Dirac electron in graphene with magnetic fields arising from first-order intertwining

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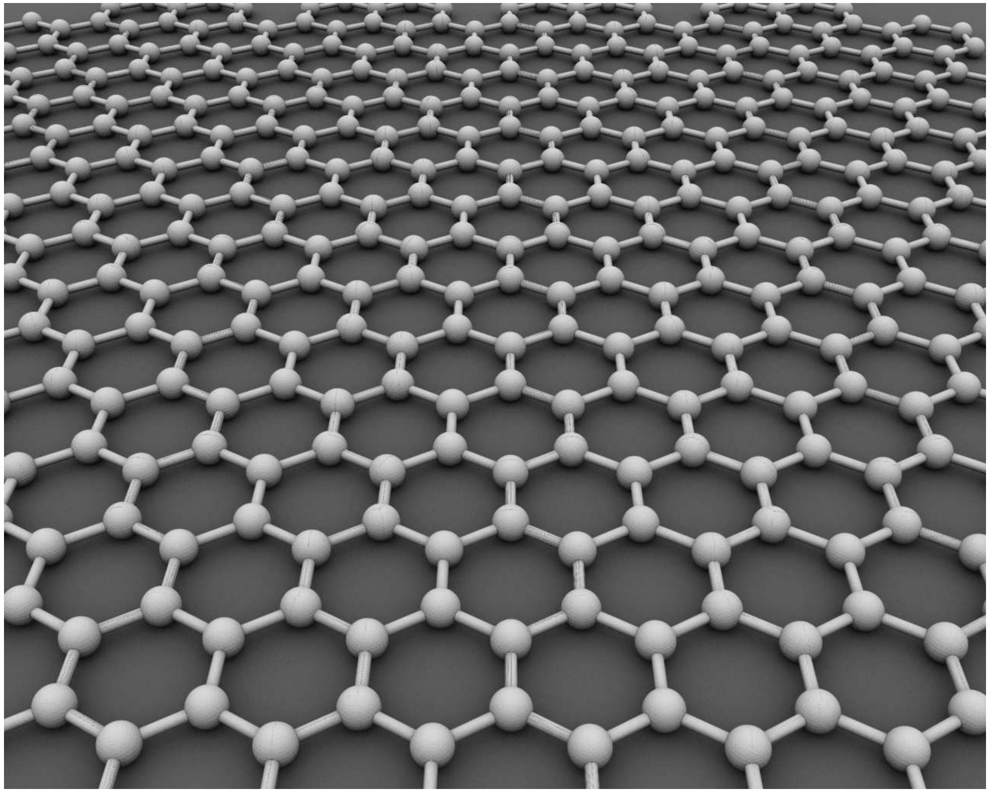
Contents

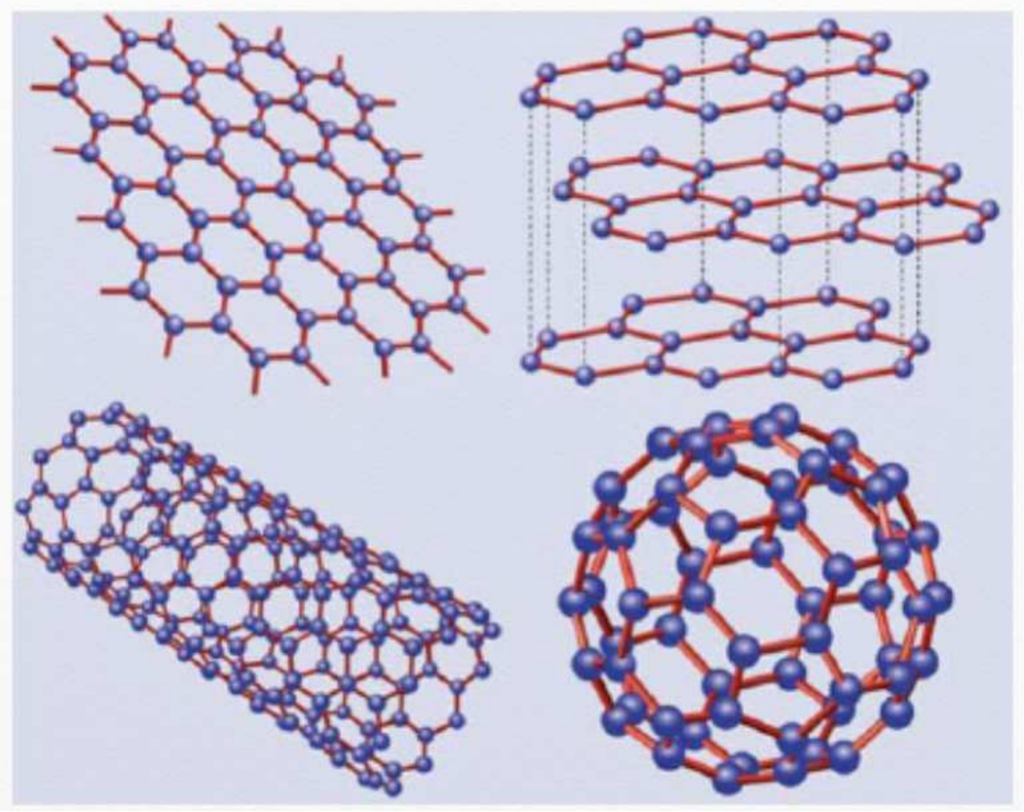
Introduction

- Graphene is a single layer of carbon atoms placed in a hexagonal configuration
- It is the thinnest material ever known, it is strong, flexible



Introduction

- Several structures can be seen as resulting from graphene: graphite, carbon nanotubes, fullerenes



Introduction

- Theoretical interest: is a two-dimensional system
- Low energy electrons in graphene behave as massles Dirac fermions
- Relativistic quantum mechanics can be imitated, with velocities 300 times lower than c
- Electron confinement can be produced through magnetic fields which are orthogonal to the layer
- Supersymmetric quantum mechanics is the natural tool to deal with the electron motion in graphene

Dirac-Weyl equation and SUSY QM

- The Dirac-Weyl equation describes low energy electrons in graphene. If magnetic fields orthogonal to the layer is applied, such equation is

$$\mathbf{H}\Psi(x,y) = v_F\boldsymbol{\sigma}\cdot\left[\mathbf{p}+\frac{e\mathbf{A}}{c}\right]\Psi(x,y) = E\Psi(x,y)$$

  - $v_F \sim 8\times 10^5 m/s$ is the Fermi velocity
  - $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ are Pauli matrices
  - $\mathbf{p} = -i\hbar(\partial_x, \partial_y)^T$ is the 2-dim momentum operator
  - $-e$ is the electron charge
  - $\mathbf{A}$ is the vector potential
  - $\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}$ is the applied magnetic field

Dirac-Weyl equation and SUSY QM

- For magnetic fields changing just along one direction the vector potential in the Landau gauge becomes $\mathbf{A} = \mathcal{A}(x)\hat{e}_y,\ \mathbf{B} = \mathcal{B}(x)\hat{e}_z,\ \mathcal{B}(x) = \mathcal{A}'(x)$
- Taking into account the translation invariance of $\mathbf{H}$ along y direction it is proposed

$$\Psi(x,y) = e^{iky} \left[\begin{array}{c} \psi^+(x) \\ i\psi^-(x) \end{array} \right]$$

