Graphene and Haldane model

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1 Graphene and Dirac points.

1. We have that:
$$\delta_{\mathbf{1}} = (0, a) \quad \text{and} \quad \delta_{\mathbf{2}} = \frac{d}{2}(\sqrt{3}, -1) \quad \text{and} \quad \delta_{\mathbf{3}} = \frac{d}{2}(-\sqrt{3}, -1)$$
Then we have that:
$$\begin{aligned} f_{\mathbf{k}} &= -t \exp\left(-\frac{id}{2}(\sqrt{3}k_x + k_y)\right)\left(1 + \exp\left(i\sqrt{3}dk_x\right) + \exp\left(\frac{id}{2}(\sqrt{3}k_x + 3k_y)\right)\right) \\ &= -t\left[\underbrace{\left(2\cos\left(\frac{\sqrt{3}}{2}dk_x\right)\cos\left(\frac{d}{2}k_y\right) + \cos(dk_y)\right)}_{h_1} + i\,\underbrace{2\left(\cos\left(\frac{\sqrt{3}}{2}dk_x\right) - \cos\left(\frac{d}{2}k_y\right)\right)\sin\left(\frac{d}{2}k_y\right)}_{h_2}\right] \end{aligned}$$
And taking $h_3 = 0$ we have that:
$$H = -t\ \mathbf{h}_{\mathbf{k}} \cdot \sigma$$
Notice that without expanding the terms we can also simply write:
$$H = \sum_{i=1}^{3} (\cos(\mathbf{k} \cdot \delta_{\mathbf{i}})\sigma_x + \sin(\mathbf{k} \cdot \delta_{\mathbf{i}})\sigma_y)$$
Then notice that similarly as in the TD we have that:
$$H^2 = t^2 ||\mathbf{h}_{\mathbf{k}}||^2\ \mathrm{Id}$$
Thus the eigenvalues of H are given by:
$$E_{\pm} = \pm t||\mathbf{h}_{\mathbf{k}}|| = \pm t\sqrt{3 + 2\cos\left(dk_x\sqrt{3}\right) + 2\cos\left(\frac{d}{2}(k_x\sqrt{3} - 3k_y)\right) + 2\cos\left(\frac{d}{2}(k_x\sqrt{3} + 3k_y)\right)}$$
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.

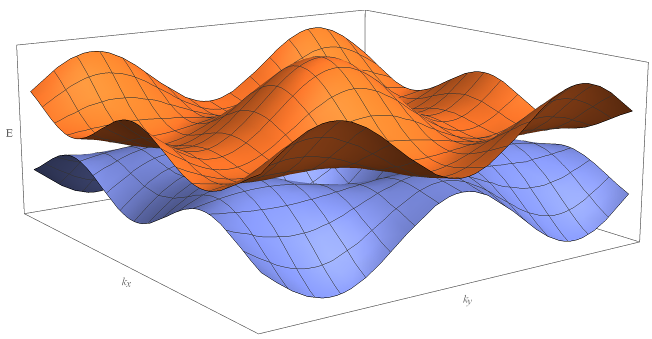

Figure 1: Plot of the positive energy levels for $k_x, k_y \in [-\frac{\pi}{d}, \frac{\pi}{d}]$.

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:

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

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

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

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:

$$u_{\pm\mathbf{k}} = \begin{pmatrix} \pm\sqrt{\varepsilon_x^2 + \varepsilon_y^2} \\ \varepsilon_x - i\varepsilon_y \end{pmatrix} = \begin{pmatrix} \pm\varepsilon \\ e^{-i\theta} \end{pmatrix} = \begin{pmatrix} \pm\varepsilon e^{i\theta} \\ 1 \end{pmatrix}$$

Where we took:

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

Hence we get:

$$\mathcal{A}_{\pm x} = u_\mp^T \frac{\partial}{\partial k_x} u_\pm = \begin{pmatrix} \mp\sqrt{\varepsilon_x^2 + \varepsilon_y^2} & \varepsilon_x - i\varepsilon_y \end{pmatrix} \begin{pmatrix} \pm\frac{\varepsilon_x}{\sqrt{\varepsilon_x^2+\varepsilon_y^2}} \\ \varepsilon_x + K_x \end{pmatrix} = -\varepsilon_x + (\varepsilon_x - i\varepsilon_y)(\varepsilon_x + K_x)$$

Similarly we get:

$$\mathcal{A}_{\pm y} = u_\mp^T \frac{\partial}{\partial k_y} u_\pm = \begin{pmatrix} \mp\sqrt{\varepsilon_x^2 + \varepsilon_y^2} & \varepsilon_x - i\varepsilon_y \end{pmatrix} \begin{pmatrix} \pm\frac{\varepsilon_y}{\sqrt{\varepsilon_x^2+\varepsilon_y^2}} \\ -i\varepsilon_y \end{pmatrix} = -\varepsilon_y - \varepsilon_y(i\varepsilon_x + \varepsilon_y) = -\varepsilon_y(1 + i\varepsilon_x + \varepsilon_y)$$

Taking $\varepsilon_x = \varepsilon\cos(\theta)$ and $\varepsilon_y = \varepsilon\sin(\theta)$ and replacing above we get:

$$\mathcal{A}_\pm = \begin{pmatrix} \frac{\varepsilon}{2}(1 - e^{i\theta} + e^{-i\theta}(1 + 2K_x) + e^{-2i\theta} \\ -\frac{\varepsilon}{2i}(e^{i\theta} - e^{-i\theta})(1 + \varepsilon e^{i\theta}) \end{pmatrix}$$

4. We therefore get for the integral:

$$\varphi_\mathcal{A} = \int_0^{2\pi} \mathcal{A}_\pm \cdot \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \varepsilon \mathrm{d}\theta$$

2 draft

Now for simplicity we write $re^{i\theta} = \varepsilon_x + i\varepsilon_y$ where $r = \sqrt{\varepsilon_x^2 + \varepsilon_y^2}$ and $\theta = \arctan(\varepsilon_y/\varepsilon_x)$. Then we can rewrite the above as:

$$H = \frac{3rdt}{4}\begin{pmatrix} 0 & e^{i\theta} e^{-i\theta} & 0 \end{pmatrix}$$

Which immediately tells us that:

$$E_\pm = \pm\frac{3rdt}{4} \quad \text{and} \quad u_\pm = \begin{pmatrix} \pm e^{i\theta} \\ 1 \end{pmatrix}$$