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Influence of Zeeman Splitting on Bandwidth in a Periodically Modulated Two Dimensional System

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Periodic electric and magnetic modulation in low dimensional systems like graphene lead to novel features in transport properties. Depending upon modulation strength, new features arises in the band structure and oscillations in the Landau level spectrum. The periodic modulation generates a set of mini bands and gaps in the energy spectrum by changing the environment. So in this regard the Zeeman splitting introduces incremental features in the band structure and the Landau levels spectrum. In this paper, we find the influence of gap opening Zeeman term on the broadening of energy spectrum induced by a weak electric modulation. We illustrate that the Landau bandwidth oscillates with Landau level index. We also present that the presence of Shubinkove-de-Haas (SdH) oscillations arise from jumps in the Fermi level index. We determine how strongly these oscillations are increased by the addition of the Zeeman term.

1. Introduction

For many years, the world of science has been fascinated by the exploration of quantum phenomena in two-dimensional (2D) systems. These types of systems have distinct electronic characteristics that make them apart from their three-dimensional counterparts, generating opportunities for new technological uses[1]. Zeeman splitting, or the splitting of energy levels in the presence of an external magnetic field, is one of the many fascinating phenomena seen in 2D systems and has a significant impact on the electrical characteristics and behavior of these materials[2]. The periodic modulation of 2D systems has been made possible by recent developments in material science, which further widens the range of potential magnetic and electronic configurations.The bandwidth, a critical factor that determines the material's magnetic and electrical properties, is effected by this periodic modulation, which generates new opportunities for the electronic band structure. For the production of next-generation quantum technologies and[3] electrical devices , it is important to comprehend how bandwidth modulation and Zeeman splitting interact in regularly modulated 2D systems.The goal of this work is to measure the effect of Zeeman splitting on bandwidth in a two-dimensional modulated system. The main physics effecting the venture of magnetic fields with modulation periods will be outlined in this study using a combination of theoretical derivations and experiments.The complexity of these systems are better understood from the concepts of quantum mechanics through more research, which can lead to the exploration of fresh insights that can benefit creative applications in quantum computing, spintronics, and advanced material design.

2. Model

Lets consider a monolayer of two dimensional graphene on which we apply magnetic field **B** perpendicularly to its plane[4].This monolayer graphene will show Zeeman splitting under the effect of external magnetic field. We also subject this graphene system to weak periodic electric modulation defined by $V(x)$ in the x-direction.The Hamiltonian comes to be [8],

$$\hat{H} = \hbar v_F \sigma.(p + eA) + \Delta_z \sigma_z + V(x) \qquad (1)$$

Where p is the momentum operator,$\sigma = \sigma_x, \sigma_y, \sigma_z$ are pauli matrices,Δ_z represents Zeeman splitting and v_F which has approximate value of $10^6 m/s$ is the electron velocity in graphene. For unmodulated graphene $V(X) = 0$ and [5] Landu gauge $A = (0, B_x, 0)$, we define the unperturbed Hamiltonian as:

$$\hat{H} = \hbar v_F \sigma.(p + eA) + \Delta_z \sigma_z \qquad (2)$$

By using eigenvalue equation $H\psi = E\psi$, we can find eigenvectors and eigenvalues

$$\begin{bmatrix} \Delta_z & \hbar v_F (p_x - i p_y) \\ \hbar v_F (p_x + i p_y) & -\Delta_z \end{bmatrix} \begin{bmatrix} \phi \\ \psi \end{bmatrix} = E \begin{bmatrix} \phi \\ \psi \end{bmatrix} \qquad (3)$$

In terms of ϕ and ψ we get two coupled equations

$$\begin{aligned} \hbar v_F (p_x - i p_y)\psi &= (E - \Delta_z)\phi \\ \hbar v_F (p_x + i p_y)\phi &= (E + \Delta_z)\psi \end{aligned} \qquad (4)$$

The Eq. (4) can be easily decoupled into two second order differential equations as;

$$[\frac{d}{dx^2} - \frac{(x_o+x)^2}{l_B^4}]\phi = \quad -a\phi$$
$$[\frac{d}{dx^2} - \frac{(x_o+x)^2}{l_B^4}]\psi = \quad -b\psi \qquad (5)$$

