University of California at San Diego – Department of Physics – Prof. John McGreevy

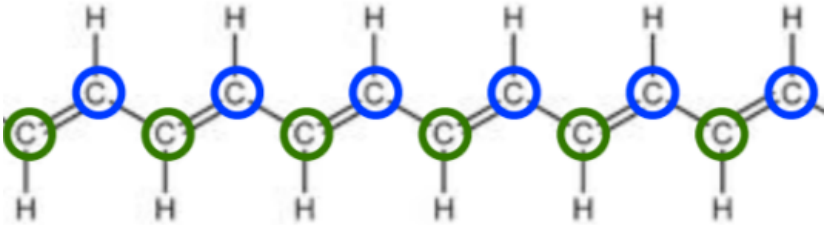
Physics 211C (239) Phases of Quantum Matter, Spring 2021
Assignment 7 – Solutions

Due 12:30pm Friday, May 28, 2021

Thanks for following the submission guidelines on hw01. Please ask me by email if you have any trouble.

---

1. **Su-Schrieffer-Heeger model as an SPT.** Consider the following system, which we can regard as protected by $G = \mathsf{U}(1) \times \mathbb{Z}_2$ in $D = 1 + 1$. It is a sort of model of polyacetylene, which looks something like this:



The Hilbert space is a representation of two complex fermion modes per unit cell (c_a and c_b – we'll ignore spin), with Hamiltonian

$$H = -\sum_j \left(t_1 c^\dagger_{ja} c_{jb} + h.c. \right) - \sum_j \left(t_2 c^\dagger_{ja} c_{(j+1)b} + h.c. \right). \tag{1}$$

(The strengths of the hopping amplitudes t_1 and t_2 model the lengths of the two kinds of bonds in the figure.)

(a) Describe the physics of an open chain at half-filling (one particle per unit cell) in the limits $(t_1, t_2) = (1, 0)$ and $(t_1, t_2) = (0, 1)$.

In the first case, it is just a bunch of molecules, each of which has a unique groundstate. In the second case one mode is left out at each end. There is therefore a fourfold degenerate groundstate, depending on whether or not we occupy the modes at each end.

(b) Diagonalize H in the momentum basis and draw the spectrum. What happens when $t_1 = t_2$?

In momentum space, the hamiltonian takes the form

$$H = \oint đk \left(c^\dagger_{ka}, c^\dagger_{kb} \right) \mathcal{H}(k) \begin{pmatrix} c_{ka} \\ c_{kb} \end{pmatrix}$$

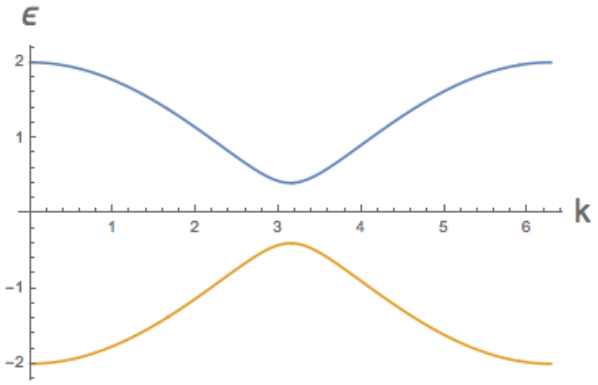
with

$$\mathcal{H}(k) = \begin{pmatrix} 0 & t_1 + t_2 e^{\mathbf{i}k} \\ t_1^\star + t_2^\star e^{-\mathbf{i}k} & 0 \end{pmatrix}$$