- k is the wavenumber in y direction
- $\psi^{\pm}(x)$ is the electron amplitude on two adjacent sites in the unit cell of graphene

Dirac-Weyl equation and SUSY QM

Thus

$$\left(\pm\frac{d}{dx} + \frac{e}{c\hbar}\mathcal{A} + k\right)\psi^{\mp}(x) = \frac{E}{\hbar\upsilon_F}\psi^{\pm}(x)$$

By decoupling this system it is obtained

$$H^{\pm}\psi^{\pm}(x) = \mathcal{E}\psi^{\pm}(x)$$

$$H^{\pm} = -\frac{d^2}{dx^2} + V^{\pm}, \quad V^{\pm} = \left(\frac{e\mathcal{A}}{c\hbar} + k\right)^2 \pm \frac{e}{c\hbar}\frac{d\mathcal{A}}{dx}$$

$$\mathcal{E} = \frac{E^2}{\hbar^2\upsilon_F^2}$$

$$SUSY\ QM!$$

Shape invariant case

The following relations are fulfilled:

$$
\begin{aligned}
H^{\pm} &= L_0^{\mp} L_0^{\pm} \\
H^{\pm} L_0^{\mp} &= L_0^{\mp} H^{\mp} \\
L_0^{\pm} &= \mp \frac{d}{dx} + W_0(x) \\
W_0(x) &= \frac{eA_y(x)}{c\hbar} + k \\
V^{\pm}(x) &= W_0^2(x) \pm W_0'(x)
\end{aligned}
$$

Shape invariant case

The eigenfunctions of $H^{\pm}$ are interconnected as

$$\psi_n^+(x) = \frac{L_0^- \psi_{n+1}^-(x)}{\sqrt{\mathcal{E}_{n+1}^-}}$$

$$\psi_{n+1}^-(x) = \frac{L_0^+ \psi_n^+(x)}{\sqrt{\mathcal{E}_n^+}}$$

$$\psi_0^-(x) \sim e^{-\int W_0(x)dx}$$

The corresponding eigenvalues are:

$$\mathcal{E}_n^+ = \mathcal{E}_{n+1}^-, \quad \mathcal{E}_0^- = 0$$

Note that

$$L_0^- \psi_0^-(x) = 0 \quad \Rightarrow \quad W_0(x) = -\frac{\psi_0^-(x)'}{\psi_0^-(x)}$$

Shape invariant case

The applied magnetic field becomes

$$B_0(x) = \frac{dA_y(x)}{dx} = \frac{c\hbar}{e}\frac{dW_0(x)}{dx} = -\frac{c\hbar}{e}\frac{d^2}{dx^2}\{\ln[\psi_0^-(x)]\}$$

The eigenfunctions and eigenvalues of the Dirac electron in graphene under $B_0(x)$ become:

$$E_0 = \hbar v_F\ \sqrt{\mathcal{E}_0^-} = 0, \qquad E_{n+1} = \hbar v_F\ \sqrt{\mathcal{E}_{n+1}^-}$$
$$\Psi_0 = e^{iky}\begin{bmatrix} 0 \\ i\ \psi_0^-(x) \end{bmatrix}, \quad \Psi_{n+1} = e^{iky}\begin{bmatrix} \psi_n^+(x) \\ i\ \psi_{n+1}^-(x) \end{bmatrix}$$

Shape invariant case

- For some special forms of $B_0(x)$ the potentials $V^{\pm}(x)$ become shape invariant
- They are exactly solvable potentials leading to magnetic fields which have been already explored [Kuru, Negro, Nieto, J. Phys. Cond. Matt. 21 (2009) 455305]
- Nothing radically new can be said from this point of view
- However ...

General case

There is a method to generate new magnetic fields for which the electron motion in graphene is exactly solvable

1. First let us displace up H^- as follows:

$$\tilde{H}_0 \equiv H^- - \epsilon_1 = -\frac{d^2}{dx^2} + V^-(x) - \epsilon_1, \quad \epsilon_1 \leq \mathcal{E}_0^- = 0$$

2. From $\tilde{H}_0$ we construct a new Hamiltonian H_1 through the requirement

$$H_1 L_1^+ = L_1^+ \tilde{H}_0$$
$$H_1 = -\frac{d^2}{dx^2} + V_1(x, \epsilon_1)$$
$$L_1^\pm = \mp \frac{d}{dx} + W_1(x, \epsilon_1)$$

General case

It turns out that

$$W_1^2(x,\epsilon_1) + W_1'(x,\epsilon_1) = \tilde{V}_0(x)$$
$$V_1(x,\epsilon_1) = \tilde{V}_0(x) - 2W_1'(x,\epsilon_1)$$

Through the change $W_1(x,\epsilon_1) = u_1^{(0)'}/u_1^{(0)}$ it is obtained

$$-u_1^{(0)''} + \tilde{V}_0(x)u_1^{(0)} = 0$$

SE for $\tilde{H}_0$

The generated magnetic field becomes

$$B_1(x,\epsilon_1) = \frac{c\hbar}{e}\frac{dW_1(x,\epsilon_1)}{dx} = -B_0(x) + \frac{c\hbar}{e}\frac{d^2}{dx^2}\left\{\ln\left[\frac{u_1^{(0)}(x)}{\psi_0^-(x)}\right]\right\}$$

General case

3. The associated eigenvalues and eigenfunctions:

$$\tilde{\mathcal{E}}_n^{(0)} = \mathcal{E}_n^- - \epsilon_1, \qquad \psi_n^-(x)$$

$$\mathcal{E}_0^{(1)} = 0, \quad \psi_0^{(1)}(x) \sim e^{-\int W_1(x,\epsilon_1)dx} = \frac{1}{u_1^{(0)}}$$

$$\mathcal{E}_{n+1}^{(1)} = \tilde{\mathcal{E}}_n^{(0)}, \quad \psi_{n+1}^{(1)}(x) = \frac{1}{\sqrt{\tilde{\mathcal{E}}_n^{(0)}}} L_1^+ \psi_n^-(x), \quad n = 0, 1, \ldots$$

Thus:

$$E_0 = \hbar v_F \sqrt{\mathcal{E}_0^{(1)}} = 0, \quad E_{n+1} = \hbar v_F \sqrt{\mathcal{E}_{n+1}^{(1)}}$$

$$\Psi_0 = e^{iky} \begin{bmatrix} 0 \\ i\ \psi_0^{(1)}(x) \end{bmatrix}, \quad \Psi_{n+1} = e^{iky} \begin{bmatrix} \psi_n^-(x) \\ i\ \psi_{n+1}^{(1)}(x) \end{bmatrix}$$

General case: iteration

- We have followed [Midya, Fernández, J. Phys. A: Math. Theor. 47 (2014) 285302], where it was taken $\tilde{H}_0 = H^+ - \epsilon_1$ with $\epsilon_1 \equiv -\delta \leq \mathcal{E}_0^- = 0$
- It remained unexplored the domain $\delta \in [-\mathcal{E}_0^+, 0)$
- Working the Riccati equation it was missed the possibility of iterating the procedure

General case: iteration

1. Let us displace now H_1:

$$\tilde{H}_1 \equiv H_1 - \epsilon_2, \quad \epsilon_2 < \epsilon_1 \quad \Rightarrow \quad \tilde{\mathcal{E}}_0^{(1)} = -\epsilon_2 \geq 0$$

