PHY801: Survey of Atomic and Condensed Matter Physics
Michigan State University

Homework 8 – equivalent to Practice Exam 2 – Solution

Common quantities:

Quantity	**Name**	**Equivalent Quantity**
1 Å	Angstrom	10^{-10} m
1 a_B	Bohr radius	0.52918 Å
1 eV	electron-Volt	1.6022×10^{-19} J
1 Ry	Rydberg	13.606 eV
1 Ha	Hartree	27.212 eV
1 amu	atomic mass unit	1.661×10^{-27} kg
h	Planck's constant	4.1357×10^{-15} eV·s
k_B	Boltzmann's constant	8.617×10^{-5} eV/K
N_A	Avogadro's number	6.0221×10^{23} mol^{-1}
e	electron charge	1.6022×10^{-19} C
m	free electron mass	9.1095×10^{-31} kg

$$R = \frac{me^4}{2\hbar^2} = 13.6 \text{ eV} \quad \text{Rydberg constant}$$
$$a_B = \frac{\hbar^2}{me^2} = 0.529 \text{ Å} \quad \text{Bohr radius}$$

8.1. Consider an electron moving in a 2-dimensional square lattice with lattice constant a.

(a) Write down the energy $E(k_x, k_y)$ of the electron in terms of the on-site energy $-\alpha$ and the nearest-neighbor hopping parameter $-\gamma$ as a function of k_x and k_y, the x and y components of the electron wave vector $\vec{k}$.

(b) What is the effective mass m_x^* of an electron with the wave vector $\vec{k}$ close to $(\pi/a, 0)$ of the 1st Brillouin zone if it is moving along the x direction?

(c) What is the effective mass m_y^* of an electron with the same wave vector if it is moving along the y direction?

Solution:

(a) $E(k_x, k_y) = -\alpha - 2\gamma(\cos k_x a + \cos k_y a)$.

(b) For $(k_x, k_y) = (\pi/a, 0)$ we find $E(\pi/a, 0) = -\alpha$. In the vicinity of this point, $\kappa_x = k_x - \pi/a$ and k_y are small. Taylor expansion yields

$$E(k_x, k_y) \approx -\alpha - \gamma\kappa_x^2 a^2 + \gamma k_y^2 a^2 = -\alpha + \frac{\hbar^2}{2m_x^*}\kappa_x^2 + \frac{\hbar^2}{2m_y^*}k_y^2 \, .$$

The effective mass of an electron moving along the $x-$direction is negative,

$$m_x^* = -\frac{\hbar^2}{2\gamma a^2} \, .$$

The effective mass of an electron moving along the $y-$direction is positive,

$$m_x^* = +\frac{\hbar^2}{2\gamma a^2} \, .$$

(c) As discussed in the lecture, k_x and k_y are small in the vicinity of $(k_x, k_y) = (0, 0)$. There, the effective masses in the $x-$ and $y-$ direction are both positive,

$$m_x^* = m_y^* = +\frac{\hbar^2}{2\gamma a^2} \, .$$

In the vicinity of $(k_x, k_y) = (\pi/a, \pi/a)$, $\kappa_x = k_x - \pi/a$ and $\kappa_y = k_y - \pi/a$ are small. Then,

$$m_x^* = m_y^* = -\frac{\hbar^2}{2\gamma a^2} \, .$$

8.2. Consider a three-dimensional crystalline lattice formed of Cu and Zn atoms. The Cu atoms form a simple cubic lattice with the lattice constant a. The Zn atoms are at the center of the cube.

(a) What is the Bravais lattice and what are the primitive Bravais lattice vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$? If there is a basis, what are the basis vectors?

(b) What are the primitive vectors $\vec{b}_1, \vec{b}_2, \vec{b}_3$ of the reciprocal lattice?

(c) If the Zn atoms are ignored, what is the volume per Cu atom?

(d) Write down the structure factor $S_{\vec{G}}$ associated with the reciprocal lattice vector $\vec{G} = \nu_1\vec{b}_1 + \nu_2\vec{b}_2 + \nu_3\vec{b}_3$ in terms of the atomic form factors f_{Cu} and f_{Zn}.

(e) If Cu and Zn atoms randomly occupy every lattice site, then the form factor associated with every lattice site can be assumed to be the same, namely the average of the two form factors. Which Bragg spots will vanish in this case?