Where a and b are constants defined as:

$$a \quad = \frac{E^2-\Delta_Z^2}{(\hbar v_F)^2} - \frac{1}{l_B^2}$$
$$b \quad = \frac{E^2-\Delta_Z^2}{(\hbar v_F)^2} + \frac{1}{l_B^2} \qquad (6)$$

where $l_B = \sqrt{\frac{\hbar}{eB}}$ is the magnetic length, and $x_0 = k_y l_B^2$ is the center of cyclotron orbit[5]. Thus normalized eigenfunctions $\Psi(x, y)$ for our hamiltonian as :

$$\Psi_n, k_y = \frac{e^i k_y y}{\sqrt{2L_y l_B}} \begin{bmatrix} -i\Phi_{(n-1)}(\frac{x+x_o}{l_B}) \\ \Phi_n \quad (\frac{x+x_o}{l_B}) \end{bmatrix} \qquad (7)$$

Where $\Phi_{(n-1)}$and Φ_n represents harmonic oscillator wave functions. They can be written explicitly as:

$$\Phi_n = \frac{e^{-\frac{x^2}{2}}}{\sqrt{2^n n!\sqrt{\pi}}} \widehat{H}_n \qquad (8)$$

Where $\widehat{H}_n$ is normalized Hermite polynomial with n being the Landau Level (LL) index. Here L_y is the length of two dimensional graphene system in y-axis. . So for finding Energy eigen values we have:

$$\left[\frac{E^2-\Delta_Z^2}{(\hbar v_F)^2} + \frac{1}{l_B^2}\right]\psi = -\left[(\frac{d}{dx})^2 - \frac{(x_o+x)^2}{l_B^4}\right]\psi \qquad (9)$$

We can write above equation as

$$\frac{1}{2}\left[\frac{E^2-\Delta_Z^2}{(\hbar v_F)^2} + \frac{1}{l_B^2}\right]\psi = \frac{1}{2}\left[p_x^2 + \frac{(x_o+x)^2}{l_B^4}\right]\psi \qquad (10)$$

Now if you compare left hand side of above equation with quantized total energy of harmonic oscillator which is $\hbar\omega_c(n + \frac{1}{2})$ then

$$\hbar\omega_c(n + \frac{1}{2}) = \frac{1}{2m}\left[\frac{E^2-\Delta_Z^2}{(\hbar v_F)^2} + \frac{1}{l_B^2}\right] \qquad (11)$$

We arrive to the result given below for the energy eigenvalues:

$$E_n = \sqrt{\Delta_z^2 + \omega_g^2 n\hbar^2} \qquad (12)$$

where $\omega_g = \sqrt{\frac{2eBv_F^2}{\hbar}}$ is cyclotron frequency of Dirac electrons in graphene.Figure 1 shows LLs spectrum as a function of magnetic field strength. In Figure 2, we show LLs spectrum[6] in the absence and presence of Zeeman splitting. The blue curves show the spectrum for $\Delta_z \neq 0$ and orange curve represents spectrum for $\Delta_z = 0$. The spectrum shows the contribution of the splitting is enhanced in the presence of Δ_z

