Physics 141 A
S. G. Louie

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Midterm Exam #2 Solutions

1. **Some short questions. (13 points)**

   Please answer the following short questions with a few sentences and/or equations.

   (a) What is the Wiedemann-Franz law? What role does this law play in our understanding of metals? **(3 pts)**

   (b) Describe the Hall effect. What can we learn about a metal from a Hall measurement? **(3 pts)**

   (c) Explain the origin of thermal expansion of solids. **(3 pts)**

   (d) Name the mechanism of crystal binding and roughly the cohesive energy (in eV/atom) for the following crystal types: van der Waals, ionic, metallic and covalent. **(4 pts)**

   Solution

   (a) The Wiedemann-Franz law states that the ratio of the thermal K to electrical conductivity σ in a metal is proportional to temperature, or

   $$\frac{K}{\sigma T} = \text{const} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$$

   and its validity supports the picture of an electron gas in metals.

   (b) The Hall effect is the development of a voltage difference across the $\vec{j} \times \vec{B}$ direction which appears when we place a conductor carrying current $\vec{j}$ in a magnetic field $\vec{B}$. The quantity measured in experiment is the Hall coefficient

   $$R_H = \frac{E_y}{j_x B} = -\frac{1}{ne}$$

   which gives us information about the sign of the charge carrier in the material (electrons or holes) and the value of the carrier number density.

   (c) Thermal expansion of solids comes from the anharmonic crystal interactions, which increase the average lattice constant as a functionof temperature.

   (d) The mechanism of crystal binding is:

   i. van der Waals: comes from mutually induced electric dipole moments between two atoms. Small cohesive energy, in the order of 10 meV/atom.

   ii. ionic: the two atoms (e.g. Na, Cl) exchange one or more electrons to fill their valence orbitals and then the ions (e.g. Na^+, Cl^-) attract each other through the Coulomb interaction. The cohesive energy is approximatelly 1 eV/atom

   iii. metallic: valence electrons escape the attraction of their atoms and delocalize (extend their wavefunction over the entire crystal), thus lowering their kinetic energy. The charge density in metals is approximatelly homogeneous. Cohesive energies are at about 1 eV/atom

iv. covalent: atomic orbitals from different atoms mix, creating bonding and antibonding molecular orbitals. The electrons lower their energy due to delocalization. The charge density is inhomogenious, mostly concentrated along the bond directions. The cohesive energy is several eVs per atom.

2. **(12 points)**

   (a) CdI_2,PbI_2 and SnS_2, each crystallizes with one molecule (three atoms) per unit cell. The elements are in the following columns of the periodic table: Cd–II, I–VII, Pb–IV, S–VI and Sn–IV. Use arguments based on band theory (assuming no band overlaps) to determine if these materials are metals or insulators. For each compound give the number of filled and half-filled bands. **(6 pts)**

   (b) At room temperature and above, the electrical resistivity $\rho(T)$ of metals in general increases linearly with increasing temperature, i.e. $\rho(T) \sim T$. using what you have learned in this class, explain the physical origin of this common phenomenon. That is, what is the dominant mechanism for resistivity at this temperature? Why does it have a linear T dependence? **(6 pts)**

Solution

(a) The index of the periodic element column gives us the number of valence electrons, i.e. Cd has 2 valence electrons, I has 7, Pb has 4, S has 6 and Sn has 4. Therefore, for the above materials:

   i. CdI_2: 2 electrons from Cd + 2 times 7 from I = 16 electrons, thus 8 filled and 0 half-filled bands, thus insulator.

   ii. PbI_2: 4 electrons from Pb + 2 times 7 from I = 18 electrons, thus 9 filled and 0 half-filled bands, thus insulator.

   iii. SnS_2: 4 electrons from Sn + 2 times 6 from S = 16 electrons, thus 8 filled and 0 half-filled bands, thus insulator.

(b) At room temperature, which is greater than the Debye temperature, the main source of resistivity in the material is the scattering of electrons by phonons. The rate of this scattering process is proportional to the density of phonons, which is proportional to temperature. Therefore $n_{\text{ph}} \propto T \Rightarrow \rho \propto T$.

3. **Two-dimensional electron gas (10 points)**

   The $2D$ electron gas systems have provided many interesting phenomena in condensed matter physics such as the quantum Hall effect. For a two-dimensional free electron gas with number density n:

   (a) What is the expression for the Fermi wavevector k_F and Fermi energy E_F? **(4 pts)**

   (b) Derive an expression for the electron density of states $D(E)$. **(3 pts)**

   (c) What is the temperature dependence for the electron heat capacity of such a system at low temperature and why? **(3 pts)**

Solution

(a) The number of states with wavevector less than k is

$$N(k) = 2\frac{V \cdot \pi k^2}{(2\pi)^2} = \frac{V}{2\pi}k^2$$

and the number of states with energy less than E is

$$N(E) = \frac{V}{2\pi}\frac{2mE}{\hbar^2}$$

Therefore, the Fermi wavevector is given by $N(k_F) = N$, or $k_F = \sqrt{2\pi N/V}$ and $E_F = \frac{\hbar^2}{2m}k_F^2 = \frac{\hbar^2\pi}{m}\frac{N}{V}$