2. From $\tilde{H}_1$ a new Hamiltonian H_2 is now constructed,

$$H_2 L_2^+ = L_2^+ \tilde{H}_1$$
$$H_2 = -\frac{d^2}{dx^2} + V_2(x, \epsilon_2)$$
$$L_2^\pm = \mp\frac{d}{dx} + W_2(x, \epsilon_2)$$

Thus

$$W_2^2(x, \epsilon_2) + W_2'(x, \epsilon_2) = \tilde{V}_1(x, \epsilon_1)$$
$$V_2(x, \epsilon_2) = \tilde{V}_1(x, \epsilon_1) - 2W_2'(x, \epsilon_2)$$

General case: iteration

By making $W_2(x,\epsilon_2) = u_2^{(1)'}/u_2^{(1)}$:

$$-u_2^{(1)''} + \tilde{V}_1(x,\epsilon_1)u_2^{(1)} = 0$$

$u_2^{(1)}$ is obtained by acting L_1^+ onto a solution of H^-:

$$u_2^{(1)} \propto L_1^+ u_2^{(0)} = -\frac{\mathsf{W}[u_1^{(0)}, u_2^{(0)}]}{u_1^{(0)}}$$

$$-u_2^{(0)''} + V^-(x)u_2^{(0)} = (\epsilon_1+\epsilon_2)u_2^{(0)}$$

The new potential:

$$V_2(x,\epsilon_2) = V^-(x) - 2\frac{d^2}{dx^2}\ln \mathsf{W}[u_1^{(0)}, u_2^{(0)}] - (\epsilon_1+\epsilon_2)$$

General case: iteration

The second-order magnetic field:

$$B_2(x,\epsilon_2) = \frac{c\hbar}{e}\frac{dW_2(x,\epsilon_2)}{dx} = -B_1(x,\epsilon_1) + \frac{c\hbar}{e}\frac{d^2}{dx^2}\{\ln[\mathrm{W}[u_1^{(0)},u_2^{(0)}]]\}$$

3. The associated eigenvalues and eigenfunctions:

$$\tilde{\mathcal{E}}_n^{(1)} = \mathcal{E}_n^{(1)} - \epsilon_2, \qquad \psi_n^{(1)}(x)$$

$$\mathcal{E}_0^{(2)} = 0, \quad \psi_0^{(2)}(x) \sim e^{-\int W_2(x,\epsilon_2)dx} = \frac{1}{u_2^{(1)}}$$

$$\mathcal{E}_{n+1}^{(2)} = \tilde{\mathcal{E}}_n^{(1)}, \quad \psi_1^{(2)}(x) = \frac{L_2^+\psi_0^{(1)}(x)}{\sqrt{\tilde{\mathcal{E}}_0^{(1)}}}, \quad \psi_{n+2}^{(2)}(x) = \frac{L_2^+\psi_{n+1}^{(1)}(x)}{\sqrt{\tilde{\mathcal{E}}_{n+1}^{(1)}}}$$

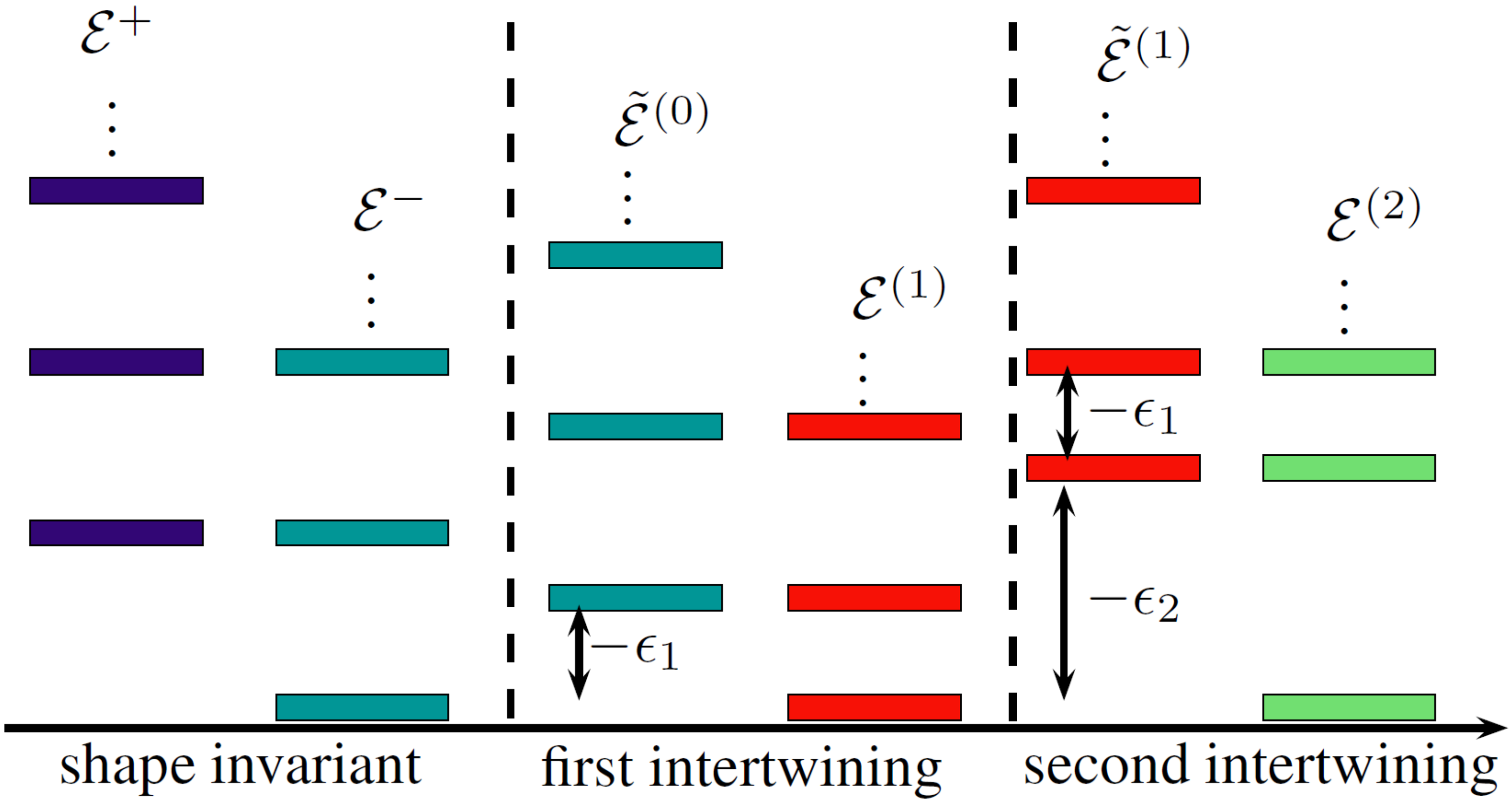
General case: iteration

$$E_0 = \hbar v_F \sqrt{\mathcal{E}_0^{(2)}} = 0, \qquad E_{n+1} = \hbar v_F \sqrt{\mathcal{E}_{n+1}^{(2)}}$$

$$\Psi_0 = e^{iky} \begin{bmatrix} 0 \\ i\,\psi_0^{(2)}(x) \end{bmatrix}, \quad \Psi_{n+1} = e^{iky} \begin{bmatrix} \psi_n^{(1)}(x) \\ i\,\psi_{n+1}^{(2)}(x) \end{bmatrix}$$

The procedure can be continued at will!