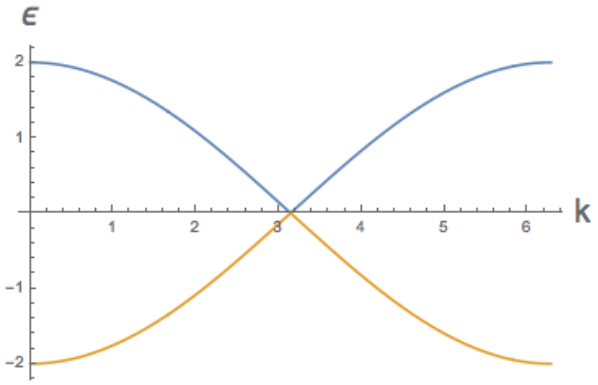
The spectrum of $\mathcal{H}(k) = \vec{h}(k) \cdot \vec{\sigma}$ is $\pm|h(k)|$. Here $\vec{h} = (h_x, h_y, h_z) = (t_1 + \cos kt_2, \sin kt_2, 0)$, so

$$\epsilon_\pm(k) = \pm\sqrt{(t_1 + t_2 \cos k)^2 + t_2^2 \sin^2 k}$$

which looks like:



for $t_1 \neq t_2$. When $t_1 = t_2$, there is a Dirac point at $k = \pi$:



(c) Check that if $t_{1,2}$ are real, then this model has an antiunitary $\mathbb{Z}_2$ particle-hole symmetry acting by

$$\mathcal{C} : c_a \leftrightarrow c_a^\dagger, c_b \leftrightarrow -c_b^\dagger, \mathbf{i} \leftrightarrow -\mathbf{i}.$$

What does this symmetry do to the single-particle hamiltonian $\mathcal{H}(k)$ defined by $H = \oint \mathrm{d}k \begin{pmatrix} c_{ka}^\dagger, c_{kb}^\dagger \end{pmatrix} \mathcal{H}(k) \begin{pmatrix} c_{ka} \\ c_{kb} \end{pmatrix}$? What does this imply for the single-particle spectrum?

This operation takes

$$tc_a^\dagger c_b \to t^\star c_a(-c_b^\dagger) = +t^\star c_b^\dagger c_a$$

which is the $+h.c.$ term as long as t is real.

Notice that it takes $\mathcal{H}(k) \to -\mathcal{H}(k)$. This is the nature of a particle-hole symmetry. It therefore guarantees that the spectrum has a level at ϵ and a level at $-\epsilon$ for each k, *i.e.* is symmetric under $\epsilon \to -\epsilon$.

I found this StackExchange answer by Ruben Verresen quite helpful in writing this problem.

(d) Compute the polarization

$$P = \frac{1}{2\pi} \oint dk \, \langle \psi_k | \, \mathbf{i}\partial_k \, | \psi_k \rangle$$

at half-filling (one particle per unit cell) as a function of t_1/t_2. (In this expression $|\psi_k\rangle$ is the occupied state.) Relate the resulting surface charge to your answer in part 1a.

We use the fact that the groundstate of $\mathcal{H}(k) = \vec{h}\cdot\vec{\sigma}$ with $\vec{h} = h(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ is

$$\psi_- = \begin{pmatrix} \sin\left(\frac{\theta}{2}\right) e^{-\mathbf{i}\varphi} \\ \cos\left(\frac{\theta}{2}\right) \end{pmatrix}.$$

Therefore its Berry connection is

$$\mathcal{A}^- = \mathcal{A}^-_\varphi d\varphi + \mathcal{A}^-_\theta d\theta$$

with

$$\mathcal{A}^-_\varphi = \sin^2\left(\frac{\theta}{2}\right), \quad \mathcal{A}^-_\theta = 0.$$

(Notice that this gives $\mathcal{F}^-_{\theta\varphi} = \partial_\theta \mathcal{A}^-_\varphi - \partial_\varphi \mathcal{A}^-_\theta = \frac{1}{2}\sin\theta$ and hence $\int_{S^2} \mathcal{F} = 2\pi$ – minimal nontrivial Berry flux. It is a minimal Dirac monopole.)

