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Exact solutions for a Dirac electron in an exponentially decaying magnetic field

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Abstract
We consider a Dirac electron in the presence of an exponentially decaying magnetic field. We obtain exact energy eigenvalues with a zero-energy state and the corresponding eigenfunctions. We also calculate the probability density and current distributions.

(Some figures in this article are in colour only in the electronic version)

The experimental realization of graphene, a two-dimensional (2D) sheet of graphite [1, 2], and of the massless Dirac nature of its electron low energy spectrum [3, 4] has given rise to a tremendous interest in this field (for recent reviews, see [5, 6]). The energy spectrum which goes linearly with the momentum and the specific density of states of the Dirac electrons [7] enabled the study of experimentally chiral tunneling and the Klein paradox in graphene [8]. This also leads to the anomalous Landau level spectrum in a uniform magnetic field, which gives rise to the half-integer quantum Hall effect [3, 9].

The discovery of the half-integer quantum Hall effect and the zero-energy Landau level [9] stimulated a lot of theoretical research interest in Dirac electrons in uniform as well as non-uniform magnetic fields. For example, the Dirac–Weyl equation has been solved numerically for a single electron in a step-like magnetic field, magnetic barrier and polytropic magnetic field with $B = B_0 y^\gamma$, where $\gamma > 0$ [10–13]. We should also mention that the Schrödinger equation has been solved numerically for spinless 2D electrons in a linearly varying magnetic field [14], step-like magnetic field and magnetic barrier [15–17]. An analytical solution has been given for an electron in the presence of an exponentially decaying magnetic field [18].

In this work, we solve analytically for the Dirac electron in graphene in the presence of an exponentially decaying magnetic field $B = B_0 e^{-\lambda x}$.

The Hamiltonian of the massless electrons in graphene near one of the Dirac K points is described by a two-component Dirac–Weyl equation

$$H = v_F \boldsymbol{\sigma} \cdot \mathbf{p}, \tag{1}$$

where $v_F \approx 10^6$ m s^{-1} is the Fermi velocity, $\boldsymbol{\sigma} = \{\sigma_x, \sigma_y\}$ are the 2×2 Pauli matrices and $\mathbf{p} = -i\hbar\nabla$ is the two-dimensional momentum operator. The pseudo-relativistic dispersion relation with Fermi velocity arises due to the sublattice structure: the basis of the graphene honeycomb lattice contains two carbon atoms, giving rise to an isospin degree of freedom. In the presence of an external magnetic field ($\mathbf{B} = \nabla \times \mathbf{A}$) perpendicular to the graphene plane, the Hamiltonian of the single Dirac electron ($-e$) is $H = v_F \boldsymbol{\sigma} \cdot (\mathbf{p} + e\mathbf{A})$.

We consider an electron in the graphene sheet in the presence of a non-uniform magnetic field $\mathbf{B}(x, y) = \{0, 0, B_0 e^{-\lambda x}\hat{z}\}$ perpendicular to the x–y plane. In the Landau gauge, the corresponding vector potential is $\mathbf{A}(x, y) = \{0, -(1/\lambda) B_0 e^{-\lambda x}\hat{y}, 0\}$. When $\lambda \to 0$, the non-uniform magnetic field becomes a constant magnetic field. The time-independent Dirac–Weyl equation is

$$v_F \boldsymbol{\sigma} \cdot (\mathbf{p} + e\mathbf{A})\Psi(x, y) = E\Psi(x, y). \tag{2}$$