Solution:

(a) Simple cubic. The primitive lattice vectors are $\vec{a}_1 = a(1,0,0)$, $\vec{a}_2 = a(0,1,0)$, $\vec{a}_3 = a(0,0,1)$. The two basis vectors are $\vec{\tau}_1 = a(0,0,0)$ and $\vec{\tau}_2 = a\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$.

(b) The primitive reciprocal lattice vectors are $\vec{b}_1 = \frac{2\pi}{a}(1,0,0)$, $\vec{b}_2 = \frac{2\pi}{a}(0,1,0)$, $\vec{b}_3 = \frac{2\pi}{a}(0,0,1)$.

(c) $V_{\mathrm{Cu}} = a^3$.

(d) $S_{\vec{G}} = f_{\mathrm{Cu}}e^{i\vec{G}\cdot\vec{\tau}_1} + f_{\mathrm{Zn}}e^{i\vec{G}\cdot\vec{\tau}_2} = f_{\mathrm{Cu}} + f_{\mathrm{Zn}}e^{i\pi(\nu_1+\nu_2+\nu_3)}$.

(e) $\bar{f} = \frac{1}{2}(f_{\mathrm{Cu}} + f_{\mathrm{Zn}})$. Then, $S_{\vec{G}} = \bar{f}\left(1 + e^{i\pi(\nu_1+\nu_2+\nu_3)}\right)$. Bragg spots will vanish when $\nu_1+\nu_2+\nu_3 =$ odd.

8.3. Consider a two-dimensional electron system, where the energy of an electron is given by $E(\vec{k}) = \hbar v k$, with v denoting the speed of the electrons and $\vec{k}$ the electron wave vector. Such an approximation is good for extremely relativistic electrons.

(a) Calculate the electronic density of states $D(E)$ as a function of the area A, of $\hbar v$ and the energy E. Include the spin degeneracy factor. Plot $D(E)$ as a function of E.

(b) Calculate the Fermi energy E_F of this system if the electron density is 10^{12} cm^{-2}. Use $v = 10^8$ cm/s.

Solution:

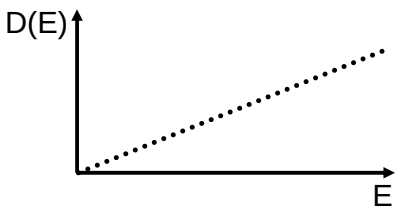
(a) Considering a square area with side length L, we obtain

$$D(E)dE = 2\frac{2\pi k dk}{\left(\frac{2\pi}{L}\right)^2} .$$

Using $E = E(\vec{k}) = \hbar v k$ and thus $dE = \hbar v dk$, we obtain

$$D(E) = \frac{A}{\pi}\left(\frac{1}{\hbar v}\right)^2 E .$$

The density of states varies linearly with energy.



(b) The total number of electrons is given by

$$N = \int_0^{E_F} D(E)dE = \frac{A}{2\pi}\left(\frac{1}{\hbar v}\right)^2 E_F^2 \ .$$

$$E_F = \hbar v\sqrt{2\pi N/A} = 2.63{\times}10^{-20} \text{ J} = 0.165 \text{ eV} \ .$$

8.4. Conduction electrons in a metal can be modeled as an ideal Fermi gas with the fermion effective mass m^*.

(a) How does the electronic heat capacity C_V vary with temperature T for $T << T_F$, where T_F is the Fermi temperature?

(b) If the effective mass m^* increases by a factor of 10 (say due to the effect of strong crystalline potential), what will be the change in C_V at a given T?

(c) Will the Pauli spin susceptibility χ_{Pauli}, which is associated with these electrons, change at low temperatures T? If so, by what factor and why?

Solution:

(a) $C_{el} \propto \gamma T$. $\gamma \propto D(E_F) \propto \frac{N}{E_F}$.

(b) $E_F \propto \frac{1}{m^*}$. Thus, $\gamma \propto m^*$. The heat capacity will increase by a factor of 10.

(c) Since χ_{Pauli} and γ are both proportional to the density of states at the Fermi energy $D(E_F)$, their ratio is a universal constant, the Wilson ratio. Therefore, χ_{Pauli} will also increase by a factor of 10.
