

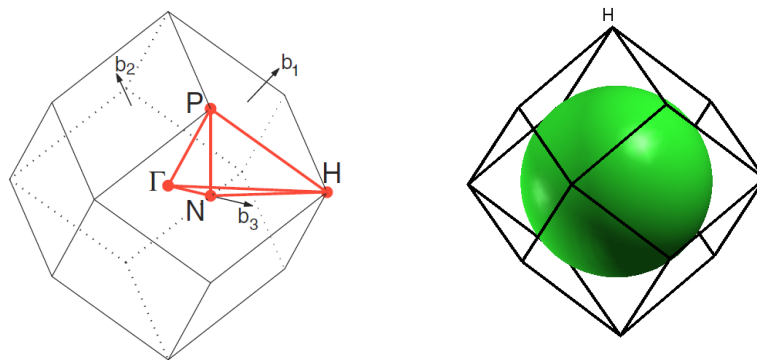
NAME: _____ SOLUTIONS

33-448 Solid State Physics Final Exam #3 Friday, May 12, 2017

Please read each question carefully before answering. Do not do unnecessary work - it will waste time and might cost you points. Feel free to take equations or other facts from the book or your notes, but only if they are directly relevant and useful. Be sure to attempt every part of every question, as many parts can be solved independently of others.

1. **Faculty course evaluation** Have you completed your FCE, or will you do so? **Yes** (1 point)/No (0 points)

2. **Brillouin zones and Fermi surfaces**



(a) Examine the body centered cubic (BCC) first Brillouin zone shown above, left. The special symmetry points H and N sit at $\mathbf{G}_H/2$ and $\mathbf{G}_N/2$, where \mathbf{G}_H and \mathbf{G}_N are reciprocal lattice vectors. State the Miller indices of \mathbf{G}_H and \mathbf{G}_N and briefly justify your assertion. Be sure to use the conventional (simple cubic) indexing, as is usual for BCC structures.

Answer: The BCC reciprocal lattice has Miller indices (hkl) such that $h + k + l$ is even. BZ boundaries will correspond to low index peaks, *e.g.* (110) , (200) , etc. The N point is closer to the zone center Γ so \mathbf{G}_N must be (110) , and \mathbf{G}_H must be (200) . This can be checked because (110) lies along a $2x$ axis, and (200) along a $4x$ axis (draw a cube to visualize this), and these are the symmetries of the corresponding special BZ points as can be seen by inspection of the figure.

(b) Now consider the Fermi surface illustrated on the right. Is the material a metal, or an insulator? What is the valence? Briefly justify your conclusions.

Answer: Because it has a Fermi surface it is a metal. Because the first Brillouin zone is 1/2-filled it is valence 1. In fact, it is the element lithium (Li).

(c) The H-point (sharp corner) sits a distance 1.91 \AA^{-1} away from the Γ -point. By visual inspection of the figure, estimate the Fermi wavenumber k_F .

Answer: The Fermi surface is nearly spherical so the Fermi wavenumber is well-defined. The radius is about 2/3 of the way to the N-point, so $k_F \approx 1.3/\text{\AA}$.

(d) In order to calculate the electron dispersion relation $E(\mathbf{k})$ of this material, which would be a more accurate starting point, a tight-binding model or the nearly-free electron approximation? Why?

Answer: Since the Fermi surface is nearly spherical, the perturbation of the electrons by the lattice must be weak, so the nearly free electron approach is more suitable.

3. Magnetoconductivity and Hall effect

(a) A p -type semiconductor with effective mass m is placed in a magnetic field $\mathbf{B} = (0, 0, B_z)$ with $B_z > 0$. In which direction do the charge carriers rotate when viewed from above, clockwise or counterclockwise?

Answer: Imagine the particle is initially traveling to the right, with speed $v_x > 0$.

Because the semiconductor is p -type, the particle is a hole with charge $q = +e > 0$. The Lorentz force $q\mathbf{v} \times \mathbf{B} = ev_x B_z (-\hat{y})$ points towards negative y , causing the particle to curve in the clockwise direction when viewed from above.

