ICFP M1 - QUANTUM MATTER - TD n°8 - Solutions
Chern numbers

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1 Berry curvature and Hall conductivity of Haldane's honeycomb model

In class, you introduced the low-energy Hamiltonian version of the Haldane model, namely

$$H = v\left(\mu^z\tau^x k_x + \tau^y k_y\right) + m_1\tau^z + m_2\mu^z\tau^z, \tag{1}$$

where the Pauli matrices mean the following:

- $\tau^z = \pm 1$: sublattices A/B,
- $\mu^z = \pm 1$: valley K/K',
- $\sigma^z = \pm 1$: spin $\pm 1/2$ (H in Eq. (1) is diagonal in spin, i.e. one should think about it as being multiplied by $\sigma^0 = \mathrm{Id}_2^{(\sigma)}$).

Using the fact that μ^z commutes with all terms in H, you found that the energy dispersions for fixed $\mu^z = \pm 1$ were

$$\epsilon_\pm(m_1, m_2) = \pm\sqrt{v^2k^2 + (m_1 + \mu^z m_2)^2}. \tag{2}$$

1. Derive this and find expressions for the corresponding eigenstates.

Let use write

$$\begin{aligned} H &= v\mu^z\tau^x k_x + v\tau^y k_y + m\tau^z \quad (3)\\ &= \mathbf{n}\cdot\boldsymbol{\tau}, \quad (4)\end{aligned}$$

where $m = m_1 + m_2\mu^z$ and

$$\mathbf{n} = (v\mu^z k_x, vk_y, m), \qquad |\mathbf{n}| = \sqrt{v^2k^2 + m^2}, \tag{5}$$

and whose eigenvalues and eigenvectors can be taken to be $\epsilon_\pm = \pm|\mathbf{n}|$,

$$\mathbf{u}_+ = \frac{1}{\sqrt{2|\mathbf{n}|(|\mathbf{n}| + n_z)}}\begin{pmatrix} n_z + |\mathbf{n}| \\ n_x + in_y \end{pmatrix}, \qquad \mathbf{u}_- = \frac{1}{\sqrt{2|\mathbf{n}|(|\mathbf{n}| + n_z)}}\begin{pmatrix} -n_x + in_y \\ n_z + |\mathbf{n}| \end{pmatrix} \tag{6}$$

2. Show that the gap vanishes (i.e. there exists at least one $\mathbf{k}_0$ such that $\epsilon_-(\mathbf{k}_0) = \epsilon_+(\mathbf{k}_0)$) if $|m_1| = |m_2|$ and in the case $\mu^z = -\mathrm{sign}(m_1/m_2)$.

We just plug that in and indeed find that the two bands touch at $k = 0$.

Assume that the system is "half-filled," i.e. that the ϵ_- band(s) are filled, and the ϵ_+ one(s) are empty. Recall the expression of the Berry phase of the lower band (ϵ_- band, also called valence band):

$$\Omega_-(\mathbf{k}) = \partial_x\mathcal{A}_-^y - \partial_y\mathcal{A}_-^x, \qquad \text{with} \qquad \mathcal{A}_-^\mu(\mathbf{k}) = i\langle u_{-\mathbf{k}}|\partial_\mu|u_{-\mathbf{k}}\rangle, \tag{7}$$

where $\partial_\mu \equiv \frac{\partial}{\partial k^\mu}$. We will derive an expression of the Berry curvature (which applies beyond the Haldane model) which will be easier to use than the definition Eq. (7).

3. Show that, for $n = \pm$,

$$\Omega_n(\mathbf{k}) = -2\mathrm{Im}[\langle\partial_x u_{n\mathbf{k}}|\partial_y u_{n\mathbf{k}}\rangle]. \tag{8}$$

$$\begin{aligned}
\Omega_n(\mathbf{k}) &= i(\partial_x\langle u_n(\mathbf{k})|\partial_y u_n(\mathbf{k})\rangle - \partial_y\langle u_n(\mathbf{k})|\partial_x u_n(\mathbf{k})\rangle) && (9)\\
&= i(\langle\partial_x u_n(\mathbf{k})|\partial_y u_n(\mathbf{k})\rangle + \langle u_n(\mathbf{k})|\partial_x\partial_y u_n(\mathbf{k})\rangle - \langle\partial_y u_n(\mathbf{k})|\partial_x u_n(\mathbf{k})\rangle - \langle u_n(\mathbf{k})|\partial_y\partial_x u_n(\mathbf{k})\rangle) && (10)\\
&= i(\langle\partial_x u_n(\mathbf{k})|\partial_y u_n(\mathbf{k})\rangle - \langle\partial_y u_n(\mathbf{k})|\partial_x u_n(\mathbf{k})\rangle) && (11)\\
&= -2\mathrm{Im}[\langle\partial_x u_{n\mathbf{k}}|\partial_y u_{n\mathbf{k}}\rangle] && (12)
\end{aligned}$$

