PHYSICS 320: Problem Set No. 1
Due: Monday Aug. 17 2009

1. A trigonal lattice is a Bravais lattice generated by three primitive vectors of equal length a and making equal angles θ with each other. Show that the reciprocal lattice of a trigonal lattice is also trigonal. Calculate the length of a primitive lattice vector of the reciprocal lattice. What is the angle between the primitive vectors of the reciprocal lattice?

2. Consider a two dimensional square lattice of spacing a. Let z be the number of conduction electrons per unit cell.

   (a) Draw the first three Brillouin zones in the extended zone scheme.

   (b) Ignoring the periodic potential due to the lattice calculate the Fermi momentum k_F.

   (c) Draw the Fermi surface for $z = 1, 2, 3$ and 4 in the extended and reduced zone schemes.

3. Consider the following dispersion relation of a d dimensional hypercubic lattice

$$E(\vec{k}) = -E_0 \sum_{\alpha=1}^{d} \cos(k_\alpha a),$$

   where k_α, $\alpha = 1, \ldots, d$ are the components of k. Calculate the density of states (DOS) for $d = 1$ and sketch it as a function of energy. You will see that there are singular points in the density of states. Identify similar singular points for $d = 2$ and obtain the DOS in their vicinity. Sketch the DOS as a function of energy.

4. Consider an electron of mass m moving in a 1D lattice of attractive delta functions of spacing a. The potential has the form

$$V(x) = -\frac{\hbar^2}{2m}\Delta \sum_n \delta(x - na),$$

   where n takes on integer values. The energy eigenstates of this system are Bloch states that can be labelled with momentum k. Consider the $k = 0$ state.

   (a) If $\psi(x)$ is the wavefunction of the state, at which values of x is $\frac{d\psi}{dx}$ discontinuous? Where is $\frac{d\psi}{dx} = 0$?

   (b) Use the above information to obtain the energy of the state as a function of Δa.

   (c) Now consider just a single δ function potential of the same strength: $V(x) = -\frac{\hbar^2}{2m}\Delta\delta(x)$ (there is no lattice anymore). What is the energy of the lowest eigenstate? What is the corresponding wavefunction?

   (d) Compare the energies obtained in (b) and (c) for $\Delta a = 5$.

5. Consider a chain of atoms of mass m such that each atom is connected to its left and right neighbour by harmonic springs of spring constant C.

   (a) Using the classical equations of motion for the atoms obtain a formula for the eigenfrequencies of oscillation of this system.

   (b) Now, suppose one of the atoms in the chain is replaced by another of mass M, what are the possible eigenfrequencies?

   (c) What is the difference between the case $m > M$ and $m < M$? (Hint: One of them is similar to the situation in problem 3 (c).)

6. A Bloch state of energy $\epsilon(\mathbf{k})$ in a band has the form $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}.\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$, where $u_{\mathbf{k}}(\mathbf{r})$ has the periodicity of the lattice. It can be shown that the semiclassical equations of motion of an electron in the presence of an electrostatic potential $\phi(\mathbf{r})$ and magnetic field $\mathbf{B}(\mathbf{r})$ are

$$\begin{aligned} \dot{\mathbf{r}} &= \frac{1}{\hbar}\nabla_{\mathbf{k}}\epsilon(\mathbf{k}) - \dot{\mathbf{k}} \times \mathbf{\Omega}(\mathbf{k}) \\ \dot{\mathbf{k}} &= e\nabla_{\mathbf{r}}\phi(\mathbf{r}) - e\dot{\mathbf{r}} \times \mathbf{B}(\mathbf{r}), \end{aligned}$$

where

$$\mathbf{\Omega}(\mathbf{k}) = i \int d\mathbf{r} \left[\nabla_{\mathbf{k}} u^*_{\mathbf{k}}(\mathbf{r}) \times \nabla_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r})\right],$$

is called the Berry curvature. $\mathbf{\Omega}(\mathbf{k})$ is generally zero but in some special cases it is not. The time evolution of a small volume of phase space $\Delta V(t)$ centred around $\mathbf{r}(t)$ and $\mathbf{k}(t)$ is given by the Liouville equation

$$\frac{1}{\Delta V}\frac{d\Delta V}{dt} = \nabla_{\mathbf{r}} \cdot \dot{\mathbf{r}} + \nabla_{\mathbf{k}} \cdot \dot{\mathbf{k}}.$$

(a) Show that $\Delta V(t)\left[1 + e\mathbf{B}.\mathbf{\Omega}/\hbar\right]$ is constant in time. Remember that $\mathbf{B}$ and $\mathbf{\Omega}$ are implicitly functions of time since they depend on $\mathbf{r}$ and $\mathbf{k}$ respectively.

