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Quantum Mechanics B (Physics 212B) Winter 2019
Worksheet 9 – Solutions

Problems

1. **Tight Binding for SSH**

Let's apply our understanding of Bloch's theorem to a simple chain involving 2 types of sites A and B. An example could be the following cartoon:

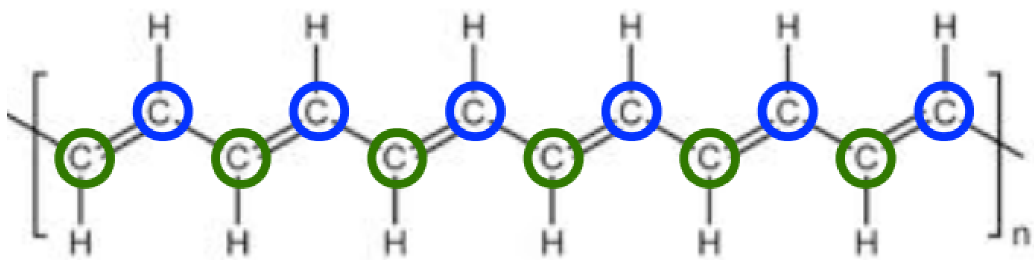

Figure 1: A cartoon of trans-polyacetalyene

Let $j \in \{0, \cdots, N-1\}$ label the number of A/B pairs. The Hilbert space is 4^N dimensional with fermionic operators $c_A^{(\dagger)}, c_B^{(\dagger)}$ representing occupation of that site.[1]

Now suppose that the particle is allowed to hop with a pair with energy cost t_1 and out of the pair with energy cost t_2. So the difference between crossing a single versus double bond above.

(a) Write a Hamiltonian for the system. Use the notation $\psi_j \equiv \begin{pmatrix} c_{j,A} \\ c_{j,B} \end{pmatrix}$ to simplify

$H = -t_1 \sum_j (c^\dagger_{j,A} c_{j,B} + c^\dagger_{j,B} c_{j,A}) - t_2 \sum_j (c^\dagger_{j+1,A} c_{j,B} + c^\dagger_{j,B} c_{j+1,A})$

$= -\sum_j (\psi^\dagger_j U \psi_j + \psi^\dagger_j V \psi_{j+1} + \psi^\dagger_{j+1} V^\dagger \psi_j)$ for $U = t_1 \sigma_x$ and $V = \begin{pmatrix} 0 & 0 \\ t_2 & 0 \end{pmatrix}$

Notice the $j \to j+1$ symmetry. This translation symmetry suggests we can define a crystal momentum k from our discussion of Bloch's theorem.

(b) Define the Fourier transform $\psi_j = \frac{1}{\sqrt{N}} \sum_k e^{\mathbf{i}kj} \psi_k$ and use this to write the Hamiltonian as $H = -\sum_k \psi^\dagger_k H(k) \psi_k$. What is $H(k)$? What is the allowed range of momentum?

We can just directly substitute the transformation in our Hamiltonian. Let's look term by term: $\sum_j \psi^\dagger_j U \psi_j = \frac{1}{N} \sum_k \sum_{k'} \psi^\dagger_k U \psi_{k'} \sum_j e^{\mathbf{i}(k'-k)j}$

[1] Assume periodic boundary conditions $|NA\rangle \equiv |0A\rangle$

$\frac{1}{N}\sum_j e^{\mathbf{i}(k'-k)j} = \delta_{k,k'}$ so we can do the sum over j and k' to get $\sum_k \psi_k^\dagger U \psi_k$

Similarly $\sum_j \psi_j^\dagger T \psi_{j+1} = \frac{1}{N}\sum_k \sum_{k'} \psi_k^\dagger T \psi_{k'} \sum_j e^{\mathbf{i}k'(j+1)} e^{-\mathbf{i}kj} = \sum_k \psi_k^\dagger T e^{\mathbf{i}k} \psi_k$

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

Because translation invariance is discrete one can see from the Fourier transform that $k \to k + 2\pi$ does nothing and therefore $k \equiv k + 2\pi$. This is the Brillouin zone; momentum lives on the circle.

(c) Diagonalize $H(k)$ to find the energies E_k. You should get two eigenvalues or *bands*. What happens when $t_1 = t_2$?

$H(k) = (t_1 + t_2\cos(k))\sigma_x + t_2\sin(k)\sigma_y$ so $E_k = \pm\sqrt{(t_1 + t_2\cos(k))^2 + (t_2\sin(k))^2}$

Or more simply $E_k = \pm\sqrt{t_1^2 + t_2^2 + 2t_1t_2\cos(k)}$

I've included a Mathematica notebook to visualize. There's an energy gap at every point in (t_1, t_2) space except $t_1 = t_2$ where $E = 0$ at $k = \pi$

So what we have is a model of an insulator with two distinct *phases*. One where $t_1 > t_2$ and another where $t_2 > t_1$. The bands cross at the *phase transition*. Is there another way to connect the regions to avoid the phase transition?

(d) Consider the number operators $N_A \equiv \sum_j c_{j,A}^\dagger c_{j,A}$ and $N_B \equiv \sum_j c_{j,B}^\dagger c_{j,B}$ to make the operator: $\Sigma \equiv N_A - N_B$. Write it in momentum space.

$\Sigma = \sum_j \psi_j^\dagger \boldsymbol{\sigma}^z \psi_j = \sum_k \psi_k^\dagger \boldsymbol{\sigma}^z \psi_k$

(e) Show that $\Sigma H(k)\Sigma = -H(k)$ it is a *chiral* symmetry. What does this imply for the spectrum of $H(k)$?

It's sufficient to check that $ZH(k)Z = -H(k)$ implying that if $H|E\rangle = E|E\rangle$ that $H\Sigma|E\rangle = -\Sigma H|E\rangle = -E\Sigma|E\rangle$

For every eigenstate of momentum k and energy E there's another with energy $-E$. This is visible in the spectrum.

(f) Apply your knowledge of avoided crossing to answer: what sort of term should you add to $H(k)$ to connect the eigenvalues?

How does this term transform under Σ?

You would need to add a term proportional to σ_z in $H(k)$ so that it commutes as opposed to anti-commuting

In this way the model is *protected* by the symmetry Σ. You can only connect the two phases by breaking the symmetry or going through a phase transition.

So what makes these phases different? Topology!

For each k there's an eigenvector of a 2-state system; a ray on the Bloch sphere. Because the Hamiltonian does not have a $\boldsymbol{\sigma}^z$ component the vectors always lie on the equator which is a circle.

The map from k to the space of eigenvectors is a map from the circle to the circle; it can have a winding number!

(g) Define $q(k) \equiv \frac{h(k)}{|E_k|}$ for $H(k) = \begin{pmatrix} 0 & h(k) \\ h^\dagger(k) & 0 \end{pmatrix}$. Convince yourself this is a map from the circle to the circle.

$q(k) = \frac{t_1 + t_2 e^{-\mathrm{i}k}}{\sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos(k)}}$ for which you can check has $|q(k)| = 1$

Since $k \in \{-\pi, \pi\}$ it is a map from $S^1 \to S^1$. See the Mathematica file

(h) Define the *winding number* of $q(k)$ to be $\nu \equiv \frac{\mathbf{i}}{2\pi} \int \mathrm{d}k \, \frac{1}{q} \partial_k q$. What is it for the different values of (t_1, t_2) ?

I've numerically evaluated it in the notebook

This is a *topological* difference between the phases; the winding number can't change continuously. The only way to break the analysis is to break the Σ symmetry (or particle number conservation). This is a *Symmetry Protected Topological Phase.*