle$ can be written in terms of the self-energy (see [24])

$$\langle G(k, z)\rangle = [G_0^{-1}(k) - \Sigma(k, z)]^{-1} \tag{10}$$

where $\langle\ldots\rangle$ means configurational averaging. In turn, it can be shown that in the self-consistent Born approximation, the self-energy at first order in the impurity concentration $c = N_i/N$ can be written as (see [24] eq.(3.59))

$$\Sigma^{SCBA}(z) = cV_0^2\sum_k\langle G(k)\rangle \tag{11}$$

where we are neglecting skeleton diagrams where impurity lines crosses and the sum in k represent the sum in all the quantum numbers of the system. In the case of graphene with magnetic field, our Hamiltonian depends on the momentum k in the x direction, the n label of the Landau levels, the spin and conduction and valence band. If we consider the sum over the Landau levels and k then last equation becomes

$$\Sigma_{\alpha,s}(z) = cV_0^2\int\frac{dk}{2\pi}\sum_{n=0}^{Q}G(\alpha, s, n, k, z) \tag{12}$$

where the self-energy depends on the conduction-valence band and spin and Q is the Landau level cutoff that is determined by the equation $\hbar\omega_Z + \hbar\omega_L\sqrt{Q} = E_C$. The impurity-averaged Green function $\langle G(\alpha, s, n, k, z)\rangle$ can be written in the spectral representation as[3]

$$\langle G(\alpha, s, n, k, z)\rangle = \frac{1}{(2-\delta_{n,0})}\frac{1}{z - \epsilon_n^{(\alpha,s)} - \Sigma_{\alpha,s}(z)} \tag{13}$$

where we have introduced the self-energy diagonal matrix elements $\Sigma_{\alpha,s}(z)$. Eq. (12) contains four independent self-consistent equations for the self-energies. Nevertheless, by following Eq. (11) we must sum over

[1] Other effects such as spin-orbit coupling has been considered (see [23]), where the spin-orbit coupling can be tuned by electric fields.

[2] The factor $(1-\delta_{n,0})$ is introduced to discriminate the ground state which contributes only in the A sublattice for the K valley. If we had considered the K' valley, the contribution is on the Bsublattice.

[3] In order to apply Eq. (10), the self-energy is considered diagonal in the spectral representation.