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:

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

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

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:

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

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

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

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.

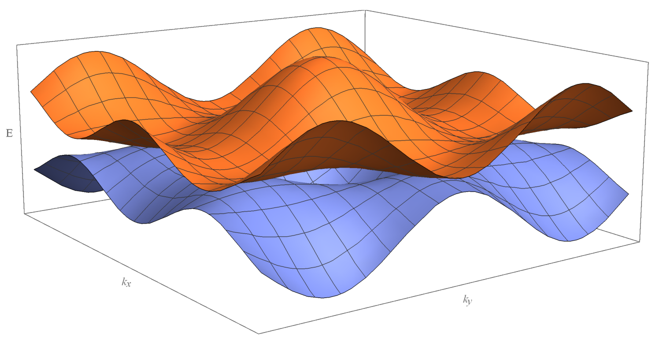

Figure 1: Plot of the positive energy levels for $k_x, k_y \in [-\frac{\pi}{d}, \frac{\pi}{d}]$.

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:

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

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:

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

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:

$$\mathcal{A}_{\pm} = i(u_{\pm})^{\star} \cdot \boldsymbol{\nabla} u_{\pm} = i\begin{pmatrix} 1 & \pm e^{i\theta} \end{pmatrix}\begin{pmatrix} \partial_{\varepsilon} \\ \frac{1}{\varepsilon}\partial_{\theta} \end{pmatrix}\begin{pmatrix} 1 & \pm e^{-i\theta} \end{pmatrix} = i\begin{pmatrix} 1 & \pm e^{i\theta} \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & \frac{\mp i}{\varepsilon}e^{-i\theta} \end{pmatrix} = \frac{1}{\varepsilon}\hat{\theta}$$

4. We then have that the Berry phase is going to be given by:

$$\varphi_{\mathcal{A}} = \int_{\mathcal{C}} \mathcal{A}_{\pm} \mathrm{d}\mathbf{l} = \int_{\mathcal{C}} \frac{1}{\varepsilon}\mathrm{d}\theta = 2\pi n \quad \text{with} \quad n \in \mathbb{Z}$$

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

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

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 2

8.

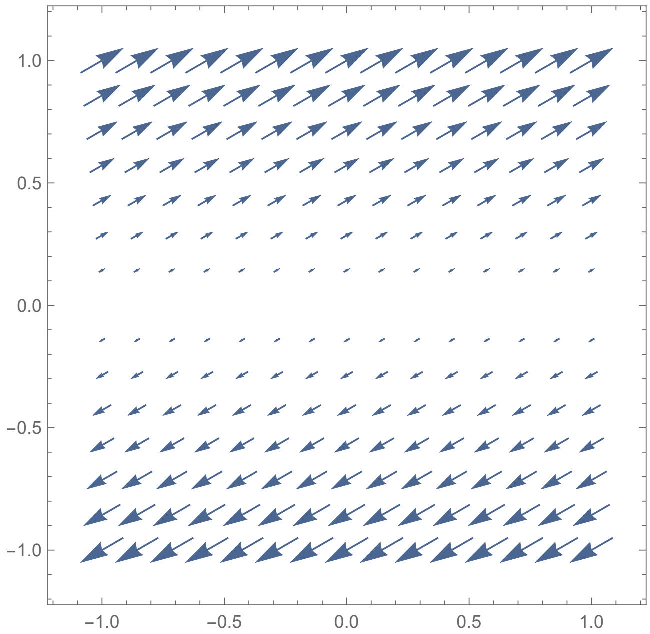

Figure 2: Orientation of $f(\mathbf{k})$

2 The Haldane Model

1. Cells can be indexed by two integers (i, j) where the i index corresponds to the horizontal position and the j to the vertical position. Then we write the orbitals $|i, j, A\rangle$ and $|i, j, B\rangle$ for A and B respectively. Then the Hamiltonian is given by:

$$
\begin{aligned}
H = \sum_{i,j} t\Big(& |i,j,B\rangle\langle i,j,A| + |i,j+1,B\rangle\langle i,j,A| + |i+1,j,B\rangle\langle i,j,A|\Big) \\
&+ t_2 e^{i\varphi}\Big(|i,j+1,A\rangle\langle i,j,A| + |i,j-1,A\rangle\langle i,j,A| + |i-1,j,A\rangle\langle i,j,A|\Big) + \frac{M}{2}|i,j,A\rangle\langle i,j,A| \\
&+ t_2 e^{-i\varphi}\Big(|i,j+1,B\rangle\langle i,j,B| + |i,j-1,B\rangle\langle i,j,B| + |i-1,j,B\rangle\langle i,j,B|\Big) - \frac{M}{2}|i,j,B\rangle\langle i,j,B| \\
&+ h.c.
\end{aligned}
$$