Here, $\Psi(x, y) = \{\Psi_+(x, y), \Psi_-(x, y)\}^T$ is the two-component wavefunction and T denotes the transpose of the column vector. Due to the translation invariance in the y-direction, the longitudinal momentum k_y is a conserved quantity. One can parameterize the wavefunction as $\Psi(x, y) = e^{ik_y y}\{\psi_+(x), \psi_-(x)\}^T$. From equation (2), one can get two coupled equations for ψ_+ and ψ_- as given below:

$$-i\hbar v_F \left[\frac{\partial}{\partial x} + \left(k_y + \frac{e}{\hbar}A_y\right)\right]\psi_-(x) = E\psi_+(x) \tag{3}$$

and

$$-i\hbar v_F \left[\frac{\partial}{\partial x} - \left(k_y + \frac{e}{\hbar}A_y\right)\right]\psi_+(x) = E\psi_-(x). \tag{4}$$

Using two coupled equations (3) and (4), we get Schrödinger-like decoupled equations for ψ_+ and ψ_-:

$$\left[-(\hbar v_F)^2 \frac{\partial^2}{\partial x^2} + V_+(x)\right]\psi_+ = E^2\psi_+ \tag{5}$$

and

$$\left[-(\hbar v_{\rm F})^2\frac{\partial^2}{\partial x^2}+V_-(x)\right]\psi_- = E^2\psi_-. \qquad (6)$$

Here, the effective potentials $V_\pm$ are given by

$$V_\pm = (\hbar v_{\rm F})^2\left[\pm\frac{e}{\hbar}\frac{\partial}{\partial x}A_y(x)+\left(k_y+\frac{e}{\hbar}A_y\right)^2\right]. \qquad (7)$$

Here, the first term on the right-hand side of the above equation is the Zeeman-like term due to the isospin degree of freedom in the presence of the magnetic field. Define the magnetic length scale as $l(x)=\sqrt{\hbar/eB(x)}$.

As seen in figure 1, the effective potentials $V_\pm(x)$ have the form of an asymmetric quantum wells formed by the exponentially decaying magnetic field. It is well known that such a well can have a bound state if the well is sufficiently deep. Figure 1 will be discussed in more detail later on.

Following the references [18, 19], we introduce two new dimensionless variables:

$$\xi(x)=\frac{1}{(l(x)\lambda)^2}=\frac{eB_0{\rm e}^{-\lambda x}}{\hbar\lambda^2} \qquad (8)$$

and

$$\xi_0=\frac{|k_y|}{\lambda}\equiv\frac{eB_0{\rm e}^{-\lambda x_0}}{\hbar\lambda^2}=\frac{1}{(l(x_0)\lambda)^2}. \qquad (9)$$

Here, $l(x_0)=\sqrt{\hbar/eB(x_0)}$ is the magnetic length scale for a given value of $x=x_0$ which depends on the conserved wavevector k_y through equation (8). Also, ξ varies from 0 to ∞ when x varies from ∞ to $-\infty$.

In the new variables, equations (5) and (6) reduce to

$$\left[\frac{{\rm d}^2}{{\rm d}\xi^2}+\frac{1}{\xi}\frac{\rm d}{{\rm d}\xi}-\frac{\beta^2}{\xi^2}+\frac{2\xi_0\mp 1}{\xi}-1\right]\psi_\pm=0, \qquad (10)$$

where $\beta^2=\xi_0^2-\epsilon^2$ and $\epsilon=E/(\hbar v_{\rm F}\lambda)$. The behavior for small and large ξ suggests that the general solution can be written as $\psi_\pm(\xi)\sim\xi^\beta{\rm e}^{-\xi}w_\pm(\xi)$. Inserting this ansatz in the previous equation, we get for $w_\pm(z=2\xi)$

$$\left[z\frac{{\rm d}^2}{{\rm d}z^2}+(\gamma-z)\frac{\rm d}{{\rm d}z}-\alpha_\pm\right]w_\pm(z)=0 \qquad (11)$$

