Magnetocapacitance of a graphene monolayer

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Abstract

We present a theoretical study of magnetocapacitance in a graphene monolayer at finite temperature taking into account the effects of disorder. The density of states (DOS) and magnetocapacitance found for graphene are compared to those found in standard two dimensional electron gas (2DEG) systems. The magnetic oscillations in DOS and magnetocapacitance are found to be enhanced and much more robust with respect to temperature damping in monolayer graphene in comparison with a 2DEG. Furthermore, we find that there is a $\pi$ phase shift between magnetic oscillations in the two systems which can be attributed to Dirac electrons in graphene acquiring a Berry’s phase as they traverse a closed path in a magnetic field.
I. INTRODUCTION

Monolayer graphene is a gapless semiconductor with conical touching of electron and hole bands. Since the quasiparticles in a graphene monolayer obey the massless Dirac equation they act as massless Dirac Fermions. This difference in the nature of the quasiparticles in graphene from conventional 2DEG has given rise to a host of new and unusual phenomena such as anomalous quantum Hall effect and a π Berry phase\[1, 2, 3\]. Besides the fundamental interest in understanding the electronic properties of graphene there are also serious suggestions that it can serve as the building block for nanoelectronic devices \[4\].

Among the most important tools in studying the electronic properties of solid state systems are capacitance measurements. Capacitance measurements can be effectively used to probe the thermodynamic density of states of an electron system. It has been successfully used to probe the density of states in a conventional 2D EG systems and references therein\[5, 6, 7\]. In the present work, we determine the magnetocapacitance of a graphene monolayer. It is possible to carry out experiments, along the lines of those carried out on conventional 2DEG systems\[5, 6, 7\] realized in semiconductor heterostructures, carbon nanotubes and graphene nanoribbons\[8\], that allow verification of the model presented here. If confirmed experimentally, our theoretical predictions provide another method of determining the density of states of a graphene monolayer in a magnetic field.

In section II, we present the formulation of the problem. Section III contains the calculation of the temperature dependent density of states and magnetocapacitance of a graphene monolayer, including the comparison with 2DEG and discussion of numerical results. The conclusions are in section IV.

II. FORMULATION

We consider two-dimensional Dirac electrons in graphene moving in the $x$-$y$-plane. The magnetic field ($B$) is applied along the $z$-direction perpendicular to the graphene plane. We employ the Landau gauge and write the vector potential as $A = (0, Bx, 0)$. The two-dimensional Dirac-like Hamiltonian\[1, 2, 3\] for an electron in the Landau gauge is $H_0 = v_D \vec{\sigma} \cdot (-i\hbar \nabla + e\vec{A})$. Here $\sigma = \{\sigma_x, \sigma_y\}$ are the Pauli matrices and $v_D$ characterizes the velocity of Dirac electron. The Landau level energy eigenvalues are given by
\[\varepsilon_n = \hbar \omega_g \sqrt{n}, \text{ where } \omega_g = v_D \sqrt{\frac{2eB}{\hbar}} \] is the cyclotron frequency of Dirac electrons and \( n \) is an integer. The Landau level spectrum for Dirac electrons is significantly different from the spectrum for electrons in a conventional 2DEG which is given as \( \varepsilon(n) = \hbar \omega_c (n + 1/2) \), where \( \omega_c \) is the cyclotron frequency. This difference between the energy dispersion of Dirac electrons and conventional electrons is also reflected in the Density of States (DOS). The oscillations in the capacitance, in the presence of a magnetic field, are directly related to the density of states at the Fermi energy. In the presence of an external magnetic field, without taking into account any disorder effects, the DOS is represented as a series of delta functions. In all practical situations, there is always some degree of disorder present in the system. The DOS delta functions broaden due to the presence of scattering centers and the DOS can be represented as a Gaussian, or a Lorentzian function to take this broadening into account. Here, we first consider the Gaussian broadening of DOS denoted by \( D_G(\varepsilon) \) given as

\[
D_G(\varepsilon) = \frac{2}{2\pi \Gamma} \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp \left[ -\frac{(\varepsilon - \varepsilon_n)^2}{2\Gamma^2} \right],
\]