In our problem, we have $h_z = 0 = \cos\theta$, so $\theta = \pi/2$, we are stuck on the equator of the Bloch sphere. And

$$h_x = h\cos\varphi = t_1 + t_2\cos k, \quad h_y = h\sin\varphi = t_2\sin k$$

or more neatly

$$h \equiv h_x + \mathbf{i}h_y = t_1 + t_2 e^{\mathbf{i}k}.$$

At half-filling only the lower eigenstate at each k is occupied. Therefore,

$$2\pi P = \oint \mathcal{A}^- = \oint \mathcal{A}^-_\varphi \frac{\partial\varphi}{\partial k} dk = \oint \sin^2\left(\frac{\theta}{2}\right) \frac{\partial\varphi}{\partial k} dk = \frac{1}{2}\oint_C d\varphi$$

(note that $\sin^2\left(\frac{\pi}{4}\right) = \frac{1}{2}$ is the origin of the factor of two) where C is the trajectory of the hamiltonian $h(k)$ in the complex plane. This is equal to half the winding number of the map $q : S^1 \to S^1$ given by $q = \frac{h(k)}{|h(k)|}$.

(e) What happens to the polarization if we allow imaginary hoppings? Can you use this to design a Thouless pump?

Actually nothing happens to it. As long as there is no σ^z term, the polarization is quantized as a half-integer.

(f) [Bonus] What happens at a domain wall between a region with $t_1/t_2 > 1$ and one with $t_1/t_2 < 1$?

See the discussion in problem 4e here.

(g) Actually, the model (1) has many symmetries. Check that the *unitary* particle-hole symmetry

$$\mathcal{S} : c_a \leftrightarrow c_a^\dagger, c_b \leftrightarrow -c_b^\dagger, \mathbf{i} \leftrightarrow \mathbf{i}$$

also preserves H. (Note that $\mathcal{C} = \mathcal{S}\mathcal{T}$ where $\mathcal{T} : c \to c, \mathbf{i} \to -\mathbf{i}$ is ordinary time reversal symmetry.) What does $\mathcal{S}$ do to $\mathcal{H}(k)$?

(h) Show that the single-particle hamiltonian $\mathcal{H}(k)$ has the form

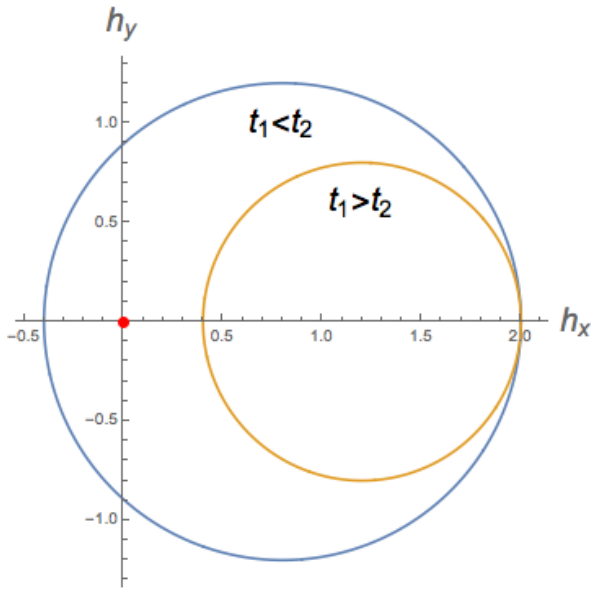
$$\mathcal{H}(k) = h_x(k)\sigma^x + h_y(k)\sigma^y = \vec{h}(k) \cdot \vec{\sigma} \tag{2}$$

with $|h(k)|^2$ nonzero for all k (where $h(k) \equiv h_x(k) + \mathbf{i}h_y(k)$). It therefore defines a map from the Brillouin zone to $\mathbb{R}^2 \setminus \{0\} \simeq S^1$

$$\mathcal{H}(k) : S^1 \to \mathbb{R}^2 \setminus \{0\}$$

which has a winding number $\nu \in \mathbb{Z}$. Respecting the symmetry $\mathcal{S}$ thus produces an integer classification of such states.

Here is a plot of the path of the hamiltonian as k varies across the BZ:



What is the physical interpretation of $\nu > 1$? Can you find an $\mathcal{S}$-invariant Hamiltonian that has $\nu > 1$?

Relate this winding number (mod two) to the polarization.