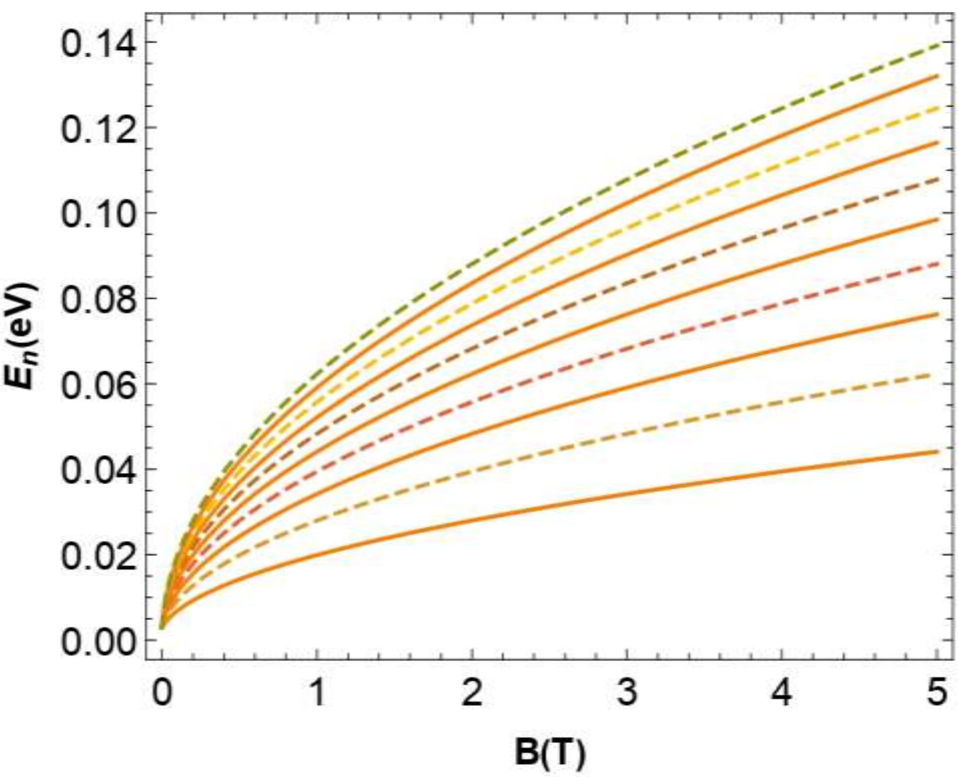

Figure 1: LLs as a function of magnetic field in the presence of Zeeman splitting.

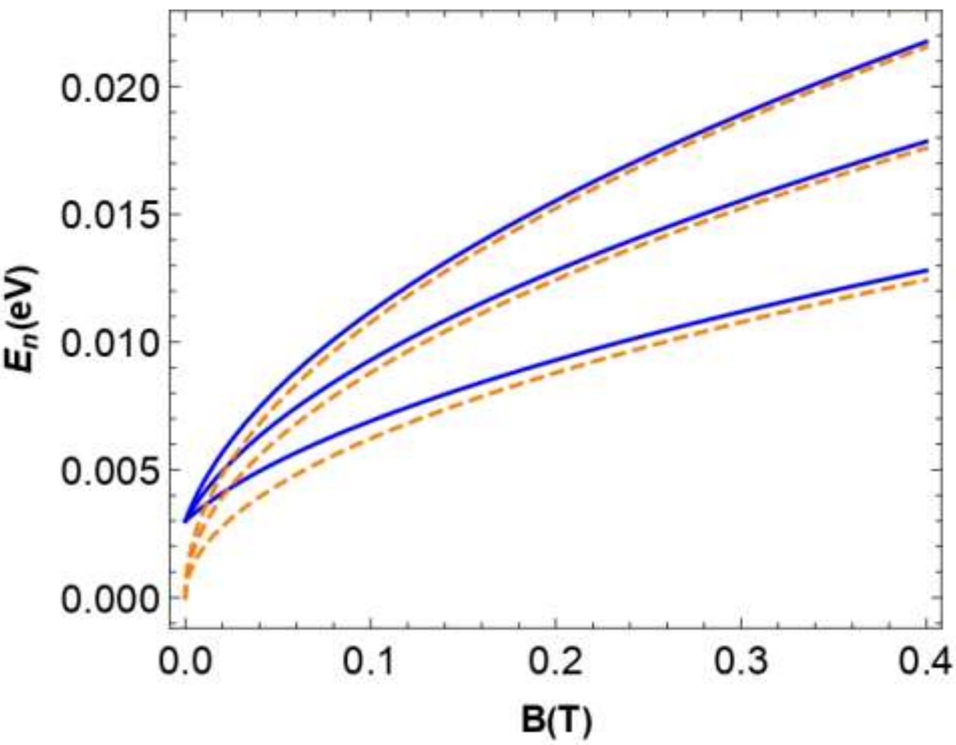

Figure 2: LLs in the presence and absence of Zeeman splitting.Blue curves show the spectrum for $\Delta_z \neq 0$ and orange curve represents spectrum for $\Delta_z = 0$. The parameter chosen are $\Delta_z = 3meVB, v_f = 3 \times 10^5 m/s$

