Graphene and Haldane model

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1 Graphene and Dirac points.

1. We have that:

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

$$H = \sum_{i=1}^{3} (\cos(\mathbf{k} \cdot \delta_{i}) \sigma_{x} + \sin(\mathbf{k} \cdot \delta_{i}) \sigma_{y})$$

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:

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

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.

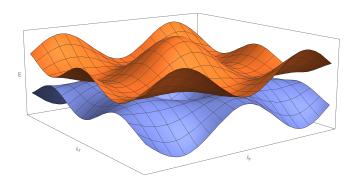


Figure 1: Plot of the positive energy levels for $k_x, k_y \in [-\frac{\pi}{d}, \frac{\pi}{d}]$.

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:

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

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

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

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 Hamitlonian 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:

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

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:

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

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.