The polarization is only defined mod one, since a rephasing of the wavefuction by $e^{\mathbf{i}k}$ shifts $\mathcal{A} \to \mathcal{A} + dk$. But $2P = \nu$ mod two.

(i) What terms can you add to H that respect $\mathcal{C}$ but break $\mathbf{S}$? What terms respect $\mathcal{S}$ but break $\mathcal{C}$? What do these do to the $\mathbb{Z}$-valued invariant?

$\mathcal{S}$ forbids terms like $c_a^\dagger c_a$ that hop from one sublattice to itself, and produce a σ^z term in $\mathcal{H}(k)$. Therefore $\mathcal{S}$ guarantees that $\mathcal{H}(k)$ is of the form (2), so it provides a map from $\mathbb{R}^2 \setminus \{0\} \to S^1$ (rather than $\mathbb{R}^3 \setminus \{0\} \simeq S^2$) and so the winding number about the origin is an invariant. Such a term is allowed by $\mathcal{C}$, as long as it has a purely imaginary coefficient:

$$\Delta H = \sum_j \mathbf{i}\lambda \left(c_{ja}^\dagger c_{(j+1)a} + h.c. - c_{jb}^\dagger c_{(j+1)b} + h.c. \right)$$

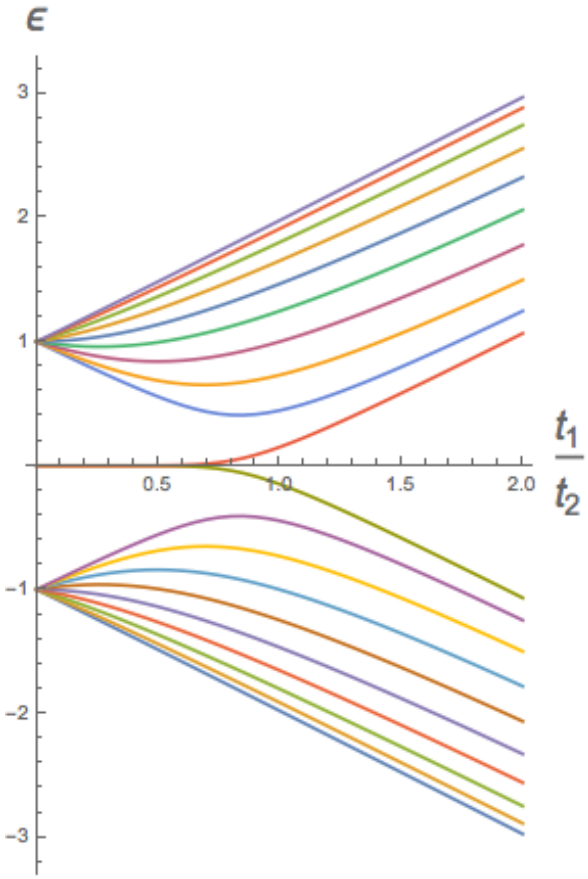
with λ real, which produces $\Delta\mathcal{H} = \lambda\sigma^z \sin k$.

(j) [Bonus] This has been a long problem, and I've still left out a crucial part of the story about polyacetylene. This is that the dimerization pattern, t_1/t_2 is a dynamical variable, a mode of the lattice. Because the energy of the electrons is lowered when $t_1/t_2 \neq 1$, the system prefers to be dimerized. But the potential for t_1/t_2 is symmetric about 1, so the dimerization pattern spontaneously breaks a $\mathbb{Z}_2$ symmetry. The domain walls of this broken