4. Using $\langle u_{n\mathbf{k}}|u_{n\mathbf{k}}\rangle = 1$ and $\langle u_{n\mathbf{k}}|u_{m\mathbf{k}}\rangle = 0$ for $m \neq n$ and differentiating, show that

$$\Omega_n(\mathbf{k}) = -i\sum_{m\neq n}(\langle u_{n\mathbf{k}}|\partial_x u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\partial_y u_{n\mathbf{k}}\rangle - \langle u_{n\mathbf{k}}|\partial_y u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\partial_x u_{n\mathbf{k}}\rangle) \quad (13)$$

$$\begin{aligned}
\Omega_n(\mathbf{k}) &= i(\langle\partial_x u_n(\mathbf{k})|\partial_y u_n(\mathbf{k})\rangle - \langle\partial_y u_n(\mathbf{k})|\partial_x u_n(\mathbf{k})\rangle) && (14)\\
&= i\sum_m(\langle\partial_x u_{n\mathbf{k}}|u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\partial_y u_{n\mathbf{k}}\rangle - \langle\partial_y u_{n\mathbf{k}}|u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\partial_x u_{n\mathbf{k}}\rangle) && (15)\\
&= i\sum_m(-\langle u_{n\mathbf{k}}|\partial_x u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\partial_y u_{n\mathbf{k}}\rangle + \langle u_{n\mathbf{k}}|\partial_y u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\partial_x u_{n\mathbf{k}}\rangle) && (16)\\
&= -i\sum_{m\neq n}(\langle u_{n\mathbf{k}}|\partial_x u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\partial_y u_{n\mathbf{k}}\rangle - \langle u_{n\mathbf{k}}|\partial_y u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\partial_x u_{n\mathbf{k}}\rangle) && (17)
\end{aligned}$$

where we used

$$\partial_\mu(\langle u_{n\mathbf{k}}|u_{m\mathbf{k}}\rangle) = 0 \Longrightarrow \langle\partial_\mu u_{n\mathbf{k}}|u_{m\mathbf{k}}\rangle = -\langle u_{n\mathbf{k}}|\partial_\mu u_{m\mathbf{k}}\rangle \quad (18)$$

as well as the cancellation of the "diagonal" terms.

5. Show that

$$\Omega_n(\mathbf{k}) = i\sum_{m\neq n}\left(\frac{\langle u_{n\mathbf{k}}|\partial_x H|u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\partial_y H|u_{n\mathbf{k}}\rangle - \langle u_{n\mathbf{k}}|\partial_y H|u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\partial_x H|u_{n\mathbf{k}}\rangle}{(E_n(\mathbf{k}) - E_m(\mathbf{k}))^2}\right). \quad (19)$$

To do so, write Schrödinger's equation for a band n

$$H|u_{n\mathbf{k}}\rangle = E_n(\mathbf{k})|u_{n\mathbf{k}}\rangle, \quad (20)$$

contract it on the left with the eigenstate for a band m

$$\langle u_{m\mathbf{k}}|H|u_{n\mathbf{k}}\rangle = E_n(\mathbf{k})\langle u_{m\mathbf{k}}|u_{n\mathbf{k}}\rangle, \quad (21)$$

and differentiate with respect to k_μ.

For $m \neq n$,

$$\begin{aligned}
\partial_\mu(\langle u_{m\mathbf{k}}|H|u_{n\mathbf{k}}\rangle) &= 0 && (22)\\
\langle\partial_\mu u_{m\mathbf{k}}|H|u_{n\mathbf{k}}\rangle + \langle u_{m\mathbf{k}}|\partial_\mu H|u_{n\mathbf{k}}\rangle + \langle u_{m\mathbf{k}}|H|\partial_\mu u_{n\mathbf{k}}\rangle &= 0 && (23)\\
E_n(\mathbf{k})\langle\partial_\mu u_{m\mathbf{k}}|u_{n\mathbf{k}}\rangle + \langle u_{m\mathbf{k}}|\partial_\mu H|u_{n\mathbf{k}}\rangle + E_m(\mathbf{k})\langle u_{m\mathbf{k}}|\partial_\mu u_{n\mathbf{k}}\rangle &= 0 && (24)\\
\langle u_{m\mathbf{k}}|\partial_\mu H|u_{n\mathbf{k}}\rangle &= (E_n(\mathbf{k}) - E_m(\mathbf{k}))\langle u_{m\mathbf{k}}|\partial_\mu u_{n\mathbf{k}}\rangle && (25)
\end{aligned}$$