where \( \Gamma \) is the Gaussian distribution broadening width of zero shift. If we use the Poisson summation formula, the summation over \( n \) in the DOS expression can be carried out by changing the variable as \( x = \frac{\varepsilon - \hbar \omega_g \sqrt{n}}{\sqrt{2\Gamma}} \) and applying the limit \( \varepsilon \sim \varepsilon_F \gg \Gamma \), where \( \varepsilon_F = v_D \hbar k_F \) denotes the Fermi energy with Fermi wavenumber \( k_F = \sqrt{2\pi n_s} \) and \( n_s \) is the number density of the system. The first integral yields \( D_0 = \frac{\varepsilon}{\pi \hbar v_D} \) which is the DOS in the absence of magnetic field and the second integral becomes proportional to

\[
\int_{-\infty}^{\infty} dx \exp \left[ -x^2 \right] \cos \left[ \frac{4\pi k_F \varepsilon \Gamma}{\hbar^2 \omega_g} \right] = \sqrt{\pi} \exp \left[ -4 \left( \frac{\pi k_F \varepsilon \Gamma}{\hbar^2 \omega_g} \right)^2 \right].
\]

The final result for the Gaussian broadened DOS can be written as

\[
D_G(\varepsilon) = D_0 \left\{ 1 - 2 \sum_{k=1}^{\infty} (-1)^k \exp \left[ -4 \left( \frac{\pi k_F \varepsilon \Gamma}{\hbar^2 \omega_g} \right)^2 \right] \cos \left[ \frac{2\pi k_F^2 \varepsilon^2}{\hbar^2 \omega_g^2} \right] \right\}.
\]

Furthermore, following the same approach we can also determine Lorentzian broadened DOS \( D_L(\varepsilon) = \frac{2}{2\pi \Gamma} \sum_{n=-\infty}^{\infty} \frac{1}{\pi (\varepsilon - \varepsilon_n)^2 + \Gamma^2} \) with the result

\[
D_L(\varepsilon) = D_0 \left\{ 1 - 2 \sum_{k=1}^{\infty} (-1)^k \exp \left[ -\frac{2\pi k_F^2 \varepsilon \Gamma}{\hbar^2 \omega_g^2} \right] \cos \left[ \frac{2\pi k_F^2 \varepsilon^2}{\hbar^2 \omega_g^2} \right] \right\}.
\]

We see that both forms of broadening yield the same numerical results in the regime \( \varepsilon \sim \varepsilon_F \gg \Gamma \). For \( \Gamma \gg \hbar \omega_g \), it is sufficient to retain only the first order term (\( k = 1 \) term).
since the contribution from the higher order terms is highly damped. Furthermore, the above result for the DOS is the same as obtained in Ref. 11 in the limit when energy gap \( \Delta = 0 \) [11].

III. MAGNETOCAPACITANCE OF A GRAPHENE MONOLAYER

We consider a top-gated graphene device in which the capacitor is formed between the top gate and the graphene sheet. In order to deposit charge on the capacitor formed by the graphene sheet and the gate, the voltage source has to do both electrostatic and chemical work on the system. The effective capacitance is the geometric capacitance in series with "chemical capacitance". In an external magnetic field, the effective capacitance \( C(B) \) can be determined from the following relation [5, 6]

\[
\frac{1}{C(B)} - \frac{1}{C_0} = \frac{1}{e^2 D_0} \left[ \frac{D_0}{D_T(B)} - 1 \right],
\]

where \( C_0 = 1168 \times 10^{-6} \, \text{F m}^{-2} \) is the capacitance at zero magnetic field and \( D_T(B) \) is the temperature dependent DOS at finite magnetic field that is determined from

\[
\frac{\partial n}{\partial \varepsilon} = \int_0^\infty d\varepsilon D_L(\varepsilon) \frac{\partial f(\varepsilon - \varepsilon_F)}{\partial \varepsilon},
\]

where \( n_s \) is the number density and \( f(\varepsilon - \varepsilon_F) \) is the Fermi Dirac distribution function. In the above expression for \( D_T(B) \), we introduce a change of variable \( \beta(\varepsilon - \varepsilon_F) = s \) and apply the low temperature limit such that \( \beta \ll \varepsilon_F \) where \( \beta = \frac{1}{k_B T} \). As a result, it can be expressed as

\[
D_T(B) = D_0 \left\{ 1 + \exp \left[ -\frac{2\pi \varepsilon_F \Gamma}{\hbar^2 \omega_g^2} \right] \cos \left[ \frac{2\pi \varepsilon_F}{\hbar^2 \omega_g^2} \right] \int_0^\infty ds \frac{\cos \left[ \frac{4\pi \varepsilon_F}{\hbar^2 \omega_g^2} \beta s \right]}{\cosh^2(s/2)} \right\}.
\]

