PCPHY552: Topological Graphene and Spin-$\frac{1}{2}$ Particle

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We introduce topology from the two inequivalent Dirac points $\mathbf{K}$ and $\mathbf{K}'$ of the graphene. The 2×2 form of the matrix Hamiltonian in $\mathbf{k}$-space allows an analogy to the Bloch sphere of a spin-1/2 particle which will be useful for the characterisation of the topology. The Hamiltonian for the spin-1/2 particle is defined as $\mathcal{H} = \sum_{\mathbf{k}} \mathcal{H}(\mathbf{k})$ with $\mathcal{H}(\mathbf{k}) = -\mathbf{d}(\mathbf{k})\cdot\boldsymbol{\sigma}$, such that the energy of the particle is minimized when aligned with the field. For graphene, we have the $\mathbf{d}$-vector

$$\mathbf{d} = \left(t\sum_{\boldsymbol{\delta}_i} \cos(\mathbf{k}\cdot\boldsymbol{\delta}_i), t\sum_{\boldsymbol{\delta}_i} \sin(\mathbf{k}\cdot\boldsymbol{\delta}_i), 0 \right),$$

where $-t$ represents the hopping term between nearest neighbors.

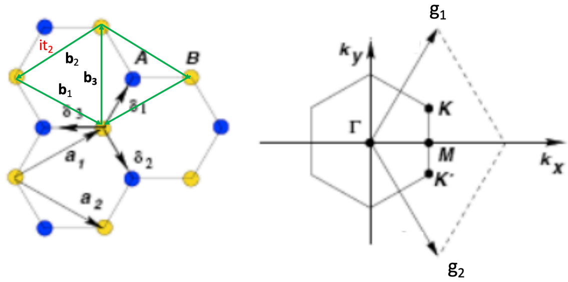

Figure 1: Haldane model on the honeycomb lattice, definition of primitive lattice vectors $\mathbf{a}_1 = \frac{a}{2}(3,\sqrt{3})$ and $\mathbf{a}_2 = \frac{a}{2}(3,-\sqrt{3})$, Brillouin zone. From the form of the nearest-neighbor vector $\boldsymbol{\delta}_3 = (-a,0)$ and the identities $\boldsymbol{\delta}_1 - \boldsymbol{\delta}_3 = \mathbf{a}_1$ and $\boldsymbol{\delta}_2 - \boldsymbol{\delta}_3 = \mathbf{a}_2$, you can determine all the $\boldsymbol{\delta}_i$s.

1. Close to the Dirac points $\mathbf{K} = \frac{2\pi}{3a}(1,\frac{1}{\sqrt{3}})$ and $\mathbf{K}' = \frac{2\pi}{3a}(1,-\frac{1}{\sqrt{3}})$, verify that the Hamiltonian takes the following form in the Hilbert space formed by the two sublattices' wavefunctions:

$$\mathcal{H}(\mathbf{k}) = -\mathbf{d}\cdot\boldsymbol{\sigma} = v_F \begin{pmatrix} 0 & \Pi^* \\ \Pi & 0 \end{pmatrix}$$

where $\mathbf{k} = \mathbf{K} + \mathbf{p}$, $\Pi = |p|e^{i\tilde{\varphi}} = p_x + ip_y$ and $v_F = \frac{3}{2}ta$ with for simplicity $\underline{\hbar = 1 \text{ or } h = 2\pi}$. Deduce $\mathcal{H}(\mathbf{k})$ close to $\mathbf{K}'$.

2. Now, we introduce the second-nearest-neighbor term $t_2 e^{i\phi}$ from the definitions of the figure with $\phi = \pi/2$ such that on a given triangle the phase accumulated is non-zero [1]. If we invert the direction on a path, then one should modify $\phi \to -\phi$. Taking into account the 6 second nearest-neighbors defined through the vectors $\mathbf{b}_1$, $\mathbf{b}_2$ and $\mathbf{b}_3$, show that the 'effective' magnetic field $\mathbf{d}$ in $\mathbf{k}$-space acquires a d_z contribution equal to $2t_2\sum_{\mathbf{b}_j}\sin(\mathbf{k}\cdot\mathbf{b_j})$. Justify that the system has a zero magnetic flux in a unit (honeycomb) cell. Justify that the system is an insulator in the bulk at the Fermi energy $E_F = 0$.

