Graphene and Haldane model

Marco Biroli

October 21, 2020

1 Graphene and Dirac points.

1. We have that:

$$\delta_1 = (0, a) \text{ and } \delta_2 = \frac{d}{2}(\sqrt{3}, -1) \text{ and } \delta_3 = \frac{d}{2}(-\sqrt{3}, -1)$$

Then we have that:

$$f_{\mathbf{k}} = -t \exp\left(-\frac{id}{2}(\sqrt{3}k_x + k_y)\right)\left(1 + \exp\left(i\sqrt{3}dk_x\right) + \exp\left(\frac{id}{2}(\sqrt{3}k_x + 3k_y)\right)\right)$$

$$= -t\left[\underbrace{\left(2\cos\left(\frac{\sqrt{3}}{2}dk_x\right)\cos\left(\frac{d}{2}k_y\right) + \cos(dk_y)\right)}_{h_1} + i\underbrace{2\left(\cos\left(\frac{\sqrt{3}}{2}dk_x\right) - \cos\left(\frac{d}{2}k_y\right)\right)\sin\left(\frac{d}{2}k_y\right)}_{h_2}\right]$$

And taking $h_3 = 0$ we have that:

$$H = -t\,\mathbf{h_k} \cdot \sigma$$

Notice that without expanding the terms we can also simply write:

$$H = \sum_{i=1}^{3}\left(\cos(\mathbf{k} \cdot \delta_\mathbf{i})\sigma_x + \sin(\mathbf{k} \cdot \delta_\mathbf{i})\sigma_y\right)$$

Then notice that similarly as in the TD we have that:

$$H^2 = t^2\|\mathbf{h_k}\|^2\,\text{Id}$$

Thus the eigenvalues of H are given by:

$$E_{\pm} = \pm t\|\mathbf{h_k}\| = \pm t\sqrt{3 + 2\cos\left(dk_x\sqrt{3}\right) + 2\cos\left(\frac{d}{2}(k_x\sqrt{3} - 3k_y)\right) + 2\cos\left(\frac{d}{2}(k_x\sqrt{3} + 3k_y)\right)}$$

Notice that solving for $E_{\pm} = 0$ we get indeed the Dirac point K, as well as $-K$ or $(K_x, -K_y)$ for example. Plotting the energy spectrum we obtain Figure 1.
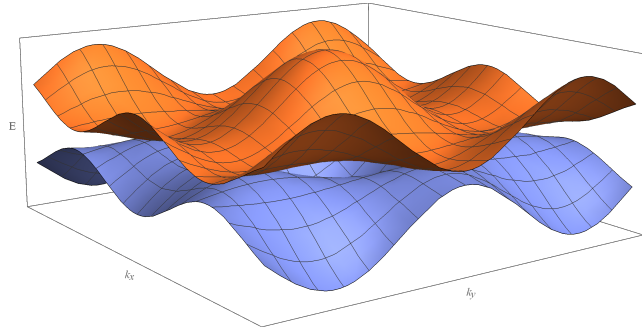

Figure 1: Plot of the positive energy levels for $k_x, k_y \in [-\frac{\pi}{d}, \frac{\pi}{d}]$.

2. We write $\mathbf{k} = \mathbf{K} + \varepsilon$. Then we know that $H_{\mathbf{K}} = 0$ and $f_{\mathbf{K}} = 0$ hence we have that:

$$f_{\mathbf{k}} = f_{\mathbf{K}} + \frac{1}{2}\varepsilon \cdot (\boldsymbol{\nabla} f_{\mathbf{k}})\Big|_{\mathbf{k}=\mathbf{K}} = \frac{1}{2}\varepsilon \cdot \left(\frac{3dt}{2}, -\frac{3}{2}idt\right) = \frac{3dt}{4}(\varepsilon_x - i\varepsilon_y)$$

Hence we also get the linearization of $\mathbf{h}$ easily as:

$$\mathbf{h_k} = \left(\frac{3dt}{4}(k_x - K_x), -\frac{3dt}{4}(k_y - K_y)\right) = \frac{3dt}{4}(\varepsilon_x, -\varepsilon_y)$$

And hence:

$$E_\pm = \pm t\frac{3dt}{4}\sqrt{\varepsilon_x^2 + \varepsilon_y^2} = \pm\frac{3dt}{4}r$$

3. Close to $\mathbf{K}$ the Hamiltlonian reads:

$$H = \frac{3dt}{4}\begin{pmatrix} 0 & \varepsilon_x + i\varepsilon_y \\ \varepsilon_x - i\varepsilon_y & 0 \end{pmatrix}$$

Hence we have that the eigenvectors are given by:

$$u_{\pm\mathbf{k}} = \begin{pmatrix} \pm\sqrt{\varepsilon_x^2 + \varepsilon_y^2} \\ \varepsilon_x - i\varepsilon_y \end{pmatrix} = \begin{pmatrix} \pm\varepsilon \\ \varepsilon e^{-i\theta} \end{pmatrix} \propto \begin{pmatrix} \pm e^{i\theta/2} \\ e^{-i\theta/2} \end{pmatrix}$$