(b) When $\mathbf{B}(\mathbf{r}) = 0$ and $\mathbf{\Omega}(\mathbf{k}) = 0$, how many states ΔN are there in a small volume of phase space ΔV centred around ($\mathbf{r}$, $\mathbf{k}$) in three dimensions? $D(\mathbf{r}, \mathbf{k}) = \Delta N/\Delta V$ is called the phase space DOS. If the number of states in a given volume does not change with time, determine $D(\mathbf{r}, \mathbf{k})$ when $\mathbf{B}(\mathbf{r}) \neq 0$ and $\mathbf{\Omega}(\mathbf{k}) \neq 0$ and write down an expression (in the form of an integral) relating the electron density to the Fermi momentum.

7. Consider a state

$$\Psi_m(\mathbf{r}, \mathbf{R}) = \sum_n \phi_{mn}(\mathbf{R})\psi_n(\mathbf{r}, \mathbf{R}),$$

of the system of ions and electrons. Here $\psi_n(\mathbf{r}, \mathbf{R})$ is an eigenfunction of just the electronic part of the Hamiltonian. $\mathbf{R} = \{\mathbf{R}_i\}$ and $\mathbf{r} = \{\mathbf{r}_j\}$ are shorthand for the entire set of ionic and electronic coordinates respectively. The partial expectation value of the ionic kinetic energy in this state obtained by integrating only over the electronic coordinates has the following three terms:

$$T^{(1)}_m(\mathbf{R}) = -\frac{\hbar^2}{2M}\sum_n \left[\phi^*_{mn}(\mathbf{R}) \sum_i \nabla^2_{\mathbf{R}_i} \phi_{mn}(\mathbf{R})\right],$$

$$T^{(2)}_m(\mathbf{R}) = -\frac{\hbar^2}{M}\sum_{n,p} \left[\phi^*_{mp}(\mathbf{R}) \int d\mathbf{r}\ \psi^*_p(\mathbf{r}, \mathbf{R}) \sum_i \{\nabla_{\mathbf{R}_i} \phi_{mn}(\mathbf{R}) \cdot \nabla_{\mathbf{R}_i} \psi_n(\mathbf{r}, \mathbf{R})\}\right],$$

and

$$T^{(3)}_m(\mathbf{R}) = -\frac{\hbar^2}{2M}\sum_{n,p} \left[\phi^*_{mp}(\mathbf{R})\phi_{mn}(\mathbf{R}) \int d\mathbf{r}\ \psi^*_p(\mathbf{r}, \mathbf{R}) \sum_i \nabla^2_{\mathbf{R}_i} \psi_n(\mathbf{r}, \mathbf{R})\right].$$

$T^{(2)}_m(\mathbf{R})$ and $T^{(3)}_m(\mathbf{R})$ are the terms that are neglected in the Born-Oppenheimer approximation. Suppose $\psi_n(\mathbf{r}, \mathbf{R}) \approx \psi_n(\mathbf{r} - \mathbf{R})$ is real.

(a) Show that sum of the diagonal terms in $\sum_{n,p}$ in the expression for $T^{(2)}_m(\mathbf{R})$ (i.e. terms with $n = p$) is zero.

(b) Show that the sum of the diagonal terms in $\sum_{n,p}$ in the expression for $T^{(3)}_m(\mathbf{R})$ gives a contribution that is proportional to m_e/M times the electronic kinetic energy. m_e is the mass of an electron.

The sum of the off-diagonal terms in $T^{(2)}_m(\mathbf{R})$ and $T^{(3)}_m(\mathbf{R})$ can also be argued to be smaller than $T^{(1)}_m(\mathbf{R})$ by powers of m_e/M but the arguments are more involved.