

Darboux transformations applied to graphene in external magnetic fields

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Introduction

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





Introduction

- Several structures arise from graphene: graphite, carbon nanotubes, fullerenes
- Theoretical interest: is a two-dimensional system
- Low energy electrons in graphene behave as massles Dirac fermions
- 6 Relativistic quantum mechanics can be imitated for velocities 300 times lower than c
- 6 Electron confinement is produced by magnetic fields which are orthogonal to the layer
- Oarboux transformation (DT) is the natural tool to address the electron motion in graphene



The graphene description is made in terms of two non-equivalent triangular lattices of atoms A and B:



The tight binding model considers that the two atoms in the unit cell of graphene interact just with its nearest neighbors



$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} 0 & \gamma_0 S(\mathbf{k}) \\ \gamma_0 \bar{S}(\mathbf{k}) & 0 \end{pmatrix}$$

where $\gamma_0 \approx -2.97 \text{ eV}$ is the hopping parameter,

$$S(\mathbf{k}) = \sum_{\delta} e^{i\mathbf{k}\cdot\delta} = 2\exp\left(\frac{ik_xa}{2\sqrt{3}}\right)\cos\left(\frac{k_ya}{2}\right) + \exp\left(\frac{-ik_xa}{\sqrt{3}}\right)$$

 $a/\sqrt{3} = 1.42$ Å is the nearest-neighbor distance. The eigenvalues of $\mathcal{H}(\mathbf{k})$ are given by

$$E(\mathbf{k}) = \pm \gamma_0 |S(\mathbf{k})| = \pm \gamma_0 \sqrt{3 + f(\mathbf{k})}$$
$$f(\mathbf{k}) = 2\cos(k_y a) + 4\cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{\sqrt{3}k_x a}{2}\right)$$





Around the so-called Dirac point \mathbf{K}^- it turns out that:

$$\mathcal{H}^{-}(\mathbf{p}) = v_F \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix} = v_F \boldsymbol{\sigma} \cdot \mathbf{p}$$



The Dirac-Weyl equation for low energy electrons in graphene placed in a magnetic field is

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

 $-v_F \sim 8 \times 10^5 m/s$ is the Fermi velocity

- $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ are the 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
- $-\mathbf{B} = \mathbf{
 abla} imes \mathbf{A}$ is the external magnetic field



For magnetic fields orthogonal to the graphene layer, which change just along x-direction, the vector potential in the Landau gauge reads

$$\mathbf{A} = \mathcal{A}(x)\hat{e}_y, \ \mathbf{B} = \mathcal{B}(x)\hat{e}_z, \ \mathcal{B}(x) = \mathcal{A}'(x)$$

6 The translation invariance of H along y-axis suggests that

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

where k is the wavenumber in y direction, $\psi^{\pm}(x)$ are the electron amplitudes on the two adjacent sites A, B in the unit cell of graphene





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

This resembles what happens in DT:

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



DT and graphene

The following relations are fulfilled:

$$\begin{split} H^- &= L_0^+ L_0^-, \quad H^+ = L_0^- L_0^+ & \text{factorizations} \\ H^+ L_0^- &= L_0^- H^-, \quad H^- L_0^+ = L_0^+ H^+ & \text{intertwining relations} \\ L_0^- &= \frac{d}{dx} + W_0(x), \quad L_0^+ = -\frac{d}{dx} + W_0(x) & \text{intertwining operators} \\ W_0(x) &= \frac{eA_y(x)}{c\hbar} + k & \text{superpotential} \\ V^-(x) &= W_0^2(x) - W_0'(x) & \text{initial potential} \\ V^+(x) &= V^-(x) + 2W_0'(x) & \text{SUSY partner potential} \end{split}$$



DT and graphene

The eigenfunctions of H^{\pm} are connected to each other 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 eigenvalues of H^{\pm} are $\mathcal{E}_n^+ = \mathcal{E}_{n+1}^-$, $\mathcal{E}_0^- = 0$. Note that

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



DT and graphene

The magnetic field applied to graphene is

$$B_0(x) = A'_y(x) = \frac{c\hbar}{e} W'_0(x) = -\frac{c\hbar}{e} \{\ln[\psi_0^-(x)]\}''$$