General case: iteration



Landau levels in graphene: shape invariant potentials

- For a uniform magnetic field $\mathcal{B} = B_0$, $B_0 > 0$ it must be taken $\mathbf{A} = \hat{e}_y B_0 x$
- The superpotential $W_0(x) = \frac{\omega}{2} x + k$, $\omega = \frac{2eB_0}{c\hbar}$
- The two shape invariant potentials $V^{\pm}(x) = \frac{\omega^2}{4}\left(x + \frac{2k}{\omega}\right)^2 \pm \frac{\omega}{2}$
- The eigenfunctions and eigenvalues of $H^{\pm}$:

$$\mathcal{E}_0^- = 0, \quad \mathcal{E}_{n+1}^- = \mathcal{E}_n^+ = \omega(n+1), \quad n = 0, 1, 2, \dots$$
$$\psi_n^- = \psi_n^+ = N_n \, e^{-\frac{\omega}{4}(x+\frac{2k}{\omega})^2} \; H_n\left[\sqrt{\frac{\omega}{2}}\left(x + \frac{2k}{\omega}\right)\right]$$

$N_n = \sqrt{\frac{1}{2^n n!}\left(\frac{\omega}{2\pi}\right)^{\frac{1}{2}}}$, H_n are the Hermite polynomials

Landau levels in graphene: general case

- The general solution of the SE for $\tilde{V}_0 = V^-(x) - \epsilon_1$ with zero energy reads ($a = -\epsilon_1/2\omega$):

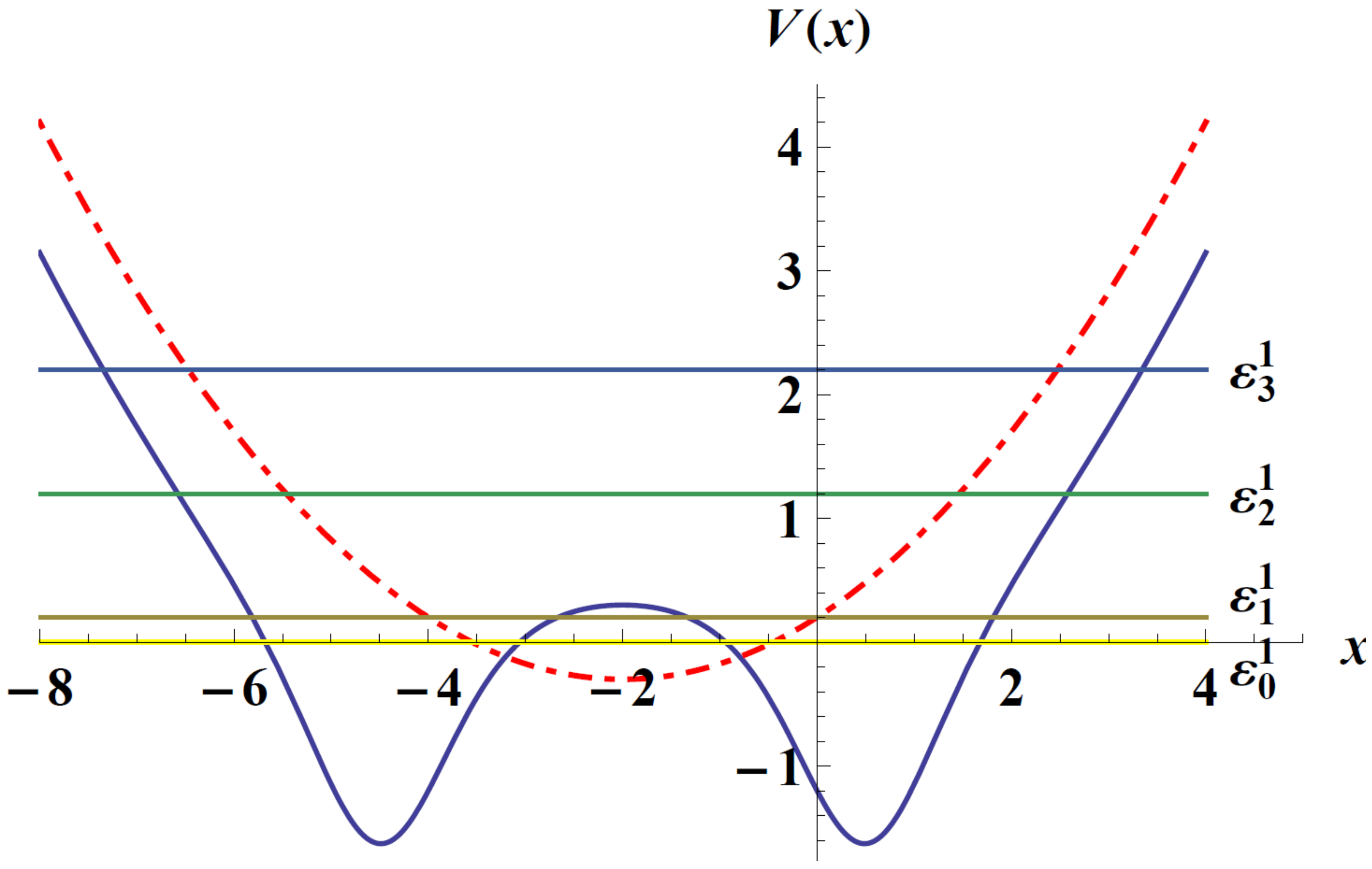
$$u_1^{(0)} = \quad e^{-\frac{\omega}{4}(x+\frac{2k}{\omega})^2}\Big({}_1F_1[a,\tfrac{1}{2},\tfrac{\omega}{2}(x+\tfrac{2k}{\omega})^2] + 2\nu_1\frac{\Gamma[a+\frac{1}{2}]}{\Gamma[a]}\sqrt{\frac{\omega}{2}}(x+\tfrac{2k}{\omega})\,{}_1F_1[a+\tfrac{1}{2},\tfrac{3}{2},\tfrac{\omega}{2}(x+\tfrac{2k}{\omega})^2]\Big)$$