3. Evaluate the d_z term at the Dirac points $\mathbf{K}$ and $\mathbf{K}'$ and show that there is an energy gap such that $d_z(\mathbf{K}) = -d_z(\mathbf{K}') = m$ with $m = 3\sqrt{3}t_2$. On the figure, we have $\mathbf{b}_1 = \frac{a}{2}(3,-\sqrt{3})$, $\mathbf{b}_2 = -\frac{a}{2}(3,\sqrt{3})$ and $\mathbf{b}_3 = (0,\sqrt{3}a)$.

All the topological properties around the Dirac points can be described through the $\mathbf{d}$ vector and the observables linked to the pseudo-spin in the sub-lattice space. We have a two-dimensional plane (k_x,k_y) which may be mapped on a torus through application of periodic boundary conditions

[1] Here, is a link to the Haldane model: F. D. M Haldane https://journals.aps.org/prl/pdf/10.1103/PhysRevLett.61.2015

or on a sphere S^2. As we show below, the sphere allows a simple calculation of the topological number and a simple understanding of adding Berry phases in the topological phase.

4. To study the topological response, we define a map from $(k_y, k_x) \to (\theta, \varphi)$ on the Riemann sphere S^2, representing here the Poincaré-Bloch sphere of the spin-1/2, such that

$$\mathcal{H}(\mathbf{k}) = -\mathbf{d}\cdot\boldsymbol{\sigma} = -|\mathbf{d}|\begin{pmatrix}\cos\theta & \sin\theta e^{-i\varphi}\\ \sin\theta e^{i\varphi} & -\cos\theta\end{pmatrix} \quad .$$

On the sphere, the two stationnary eigenstates $|\psi_+\rangle$ and $|\psi_-\rangle$ are:

$$\begin{aligned}|\psi_+\rangle &= e^{-i\varphi/2}\cos\theta/2|a\rangle + e^{i\varphi/2}\sin\theta/2|b\rangle\\ |\psi_-\rangle &= -e^{-i\varphi/2}\sin\theta/2|a\rangle + e^{i\varphi/2}\cos\theta/2|b\rangle.\end{aligned}$$

We have simplified the notations $|\psi_{A\mathbf{k}}\rangle = |a\rangle$ and $|\psi_{B\mathbf{k}}\rangle = |b\rangle$.

Justify why the $\mathbf{K}$ and $\mathbf{K}'$ points can be described by $\theta = 0$ and $\theta = \pi$ respectively on S^2. What is the lowest energy state on the sphere and give an interpretation on the lattice.

5. From Amphi[2], we introduce the topological number or Chern number

$$C = \frac{1}{2\pi}\int_{S^2}\nabla\times\mathbf{A}\cdot\mathbf{e}_r d^2s = \frac{1}{2\pi}\int_0^{2\pi}d\varphi\int_0^{\pi}d\theta F_{\theta\varphi},$$

where $\mathbf{e}_r$ is the unit vector along the radial direction with $d^2s = d\varphi d\theta$, $\mathbf{A} = \langle\psi|i\nabla|\psi\rangle$ is related to the Berry phase with $|\psi\rangle = |\psi_+\rangle$ or $|\psi_-\rangle$ and $\nabla = (\partial/\partial\varphi, \partial/\partial\theta)$ and $F_{\theta\varphi} = \partial_\theta A_\varphi - \partial_\varphi A_\theta$. Calculate $A_\varphi(\theta)$ and verify that $A_\theta = 0$. Evaluate directly C for the lowest energy band and check that it is equal to $C = A_\varphi(0) - A_\varphi(\pi) = 1$ where $A_\varphi(0) = \lim_{\theta\to 0} A_\varphi(\theta)$ and $A_\varphi(\pi) = \lim_{\theta\to\pi} A_\varphi(\theta)$.

6. Justify that one can measure C from the spin magnetization at the poles and averaging on an ensemble of spins.

7. Here, we discuss transport properties and apply an electric field along the polar angle. Write Newton's equation for a charge e particle and verify the Karplus-Luttinger velocity from the definition of the topological number (see Amphi). Evaluate the quantum Hall conductivity for the crystal.

[2] See Introduction in Review K. Le Hur, arXiv:2209.15381