The eigenfunctions and eigenvalues for the Dirac electron in graphene are

$$E_{0} = \hbar v_{F} \sqrt{\mathcal{E}_{0}^{-}} = 0, \quad E_{n+1} = \hbar v_{F} \sqrt{\mathcal{E}_{n+1}^{-}}$$
$$\Psi_{0} = e^{iky} \begin{bmatrix} 0\\ i \psi_{0}^{-}(x) \end{bmatrix}, \quad \Psi_{n+1} = e^{iky} \begin{bmatrix} \psi_{n}^{+}(x)\\ i \psi_{n+1}^{-}(x) \end{bmatrix}$$





- For some special forms of $B_0(x)$ the auxiliary potentials $V^{\pm}(x)$ become shape invariant (Infeld-Hull, Gendenshtein), i.e., when deleting the ground state of $V^-(x)$ the produced potential $V^+(x)$ can be obtained as well from V^- by just changing their parameters (up to an energy displacement)
- 6 This approach was explored by Kuru, Negro, Nieto [J. Phys. Cond. Matt. 21 (2009) 455305]



Shape invariant case

- Solution Example. For a constant homogeneous magnetic field $\mathcal{B} = B_0 > 0$ we must take $\mathbf{A} = \hat{e}_y B_0 x$
- 6 The superpotential is $W_0(x) = \frac{\omega}{2}x + k$, $\omega = \frac{2eB_0}{c\hbar}$
- 6 The two shape invariant potentials are $V^{\pm}(x) = \frac{\omega^2}{4} \left(x + \frac{2k}{\omega}\right)^2 \pm \frac{\omega}{2}$
- 5 The eigenfunctions and eigenvalues of H^{\pm} are

$$\mathcal{E}_{0}^{-} = 0, \quad \mathcal{E}_{n+1}^{-} = \mathcal{E}_{n}^{+} = \omega(n+1), \quad n = 0, 1, 2, \dots$$
$$\psi_{n}^{-} = \psi_{n}^{+} = N_{n} \ e^{-\frac{\omega}{4}(x+\frac{2k}{\omega})^{2}} \ H_{n} \left[\sqrt{\frac{\omega}{2}} \left(x+\frac{2k}{\omega}\right)\right]$$

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



Next we follow [Midya, Fdez, J Phys A 47 (2014) 285302], [Castillo-Celeita, Fdez, J Phys A 53 (2020) 035302], based on [Mielnik, J Math Phys 25 (1984) 3387]

In order to generate new magnetic fields for which the problem is exactly solvable, let us displace up H^- :

1.
$$\tilde{H}_0 \equiv H^- - \epsilon_1 = -\frac{d^2}{dx^2} + V^-(x) - \epsilon_1, \quad \epsilon_1 \le \mathcal{E}_0^- = 0$$

2. From \tilde{H}_0 we build a new Hamiltonian H_1 through

$$H_{1}L_{1}^{+} = L_{1}^{+}\tilde{H}_{0}$$
$$H_{1} = -\frac{d^{2}}{dx^{2}} + V_{1}(x,\epsilon_{1})$$
$$L_{1}^{+} = -\frac{d}{dx} + W_{1}(x,\epsilon_{1})$$





Thus

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

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

By changing $W_1(x, \epsilon_1) = u_1^{(0)'}/u_1^{(0)}$ it is obtained

$$-u_1^{(0)''} + \tilde{V}_0(x)u_1^{(0)} = 0 \qquad \qquad \text{SE for } \tilde{H}_0$$

The generated magnetic field becomes

$$B_1(x,\epsilon_1) = \frac{c\hbar}{e} W_1'(x,\epsilon_1) = -B_0(x) + \frac{c\hbar}{e} \left\{ \ln\left[\frac{u_1^{(0)}(x)}{\psi_0^-(x)}\right] \right\}''$$