So, for $E_m \neq E_n$,

$$\langle u_{m\mathbf{k}}|\partial_\mu u_{n\mathbf{k}}\rangle = \frac{\langle u_{m\mathbf{k}}|\partial_\mu H|u_{n\mathbf{k}}\rangle}{E_n(\mathbf{k}) - E_m(\mathbf{k})}, \quad (26)$$

and substituting twice, we obtain

$$\begin{aligned}
\Omega_n(\mathbf{k}) &= -i\sum_{m\neq n}\left(\frac{\langle u_{n\mathbf{k}}|\partial_x H|u_{m\mathbf{k}}\rangle}{E_m(\mathbf{k}) - E_n(\mathbf{k})}\frac{\langle u_{m\mathbf{k}}|\partial_y H|u_{n\mathbf{k}}\rangle}{E_n(\mathbf{k}) - E_m(\mathbf{k})} - \frac{\langle u_{n\mathbf{k}}|\partial_y H|u_{m\mathbf{k}}\rangle}{E_m(\mathbf{k}) - E_n(\mathbf{k})}\frac{\langle u_{m\mathbf{k}}|\partial_x H|u_{n\mathbf{k}}\rangle}{E_n(\mathbf{k}) - E_m(\mathbf{k})}\right) && (27)\\
&= i\sum_{m\neq n}\left(\frac{\langle u_{n\mathbf{k}}|\partial_x H|u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\partial_y H|u_{n\mathbf{k}}\rangle - \langle u_{n\mathbf{k}}|\partial_y H|u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|\partial_x H|u_{n\mathbf{k}}\rangle}{(E_n(\mathbf{k}) - E_m(\mathbf{k}))^2}\right). && (28)
\end{aligned}$$

6. Let us now go back to the specific case of the Haldane model. Writing $H = v\mu^z\tau^x k_x + v\tau^y k_y + m\tau^z$ (think $m = m_1 + \mu^z m_2$) and noticing that

$$|u_{\pm\mathbf{k}}\rangle\langle u_{\pm\mathbf{k}}| = \frac{1}{2}\left(\tau^0 \pm \frac{H}{\epsilon_{+\mathbf{k}}}\right), \quad (29)$$

recover the result for the Berry phase of the lower band of the Haldane model given in class, i.e.

$$\Omega_-(\mathbf{k}) = \mu^z \frac{mv^2}{2(v^2k^2+m^2)^{3/2}}. \tag{30}$$

We first compute $\partial_\mu H$:

$$\partial_x H = v\mu^z\tau^x \tag{31}$$
$$\partial_y H = v\tau^y \tag{32}$$

The Berry phase is now:

$$\begin{aligned}
\Omega_- &= \frac{i}{4\epsilon_+^2}\left[\langle u_{-\mathbf{k}}|\partial_x H|u_{+\mathbf{k}}\rangle\langle u_{+\mathbf{k}}|\partial_y H|u_{-\mathbf{k}}\rangle - \langle u_{-\mathbf{k}}|\partial_y H|u_{+\mathbf{k}}\rangle\langle u_{+\mathbf{k}}|\partial_x H|u_{-\mathbf{k}}\rangle\right] &(33)\\
&= \frac{i}{16\epsilon_+^2}\mathrm{Tr}\left[\partial_x H\left(\tau^0+\frac{H}{\epsilon_{+\mathbf{k}}}\right)\partial_y H\left(\tau^0-\frac{H}{\epsilon_{+\mathbf{k}}}\right) - \partial_x H\left(\tau^0-\frac{H}{\epsilon_{+\mathbf{k}}}\right)\partial_y H\left(\tau^0+\frac{H}{\epsilon_{+\mathbf{k}}}\right)\right] &(34)\\
&= \frac{i}{8\epsilon_+^3}\mathrm{Tr}\left[\partial_x H H \partial_y H - \partial_x H \partial_y H H\right] &(35)\\
&= \frac{iv^2\mu^z m}{8\epsilon_+^3}\mathrm{Tr}\left[\tau^x\tau^z\tau^y - \tau^x\tau^y\tau^z\right] &(36)\\
&= -\frac{iv^2\mu^z m}{4\epsilon_+^3}\mathrm{Tr}\left[\tau^x\tau^y\tau^z\right] &(37)\\
&= \frac{v^2\mu^z m}{2\epsilon_+^3} &(38)
\end{aligned}$$

where we have used that $\tau_\alpha^2 = \tau^0$ and $\mathrm{Tr}[\tau_\alpha] = 0$ for $\alpha \in \{x, y, z\}$, and $\tau^x\tau^y\tau^z = i\tau^0$.

