Problem Set 5
Theoretical Solid State Physics (SoSe2017)

Due: Due Friday, May 26, 2017; **in Yang Peng's mailbox**

Problem 1: Kronig Penney Modell

A simple band structure problem considers a periodic chain of δ-function potentials in one dimension. The resulting Hamiltonian

$$H = \frac{p^2}{2m} + \alpha \sum_j \delta(x - x_0 - ja) \tag{1}$$

is referred to as Kronig-Penney model. Here, x_0 is included since we will use it in problem 2 and a denotes the lattice constant. For definiteness, assume that the potential is repulsive, i.e., $\alpha > 0$.

(a) To calculate the band structure, consider the unit cell $x \in [-a/2, a/2]$ with a single δ-function located at x_0. Make the ansatz

$$\psi(x) = \begin{cases} Ae^{i\kappa x} + Be^{-i\kappa x} & x < x_0 \\ Ce^{i\kappa x} + De^{-i\kappa x} & x > x_0 \end{cases} \tag{2}$$

for the wavefunction of energy $E = \hbar^2\kappa^2/2m$. Use the appropriate boundary conditions for the wavefunction and its derivative at $x = x_0$ to compute the S-matrix of the δ-function which relates the amplitudes of the outgoing waves C and B to the amplitudes of the incoming waves D and A,

$$\begin{pmatrix} C \\ B \end{pmatrix} = S \begin{pmatrix} D \\ A \end{pmatrix}. \tag{3}$$

You should find

$$S = \frac{1}{i\kappa - \lambda} \begin{pmatrix} \lambda e^{-2i\kappa x_0} & i\kappa \\ i\kappa & \lambda e^{2i\kappa x_0} \end{pmatrix} \tag{4}$$

(b) According to Bloch theory, the wavefunction should satisfy the additional boundary condition

$$\psi(x + a) = e^{ika}\psi(x), \tag{5}$$

which also implies

$$\psi'(x + a) = e^{ika}\psi'(x) \tag{6}$$

for the derivative of the wavefunction. Use these relations to again find a relation between incoming and outgoing waves,

$$\begin{pmatrix} D \\ A \end{pmatrix} = \begin{pmatrix} 0 & e^{ika} \\ e^{-ika} & 0 \end{pmatrix} \begin{pmatrix} C \\ B \end{pmatrix}. \tag{7}$$

(c) Combine your results from parts (a) and (b) to derive a relation between the parameter κ and the Bloch wavevector k, and use this relation to plot the bandstructure of the Kronig Penney model. (This last step of plotting can only be done numerically.)

Problem 2: Chern number for Kronig Pennig model

Consider now a Kronig-Penney model with a slowly sliding potential by setting $x_0 = vt$ with sliding velocity v. Use your result in the first problem to compute the Berry curvature for the lowest band and hence the corresponding Chern number when the lowest band is completely filled. Specifically, this requires you to find explicit expressions for the periodic part of the Bloch wavefunctions of the Kronig-Penney model which you essentially computed in problem 1.

This is a bit of a research problem in that I have not actually done this calculation myself, although I believe that it should be possible to do in principle. Grading is on the basis of effort, without regard to whether you fully solve this problem or not.

Problem 3: Quantization of Chern number for tori

We proved that the integral of the Berry curvature over a closed sphere-like manifold is equal to 2π times an integer which is known as a Chern number. In the context of adiabatic transport, we encountered a Berry curvature integrated over a torus. Prove that this is again quantized in the same manner by cutting the torus open into a rectangle, changing the surface area into a line integral along the boundary of the rectangle, and using opposite boundaries of the rectangle should be identified.

The argument is summarized in the lecture notes and also in the references included there. Your job is simply to go through this argument in detail and write it up in your own words.