3. The auxiliary eigenvalues and eigenfunctions are

$$\tilde{\mathcal{E}}_{n}^{(0)} = \mathcal{E}_{n}^{-} - \epsilon_{1}, \quad \psi_{n}^{-}(x)
\mathcal{E}_{0}^{(1)} = 0, \qquad \psi_{0}^{(1)}(x) \sim e^{-\int W_{1}(x,\epsilon_{1})dx} = \frac{1}{u_{1}^{(0)}}
\mathcal{E}_{n+1}^{(1)} = \tilde{\mathcal{E}}_{n}^{(0)}, \qquad \psi_{n+1}^{(1)}(x) = \frac{1}{\sqrt{\tilde{\mathcal{E}}_{n}^{(0)}}} L_{1}^{+} \psi_{n}^{-}(x), \quad n = 0, 1, \dots$$

The new solutions for graphene become

$$E_{0} = \hbar v_{F} \sqrt{\mathcal{E}_{0}^{(1)}} = 0, \quad E_{n+1} = \hbar v_{F} \sqrt{\mathcal{E}_{n+1}^{(1)}}$$
$$\Psi_{0} = e^{iky} \begin{bmatrix} 0\\ i \psi_{0}^{(1)}(x) \end{bmatrix}, \quad \Psi_{n+1} = e^{iky} \begin{bmatrix} \psi_{n}^{-}(x)\\ i \psi_{n+1}^{(1)}(x) \end{bmatrix}$$



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

$$u_{1}^{(0)} = e^{-\frac{\omega}{4}(x + \frac{2k}{\omega})^{2}} \left\{ {}_{1}F_{1}\left[a, \frac{1}{2}, \frac{\omega}{2}(x + \frac{2k}{\omega})^{2}\right] + 2\nu_{1}\frac{\Gamma(a + \frac{1}{2})}{\Gamma(a)}\sqrt{\frac{\omega}{2}}(x + \frac{2k}{\omega})_{1}F_{1}\left[a + \frac{1}{2}, \frac{3}{2}, \frac{\omega}{2}(x + \frac{2k}{\omega})^{2}\right] \right\}$$

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

$$V_{1}(x,\epsilon_{1}) = \tilde{V}_{0} - 2\left[\frac{\omega}{2}\left(x + \frac{2k}{\omega}\right)\left(-1 + \frac{2}{5}\frac{1F_{1}\left[\frac{11}{10}, \frac{3}{2}, \frac{\omega}{2}\left(x + \frac{2k}{\omega}\right)^{2}\right]}{1F_{1}\left[\frac{1}{10}, \frac{1}{2}, \frac{\omega}{2}\left(x + \frac{2k}{\omega}\right)^{2}\right]}\right)\right]'$$
$$B_{1}(x,\epsilon_{1}) = -B_{0} + \frac{2B_{0}}{5}\left[\left(x + \frac{2k}{\omega}\right)\frac{1F_{1}\left[\frac{11}{10}, \frac{3}{2}, \frac{\omega}{2}\left(x + \frac{2k}{\omega}\right)^{2}\right]}{1F_{1}\left[\frac{1}{10}, \frac{1}{2}, \frac{\omega}{2}\left(x + \frac{2k}{\omega}\right)^{2}\right]}\right]'$$









1. Now let us displace up H_1 as

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

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

$$H_{2}L_{2}^{+} = L_{2}^{+}\tilde{H}_{1}$$
$$H_{2} = -\frac{d^{2}}{dx^{2}} + V_{2}(x,\epsilon_{2})$$
$$L_{2}^{+} = -\frac{d}{dx} + W_{2}(x,\epsilon_{2})$$

Thus

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



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

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

 $u_2^{(1)}$ arises from acting L_1^+ onto an appropriate solution of H^- :

$$u_2^{(1)} \propto L_1^+ u_2^{(0)} = -\mathsf{W}(u_1^{(0)}, u_2^{(0)}) / u_1^{(0)}$$
$$-u_2^{(0)''} + V^-(x)u_2^{(0)} = (\epsilon_1 + \epsilon_2)u_2^{(0)}$$

The new potential and external magnetic field are

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

$$B_2(x,\epsilon_2) = \frac{c\hbar}{e} W_2'(x,\epsilon_2) = -B_1(x,\epsilon_1) + \frac{c\hbar}{e} \{\ln[\mathsf{W}(u_1^{(0)}, u_2^{(0)})]\}''$$