7. What is the sign of $\Omega_+(\mathbf{k})$ compared to that of $\Omega_-(\mathbf{k})$?

It's opposite.

8. Check that

$$\int d^2k\,\Omega_-(\mathbf{k}) = \pi\mu^z \mathrm{sign}(m). \tag{39}$$

To do so, extend the integral over the BZ to infinity and recall $\int_0^\infty dx\, x/(x^2+b^2)^{3/2} = 1/\sqrt{b^2}$.

$$\begin{aligned}
\int d^2k\,\Omega_-(\mathbf{k}) &= \int d^2k \mu^z \frac{mv^2}{2(v^2k^2+m^2)^{3/2}} &(40)\\
&= \int_0^{2\pi} d\theta \int_0^\infty dk \frac{\mu^z m}{2|v|}\frac{k}{(k^2+(m/v)^2)^{3/2}} &(41)\\
&= \frac{\pi\mu^z m}{|v|}\left|\frac{v}{m}\right| &(42)\\
&= \pi\mu^z \mathrm{sign}(m). &(43)
\end{aligned}$$

9. Note the appearance of μ^z. This appears because the valley determines the sense of winding of the Dirac point, or chirality. For a given sign of mass, opposite chirality gives opposite Berry curvature. The integrand is strongly peaked in a region of width m/v in momentum space around the Dirac point. So when the Fermi level lies in the gap formed by the mass, we can say, using the general formula $C_n = \frac{1}{2\pi}\int_{BZ} d^2k\Omega_n(\mathbf{k})$, that each Dirac point contributes plus or minus half an integer to the Chern number. This must be added for every distinct Dirac point, i.e. for each spin and valley. Therefore there is a general formula for the Chern number for a set of massive Dirac points with the Fermi level in the gap:

$$C = \sum_i \frac{1}{2}\mathrm{sign}(m_i\mu_i^z) \tag{44}$$

Here the sum is over all Dirac points, i.e. for our model of graphene it includes four such points, for spin and valley. One might be worried about Eq. (44), because it looks like it can give a half-integer quantum Hall effect. However, for any physical two dimensional system, there is a famous theorem (Nielsen-Ninomiya) that there must always be an even number of Dirac points. This guarantees an integer result for an insulator.

10. Let's apply the formula Eq. (44) to two limit cases.

(a) Apply Eq. (44) in the limit $m_2 = 0$.

In this case, we have the mass m_1, which is the same for both valleys:

$$C^{\text{CDW}} = 2_{\text{spin}} \times \left(\frac{1}{2}\text{sign}(m_1) - \frac{1}{2}\text{sign}(m_1)\right) = 0. \tag{45}$$

As mentioned in class, CDW stands for "charge density wave" and represents a state which has a nonuniform ("wave") charge density because of the two valleys have different chemical potential. As mentioned below, it has zero Hall conductivity because the contributions from the two valleys have opposite sign, as expected since it is time-reversal invariant ($\tau^z \to \tau^z$ under time-reversal).

(b) Now consider the limit $m_1 = 0$.

Now we have mass m_2 which is opposite for the two valleys. We obtain

$$C^{\text{QAHE}} = 2_{\text{spin}} \times \left(\frac{1}{2}\text{sign}(m_2) + \frac{1}{2}\text{sign}(m_2)\right) = 2\text{sign}(m_2). \tag{46}$$

QAHE stands for "quantum anomalous Hall effect". As mentioned below, this state, which has a non-zero Chern number, in turn has edge states and a nonzero Hall conductivity. This is also consistent with the fact that the m_2 mass term is odd under time-reversal (TR), since $\mu^z\tau^z \to -\mu^z\tau^z$ under TR.

Remark: Can these insulators be distinguished experimentally? Yes! The nontrivial ($C \neq 0$ in this case) insulators have edge states and a nonzero (and quantized) Hall conductivity, which the "trivial" ($C = 0$ here) insulators do not have. In fact, one can show that

$$C = N_R - N_L, \tag{47}$$

where N_R and N_L are the number of "right" and "left" movers respectively at a boundary. This is an instance of the "bulk-boundary correspondence";

$$\sigma_H = \frac{\sigma_{yx} - \sigma_{xy}}{2} = e^2 \sum_{n\,\text{occupied}} \int \frac{d^2k}{(2\pi)^2}\Omega_n(\mathbf{k}) = \frac{e^2}{2\pi} \sum_{n\,\text{occupied}} C_n = \frac{e^2}{h}C, \tag{48}$$

where we restored the factor $\hbar$ to get physical units. This is the TKNN formula. (One can also understand it from the bulk-boundary correspondence.) We have therefore shown that one can have a nonzero Hall conductivity in the absence of a magnetic field.