Thermodynamic Properties of electrically modulated monolayer Graphene: Theory

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Abstract

Theoretical investigation of thermodynamic properties of electrically modulated monolayer graphene in the presence of a perpendicular magnetic field $B$ is presented. The results obtained are compared with those of the conventional 2DEG. The one-dimensional periodic potential due to electric modulation lifts the degeneracy of the Landau Levels and converts them into bands whose width oscillates as the function of $B$. We find Weiss type oscillations for small values of $B$ and dHvA type oscillations at larger values values of $B$. These oscillations are more pronounced in Graphene than in conventional 2DEG system. These oscillations are less damped with temperature in Graphene compared with conventional 2DEG systems.
I. INTRODUCTION

Graphene is a 2D-honeycomb lattice of carbon atoms. Its experimental realization has opened up new horizons in the field of condensed matter physics and material sciences. Unique electronic properties of Graphene make it substantially different from conventional 2DEG systems. The quasi particles in graphene at low energies have a linear dispersion relation $\epsilon_k = \hbar v_F k$ with characteristic velocity of $v_F = 10^6 \text{m/s}[1]$. These quasi particles called massless Dirac Fermions, can be treated as electrons with zero mass or neutrinos having electronic charge. The zero mass property of charge carriers in graphene along with charge conjugation symmetry, results in many unusual transport phenomena such as anomalous Quantum Hall Effect, Chiral Tunneling and non-zero Berry’s Phase[2–6]. The 2D Dirac like spectrum was also confirmed recently by cyclotron resonance measurements in monolayer Graphene[1] and also by angle resolved photo electron spectroscopy[7].

Weiss oscillations[8, 9] appear in magnetoresistance when conventional 2DEG is subjected to artificially created periodic potentials (either electric or magnetic) in submicron range. Electrical modulation can be carried out by depositing an array of parallel metallic strips on the surface[12] or through two interfering laser beams[13]. These Oscillations are the direct consequence of the commensurability of two different length scales namely the cyclotron orbit radius $R_c = \sqrt{2\pi n_e l^2}$ (where $n_e$ is the density of electrons, and $l = \sqrt{\hbar/eB}$ is the magnetic length) and the period of modulation $a$. Weiss oscillations occur in the small magnetic field range[10, 11] and are separate from dHvA(de Hass van Alphen) and SdH(Subnikov de Hass) type oscillations which occur at larger values of magnetic field. These oscillations are found to be periodic in the inverse magnetic field. It is interesting to study the effects of electrical modulation on Dirac electrons in graphene. Theoretical studies of transport properties of Dirac electron in graphene subjected to electrical modulation were recently carried out and showed the appearance of Weiss oscillations in magnetoconductivity. In addition, the magnetoplasmon spectrum of monolayer graphene in the presence of electrical modulation was recently investigated[14].

In this work we investigate the effects of electrical modulation on thermodynamic properties of monolayer graphene and compare the results obtained with those of conventional 2DEG system found in semiconductor heterostructures. To this end, we have determined the following thermodynamic quantities: The chemical potential, Helmholtz free energy, orbital
magnetization, orbital magnetic susceptibility and electronic specific heat. The results are compared with those of the conventional 2DEG studied in[15] and[16].

This paper is arranged as follows. In section II, we give the formulation of the problem. The calculation of the thermodynamic quantities is given in section III and numerical results with discussion are presented in section IV. Finally the Conclusions are drawn at the end.

II. FORMULATION

We consider monolayer graphene in the xy-plane subjected to a magnetic field B along the z-direction. In the Landau gauge, the unperturbed Dirac like Hamiltonian for single electron may be written as[6]

$$\hat{H}_o = v_F \sigma \cdot \left( -i\hbar \nabla + eA \right). \tag{1a}$$

Here, $\sigma = \{\sigma_x, \sigma_y\}$ are the Pauli matrices and $v_F = 10^6 m/s$ characterizes the electron velocity. and $A = (0, Bx, 0)$ is the vector potential. The normalized eigenfunctions of the Hamiltonian given in Eq.(1)[17]

$$\Psi_{n,k_y} = \frac{e^{ik_y y}}{\sqrt{2L_y^l}} \left( \phi_n \frac{[(x + x_o)/l]}{\phi_n [((x + x_o)/l]} \right), \tag{2}$$

