8.514 Strongly Correlated Electrons in Condensed Matter Physics, Spring 2023

Prob Set 1

Due by March 2

1. Let $|n\vec{R}\rangle$ be Wannier states and let $|\psi_{n\vec{k}}\rangle$ be the Bloch states. Thus

$$|n\vec{R}\rangle = \frac{1}{\sqrt{N}}\sum_k e^{-i\vec{k}\cdot\vec{R}}|\psi_{n\vec{k}}\rangle \tag{1}$$

Write $|\psi_{n\vec{k}}\rangle = \frac{1}{\sqrt{N}}e^{i\vec{k}\cdot\vec{r}}|u_{n\vec{k}}\rangle$. Then define the Wannier center $\vec{r}_n$ corresponding as the expectation value

$$\vec{r}_n = \langle n\vec{R}|\vec{r}-\vec{R}|n\vec{R}\rangle \tag{2}$$

In this problem you will prove the formula mentioned in class expressing the Wannier centers as a k-space integral.

(a) First show that

$$\left(\vec{r}-\vec{R}\right)|n\vec{R}\rangle = \frac{1}{N}\frac{V}{(2\pi)^d}\int d^dk\left(-i\frac{d}{d\vec{k}}e^{i\vec{k}\cdot(\vec{r}-\vec{R})}\right)|u_{n\vec{k}}\rangle \tag{3}$$

Here d is the space dimension, V is the volume of the system, and we converted the momentum sum to an integral (assuming a large volume). The momentum integral is over the Brillouin zone.

(b) Integrate by parts and take the inner product with $\langle n\vec{R}|$ to express $\vec{r}_n$ in the form

$$\vec{r}_n = \frac{V^2}{(2\pi)^{2d}N^2}\int d^drd^dkd^dk'e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}\vec{f}(\vec{r};\vec{k},\vec{k}') \tag{4}$$

Determine the (vector-valued) function $\vec{f}$ in terms of the $|u_{n\vec{k}}\rangle$, and show that it is a periodic function of $\vec{r}$ in the real space unit cell.

(c) Use the periodicity in $\vec{r}$, and the restriction of $\vec{k}, \vec{k}'$ to the Brillouin Zone to do the $\vec{r}$ integral. Thus obtain the needed formula for the Wannier center

$$\vec{r}_n = \frac{V}{N} \int \frac{d^d k}{(2\pi)^d} \langle u_{n\vec{k}} | i \frac{d}{d\vec{k}} | u_{n\vec{k}} \rangle \tag{5}$$

2. Here you will explore some of the physics of the SSH model in the presence of the particle-hole symmetry C defined in class. This takes

$$c_{iA} \to c_{iA}^\dagger; \quad c_{iB} \to -c_{iB}^\dagger \tag{6}$$

(a) First verify that C is a symmetry of the Hamiltonian.

(b) Show that C is implemented in the one-particle Hamiltonian $H(k)$ through the relation[1]

$$\sigma^z H(k) \sigma^z = -H(k) \tag{7}$$

Hence argue that energy eigenstates come in pairs $(E, -E)$.

(c) Write $H(k) = h^i(k)\sigma^i$ for $i = x, y, z$. The $h^i(k)$ can be regarded as a vector in the A-B sublattice "pseudospin" space. Notice that the closing of a band gap requires that $|h(k)| = \sqrt{\sum_i (h^i(k))^2}$ is zero. For the SSH model the condition above implies that $h^z(k) = 0$. Thus h^i lies in the equatorial plane of pseudospin space. Plot the shape of $h^i(k)$ in this equatorial plane in either of the two insulators. What is the qualitative difference between the two plots?

(d) Either based on the plot above, or if you prefer, through explicit calculation, what can you conclude on the phase winding of the Bloch wavefunctions on going through the Brillouin zone? This

[1] A direct application of C actually leads to the condition $\sigma^z H^*(-k)\sigma^z = -H(k)$. You must then use the reality of the hopping matrix elements which implies that $H^*(-k) = H(k)$ to obtain the equation below which is what you will use. This condition on $H(k)$ is referred to as a "chiral symmetry" and is satisfied by any bipartite structure of hopping matrix elements.

winding is of course measured precisely by the Berry phase defined in class. Again, if you prefer, you may wish to explicitly calculate the Berry phase using the Bloch functions, and then relate them later to the plot of $h^i(k)$.

(e) Argue that the polarization P is quantized in the presence of C (just as it was due to inversion symmetry), and hence conclude that the two phases are sharply distinct so long as C is preserved.

3. An interesting feature of the SSH model is the structure of domain walls where the dimerization pattern flips. Here you will study this within the continuum Dirac fermion model. The single particle Hamiltonian in the continuum approximation is

$$H = -i\sigma^y v \frac{d}{dx} + m\sigma^x \tag{8}$$

Assume the system has the particle-hole C symmetry. As the sign of mass distinguishes the two dimerization patterns, a domain wall may be described by a space dependent mass $m(x)$ that smoothly interpolates between $+m$ as $x \to +\infty$ and $-m$ as $x \to -\infty$.

(a) Show that the eigenvalue equation

$$Hf(x) = Ef(x) \tag{9}$$

has a normalizable zero mode solution ($i.e$, where $E = 0$).

(b) In the *many body* ground state this zero mode can either be empty or occupied. Show that these two possibilities are related by the particle-hole transformation C. However argue that the deviation of the total charge measured from the ground state of the system without the domain wall is odd under C. Show that this implies that the domain wall carries fractional charge $\pm\frac{e}{2}$.

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4. Using the continuum low energy Dirac model, calculate the low temperature heat capacity $C(T)$ as a function of temperature T right at the quantum critical point of the SSH model. As you change parameters to move into either of the two insulating phases, indicate qualitatively

the change in the behavior of the low-T specific heat. (You do not need to calculate the 'crossover' of the function $C(T; m)$ explicitly but are welcome to do so if you are upto it).

5. **Optional: do not submit**

   (a) Suppose we consider a 1d lattice system with translation invariance, charge conservation and inversion symmetries. Argue that it is still true that the polarization can only take two discrete values.

   (b) To explore this concretely, consider a bosonic version of the SSH model with Hamiltonian

   $$\mathcal{H} = -\sum_i \left(t_1 b^\dagger_{iA} b_{iB} + t_2 b^\dagger_{iB} b_{i+1,A} \right) + h.c \tag{10}$$

   at a lattice filling of 1 particle per unit cell. Here $b_{iA/B}$ is the destruction operator of a *hard-core* boson, *i.e* one whose number at that site is either 0 or 1.

   Argue that in the two extreme limits of $t_1 \gg t_2$ and $t_2 \gg t_1$ the respective ground states realize the two distinct allowed polarizations.

   (c) Clearly there needs to be a phase transition between these two distinct ground states. What can you say about this phase transition?

   (Hint: Map it to the corresponding transition of free fermions using what is known as the Jordan-Wigner transformation. Search it up if you haven't seen it before) A further challenge is to calculate, at the critical point, the boson Green's function at long distances/times. This is most readily done using what is known as bosonization which you may have seen before.