which has the form of a confluent hypergeometric equation, where $\gamma=2\beta+1$ and $\alpha_\pm=-\xi_0+\beta+\frac{1}{2}\pm\frac{1}{2}$. Two linearly independent solutions can be chosen as $F[\alpha_\pm,\gamma;z]$ and $U[\alpha_\pm,\gamma;z]$, so the general solution can be written as $w_\pm(z)=A_1F[\alpha_\pm,\gamma;z]+A_2U[\alpha_\pm,\gamma;z]$. Here, F and U are the first and second kinds of confluent hypergeometric functions, respectively. However, U is not regular at the origin and has to be discarded. The requirement of normalizability implies that the solution is acceptable if $\alpha_\pm$ is a negative integer, $\alpha_\pm=-\nu$, $\nu=0,1,2,\ldots$. This constraint produces the quantization of the energy:

$$E_\pm=\frac{\hbar v_{\rm F}\lambda}{2}\sqrt{(2\xi_0)^2-(2\xi_0-(2\nu+1\pm 1))^2}. \qquad (12)$$

The energy eigenvalues are then conveniently written as

$$E_n=\hbar v_{\rm F}\lambda\sqrt{(\xi_0)^2-(\xi_0-n)^2}. \qquad (13)$$

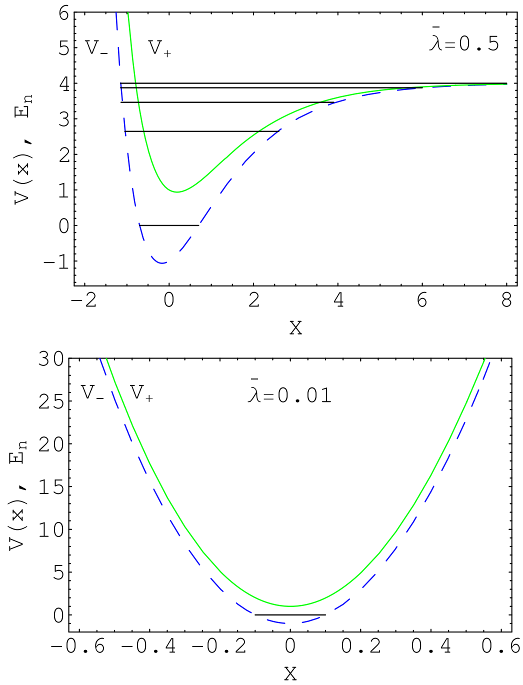

Figure 1. Plots of the effective potential $V_\pm(x)$ (in units of $(\hbar\omega_{\rm c})^2$) versus X together with the energy eigenvalues E_n (in units of $\hbar\omega_{\rm c}$) for $\bar\lambda=0.5$ and $\bar\lambda=0.01$ (only the zero-energy level is shown in this case).

For E_+, $\nu=n-1$ and for E_-, $\nu=n$. For $n=0$ and E_+, $\nu=-1$, but ν cannot be negative. For $n=0$ and E_-, $\nu=0$. Therefore, the $n=0$ state is not degenerate. For $n=0$, the solution w_+ does not exist. We will consistently incorporate this fact by defining $w_{n-1}=0$. The corresponding wavefunction is given by

$$w_\pm(2\xi)={}_1F_1[-(n-\tfrac{1}{2}\mp\tfrac{1}{2}),2\beta+1,2\xi], \qquad (14)$$

where ${}_1F_1[-n,\alpha,x]$ is the confluent hypergeometric function.

Equation (13) can be rewritten as

$$E_n^2=\hbar^2\omega_{\rm c}^2(x_0)2n\left(1-\frac{n}{2\xi_0}\right), \qquad (15)$$

where the local cyclotron frequency is $\omega_{\rm c}(x_0)=(v_{\rm F})/l(x_0)$. Note that when $\bar\lambda\to 0$ ($\xi_0\to\infty$), the energy eigenvalues reduce to the well known relativistic Landau level structure for uniform magnetic field: $E_n=(\hbar v_{\rm F}/l(x_0))\sqrt{2n}$.

When $\bar\lambda$ is very large, the effect of inhomogeneous magnetic field vanishes and the Dirac electron feels no effective potential. It behaves like a free particle. In this limit, the energy spectrum becomes $E_n\propto n$ which agrees with the known result for the free Dirac electron [20].