3. Energy eigen values calculation

Next we focus our attention to the modulated potential V_x which we approximate by the first Fourier component of periodic potential $V(x) = V_e \cos kx$, where $k = \frac{2\pi}{a}$ and "a" being a modulation period. Here V_e is the modulation constant amplitude also known as modulation strength .The modulation potential $V(x)$ lifted the degeneracy of landau levels and the energy becomes dependent on position x_o of guiding centre.Since modulation is weak($V_e < < E_F$),we use the standard first order perturbation theory to evaluate the energy eigenvalues of a weakly modulated graphene system such that;

$$\Delta E_n, k_y = \int_{-\infty}^{\infty} dx \int_0^{L_y} dy \Psi_n^*, k_y(x,y) V(x) \Psi_n, k_y(x,y) \quad (13)$$

Solve the above equation by using Eq. (7) and Eq. (8),we arrive at the expression:

$$\Delta E_n, k_y = \frac{V_e}{2l} \int_{-\infty}^{\infty} e^{-}(\frac{x+x_o}{l}) \cos Kx \{\frac{1}{2^n n! \sqrt{\pi}} [H_n(\frac{x+x_o}{l})]^2 + \frac{1}{2^{n-1}(n-1!)\sqrt{\pi}} [H_{n-1}(\frac{x+x_o}{l})]^2\} dx \quad (14)$$

We can define new variable $x' = (\frac{x+x_o}{l})$ and after solving the above equation,we arrive at the following relation

$$\Delta E_n, k_y = V_e \cos Kx_o \int_{-\infty}^{\infty} e^{-x'^2} \cos lKx' \{\frac{1}{2^n n! \sqrt{\pi}} [H_n(x')]^2 + \frac{1}{2^{n-1}(n-1!)\sqrt{\pi}} [H_{n-1}(x')]^2\} dx' \quad (15)$$

The above integrals are of the following type;

$$\int_0^{\infty} e^{-x^2} \cos(bx) [H_n(x)]^2 dx = 2^{n-1} \sqrt{\pi} n! \, e^{\frac{-b^2}{4}} L_n(\frac{b^2}{2}) \quad (16)$$

Hence solving second last equation ,we reach the following expression;

$$\Delta E_{n,k_y} = V_e \cos kx_o e^{\frac{-u}{2}} [\frac{L_n(u) + L_{n-1}(u)}{2}] \quad (17)$$

Thus energy eigenvalues for weak electric modulation is

$$E_{n,k_y} = E_n + V_{n,B} \cos kx_o \quad (18)$$

Where $V_{n,B} = \frac{V_e}{2} e^{-\frac{u}{2}} [L_n(u) + L_{n-1}(u)]$ is Landau bandwidth and both $L_{n-1}(u)$ and L_n are Lauguerre polynomial,here $u = \frac{k^2 l^2}{2}$. As weak modulation having amplitude of $V_(x)$ is much smaller than the cyclotron energy $\hbar\omega_g$ is taken,so Landau levels mixing can be ignored at these weak B fields.In this system,it is important to note that we have taken Fermi level to be moveup from Dirac point which explain this system related to n-doped graphene. As we know that,for the graphene which is undoped,the Fermi level is at Dirac point and density of electron in conduction band will become zero. However we can doped real graphene samples.We also observe the energy spectrum broadening which is induced by weak electric modulation is nonuniform.Now if we approximate $\cos kx_o \approx 1$ then Figure 3 can present the total energy eigen values in the presence and absence of zeeman splitting.