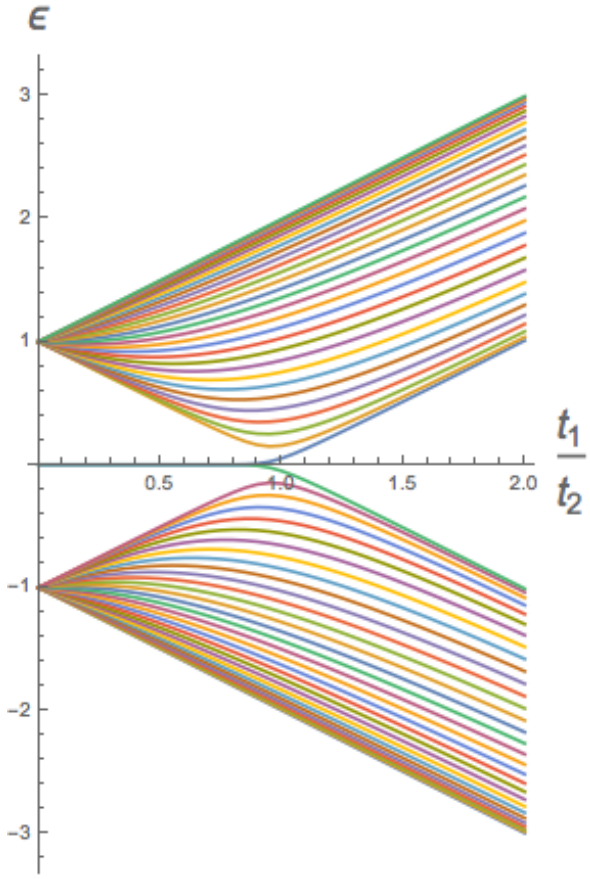
symmetry are the ones in part 1f. They carry charge but not spin, unlike the electron. (Pretend that we included the spin degree of freedom of the electron in all of the above.) Use this to explain the observation that upon doping in extra charge, the conductivity of polyacetylene increases rapidly, but the magnetic susceptibility does not.

(k) [Bonus] Find the spectrum of an open chain (of, say, 10 or 15 unit cells), and plot it as a function of t_1/t_2. Watch the edge states get absorbed into the continuum near the phase transition. Plot the wavefunctions of the edge states and compare them to generic states.

Here is the spectrum for $N = 10$ unit cells:

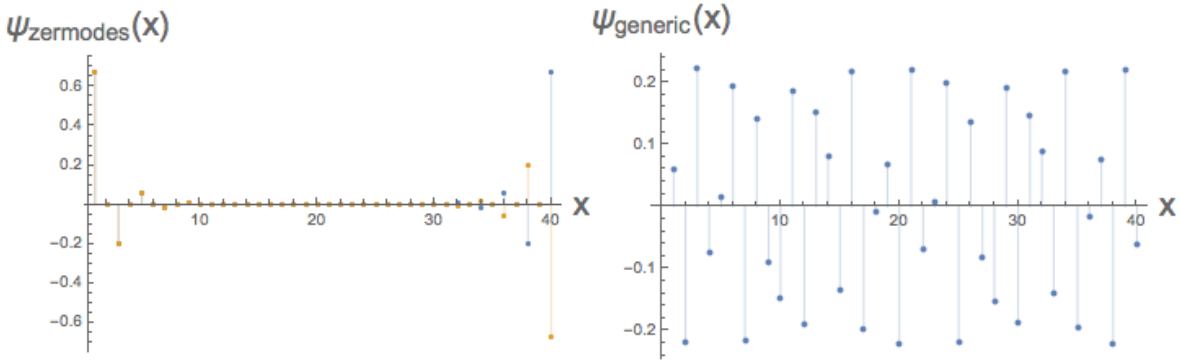


Here's a plot for $N = 30$ unit cells:



that shows that the hybridization of the edge states happens closer to the transition at $t_1/t_2 = 1$ as we increase the system size.

Here is a plot of the two mid-gap modes for $N = 20$ (left) and a generic mode (right):



Notice that the mid-gap modes are (a) localized at the two ends, as expected from the continuum analysis, and (b) supported on only one of the two sublattices.

2. **Chern-number changing transition.**

Consider the following approximate single-particle Hamiltonian for a particle in $D = 2 + 1$:

$$\mathcal{H}(k) = v(k_x\sigma_x + k_y\sigma_y) + m\sigma_z$$

(valid near $\vec{k} = 0$), describing a single Dirac cone as $m \to 0$.