The complete normalized wavefunctions can be written as

$$\Psi_+^{(n)}=\frac{{\rm e}^{{\rm i}k_y y}}{\sqrt{2L_y l(x_0)}}(2\xi_0)^\beta{\rm e}^{-\bar\lambda\beta X}{\rm e}^{-\xi_0{\rm e}^{-\bar\lambda X}}w_{n-1} \qquad (16)$$

and

$$\Psi_-^{(n)}=\frac{{\rm i}c_n{\rm e}^{{\rm i}k_y y}}{\sqrt{2L_y l(x_0)}}(2\xi_0)^\beta{\rm e}^{-\bar\lambda\beta X}{\rm e}^{-\xi_0{\rm e}^{-\bar\lambda X}}w_n, \qquad (17)$$

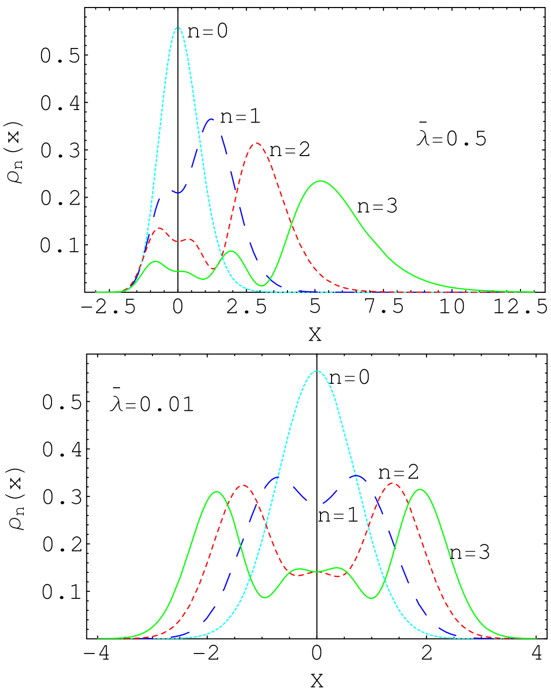

Figure 2. Plots of the probability density distribution $\rho_n(x)$ (in units of $1/(L_y l(x_0))$) versus X for various values of n with $\bar{\lambda} = 0.5$ and 0.01.

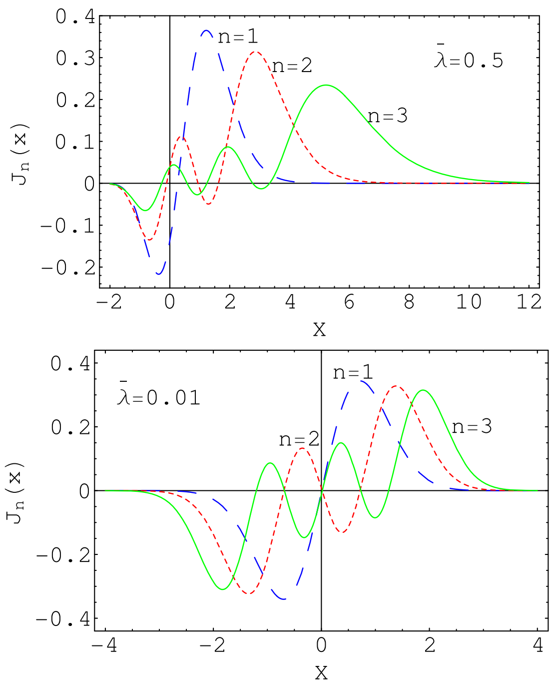

Figure 3. Plots of the probability current density $J_n(x)$ (in units of $ev_F/(L_y l(x_0))$) versus X for various values of n with fixed $\bar{\lambda} = 0.5$ and 0.01.