- In particular, for $\epsilon_1 = -\omega/5$, $\nu_1 = 0$ it is obtained

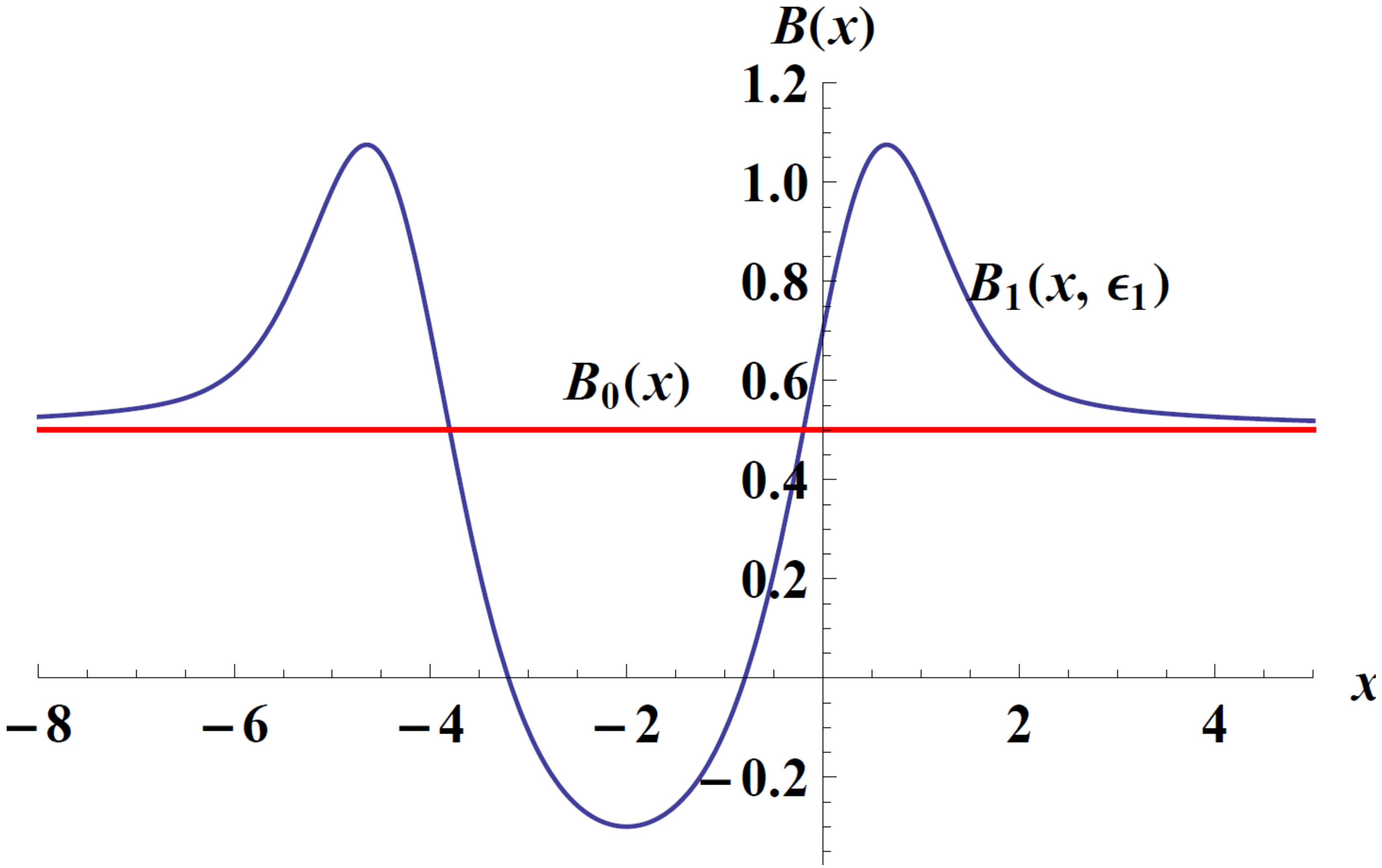
$$V_1(x,\epsilon_1) = \tilde{V}_0 - 2\frac{d}{dx}\left[\frac{\omega}{2}(x+\frac{2k}{\omega})\left(-1+\frac{2}{5}\frac{{}_1F_1[\frac{11}{10},\frac{3}{2},\frac{\omega}{2}(x+\frac{2k}{\omega})^2]}{{}_1F_1[\frac{1}{10},\frac{1}{2},\frac{\omega}{2}(x+\frac{2k}{\omega})^2]}\right)\right]$$

$$B_1(x,\epsilon_1) = -B_0 + \frac{2B_0}{5}\frac{d}{dx}\left[(x+\frac{2k}{\omega})\frac{{}_1F_1[\frac{11}{10},\frac{3}{2},\frac{\omega}{2}(x+\frac{2k}{\omega})^2]}{{}_1F_1[\frac{1}{10},\frac{1}{2},\frac{\omega}{2}(x+\frac{2k}{\omega})^2]}\right]$$