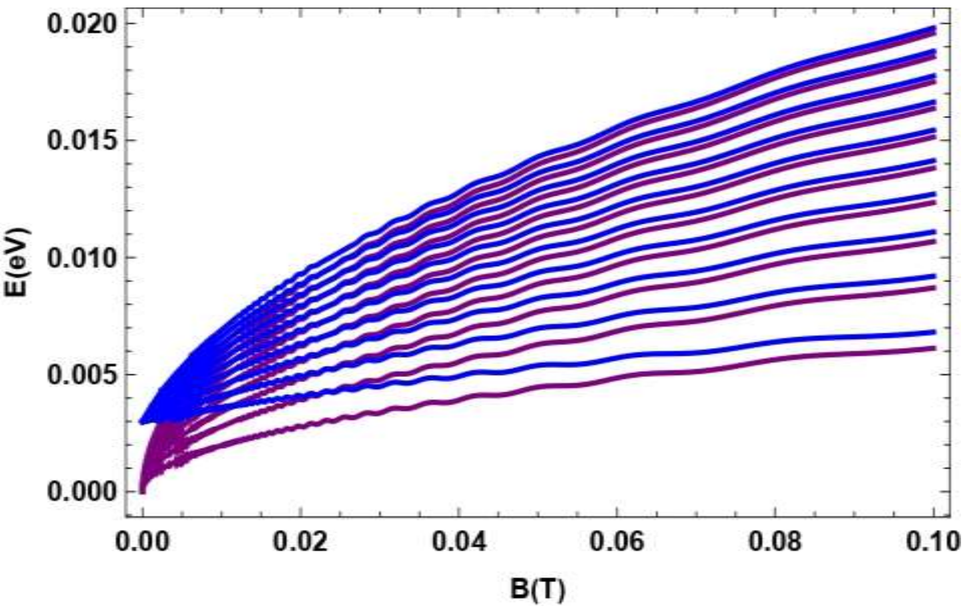

Figure 3 : Energy eigen values in the presence of Electric Modulation.Blue curves show thespectrum for $\Delta_z \neq 0$ and purple curve represents spectrum for $\Delta_z = 0$

In Figure 3, we can see a splitting because of electrons magnetic moment interaction with external magnetic field. In the presence of Zeeman splitting term, we can observe the shift in energy levels . Landau bandwidth oscillates with Landau level index because Laguerre polynomials are oscillatory functios of n.So by using an asymptotic expression for $n >> 1$, $V_{n,B}$ can be approximated at Fermi energy which is suitable for low magnetic field range and it is also coincide to present study,as

$$V_B = V_e \sqrt{\frac{2}{\pi k R_c}} \cos(kR_c - \frac{\pi}{4}) \quad (19)$$

Where $R_C = k_F l^2$ is classical cyclotron orbit[7],$k_F = \sqrt{2\pi n_e}$ and n_e is the electron number density.The above expressions shows thatV_B oscillates with magnetic field,through R_C and maxima of Landau bandwidth $2|V_B|$ occurs at;

$$\frac{2R_c}{a} = i + \frac{1}{4}(i = 1,2,3,\ldots..) \qquad (20)$$

And bandwidth vanishes at;

$$\frac{2R_c}{a} = i - \frac{1}{4}(i = 1,2,3,\ldots..) \qquad (21)$$

Eq. (20) is called broad band condition while Eq. (21) is called as flat band condition.The origin of commensurability (Weiss) oscillations[8] are caused by the oscillations of Landau bandwidth $2|V_B|$. This Landau bandwidth are also responsible for phase of Shubnikov-de Haas (Sdh) oscillations[9] and amplitude modulation. So, the half Landau bandwidth of the Fermi energy of periodically modulated graphene as a magnetic field function is shown in Figure 4.