(b) The density of states is given by

$$D(E) = \frac{dN(E)}{dE} = \frac{V}{\pi}\frac{m}{\hbar^2} = \text{const}$$

(c) At low temperatures, the number of electrons which are thermally active is $N\frac{T}{T_F}$. These electrons are the ones near the Fermi level. The other electrons at lower energies are frozen out and do not contribute to thermal motion. The average energy for each of these particles is k_BT, thus $U \approx N\frac{T^2}{T_F} \propto T^2$ and $C_V \propto T$.

4. **Electronic band structure (12 points)**

(a) The Kronig-Penney model **(8 pts)**
In the text and in class we derived the following expression for the energy disparsion relation $E(k)$ for an electron moving in a one-dimensional periodic potential

$$\left(\frac{P}{Ka}\right)\sin Ka + \cos Ka = \cos ka$$

where a is the lattice constant, P is a positive parameter and $K = \sqrt{\frac{2mE}{\hbar^2}}$.
Assuming $P \ll 1$, obtain an explicit relation for E vs. k in the limit $k \to 0$. How is it different from the free electron dispersion relation?

(b) Bands of a simple square lattice **(7 pts)**
For a two-dimensional simple square lattice with lattice constant a, use the empty lattice approximation to draw the energy band structure (i.e. E vs. $\vec{k}$) in the reduced zone scheme along the (10) and the (11) directions for the lowest few bands.

Solution

(a) Starting from

$$\left(\frac{P}{Ka}\right)\sin Ka + \cos Ka = \cos ka$$

and given $P \ll 1$ and $k \to 0$ we find that $0 + \cos Ka = 1$, or $Ka \approx 0$, therefore Ka is small and we can Taylor expand the sine and cosine terms near zero:

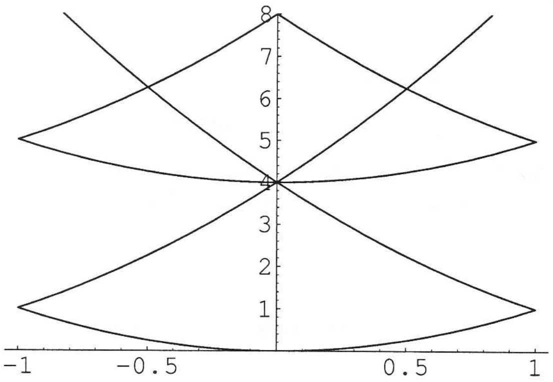
$$\left(\frac{P}{Ka}\right)Ka + 1 - \frac{(Ka)^2}{2} = 1 - \frac{(ka)^2}{2} \Rightarrow$$

$$P - \frac{(Ka)^2}{2} = -\frac{(ka)^2}{2} \Rightarrow \frac{(Ka)^2}{2} = \frac{(ka)^2}{2} + P \Rightarrow \frac{2mE}{\hbar^2} = k^2 + \frac{2P}{a^2} \Rightarrow E = \frac{\hbar^2k^2}{2m} + \frac{\hbar^2 P}{ma^2}$$

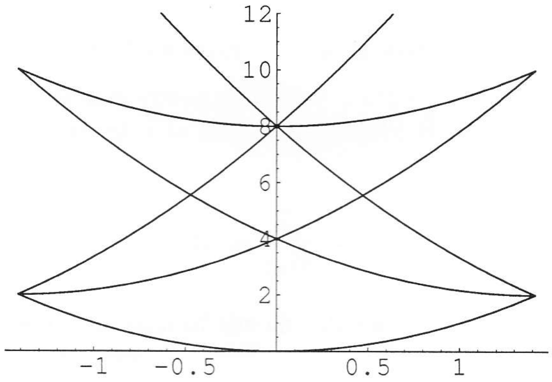
(b) For a $2D$ lattice and in the repeated zone scheme, the energy bands are going to be given by $E_{k,G} = \frac{\hbar^2}{2m}(\vec{k} - \vec{G})^2$ where $\vec{G} = \frac{2\pi}{a}(n\hat{x} + l\hat{y})$. Therefore

$$E_{k,n,l} = \frac{\hbar^2}{2m}\left[\left(k_x - \frac{2\pi n}{a}\right)^2 + \left(k_y - \frac{2\pi l}{a}\right)^2\right]$$

For the lowest bands, we need to consider the lowest $\vec{G}$ vectors, i.e. the set (n, l) where $n = -1, 0, 1$ and $l = -1, 0, 1$. For these values, the band structure along the (10) direction is plotted in the graph below:



and along the (11) direction is plotted in the graph below:



The x-axis (magnitude of k-vector) has units $\frac{\pi}{a}$ and the y-axis (energy) has units $\frac{\hbar^2\pi^2}{2ma^2}$.