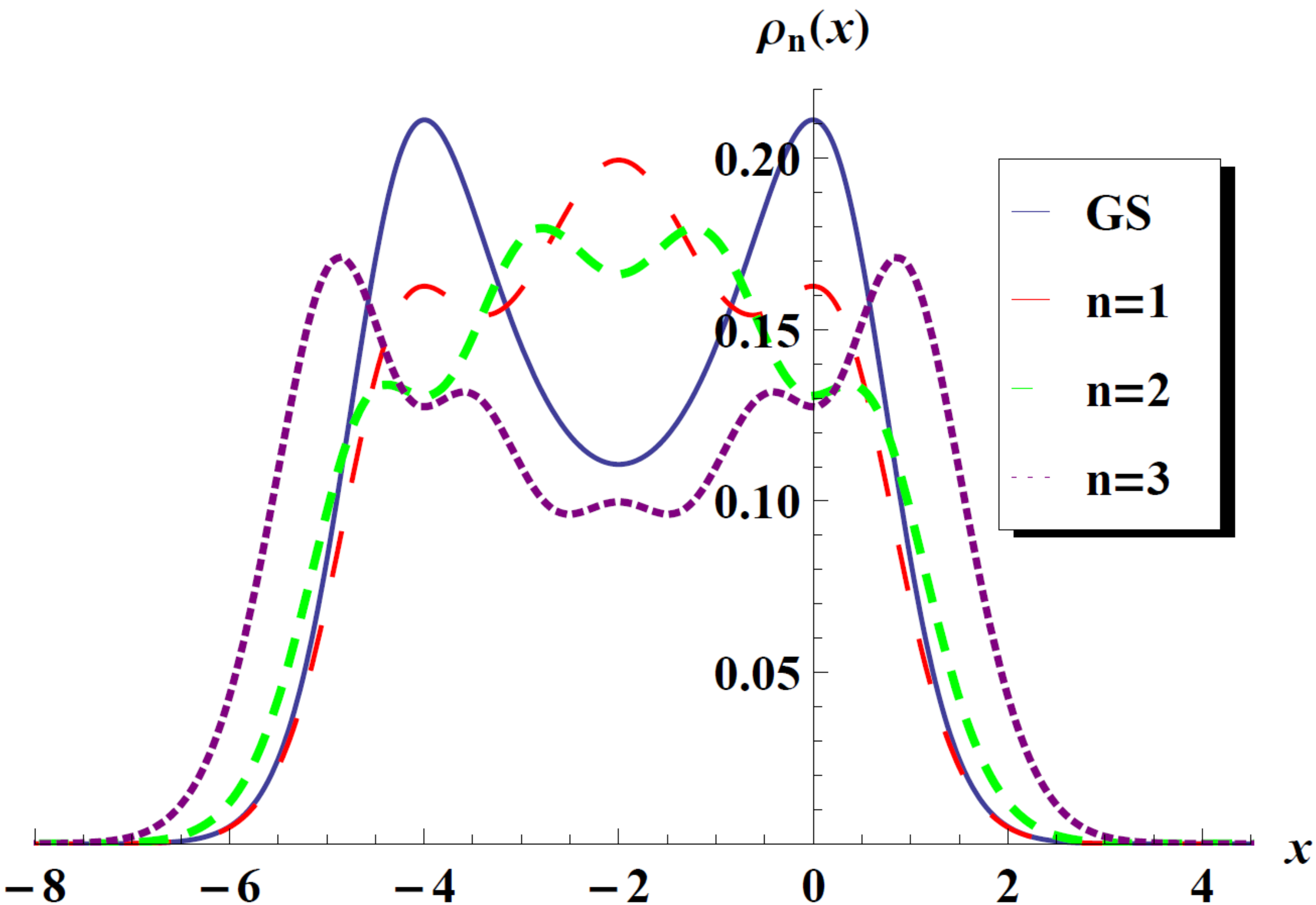
Landau levels in graphene: general case



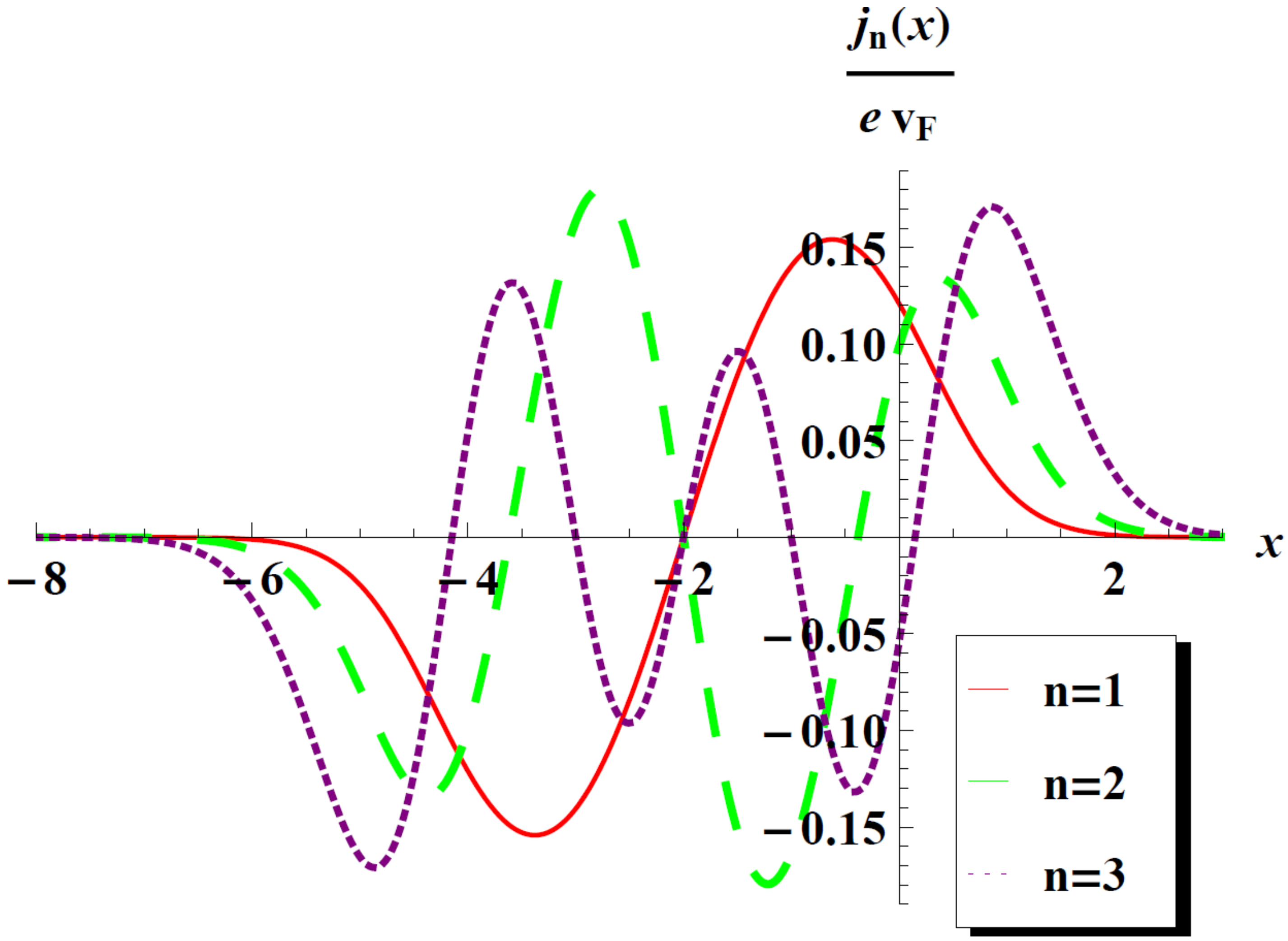
Landau levels in graphene: general case



Landau levels in graphene: general case



Landau levels in graphene: general case



Landau levels in graphene: second-order case

- For the second step $V_1(x)$ is moved up by $-\epsilon_2$:

$$\tilde{V}_1(x,\epsilon_1) = \left[\frac{\omega^2}{4}\left(x+\frac{2k}{\omega}\right)^2 - \frac{\omega}{2} - \epsilon_1 - 2\frac{d}{dx}W_1(x,\epsilon_1)\right] - \epsilon_2$$

- Then it is built the second-order potential and magnetic field:

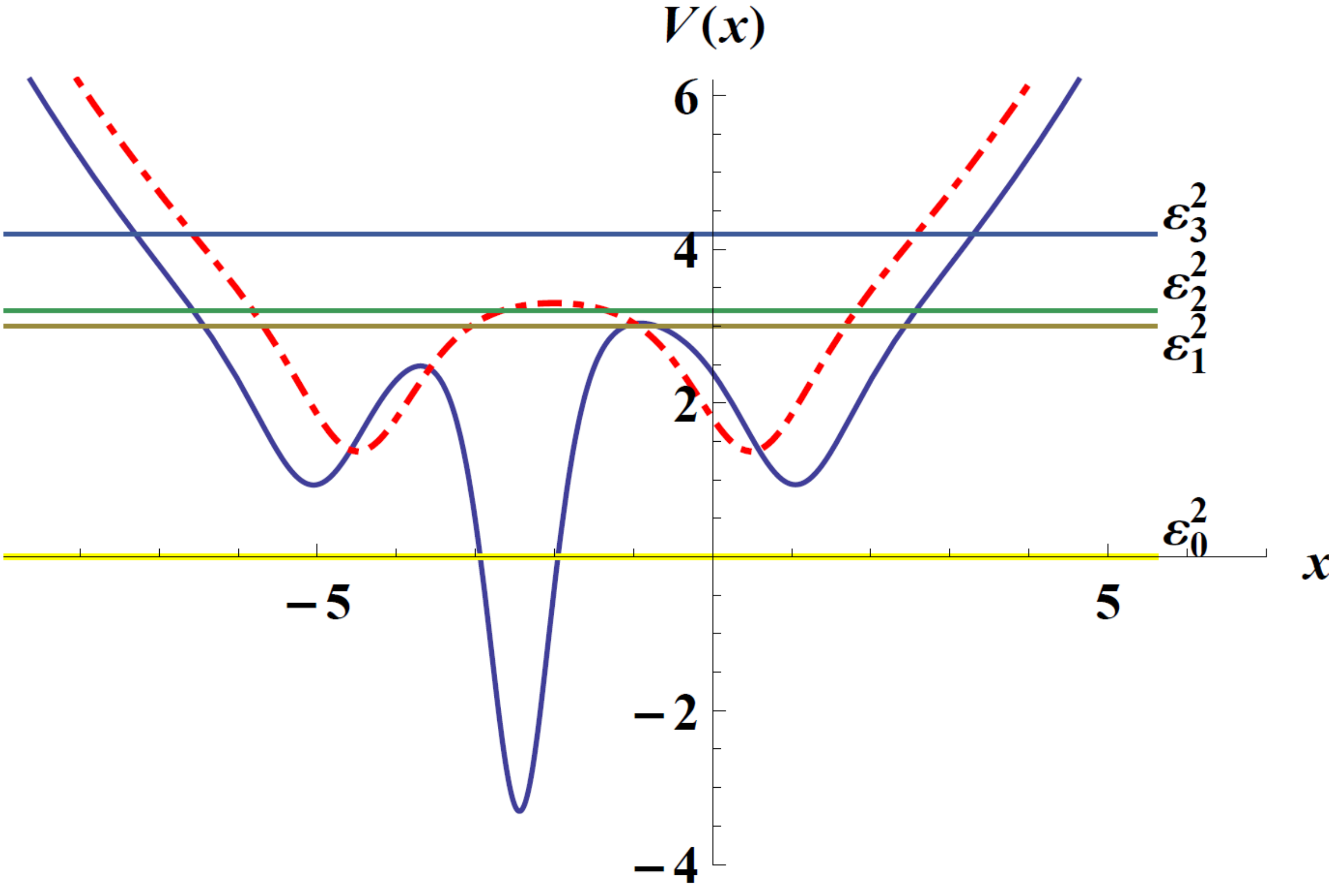
$$V_2(x,\epsilon_2) = \tilde{V}_0 - 2\frac{d^2}{dx^2}\ln \mathrm{W}[u_1^{(0)}, u_2^{(0)}] - \epsilon_2$$