(a) [Bonus] Argue that, up to relabellings and rescalings, this is the generic form for the single-particle Hamiltonian near a point in parameter space where two bands are colliding.

(b) Compute the Chern number of the bands as a function of m.

Again we use the formula for the Berry connections of the two states of the hamiltonian $\mathcal{H} = \vec{h} \cdot \vec{\sigma}$, which are (for $\mathcal{H}|\pm\rangle = \pm|h||\pm\rangle$) :

$$\mathcal{A}^{\pm} = \frac{1 \pm \cos\theta}{2} d\varphi, \quad \mathcal{F}^{\pm} = \pm\frac{\sin\theta}{2} d\theta d\varphi$$

with

$$\vec{h} = h(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta) = (vk_x, vk_y, m).$$

Here $h \equiv |h| = \sqrt{v^2k^2 + m^2}$. We therefore identify

$$h(k) = \frac{m}{\cos\theta}, \quad \sin\theta e^{\mathbf{i}\varphi} = \frac{v}{h}(k_x + \mathbf{i}k_y) = \frac{vk}{h}e^{\mathbf{i}\varphi}$$

and therefore we can identify the angle in the k_x, k_y plane with φ. The relationship between k and θ is a little more complicated:

$$\cos\theta = \frac{m}{h}, \sin\theta = \frac{vk}{h}$$

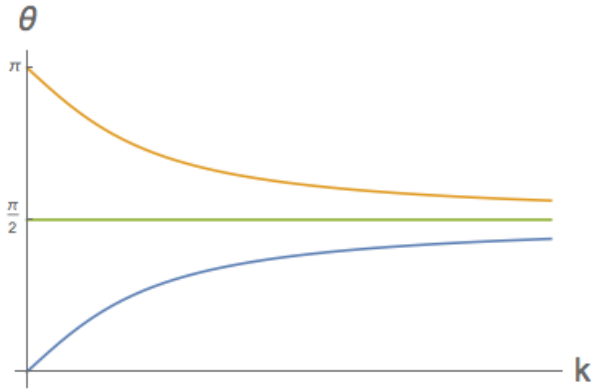
so

$$\cos\theta d\theta = \partial_k(vk/h)dk$$

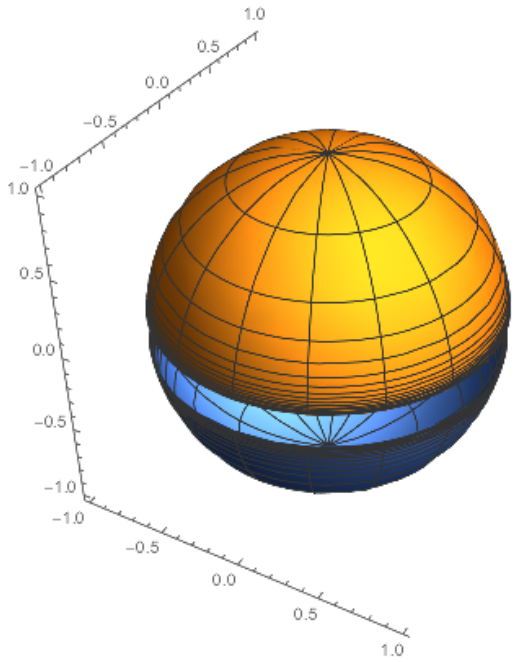
and therefore

$$\frac{d\theta}{dk} = \frac{mv}{h^2}.$$

As a function of k the polar angle looks like this for $m > 0$ and $m < 0$ respectively:



For $m > 0$ and $m < 0$ respectively, the images on the Bloch sphere of a disk around the origin in k space is the upper and lower hemisphere:



In each case, $k = 0$ is at the pole (north or south, respectively) and as k increases, we approach the equator. Thus the two hemispheres are traversed with opposite orientation, and we can already conclude from this that $\int_{D_K} \mathcal{F}^- \overset{K\to\infty}{\to} \pm\pi$ for the two cases (where D_K is a disk of radius K centered at the Dirac point).