where L_y is the length of the system along the y axis, $c_0 = \sqrt{2}$ and $c_{n>0} = 1$. Also, $X = (x - x_0)/l(x_0)$, $\bar{\lambda} = \lambda l(x_0)$, and w_n is given by

$$w_n = \sqrt{\frac{\Gamma[2\beta + n + 1]\bar{\lambda}}{\Gamma[2\beta + 1]\Gamma[2\beta]\Gamma[n + 1]}}\,{}_1F_1[-n, 2\beta + 1, 2\xi_0 \mathrm{e}^{-\bar{\lambda}X}]. \tag{18}$$

We have also checked that the wavefunctions (16) and (17) reduce to that of the Dirac Landau level for constant magnetic field (i.e. a Hermite polynomial multiplied with a Gaussian factor) when $\bar{\lambda} \to 0$. The phase factor i in the lower component wavefunction (17) is obtained from equation (4), which is crucial for calculating the probability current density.

The effective potential (7) can be rewritten as

$$V_\pm = (\hbar\omega_c(x_0))^2[\pm \mathrm{e}^{-\bar{\lambda}X} + \xi_0(1 - \mathrm{e}^{-\bar{\lambda}X})^2]. \tag{19}$$

For weak inhomogeneity ($\bar{\lambda} \ll 1$), the effective potentials are almost symmetric around the $X = 0$ point. For strong inhomogeneity ($\bar{\lambda} \gg 0$), there is a strong asymmetry of the effective potentials. The effective potentials for negative k_y do not have any global minimum. Therefore, the bound state does not exist for negative k_y. The effective potentials together with the energy eigenvalues for various values of $\bar{\lambda}$ are shown in figure 1. Both the effective potentials get saturated to $(\hbar\omega_c(x_0))^2\xi_0$ at large X. The zero-energy state ($n = 0$) always lies inside the potential V_- but outside the potential V_+. However, all other discrete energy levels ($n > 0$) are lying inside both the potentials $V_\pm$, which is expected from the solution of the Dirac–Weyl equation. The number of energy levels decreases as we increase $\bar{\lambda}$. For example, there are five energy levels including the zero-energy state when $\bar{\lambda} = 0.5$. On the other hand, the number of energy levels is quite large when $\bar{\lambda} = 0.01$. There are a finite number of discrete energy levels for a given asymmetric parameter $\bar{\lambda}$. The total number of discrete energy levels including the zero-energy level can be calculated easily from the condition that $E_n^2 \leqslant V_\pm(X \to \infty)$ and it is given by $N = \mathrm{Int}[\xi_0] + 1$. Here, Int[$b$] means the integer that is just smaller than b. In figure 1, only the zero-energy level is shown for the $\bar{\lambda} = 0.01$ case.

The probability density distribution of Dirac electrons in a given level n is $\rho_n(x) = \Psi^{(n)\dagger}(x)\Psi^{(n)}(x)$. The probability density distributions ρ_n for different values of n and $\bar{\lambda}$ are shown in figure 2. The velocity operator that follows from the Heisenberg equation is given by $\mathbf{v} = v_F\boldsymbol{\sigma}$. The probability current distribution is $J_n(x) = ev_F\Psi^{(n)\dagger}(x)\sigma_y\Psi^{(n)}(x) = -\mathrm{i}ev_F(\Psi_+^{(n)*}(x)\Psi_-^{(n)}(x) - \Psi_-^{(n)*}(x)\Psi_+^{(n)}(x))$. The probability current distributions for various values of n and $\bar{\lambda}$ are shown in figure 3. The zero-energy state does not carry any current, irrespective of the nature of the magnetic field. When $\bar{\lambda} \to 0$, ρ_n and J_n are symmetric around the point $X = 0$. When $\bar{\lambda} \gg 0$, ρ_n and J_n are strongly asymmetric, as is expected from the effective potentials.

In summary, we have obtained exact energy eigenvalues and the corresponding eigenfunctions for a Dirac electron in the presence of an exponentially decaying magnetic field. We have also provided the probability density and current distributions for each band.

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