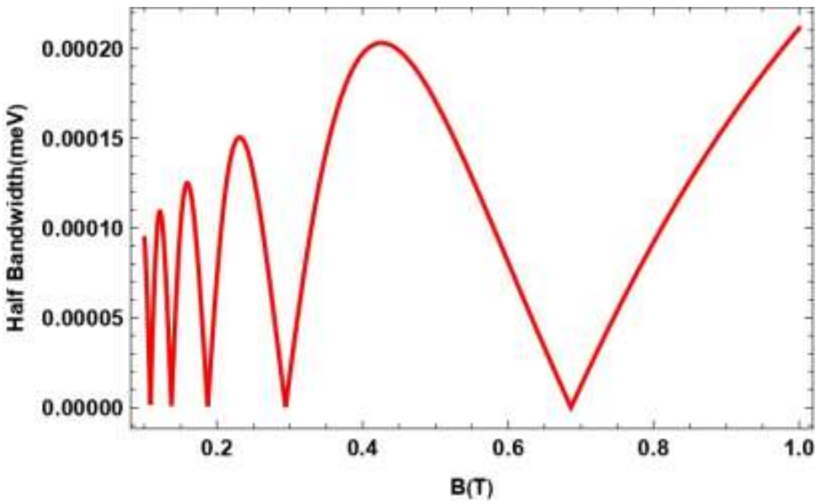

Figure 4: The Landau level bandwidth in an electrically modulated graphene at Fermi energy as a function of magnetic field.

The curve shows the exact numerical result of the bandwidth which is $V_{n,B} = \frac{V_e}{2} e^{-\frac{u}{2}}[L_n(u) + L_{n-1}(u)]$ for $n = n_F$.Here $n_F = (\frac{E_F}{\hbar\omega_g})^2$ which gives the LL index at the Fermi energy. The jumps in the curves show the presence of Shubnikov-de Haas oscillations, and the integer n_f varies discontinuously with magnetic field.

4. Density of State

Here we introduced the Density of States(DOS) which can be expressed as $\hat{\delta}$ function sum as ;

$$D(E) = \frac{1}{\Omega^*}\Sigma_{n,\alpha,s}\hat{\delta}(E - E_{n\alpha s}) \qquad (22)$$

Where $\Omega *= L_X \times_Y^L$ is system area.For plotting DOS we take Gaussian broadening for LLs so Eq. (22) becomes;

$$D(E) = \frac{1}{D_o}\frac{1}{\hat{\Gamma}\sqrt{2\pi}}\Sigma_{n,\alpha,s}\exp[\frac{E-E_{n\alpha s}}{2\hat{\Gamma}^2}] \ (23)$$

Where $\hat{\Gamma}$ is the LLs broadening term due to disorder and $D_o = \frac{1}{2\pi l_b}$.The impurity induced broadening in 2D materials which are proportional to $\sqrt{B}$.We can obtain Fermi energy by using density of states from the following relation;

$$n_C = \int_{-\infty}^{-\infty} D(E)F(E)dE = \frac{1}{D_o}\Sigma_{n,\alpha,s}F(E_{n\alpha s}) \ (24)$$

Here $D(E)$ is termed as states density,$D_o = \frac{1}{2\pi l_b}$,here Fermi-Dirac function is $F(E_{n\alpha s}) = \frac{1}{(1+e^{\beta(E_{n\alpha s}-E)}}$, $\beta = \frac{1}{K_b T}$ and n_c is concentration of electron.We calculate the Fermi energy numerically as a function of magnetic field from Eq. (23), shown in Figure 5.