Pulled back to k-space, the Berry flux density is

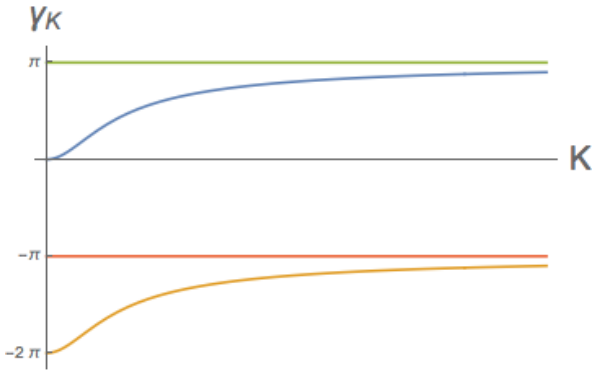
$$\mathcal{F}^{\pm} d\theta d\varphi = \pm \frac{\sin\theta}{2} d\theta d\varphi = \pm \frac{vk}{2h} \frac{mv}{h^2} dk d\varphi = \pm \frac{mv^2}{2} \frac{k dk d\varphi}{h^3}.$$

Notice that the two bands have equal and opposite Berry flux. And notice that the Berry flux is proportional to m and changes sign if m changes sign.

For the integrated flux through this disk of radius K, we find therefore

$$\gamma_K \equiv \int_{D_K} \mathcal{F}^{\pm} = \pm \frac{mv^2}{2} \int_0^K \frac{k dk}{(m^2 + k^2 v^2)^{3/2}} = \pm\pi \frac{m}{|m|} \left(1 - \frac{|m|}{\sqrt{m^2 + v^2 K^2}} \right).$$

For the lower band, as a function of K this looks like:

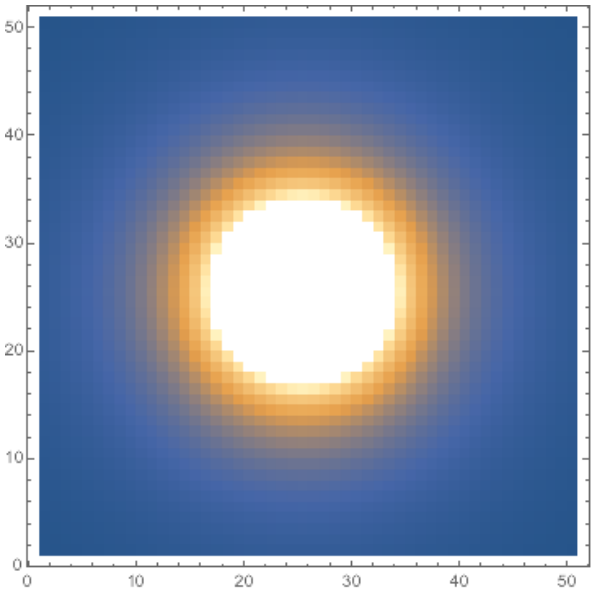


(the two curves are for $m > 0$ and $m < 0$. Notice that the Berry flux asymptotes to $\pi \pmod{2\pi}$.

Actually the relationship between h and k is unnecessary if we use Stokes' theorem. The Berry flux (of the lower band) in a disk of radius K about the origin in k space is

$$\int_{D_K} \mathcal{F}^- \overset{\text{Stokes}}{=} \oint_{\partial D_K} \mathcal{A}^-.$$

Here is a density plot of the Berry flux (the origin of k-space is in the middle of the picture) for $m \neq 0$:



(c) Argue that such an $\mathcal{H}$ cannot arise from a local lattice model, without additional contributions to the Berry curvature elsewhere in the Brillouin zone.

We found that a loop around the Dirac point sees π Berry flux: $\oint_{\partial D_K} \mathcal{A}^- = \pi$. But in a lattice model, we can deform this contour so that it reaches the boundary of the Brillouin zone and annihilates itself and therefore should subtend no flux.