3. The auxiliary eigenvalues and eigenfunctions are

$$\tilde{\mathcal{E}}_{n}^{(1)} = \mathcal{E}_{n}^{(1)} - \epsilon_{2}, \qquad \psi_{n}^{(1)}(x)$$
$$\mathcal{E}_{0}^{(2)} = 0, \quad \psi_{0}^{(2)}(x) \sim e^{-\int W_{2}(x,\epsilon_{2})dx} = \frac{1}{u_{2}^{(1)}}$$
$$\mathcal{E}_{n+1}^{(2)} = \tilde{\mathcal{E}}_{n}^{(1)}, \quad \psi_{1}^{(2)}(x) = \frac{L_{2}^{+}\psi_{0}^{(1)}(x)}{\sqrt{\tilde{\mathcal{E}}_{0}^{(1)}}}, \quad \psi_{n+2}^{(2)}(x) = \frac{L_{2}^{+}\psi_{n+1}^{(1)}(x)}{\sqrt{\tilde{\mathcal{E}}_{n+1}^{(1)}}}$$

The new solutions for graphene are

$$E_{0} = \hbar v_{F} \sqrt{\mathcal{E}_{0}^{(2)}} = 0, \quad E_{n+1} = \hbar v_{F} \sqrt{\mathcal{E}_{n+1}^{(2)}}$$
$$\Psi_{0} = e^{iky} \begin{bmatrix} 0\\ i \psi_{0}^{(2)}(x) \end{bmatrix}, \quad \Psi_{n+1} = e^{iky} \begin{bmatrix} \psi_{n}^{(1)}(x)\\ i \psi_{n+1}^{(2)}(x) \end{bmatrix}$$

The procedure can be continued at will!



Iterative DT





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• Example. In the second SUSY step $V_1(x)$ is moved up by $-\epsilon_2$:

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

The second-order potential and magnetic field are

$$V_2(x,\epsilon_2) = \tilde{V}_0 - 2\{\ln[\mathsf{W}(u_1^{(0)}, u_2^{(0)})]\}'' - \epsilon_2$$
$$B_2(x,\epsilon_2) = -B_1(x,\epsilon_1) + \frac{c\hbar}{e}\{\ln[\mathsf{W}(u_1^{(0)}, u_2^{(0)})]\}''$$

 $u_2^{(0)}$ arises from $u_1^{(0)}$ by changing $\epsilon_1 \rightarrow \epsilon_1 + \epsilon_2$

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







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- 6 Real seed solutions with nodes can be used in the first step \Rightarrow singularities arise in $W_1(x, \epsilon_1)$, $V_1(x, \epsilon_1)$ and $B_1(x, \epsilon_1)$
- 6 An appropriate transformed seed solution of H^- with nodes is used in the second step to cancel some singularities induced in the first step. At the end singularities still appear in $W_2(x, \epsilon_2)$ and in $B_2(x, \epsilon_2)$ but disappear from $V_2(x, \epsilon_2)$
- A third non-singular Darboux transformation is required to cancel completely the singularities remaining of the second step







Singular DT





 $\epsilon_1 = 1.7, \quad \nu_1 = 0.1$ $\epsilon_2 = 1.5, \quad \nu_2 = 1.1$ $\epsilon_3 = -0.5, \quad \nu_3 = 0.5$





Complex DT

Seed solutions for $\epsilon \in \mathbb{C}$ can be used, such that after 3 steps a Hermitian graphene Hamiltonian is obtained:

– A complex seed solution $u^{(0)}$ for $\epsilon \in \mathbb{C}$, vanishing at one of the ends of the *x*-domain, is chosen

– Then, the (transformed) seed solution $-iu^*(x)$ associated to ϵ^* is used, such that $-iW(u^{(0)}, u^{*(0)})$ is real nodeless