where $\phi_n = \frac{\exp(-x^2/2)}{\sqrt{2^n n! \sqrt{\pi}}} \sqrt{2} \mathcal{H}_n(x)$, $\mathcal{H}_n(x)$ are the Hermite Polynomials, $L_y$ is the normalization length in the y-direction, $n$ is an integer corresponding to the Landau Level index and $x_o = k_y l^2$, is the center of the cyclotron orbit. The energy eigenvalues are

$$\varepsilon_n = \frac{v_F \hbar \sqrt{2n}}{l} = \sqrt{n} \hbar \omega_c \tag{3}$$

where $\omega_c = v_F \sqrt{\frac{2eB}{\hbar}}$ is the cyclotron frequency of the Dirac electrons in graphene. To investigate the effects of modulation we write the Hamiltonian in the presence of modulation as

$$H = H_o + U(x) \tag{4}$$

where $U(x)$ is the one-dimensional periodic modulation potential along the x-axis and is given by

$$U(x) = V_o \cos Kx. \tag{5}$$
\[ K = \frac{2\pi}{a}, \quad a \text{ is the period of modulation and } V_o \text{ is the constant modulation amplitude.} \]

To account for the weak modulation we take \( V_o \) to be an order of magnitude smaller than the Fermi Energy \( \varepsilon_F^e = v_F \hbar k_F \), where \( k_F = \sqrt{2\pi n_s} \) is the magnitude of Fermi wave vector. Hence we can apply standard first order perturbation theory to determine the energy eigenvalues in the presence of modulation. The first order energy correction is

\[ \varepsilon_{n,x_o} = \varepsilon_n + U_n \cos K x_o \]  

Here, \( U_n = \frac{V_o}{2} \exp\left(-\frac{\chi^2}{2}\right)[L_n(\chi) + L_{n-1}(\chi)], \quad \chi = \frac{K^2}{2} \) and, \( L_n(\chi) \) and \( L_{n-1}(\chi) \) are Laguerre polynomials.

Although similar features in the energy spectrum have also been found in the 2DEG system under similar conditions, there are substantial differences between the two systems. Landau level spectrum of Dirac electrons depends on the square root of both magnetic field \( B \) and the Landau band index \( n \) against linear dependence in the case of conventional electrons in 2DEG. The energy eigenvalues in the presence of modulation given by Eq.(6) contains a term which is a linear combination of two successive Laguerre polynomials with indices \( n \) and \( n - 1 \), while conventional electrons obey a relation containing one Laguerre polynomial with index \( n \).

The modulation potential lifts the degeneracy of the Landau levels and broadens the formerly sharpe levels into electric Landau bands. The electric modulation induced broadening of the energy spectrum is nonuniform. The Landau band width \( U_n \) oscillates as a function of \( n \) since \( L_n(\chi) \) is an oscillatory function of the index \( n \). These landau bands become flat for different values of \( B \). Flat bands occur for those values of \( B \) for which modulation strength becomes zero. By putting \( U n = 0 \) one can get the flat band condition.

\[ \exp\left(-\frac{\chi^2}{2}\right)[L_n(\chi) + L_{n-1}(\chi)] = 0 \] 

Using the asymptotic expression \[ \text{[17]} \]

\[ \exp\left(-\frac{\chi^2}{2}\right)L_n(\chi) \simeq \frac{1}{\sqrt{\pi} \sqrt{n\chi}} \cos\left(2\sqrt{n\chi} - \frac{\pi}{4}\right) \] 

and \( L_n(\chi) = L_{n-1}(\chi) \), one obtains from Eqs (6) and (7) the following condition

\[ 2R_c = a(i - 1/4), \quad i = 1, 2, 3, \ldots \ldots \]  

where, \( R_c = k_F l^2 \), is the classical cyclotron orbit. From Eqs (6) and (8) it can be observed that, in the large \( n \) limit electron bandwidth oscillates sinusoidally and is periodic in \( 1/B \).
for fixed values of $n$ and $a$. When $n$ is small bandwidth still oscillates, but the condition (9) no longer holds because neither eq. (8) nor $L_n(\chi) \simeq L_{n-1}(\chi)$ is valid. Interestingly, for low values of $B$, when many Landau levels are filled, both the systems have the same flat band condition[15].