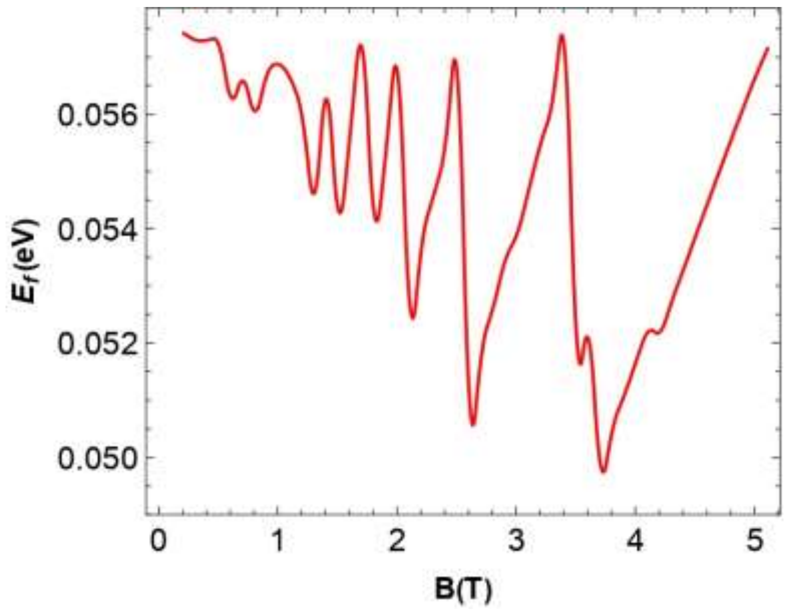

Figure 5: LLs with Fermi level(E_F) as a function of magnetic field

In Figure 5,we draw LLs with Fermi level (E_F) as a magnetic field function for Bi_2Te_3.The Fermi level vibrates between two consecutive LLs as strenght of magnetic field is increased.we notice an increase in amplitude of fluctuations with increasing B strength as a result of increased LLs[10] splitting between consecutive n.The huge fluctuations in Fermi level at stronger magnetic field resulted from some LLs contributing keeping n_c constant.

Here Figure 6 represents states density as a function of magnetic field.DOS depicts SdH oscillations in the absence of gap opening terms for low magnetic field and huge splitting at higher B values.In the presence of Zeeman splitting term,we notice SdH oscillations showing doubly split peaks at $1.4T$.This will happen because of doubly split landau levels in the spectrum.We also see that,in the presence of higher magnetic field oscillations amplitude decays rapidly.

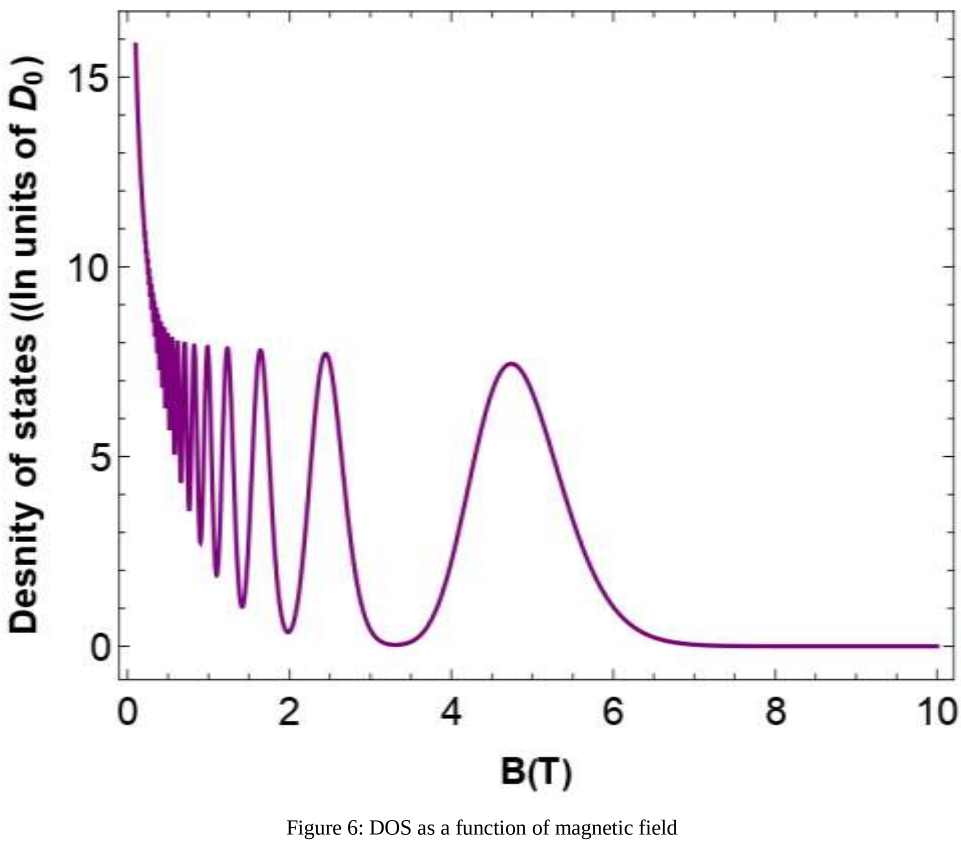

Figure 6: DOS as a function of magnetic field

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