$$B_2(x,\epsilon_2) = -B_1(x,\epsilon_1) + \frac{c\hbar}{e}\frac{d^2}{dx^2}\{\ln[\mathrm{W}[u_1^{(0)}, u_2^{(0)}]]\}$$

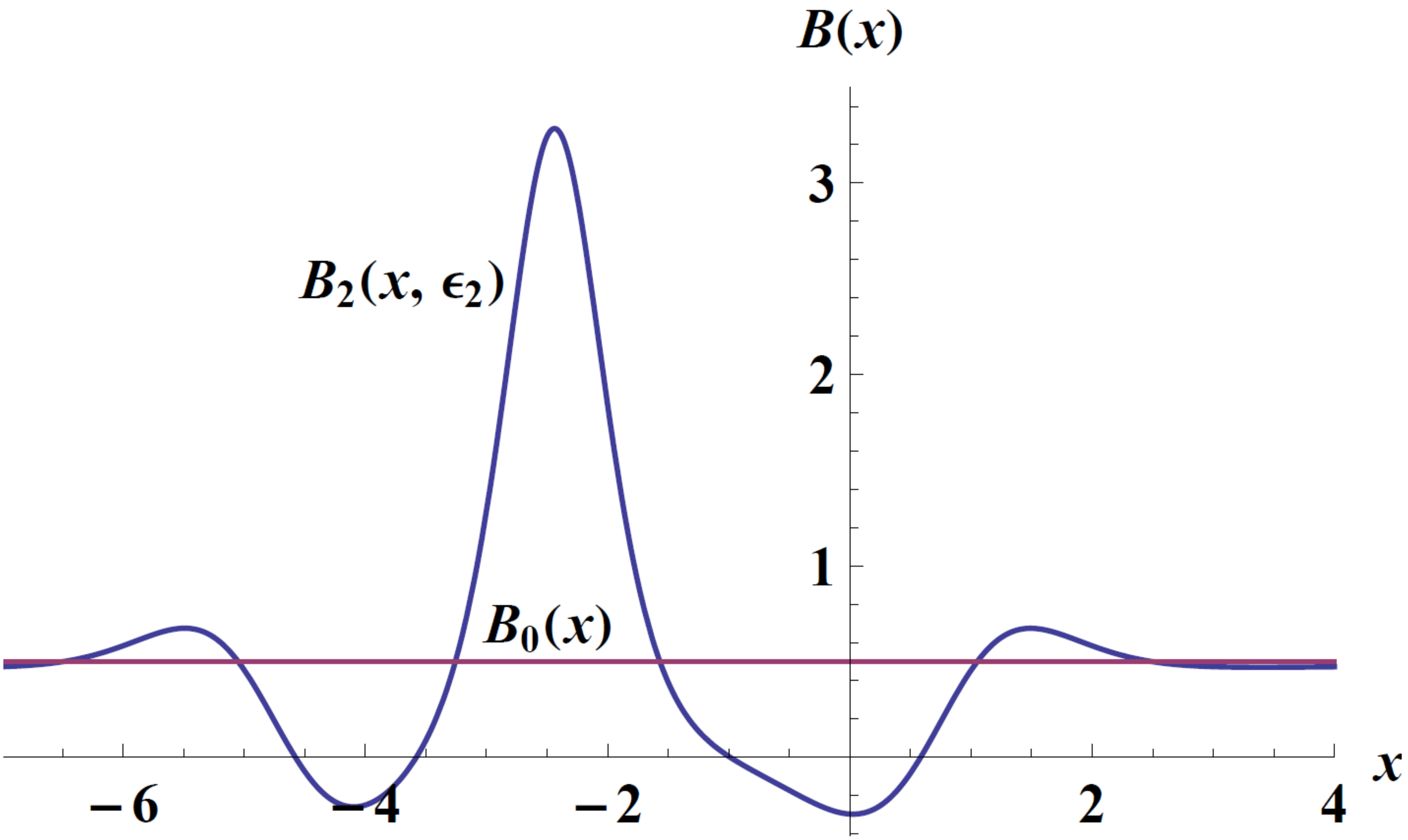
$u_2^{(0)}$ arises from $u_1^{(0)}$ with the change $\epsilon_1 \to \epsilon_1 + \epsilon_2$

- In particular, for $\epsilon_1 = -\omega/5$, $\epsilon_2 = -3\omega$, $\omega = 1$, $\nu_1 = 0$, $\nu_2 = \frac{3}{2}$:

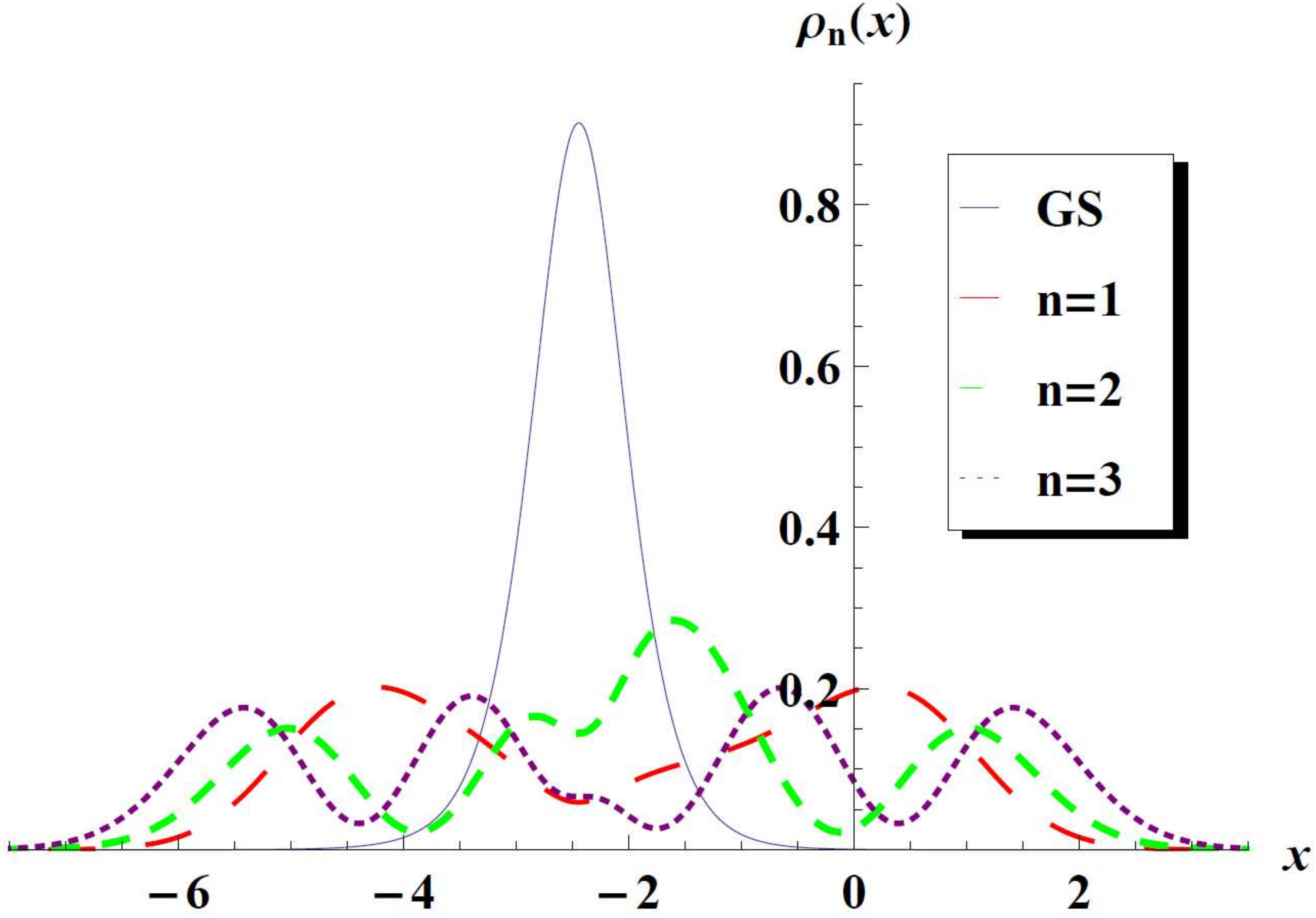
Landau levels in graphene: second-order case



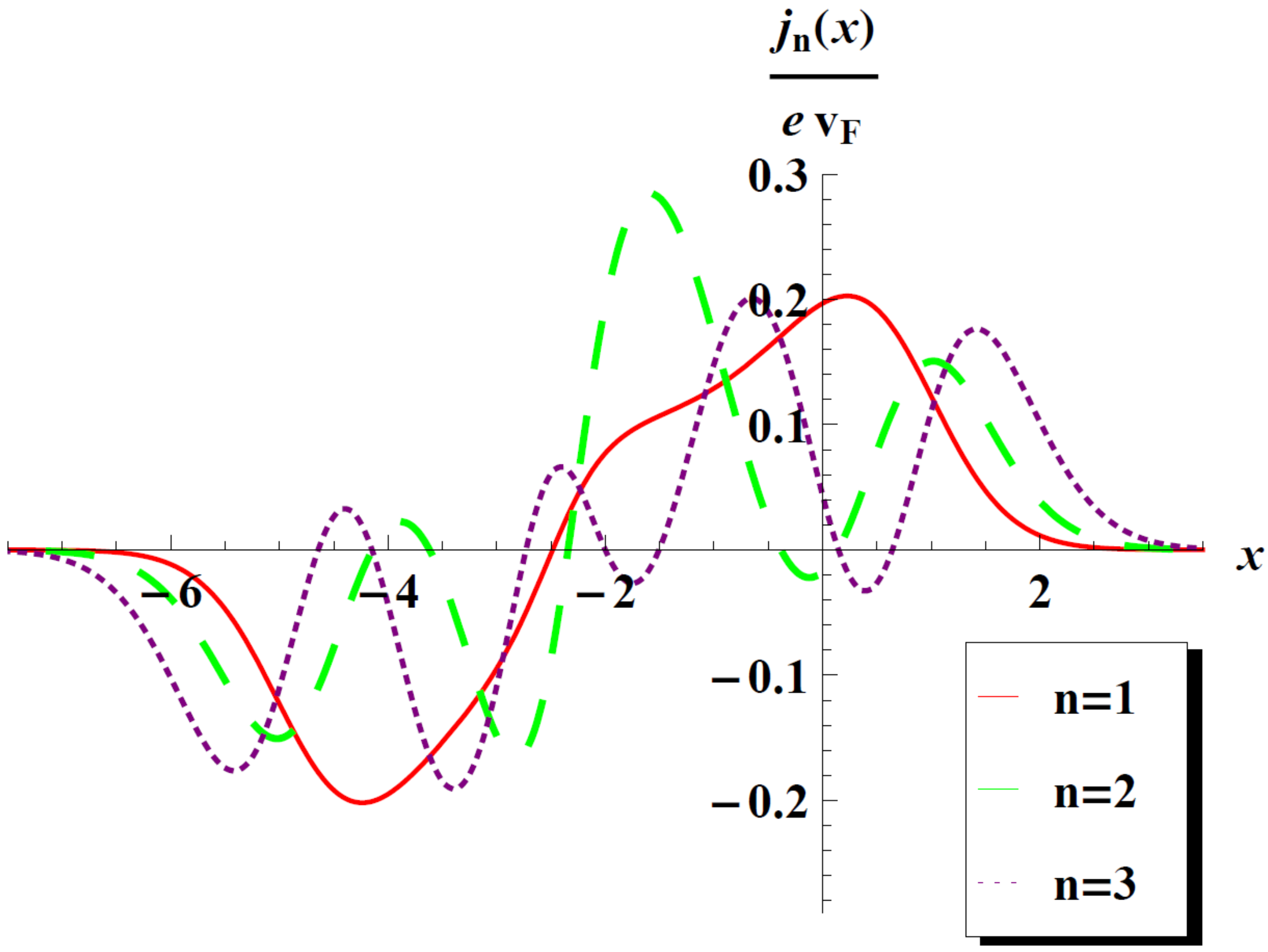
Landau levels in graphene: second-order case



Landau levels in graphene: second-order case



Landau levels in graphene: second-order case



Conclusions

- We have generalized the shape invariant method addressed by Kuru, Negro and Nieto to study the electron motion in graphene in external magnetic fields orthogonal to the layer
- The ideas introduced by Midya and Fernández to generate new magnetic fields for which the system is exactly solvable were taken into account
- The iterations of the method, to generate higher-order exactly solvable magnetic fields, have been implemented
- This is an interesting topic in which the ideas of SUSY QM will be applied in the near future

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