(b) The semiconductor is now placed in an electric field $\mathbf{E} = (E_x, E_y, 0)$. Determine the resulting steady-state current density \mathbf{j} . Please express your result in terms of the Drude conductivity $\sigma_0 = pe^2\tau/m$, the cyclotron frequency $\omega_c = eB_z/m$ and the relaxation time τ . The matrix relating \mathbf{j} to \mathbf{E} is known as the magnetoconductivity tensor $\boldsymbol{\sigma}$. You only need concern yourself with the x and y components of \mathbf{j} and \mathbf{E} .

Answer: In the relaxation time approximation the equation of motion is $d\mathbf{p}/dt = e(\mathbf{E} + (\mathbf{p}/m) \times \mathbf{B}) - \mathbf{p}/\tau$. In steady-state the time derivative vanishes. We may relate the current to the momentum as $\mathbf{j} = pe\mathbf{p}/m$. Substituting yields

$$\mathbf{E} = \frac{1}{\sigma_0}\mathbf{j} - \frac{1}{pe}\mathbf{j} \times \mathbf{B},$$

or, in components,

$$\begin{aligned}\sigma_0 E_x &= j_x - \omega_c \tau j_y \\ \sigma_0 E_y &= j_y + \omega_c \tau j_x.\end{aligned}$$

Solving the simultaneous equations we obtain

$$\mathbf{j} = \boldsymbol{\sigma}\mathbf{E}, \quad \boldsymbol{\sigma} = \frac{\sigma_0}{1 + \omega_c^2 \tau^2} \begin{pmatrix} 1 & \omega_c \tau \\ -\omega_c \tau & 1 \end{pmatrix}.$$

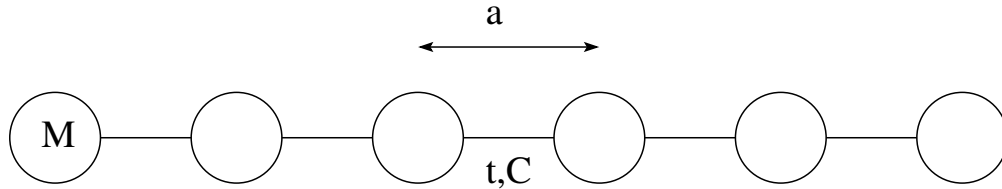
(c) In the Hall geometry, a current j_x is passed through the sample and an electric field E_y results. What is the physical origin of E_y ? Derive the value of E_y as a function of j_x , B , and any other relevant quantities.

Positive charge deflects downward toward negative y , leading to an accumulation of positive charge at the bottom and leaving negative charge at the top. This creates an upward-pointing field component $E_y > 0$. Because $j_y = 0$ in steady state, we must have

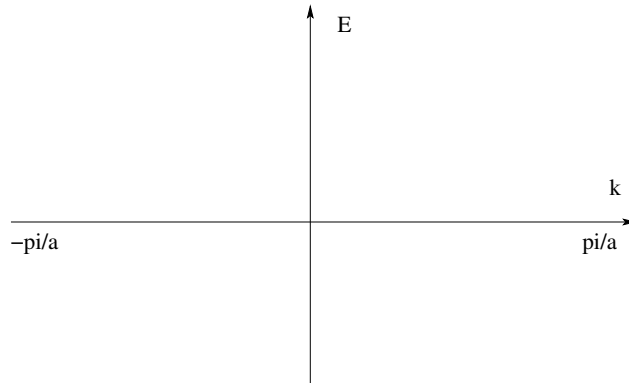
$$E_y = B_z j_x / pe.$$

4. Peierls transition

An infinite one dimensional chain of monovalent atoms has bonds of length a and spring constant C . The electronic band structure can be described by a tight-binding model with onsite energy $\epsilon_0 = 0$ and nearest neighbor electron hopping amplitude (matrix element) $-t$ (with $t > 0$).



(a) Sketch the electron dispersion relation on the axes provided, and label the Brillouin zone boundaries, the Fermi energy E_F , and the Fermi wavevector k_F .

