Physics 295a

Problem Set 2

Due: Wednesday, October 10, 2018

Problem 1

Consider a two-dimensional nearly free-electron system on a square lattice of lattice spacing \( a \). The Fourier transform of the weak lattice potential is \( V(\vec{G}) \). We want to investigate the band structure around the \( (\frac{\pi}{a}, \frac{\pi}{a}) \) point in the reciprocal lattice. The unperturbed spectrum has a fourfold degeneracy at this point. Only the components \( V(0, 2\pi/a) = V_0 \) and \( V(2\pi/a, 2\pi/a) = V_1 \), as well as components such as \( V(2\pi/a, 0) \) that are related by symmetry, are important. Find the electron energies at \( k = (\frac{\pi}{a}, \frac{\pi}{a}) \) if:

a) \( V_1 = 0, V_0 \neq 0 \)

b) \( V_0 = 0, V_1 \neq 0 \).

Problem 2

An electron of mass \( m \) moves in a square lattice of lattice spacing \( a \). The nearly free electron approximation applies.

(a) With one electron per site in the crystal, draw the Fermi surface in the \( k_x, k_y \) plane. Is this a metal or an insulator?

(b) If there are two electrons per site is this a metal or an insulator? If possible, draw the Fermi surface.

Problem 3

Consider electrons on a two-dimensional square lattice (lattice constant \( a \)) in the tight binding approximation with band structure \( E = -E_0(\cos k_x a + \cos k_y a) \). With one electron per site in this crystal, draw the Fermi surface and explain your reasoning. Is this a metal or an insulator?

Problem 4

(a) The density of states for a two-dimensional system of electrons with the tight binding band structure \( E(k) = -E_0(\cos k_x a + \cos k_y a) \) has the asymptotic form \( g(E) \sim c + \alpha |E|^{\beta} \) as \( E \to 0 \). Find \( \alpha \) and \( \beta \).

(b) What feature of the band structure caused the singular cusped behavior at \( E = 0 \)? Do you expect singularities at other energies? Why or why not?

Problem 5

For the problem 4c from PS1, consider the case of a strong attractive potential: \( V_0 < 0, |V_0| \gg \frac{\hbar^2}{ma^2} \). Calculate the bandwidth and compare the result to the bandwidth obtained in the tight-binding approximation. Note that you will have to modify part 4a as well. In PS1 we dealt with positive-energy sinusoidal solutions, while here we are dealing with negative-energy states.

Problem 6 Extra credit

Consider a one-dimensional tight-binding model with dimerized hopping (the SSH model) that we considered in class.

Here we will investigate how the topological difference between the band structure of the cases \( t > t' \) and \( t < t' \), which we found for periodic boundary conditions, leads to the existence or non-existence of edge states in a finite chain with more realistic boundary conditions.

We can build states of the finite chain as follows: For a periodic chain with \( M \) unit cells \( m = 1, 2, \ldots M \) we obtained the explicit Bloch eigenstates \( |\psi_k^\pm\rangle \), where the quasimomentum \( k \) takes on \( M \) different values in the set \([-\pi/a, \pi/a]\) and the \( \pm \) sign denotes the upper/lower band. We construct extended (also called “bulk” or “delocalized”) states of the extended eigenstates of the finite chain by taking linear combinations of the Bloch eigenstates. Since the only degeneracies are \( E_k^\pm = E_{-k}^\mp \), the extended eigenstates of the finite chain must have the form \( |\Psi_k^\pm\rangle = a_k^\pm |\psi_k^\pm\rangle + b_k^\pm |\psi_{-k}^\mp\rangle \).

a) Now we will deal with the fact that the solid is not actually periodic. Impose the boundary condition that \( |\Psi_k^\pm\rangle \) vanishes at the ‘B’ atom of unit cell \( m = 0 \) and determine the coefficients \( a_k^\pm \) and \( b_k^\pm \) up to a normalization constant.

b) Now impose the second boundary condition that \( |\Psi_k^\pm\rangle \) vanishes at the ‘A’ atom of site \( m = M + 1 \). How many different \( k \in [-\pi/a, \pi/a] \) satisfy the boundary condition? You should find that the topological case \( t' < t \) has two fewer solutions than the non-topological case. The difference will depend crucially on the different winding numbers of the phase \( \theta(k) \).

c) The total number of states must be \( 2M \). Find the “missing” eigenstates of the topological case, which are wavefunctions localized at the edges of the chain. \( \text{Hint:} \) Try to satisfy the boundary equations with a complex wavevector \( k = \pi/a + i\lambda \). Discuss the physical meaning of \( \lambda \).
FIG. 1: Figure for problem 4

FIG. 2: Figure for problem 6