The integration can be performed by using the following identity [12]:

\[
\int_0^\infty dx \frac{\cos ax}{\cosh^2 bx} = \frac{a \pi}{2bx^2 \sinh(a \pi/2b)},
\]

with the result that the temperature dependent DOS is

\[
D_T(B) = D_0 \left\{ 1 + 2 \frac{\alpha}{\sinh \alpha} \exp \left[ -\frac{2\pi \varepsilon_F \Gamma}{\hbar^2 \omega_g^2} \right] \cos \left[ \frac{2\pi \varepsilon_F^2}{\hbar^2 \omega_g^2} \right] \right\},
\]

where \( \alpha = \frac{4\pi \varepsilon_F}{\hbar^2 \omega_g^2} \) is a dimensionless parameter which expresses the characteristic temperature for damping of oscillations in \( D_T(B) \).
Following the same approach as given above for graphene monolayer, we can obtain the temperature dependent DOS for conventional 2DEG with the result

\[ D_T(B) = D_s \left\{ 1 + 2 \frac{\alpha_s}{\sinh \alpha_s} \exp \left[ -\frac{2\pi \Gamma}{\hbar \omega_c} \right] \cos \left[ \frac{2\pi \varepsilon_F}{\hbar \omega_c} - \pi \right] \right\}, \]

where \( D_s = \frac{m^*}{2\pi \hbar^2} \) and \( \alpha_s = \frac{2\pi^2}{\hbar \omega_c^2}. \)

Now, we are in a position to compare the results for the temperature dependent DOS for monolayer, given by Eq.(4), with the result for 2DEG, shown in Eq. (5). The following differences in temperature dependent DOS in the two systems are found:

i)- The argument of the oscillatory cosine term, \( \cos \left[ \frac{2\pi \varepsilon_F}{\hbar \omega_c} - \pi \right] \) responsible for the \( \pi \)-Berry phase shift, in 2DEG depends on the ratio of the Fermi energy to the cyclotron frequency while for monolayer graphene the argument of the cosine depends on the square of the ratio of the Fermi energy to the corresponding cyclotron frequency without an extra \( \pi \).

ii)- The exponential term, \( \exp \left[ -\frac{2\pi \Gamma}{\hbar \omega_c} \right] \), responsible for the exponential decay of the amplitude of the oscillatory DOS for 2DEG depends on the ratio of \( \Gamma \) to the cyclotron frequency \( \omega_c \). From Eq.(4), in monolayer graphene the exponential term depends on the ratio of the product of \( \Gamma \) and \( \varepsilon_F \) to the square of the corresponding cyclotron frequency \( \omega_g \). The magnitude of the argument of the exponential term is 1.84 in GaAs 2DEG while 0.22 in Graphene at fixed value of the magnetic field (1 Tesla) and disorder (0.5 meV). Therefore, we expect that for experimentally relevant parameters as considered here, disorder will cause less damping of DOS oscillations in a graphene monolayer compared to a standard 2DEG.