- A real nodeless (transformed) seed solution $u_3^{(0)}$ for $\epsilon_3 \leq \mathcal{E}_0^- = 0$ is used. At the end a real potential and magnetic field are obtained,

$$V_{3}(x,\epsilon_{3}) = V^{-}(x) - 2\left\{\ln\left[\mathsf{W}\left(u^{(0)}, -iu^{*(0)}, u^{(0)}_{3}\right)\right]\right\}^{\prime\prime} - \epsilon_{3}$$
$$B_{3}(x,\epsilon_{3}) = \frac{c\hbar}{e}\left\{\ln\left[\frac{\mathsf{W}(u^{(0)}, -iu^{*(0)}, u^{(0)}_{3})}{\mathsf{W}(u^{(0)}, -iu^{*(0)})}\right]\right\}^{\prime\prime}$$



Complex DT



$$\epsilon_{1} = -\frac{1}{2} + \frac{i}{10}$$

$$\epsilon_{2} = -\frac{1}{2} - \frac{i}{10}$$

$$\epsilon_{3} = -\frac{1}{2}, \quad \Lambda = \frac{1}{10}$$



Periodic DT

Finally, let us consider a periodic magnetic field,

$$\mathcal{B}(x) = B_0 \frac{m - 1 + \operatorname{dn}(x|m)^4}{\operatorname{dn}(x|m)^2}$$

The superpotential is,

$$W_0(x) = m \frac{\operatorname{sn}(x|m)\operatorname{cn}(x|m)}{\operatorname{dn}(x|m)}$$

6 The two self-isospectral periodic Lamé potentials are:

$$V^{-}(x) = 2m \operatorname{sn}(x|m)^{2} - m$$
$$V^{+}(x) = 2m \operatorname{sn}(x + K|m)^{2} - m$$



Periodic DT

The bande edge eigenfunctions and eigenvalues are

$$\begin{aligned} \mathcal{E}_0^- &= 0 & \mathcal{E}_1^- &= 1 - m & \mathcal{E}_{1'}^- &= 1 \\ \psi_0^- &= \mathrm{dn}(x|m) & \psi_1^- &= \mathrm{cn}(x|m) & \psi_{1'}^- &= \mathrm{sn}(x|m) \\ \psi_0^+ &= \mathrm{dn}(x+K|m) & \psi_1^+ &= \mathrm{cn}(x+K|m) & \psi_{1'}^+ &= \mathrm{sn}(x+K|m) \end{aligned}$$

The band edge solutions for electrons in the graphene periodic magnetic superlattice:

$$E_0^- = 0 \qquad \Psi_0 = e^{iky} \begin{bmatrix} A_1 \operatorname{dn}(x+K|m) \\ i A_2 \operatorname{dn}(x|m) \end{bmatrix}$$
$$E_1^- = \sqrt{1-m} \quad \Psi_1 = e^{iky} \begin{bmatrix} \operatorname{cn}(x+K|m) \\ i \operatorname{cn}(x|m) \end{bmatrix}$$
$$E_{1'}^- = 1 \qquad \Psi_{1'} = e^{iky} \begin{bmatrix} \operatorname{sn}(x+K|m) \\ i \operatorname{sn}(x|m) \end{bmatrix}$$



Quasi-periodic DT

By applying the general DT, it is possible to create a bound state at zero energy departing from $\tilde{V}_0 = V^- - \epsilon_1$. Thus, a new potential $V_1(x, \epsilon_1)$ is generated, which is not longer periodic but it is quasiperiodic. The same property is acquired by the new magnetic field





Conclusions

- We have analyzed the behavior of graphene in external magnetic fields orthogonal to the layer through DT. The seed solutions employed can produce either shape invariant or more general potentials
- Non-singular DT and their iterations have been proposed as an algorithm to generate magnetic field for which the graphene Hamiltonian admits exact solutions
- Singular DT and their iterations producing non-singular potentials and associated magnetic field (after 3 steps) have been explored
- Complex DT and their iterations generating real SUSY partner potentials and associated magnetic field (after 3 steps) have been studied



Conclusions

- Complex DT involving complex magnetic fields and leading to non-Hermitian graphene Hamiltonians start to be explored
- 6 The second-order DT emerges as the natural tool to address a similar study for bilayer graphene in the so-called Bernal stacking
- We would like to explore if for twisted bilayer graphene it is possible to implement a similar study
- The coherent states approach to graphene is a feasible study, that we started in 2017 and it is still in progress



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