Where we took:

$$\cos\theta = \frac{\varepsilon_x}{\varepsilon} \quad \text{and} \quad \sin\theta = \frac{\varepsilon_y}{\varepsilon} \quad \text{and} \quad \varepsilon = \sqrt{\varepsilon_x^2 + \varepsilon_y^2}$$

Now however notice that at the origin i.e. $\varepsilon_x = \varepsilon_y = 0$ we have that θ is not well defined. Now for the Berry connection we see that there is only an angular dependency hence we have:

$$\mathcal{A}_\pm = i(u_\pm^T)^\star \frac{\partial}{\partial} u_\pm = \begin{pmatrix} 1 & e^{i\theta} \end{pmatrix} \begin{pmatrix} 0 \\ -ie^{-i\theta} \end{pmatrix} = \frac{1}{\varepsilon}\hat{\theta}$$

4. From an immediate application of the residue theorem we know that the Berry phase will be given by the residue of $\frac{1}{\varepsilon}$ at $\varepsilon = 0$ which is 1 times $2\pi i n$ where $n \in \mathbb{Z}$. The Berry phase around $\tilde{K}$ would be given by the conjugate of the one around K.

5. We are now modifying $f_{\mathbf{k}}$ to:

$$f'_{\mathbf{k}} = -t'e^{i\mathbf{k}\cdot\delta_1} - t\sum_{i=2}^{3} e^{i\mathbf{k}\cdot\delta_i}$$

Which then gives for the energies:

$$E'_\pm = \sqrt{2t^2 + t'^2 + 2t\left(t\cos\left(dk_x\sqrt{3}\right) + t'\left(\cos\left(\frac{d}{2}(k_x\sqrt{3} - 3k_y)\right) + \cos\left(\frac{d}{2}(k_x\sqrt{3} + 3k_y)\right)\right)\right)}$$

6. Similarly as before by taking $\mathbf{k} = \mathbf{M} + \varepsilon$ and making an expansion of $f'_{\mathbf{k}}$ we obtain:

$$f'_{\mathbf{k}} \approx e^{i\frac{\pi}{6}}(2it - it' + d(t + t')\varepsilon_y)$$

Hence the Hamiltonian is given by:

$$H = \begin{pmatrix} 0 & e^{-i\frac{\pi}{6}}(it' - 2it + d(t + t')\varepsilon_y) \\ e^{i\frac{\pi}{6}}(2it - it' + d(t + t')\varepsilon_y) & 0 \end{pmatrix}$$
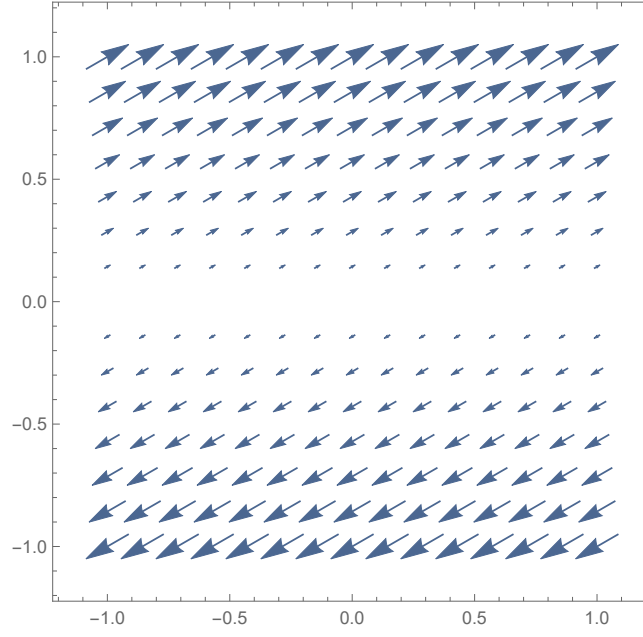
7. See Figure 7

8.

Figure 2: Orientation of $f(\mathbf{k})$

2   The Haldane Model

1. In the case of a crystal with one atom per unit cell the Hamiltonian can be written:

$$...$$

2. We have that the hoping term from an A state to an A state is given by:

$$A = 2\operatorname{Re}\left(t_2 e^{i\varphi} \sum_{j=1}^{d} e^{i\mathbf{k}\cdot\mathbf{b_j}} \right)$$

Similarly the one for B is given by:

$$B = 2\operatorname{Re}\left(t_2 e^{-i\varphi} \sum_{j=1}^{d} e^{i\mathbf{k}\cdot\mathbf{b_j}} \right)$$

Then we have that:

$$H_{\mathbf{k}} = \begin{pmatrix} A + M & (f_{\mathbf{k}})^\star \\ f_{\mathbf{k}} & B - M \end{pmatrix} = \begin{pmatrix} 0 & (f_{\mathbf{k}})^\star \\ f_{\mathbf{k}} & 0 \end{pmatrix} + M\sigma_{\mathbf{3}} + 2t_2 \left(\cos\varphi \sum_{j=1}^{3} \cos(\mathbf{k}\cdot\mathbf{b_j}) + i\left(\cos\varphi \sum_{j=1}^{3} \sin(\mathbf{k}\cdot\mathbf{b_j}) \right) \right) \operatorname{Id} = ...$$

3.