iii)- The temperature dependence of the oscillation amplitude of DOS is given by the factor \( \lim_{\alpha \to \infty} \frac{\alpha}{\sinh(\alpha)} = 2\alpha e^{-\alpha} \). The amplitude of the oscillatory DOS decays exponentially as the temperature is raised. From this temperature dependent coefficient the characteristic temperature for damping of oscillations in DOS, \( T_D \), can be identified such that \( k_B T_D = \frac{v_F \hbar}{2\pi \varepsilon_F} \), with \( v_F \) being the Fermi wavenumber, equal to \( \sqrt{2\pi n_s} \), while in a standard 2DEG the corresponding expression is \( k_B T_s = \frac{\hbar \omega_c}{2\pi^2} = \frac{\hbar eB}{2\pi^2 m^*}. \) Here \( m^* = 0.068 m_e \) in GaAs and \( m_e \) is the usual electron mass. These characteristic temperatures determine the robustness with respect to temperature of magnetic oscillations in DOS. The relative magnitudes of the characteristic temperatures for damping in 2DEG and graphene monolayer is \( \frac{T_D}{T_s} = \frac{v_F}{v_p} \), the ratio of the characteristic temperatures is equal to the ratio of the corresponding Fermi velocities in the two systems, where \( v_p = \frac{\hbar k_F}{m^*} \) is the Fermi velocity in a 2DEG. Typically, the
Fermi velocity of 2DEG systems (∼10^5 m/s) is an order of magnitude smaller than that of Graphene (∼10^6 m/s). An estimate of this ratio of temperatures is given by \( \frac{T_s}{T_D} = \frac{\hbar k_F}{m^* v_{Dm}} \). For GaAs, For Ge is \( \approx 0.03 \) and \( \approx 0.015 \) for Si with a fixed value of the number density \( n_s = 3.2 \times 10^{15} \text{ m}^{-2} \). For comparison for an equal temperature scale the effective mass should be \( \approx 0.016 m_e \), which is smaller than that for most 2DEG systems such as Si, Ge, GaAs.

From the discussion of the DOS expressions in the two systems given above, we expect that the oscillations in the magnetocapacitance will be affected less by temperature in a monolayer graphene compared to a 2DEG (GaAs is considered for comparison in the numerical results) due to the higher damping temperature in the monolayer. On varying the magnetic field, changes in the DOS are reflected by oscillations of the magnetocapacitance. Since magnetocapacitance is directly related to the DOS, the exponential decay in the amplitude of the magnetocapacitance oscillations with temperature and disorder is expected. Before we present results for the magnetocapacitance, the dimensionless DOS \( D_T(B)/D_0 \) for the two systems is shown in Fig.(1). The DOS is plotted as function of the inverse magnetic field. The dimensionless magnetic field \( B_0/B \) is introduced through the characteristic magnetic field \( B_0 = \hbar k_F^2 \). \( B_0 = 13.25 \text{ T} \) for \( n_s = 3.2 \times 10^{15} \text{ m}^{-2} \). The temperature is 1.2 K and the disorder energy \( \Gamma = 0.5 \text{ meV} \) in Fig.(1). The magnetic oscillations, with \( \pi \)-Berry phase difference, are clearly visible in the DOS of the two systems. Furthermore, the oscillation in the DOS in the graphene monolayer are found to be enhanced and less damped with temperature compared to those in a 2DEG. In order to study the effects of temperature on the magnetocapacitance in the monolayer and 2DEG, we show in Figs. (2, 3) the temperature dependent magnetocapacitance as a function of the magnetic field at two different temperatures: 1.5 K and 22 K. In these figures, \( \Gamma \) is held constant at 0.5 meV. We observe, as expected from the above discussion, that oscillations in magnetocapacitance are less damped by temperature and there is a \( \pi \)-Berry phase difference in graphene monolayer compared with the same oscillations found in a 2DEG. For the parameters considered here and with constant disorder, the oscillations found in the magnetocapacitance in a 2DEG become completely damped at 22 K whereas they are found to persist up to a temperature of 60 K in a graphene monolayer. Therefore, we have found that magnetocapacitance oscillations are more robust with respect to temperature damping in a graphene monolayer compared to a 2DEG. Furthermore, these magnetic oscillations have a \( \pi \)-Berry phase difference in the
two systems.

IV. CONCLUSIONS

We have investigated the finite temperature density of states and magnetocapacitance in a graphene monolayer taking into account finite temperature as well as disorder. The results obtained are compared to those found for conventional 2DEG systems. We have found that magnetic oscillations in the DOS and magnetocapacitance in a graphene monolayer are enhanced, are more robust against temperature and have a $\pi$-Berry phase difference compared to a 2DEG.

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[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, Nature 438, 197 (2005); Y. Zhang, Y. W. Tan, H. L. Stormer, and P. Kim, Nature 438, 201 (2005).