2. The first line and it's Hermitian conjugate of the above definition of the Hamiltonian corresponds to the one studied in part one and we will denote it by H_0 which we already know can be expressed as $H_0 = \mathbf{h}\cdot\sigma$. Now we study the two remaining lines of the Hamiltonian. The first one (resp. second one) corresponds to the contribution from clock-wise hoping on $A - A$ terms plus the staggered potential (resp. $B - B$ terms with the staggered potential). Which we can re-write as:

$$
|i,j,A\rangle\left(\frac{M}{2} + t_2 e^{i\varphi}\sum_{j=1}^{3} e^{i\mathbf{k}\cdot\mathbf{b_j}}\right)\langle i,j,A| \quad \text{and} \quad |i,j,B\rangle\left(\frac{-M}{2} + t_2 e^{-i\varphi}\sum_{j=1}^{3} e^{i\mathbf{k}\cdot\mathbf{b_j}}\right)\langle i,j,B|
$$

Then adding these with their conjugates will give:

$$
\begin{pmatrix}|i,j,A\rangle & |i,j,B\rangle\end{pmatrix}\begin{pmatrix} 2\,\mathrm{Re}\left(t_2 e^{i\varphi}\sum_{j=1}^{3} e^{i\mathbf{k}\cdot\mathbf{b_j}}\right) + M & 0 \\ 0 & 2\,\mathrm{Re}\left(t_2 e^{-i\varphi}\sum_{j=1}^{3} e^{i\mathbf{k}\cdot\mathbf{b_j}}\right) - M\end{pmatrix}\begin{pmatrix}\langle i,j,A| \\ \langle i,j,B|\end{pmatrix}
$$

Now from the properties:

$$
\mathrm{Re}(ab) = \mathrm{Re}(a)\,\mathrm{Re}(b) - \mathrm{Im}(a)\,\mathrm{Im}(b) \quad \text{and} \quad \mathrm{Re}(a) = \mathrm{Re}(a^\star) \quad \text{and} \quad \mathrm{Im}(a) = -\,\mathrm{Im}(a^\star)
$$

We can simplify the above (calling $a = t_2 e^{i\varphi}$ and b the sum):

$$\begin{aligned}
&\begin{pmatrix}|i,j,A\rangle & |i,j,B\rangle\end{pmatrix}\begin{pmatrix}2\,\mathrm{Re}\,(ab)+M & 0\\ 0 & 2\,\mathrm{Re}\,(a^\star b)-M\end{pmatrix}\begin{pmatrix}\langle i,j,A|\\ \langle i,j,B|\end{pmatrix}\\
&=\begin{pmatrix}|i,j,A\rangle & |i,j,B\rangle\end{pmatrix}\begin{pmatrix}2\,\mathrm{Re}(a)\,\mathrm{Re}(b)-2\,\mathrm{Im}(a)\,\mathrm{Im}(b)+M & 0\\ 0 & 2\,\mathrm{Re}(a^\star)\,\mathrm{Re}(b)-2\,\mathrm{Im}(a^\star)\,\mathrm{Im}(b)-M\end{pmatrix}\begin{pmatrix}\langle i,j,A|\\ \langle i,j,B|\end{pmatrix}\\
&=\begin{pmatrix}|i,j,A\rangle & |i,j,B\rangle\end{pmatrix}\begin{pmatrix}2\,\mathrm{Re}(a)\,\mathrm{Re}(b)+(-2\,\mathrm{Im}(a)\,\mathrm{Im}(b)+M) & 0\\ 0 & 2\,\mathrm{Re}(a)\,\mathrm{Re}(b)-(-2\,\mathrm{Im}(a)\,\mathrm{Im}(b)+M)\end{pmatrix}\begin{pmatrix}\langle i,j,A|\\ \langle i,j,B|\end{pmatrix}\\
&=\begin{pmatrix}|i,j,A\rangle & |i,j,B\rangle\end{pmatrix}\left(2Re(a)Re(b)\mathrm{Id}+\Big(M-2\,\mathrm{Im}(a)\,\mathrm{Im}(b)\Big)\sigma_z\right)\begin{pmatrix}\langle i,j,A|\\ \langle i,j,B|\end{pmatrix}
\end{aligned}$$

Hence now we write:

$$\varepsilon_0(\mathbf{k}) = 2\,\mathrm{Re}(a)\,\mathrm{Re}(b) = 2\cos\varphi\sum_{j=1}^{3}\cos(\mathbf{k}\cdot\mathbf{b_j})$$

As well as:

$$d_z(\mathbf{k}) = M - 2\,\mathrm{Im}(a)\,\mathrm{Im}(b) = M - 2t_2\sin(\varphi)\sum_{j=1}^{3}\sin(\mathbf{k}\cdot\mathbf{b_j})$$

Then we define:

$$\mathbf{d}(\mathbf{k}) = \mathbf{h}(\mathbf{k}) + d_z(\mathbf{k})\hat{\mathbf{z}}$$