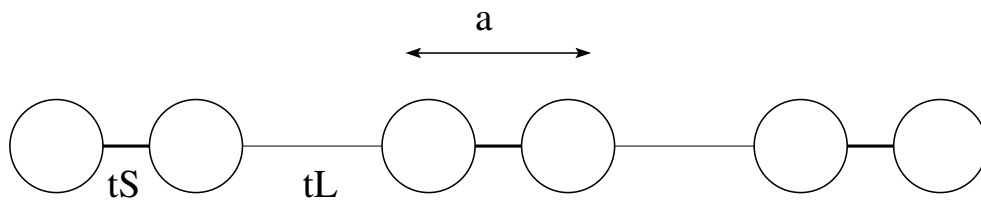


(b) Calculate the band energy E_b , defined as the energy per atom.

Answer: We know the dispersion relation is $E(k) = -2t \cos ka$, and the states are filled with $-k_F \leq k \leq k_F$. Integrating over the occupied states to get the band energy, we have

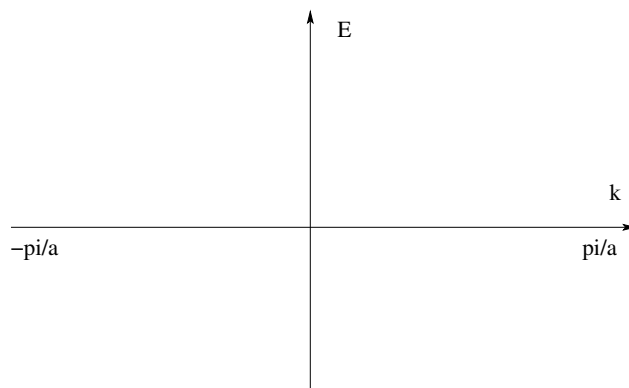
$$E_b = \frac{1}{N} \int_{-k_F}^{k_F} \frac{dk}{2\pi/(Na)} E(k) = -\frac{2t}{\pi} \quad (1)$$

(c) The chain distorts causing alternating displacements of $\pm\delta$ as shown. What is the wavenumber K of this distortion? What is the elastic energy per atom E_d given the distortion amplitude δ ?



Answer: Each bond energy grows by $(1/2)C(\pm\delta)^2$, and there is one bond per atom. Hence, $E_d = C\delta^2/2$.

(d) Due to the displacement, the bond lengths alternate short and long, with hopping amplitudes $t_{S,L} = t \pm \delta$. Sketch the electron dispersion relation on the axes provided, and label the Brillouin zone boundaries, the Fermi energy E_F , and the Fermi wavevector k_F . Your sketch should be accurate, but need not be exact.



(e) Which energy greater had the greater change in magnitude ($|E_b|$ or $|E_d|$) for small δ ? Will the chain spontaneously distort? Briefly justify your answer. Hint, the band gap is linear in δ .

Answer: Because E_d grows as δ^2 , while E_b drops linearly as δ^1 , the decrease wins and the chain spontaneously distorts. This is the Peierls instability. Note that the actual drop in E_b is of order $\delta^2 \log \delta$ when the full band energy is evaluated, but the effect is the same.

(f) Calculate the band gap E_g exactly. Hint: this easiest if you can *guess* the eigenstates at the band edges.

Answer: The band edge lies at $k = \pi/2a$, so the eigenstates must reverse sign from one unit cell to the next. Let the vertical bar “|” represent the cell boundary, and spaces represent the long bond. By symmetry the eigenstates must be:

$|\text{Sym}\rangle = | ++ | -- | ++ | -- |$ and $|\text{Anti}\rangle = | +- | -+ | +- | -+ |$.

We can check this by applying the Hamiltonian

$$H = -t_S \sum_n (|An\rangle\langle Bn| + |Bn\rangle\langle An|) - t_L \sum_n (|An\rangle\langle Bn-1| + |Bn\rangle\langle An+1|)$$

where A and B represent the two atoms in the cell. We confirm that

$H|\text{Sym}\rangle = E_{\text{Sym}}|\text{Sym}\rangle$ and $H|\text{Anti}\rangle = E_{\text{Anti}}|\text{Anti}\rangle$, with $E_{\text{Sym}} = t_L - t_S = -2\delta$ and $E_{\text{Anti}} = t_S - t_L = +2\delta$. Hence the gap is $E_g = 4\delta$.