It is well known that in the absence of modulation the density of states (DOS) consists of a series of delta functions at energies equal to $\varepsilon_n$. The addition of a weak periodic electric modulation however modifies the former delta functions leading to DOS broadening. The density of states $D(\varepsilon)$ are given by [18]

$$D(\varepsilon) = \frac{A}{\pi l^2} \sum_{n,x_o} \delta (\varepsilon - \varepsilon_{n,x_o}) = \frac{A}{\pi l^2} \sum_{n,x_o} \theta (|U_n| - |\varepsilon - \varepsilon_{n,x_o}|) \sqrt{|U_n|^2 - (\varepsilon - \varepsilon_{n,x_o})^2}$$

(10)

where, $\theta(x)$ is a unit Heaviside step function and $A$ is the area of the sample.

### III. EQUILIBRIUM THERMODYNAMIC QUANTITIES

We have determined the electronic contribution to the equilibrium thermodynamic properties of monolayer graphene subjected to a perpendicular magnetic field and weak electric modulation. The thermodynamic quantities calculated are chemical potential, Helmholtz free energy, electronic specific heat, orbital magnetization and orbital magnetic susceptibility.

The magnetic field ($B$) and temperature ($T$) dependent chemical potential $\mu \equiv \mu(B,T)$ of a system can be determined by inverting the following relation

$$N = \int_0^\infty D(\varepsilon) f(\varepsilon)d\varepsilon$$

(11)

where the Fermi Dirac distribution function $f(\varepsilon)$ is

$$f(\varepsilon) = \left[ \exp \left( \frac{\varepsilon - \mu}{k_B T} \right) + 1 \right]^{-1},$$

(12)

$k_B$ is the Boltzmann’s constant and $N$ is the total number of electrons. Hence change in the $D(\varepsilon)$ will affect $\mu(B,T)$. Substituting Eq.(9) into Eq.(11) we obtain

$$N = \frac{A}{\pi l^2} \sum_{n=0}^\infty \int_{-1}^1 \frac{dx}{\sqrt{1-x^2}} (1 + \chi_n \exp[z_n x])^{-1}$$

(13)
Here $\chi_n = \exp \left[ \frac{\varepsilon_n - \mu}{k_B T} \right]$ and $z_n = |U_n|/(k_B T)$. Eq. (12) can be used for both modulated and unmodulated systems ($z_n = 0$). We solve this equation numerically in order to obtain the chemical potential $\mu(B, T)$. We are able to determine the change in the chemical potential due to the electric modulation. Once the chemical potential and the density of states are known, the free energy $F$ of the system can be calculated. From there on the thermodynamic properties of the system can be obtained from the free energy by taking the appropriate derivatives. For a system of non-interacting fermions, the Helmholtz free energy is given by [19]

$$F = \mu N - k_B T \int_0^\infty D(\varepsilon) \ln \left[ 1 + \exp \left( \frac{\mu - \varepsilon}{k_B T} \right) \right] d\varepsilon$$

The density of states $D(\varepsilon)$ is the central quantity in the above expression. The expression for $D(\varepsilon)$ in graphene is different from that in conventional 2DEG due to the difference in the energy spectrum in the two cases. This difference will affect the electronic contribution in the thermodynamic properties in the two systems determined from the following free energy for the electrically modulated graphene system

$$F = \mu N - k_B T A \pi^2 l^2 \sum_{n=-\infty}^{\infty} \int_{-1}^{1} \frac{dx}{\sqrt{1-x^2}} \ln \left[ 1 + \chi_n^{-1} \exp (-z_n x) \right]$$

From Eq. 15, one can calculate the electronic contribution of magnetization for both graphene and 2DEG systems as $M = - \left( \frac{\partial F}{\partial B} \right)_{A, N}$ and specific heat as $C_v = - T \left( \frac{\partial^2 F}{\partial T^2} \right)_{A, N}$. The electronic contribution to susceptibility is obtained directly from $\chi = - \left( \frac{\partial^2 F}{\partial B^2} \right)_{A, N}$.