Which allows us to re-write:

$$H = \sum_{\mathbf{k}}\begin{pmatrix}|\mathbf{k},A\rangle & |\mathbf{k},B\rangle\end{pmatrix}\underbrace{\Big(\varepsilon_0(\mathbf{k})\mathrm{Id}+\mathbf{d}(\mathbf{k})\cdot\sigma\Big)}_{H_{\mathbf{k}}}\begin{pmatrix}\langle\mathbf{k},A|\\ \langle\mathbf{k},B|\end{pmatrix}$$

3. We have immediately that the eigenvalues of $H_{\mathbf{k}}$ are going to be given by:

$$E_{\pm\mathbf{k}} = \varepsilon_0(\mathbf{k}) \pm ||\mathbf{d}(\mathbf{k})||$$

Hence we have that:

$$\Delta E_{\pm\mathbf{k}} = E_{+\mathbf{k}} - E_{-\mathbf{k}} = 2||d(\mathbf{k})||$$

Hence gaps close if and only if:

$$2||\mathbf{d}(\mathbf{k})|| = 0 \Leftrightarrow ||\mathbf{h}(\mathbf{k})||^2 + d_z(\mathbf{k})^2 = 0 \Leftrightarrow \begin{cases}||h(\mathbf{k})||^2 = 0\\ d_z(\mathbf{k})^2 = 0\end{cases} \Rightarrow d_z(\mathbf{K}) = 0$$

Furthermore from the relation that we are given we have that:

$$d_z(\mathbf{K}) = M + 3t_2\sin(\varphi)\sqrt{3}$$

Hence we will have conduction only along the line (in the $(\sin\varphi, M)$ plane):

$$M = -3t_2\sqrt{3}\sin(\varphi)$$

4. Notice that $d_3(\tilde{\mathbf{K}}) = d_3(-\mathbf{K}) = -d_3(\mathbf{K})$, furthermore $\mathbf{n}(\tilde{K}) = -\hat{\mathbf{z}}$ hence the two opposite signs cancel and we get that:

$$\nu = 2\mathrm{sign}(d_3(\mathbf{K}))$$

5. At the transition the gap will be close to the Dirac points hence:

$$\Delta E_{\pm\mathbf{k}} = 2||\mathbf{d}(\mathbf{k})|| = 2|d_z(\mathbf{K})|$$

6. In order to linearize we can use the following simplification: $\cos(\mathbf{q}\cdot\mathbf{b_j}) = 1 + \mathcal{O}(||\mathbf{q}||^2)$ and $\sin(\mathbf{q}\cdot\mathbf{b_j}) = \mathbf{q}\cdot\mathbf{b_j} + \mathcal{O}(||\mathbf{q}||^3)$. Then we can re-write:

$$\varepsilon_0(\mathbf{K}+\mathbf{q}) = 2\cos\varphi\sum_{j=1}^{3}\cos(\mathbf{K}\cdot\mathbf{b_j}+\mathbf{q}\cdot\mathbf{b_j}) = 2\cos\varphi\sum_{j=1}^{3}\Big(\cos(\mathbf{K}\cdot\mathbf{b_j})\cdot 1 - (\mathbf{q}\cdot\mathbf{b_j})\sin(\mathbf{K}\cdot\mathbf{b_j})\Big)$$

Now we can simplify this as follows:

$$\varepsilon_0(\mathbf{K}+\mathbf{q}) = \underbrace{\varepsilon_0(\mathbf{K})}_{-3\cos\varphi} + 3\sqrt{3}(\mathbf{q}\cdot\mathbf{b_j})\cos\varphi$$

Similarly we get:

$$\begin{aligned} d_z(\mathbf{K}+\mathbf{q}) &= M - 2t_2\sin(\varphi)\sum_{j=1}^{3}(\mathbf{q}\cdot\mathbf{b_j})\cos(\mathbf{K}\cdot\mathbf{b_j}) + \sin(\mathbf{K}\cdot\mathbf{b_j}) \\ &= d_z(\mathbf{K}) - 2t_2\sin(\varphi)\mathbf{q}\cdot\underbrace{\sum_{j=1}^{3}\mathbf{b_j}\cos(\mathbf{K}\cdot\mathbf{b_j})}_{=0} = d_z(\mathbf{K}) \end{aligned}$$

Then from the expression of $\mathbf{h}$ we have that:

$$d_x(\mathbf{K}+\mathbf{q}) = \overbrace{d_x(\mathbf{K})}^{=0} + t\mathbf{q}\cdot\underbrace{\sum_{j=1}^{3}\delta_\mathbf{j}\sin(\mathbf{K}\cdot\delta_\mathbf{j})}_{=3d/2\hat{\mathbf{x}}} \quad \text{and} \quad d_y(\mathbf{K}+\mathbf{q}) = \overbrace{d_y(\mathbf{K})}^{=0} + t\mathbf{q}\cdot\underbrace{\sum_{j=1}^{3}\delta_\mathbf{j}\cos(\mathbf{K}\cdot\delta_\mathbf{j})\,\delta_\mathbf{j})}_{=3d/2\hat{\mathbf{y}}}$$

So in total we obtain:

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