[2] Y. Zheng and T. Ando, Phys. Rev. B 65, 245420 (2002); V. P. Gusynin and S. G. Sharapov, Phys. Rev. Lett. 95, 146801 (2005); N. M. R. Perez F. Guinea, and A. H. Castro Neto, Phys. Rev. B 73, 125411 (2006); M. I. Katsnelson, K. S. Novoselov, and A. K. Geim, Nat. Phys. 2, 620 (2006).

[3] K. S. Novoselov, E. McCann, S. V. Morozov, V. I. Fal’ko, M. I. Katsnelson, U. Zeitler, D. Jiang, F. Schedin, and A. K. Geim, Nat. Phys. 2, 177 (2006); J. B. Oostinga, H. B. Heersche, X. Liu, A. F. Morpurgo and L. M. K. Vandersypen, Nat. Mat. 7, 151 (2008); T. Ohta, A. Bostwick, T. Seyller, K. Horn and E. Rotenberg, Science 313, 951 (2006).

[4] C. Berger, et al, Science 312, 1191 (2006); R. S. Deacon, K-C. Chuang, R. J. Nicholas, K. S. Novoselov, and A. K. Geim, Phys. Rev. B 76, 081406(R) (2007); S. Y. Zhou, G.-H. Gweon, J. Graf, A. V. Fedorov, C. D. Spataru, R. D. Diehl, Y. Kopelevich, D. H. Lee, S. G. Louie, and A. Lanzara, Nat. Phys. 2, 595 (2006).

[5] T. P. Smith, B. B. Goldberg, P. J. Stiles, and M. Heiblum, Phys. Rev. B 32, 2696 (1985); V. Mosser, D. Weiss, K. von Klitzing, K. Ploog, and G. Weimann, Solid State Commun.
58, 5 (1986); H.-z. Zheng, A. Song, F.-h. Yang, Y.-z. Li, Phys. Rev. B 49, 1802 (1994); T. Jungwirth, L. Smrcka, Phys. Rev. B 51, 10181 (1995); D. Weiss, C. Zhang, R. R. Gerhardts, K. von Klitzing, G. Weimann, Phys. Rev. B 39, 13020 (1989); T. Ando, Y. Uemura, J. Phys. Soc. Jpn 36, 959 (1974); D. Weiss and K. von Klitzing in High magnetic fields in semiconductor physics, edited by G. Landwehr, Springer series in Solid State Sciences, Vol. 71 (Springer-Verlag, Berlin, 1987).

[6] V. S. Khrapai, A. A. Shashkin, M. G. Trokina, V. T. Dolgopolov, V. Pellegrini, F. Beltram, G. Biasiol, and L. Sorba, Phys. Rev. Lett. 99, 086802 (2007); V. S. Khrapai, A. A. Shashkin, M. G. Trokina, V. T. Dolgopolov, V. Pellegrini, F. Beltram, G. Biasiol, and L. Sorba, Phys. Rev. Lett. 100, 196805 (2008).

[7] T. Ando, A. B. Fowler and F. Stern, Rev. Mod. Phys. 54, 437 (1982); Akira Isihara and Ludvig Smrcka, J. Physics. C: Solid State Phys. 19, 6777 (1986); A. Alsihara, Physica Scripta. Vol. 32, 26 (1985).

[8] S. Ilani, L. A. K. Donev, M. Kindermann and P. L. McEuen, Nat. Phys. 2, 687 - 691 (2006); Jing Guo, Youngki Yoon, and Yijian Ouyang, Nano Lett., 7 (7), 1935 (2007).

[9] R. B. Dingle, Proc. R. Soc. A 211, 517(1952); Akira Isihara and Ludvig Smrcka, J. Physics. C: Solid State Phys. 18, 4703(1985).

[10] Akira Endo and Yasuhiro Iye, J. Phys. Soc. Jpn 77, 064713 (2008), and references therein.

[11] V. P. Gusynin and S. G. Sharapov, Phys. Rev. Lett. 95 146801 (2005); V. P. Gusynin and S. G. Sharapov, Phys. Rev. B 71 125124 (2005); S. G. Sharapov, V. P. Gusynin and H. Beck, Phys. Rev. B 69 075104 (2004).

[12] I. S. Gradshteyn and I. M. Ryzhik, Table of Integrals, Series and Products (Academic Press, New York, 1980).