### IV. RESULTS AND DISCUSSION

Numerical study of thermodynamic properties for monolayer graphene system subjected to electrical modulation is presented. We have also plotted the same quantities for the 2DEG system. This is to facilitate comparison and was also a check on our numerical program. For the 2DEG parameters for GaAs are used. We have taken $n_s = 3.16 \times 10^{15} m^{-2}$ and $a = 382 nm$. For electrical modulation we have taken $V_0 = 1 meV$. Thus our 2DEG results are those already given in [16? ]. Modulation induced effects on thermodynamic quantities can be highlighted by calculating the difference between the modulated case and the unmodulated case in each system.
In Figures 1 – 5 we have plotted the change in various thermodynamic properties due to electric potential at temperatures of $T = 2K$ (full curve) and $T = 6K$ (broken curve). for both conventional 2DEG system and graphene system. These figures were scaled to appropriate values to make them appear dimensionless.

In Fig. (1), we have plotted the change in chemical potential versus magnetic field at temperatures $2K$ (straight) and $6K$ (broken). For Conventional 2DEG system for $B < 0.3T$, oscillations depend very weakly on temperature, which is a clear signature of Weiss type Oscillations. Where as for $B > 0.3T$, the oscillations depends strongly on temperature, in particular they die out at $6K$, a clear signature of dHvA type oscillations. Furthermore, the zeros in the chemical potential are in close agreement as predicted by the flat band condition Eq.(9). A similar behavior is expected for Graphene system. But for Graphene the value of $B$ defining the boundary between the two oscillatory phenomena is quite low (It lies some where between 0.1 and 0.15T). For smaller values of $B$ Weiss type oscillations are present and the amplitude of the oscillations remain essentially the same at different temperatures. For larger values of $B$, the familiar dHvA-type oscillations are present, as the amplitude of oscillations is reduced considerably at comparatively higher temperature. However the oscillatory phenomenon still persists, contrary to the conventional 2D system in which oscillations completely die out at $6K$. In comparison we can say, Graphene system is more sensitive to the magnetic field and less sensitive to temperature, than the conventional 2DEG system. This difference arises mainly due to the difference in the Landau level energies of the two systems and due to the presence of an additional Laguerre Polynomial term in the modulation contribution to the energy spectrum for Graphene system.

The Free energy is shown in Fig. (2), for the two systems. To make $y$-axis dimensionless, Free energy has been scaled using $F_0 = \frac{1}{2}NE_F$. It can be seen that at small values of $B$ periodically modulated potential induces temperature independent Weiss type oscillations, with zeros occurring at their respective flat band conditions. Weiss Oscillations are more pronounced in Graphene system, significantly the amplitude of Weiss oscillations for the graphene system remains unchanged at higher temperature, contrary to the 2DEG in which damping may be observed. The familiar dHvA type oscillations are observed for higher values of $B$. As in the case of the Chemical Potential, again the dHvA type oscillations starts quite early. The first period for the dHvA type oscillations starts from $B = 0.3T$ and extends up to $0.6T$ for the standard 2DEG system, while for graphene the first period of
dHvA type starts near $B = 0.175T$ and terminates at $0.27T$.

In Figs.(3) and (4) we have plotted the changes in the magnetization $\Delta M$ and the susceptibility $\Delta \chi$ against the magnetic field. Both the quantities has been appropriately scaled to appear dimensionless. At low $B$ oscillations having their origin in the commensurability of two length scales, and are effected weakly by temperature, having zeros as given by their respective flat band conditions. For higher values of $B$, dHvA oscillations are present at lower temperature ($2K$), with amplitude becoming zero for the conventional 2DEG system while reduced considerably for the Graphene system at higher temperature ($6K$).

In fig.5 we plot change in the electronic specific heat capacity against magnetic field. $y$-axis has been scaled using $C_{el} = Nk_B$, to appear dimensionless. In both systems the Weiss type oscillations are not large effects, however the damping behavior of dHvA type oscillations is clearly observable.

V. CONCLUSIONS

We have presented a study of the thermodynamic properties of monolayer graphene system and compared the results with those of the conventional 2DEG. The commensurability oscillations (Weiss type) and dHvA type oscillations are reflected in all the thermodynamic quantities under consideration in this work for the two systems. However, these effects are more pronounced in graphene system in the sense that the oscillations in the thermodynamic quantities are more robust against temperature. We can therefore say that Graphene system is less sensitive to temperature and more sensitive to the magnetic field. This difference arises because of the different nature of the quasiparticles in the two systems.

VI. REFERENCES

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