FACULTY OF SCIENCE

PHYSICS	**AUCKLAND PARK KINGSWAY CAMPUS**

PHY8X13
Advanced Solid State Physics A

EXAMINATION

June 2019

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TIME: 3 Hours **MARKS: 110**

Please read the following instructions carefully:

1. Answer all the questions.
2. No programmable calculators allowed.
3. All symbols have their normal meaning.

Question 1 [5]

Accept that the electron density, *n(**r**)*, associated with the crystal lattice can be expanded in the following Fourier series:

$$n(\overline{r}) = \sum_{\overline{G}} e^{-i\overline{G}\bullet\overline{r}} \ .$$

The primitive reciprocal lattice vectors are:

$$\overline{b_1} = 2\pi \frac{\overline{a_2} \times \overline{a_3}}{\overline{a_1} \bullet \overline{a_2} \times \overline{a_3}} \ , \ \overline{b_2} = 2\pi \frac{\overline{a_3} \times \overline{a_1}}{\overline{a_1} \bullet \overline{a_2} \times \overline{a_3}} \ , \ \overline{b_3} = 2\pi \frac{\overline{a_1} \times \overline{a_2}}{\overline{a_1} \bullet \overline{a_2} \times \overline{a_3}} \ .$$

Show that *n(**r**)* is invariant under a crystal translation ***T***. [5]

Question 2 [20]

The primitive translation vectors of the hexagonal space lattice are given by:

$$\overline{a_1} = \frac{\sqrt{3}a}{2}\hat{x} + \frac{a}{2}\hat{y}; \qquad \overline{a_2} = \frac{-\sqrt{3}a}{2}\hat{x} + \frac{a}{2}\hat{y}; \qquad \overline{a_3} = c\hat{z} \ .$$

(a) Show that the volume of the primitive cell is given by $\sqrt{3}a^2c/2$. [4]

(b) Show that the primitive translations of the reciprocal lattice are given by:

$$\overline{b_1} = \frac{2\pi}{\sqrt{3}a}\hat{x} + \frac{2\pi}{a}\hat{y}; \qquad \overline{b_2} = \frac{-2\pi}{\sqrt{3}a}\hat{x} + \frac{2\pi}{a}\hat{y}; \qquad \overline{b_3} = \frac{2\pi}{c}\hat{z} \ .$$ [9]

(c) Describe the first Brillouin zone of the bcc lattice. [7]

Question 3 [12]

Consider X-rays with wave vector ***k*** falling onto a crystal. The rays are elastically scattered in the direction ***k'*** the wave vector of the reflected beams. Making use of a sketch, derive the diffraction condition: [12]

$$2\overline{k} \bullet \overline{G} + G^2 = 0 \ .$$

Question 4 [5]

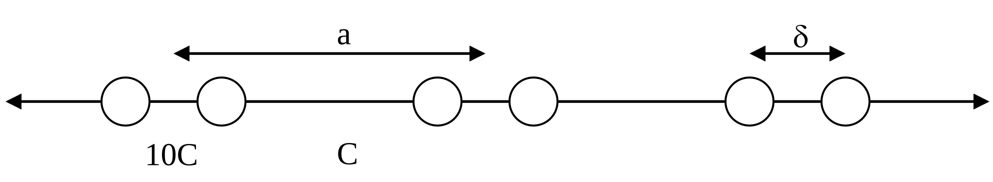
Accept that the scattering amplitude in the direction $\Delta\overline{k} = \overline{k'} - \overline{k} = \overline{G}$ is directly proportional to the geometric structure factor:

$$S_{\overline{G}} = \sum_j^s f_j e^{i\overline{G}\cdot\overline{r_j}} \ ,$$

where *j* is over the *s* atoms in the basis and f_j the atomic form factor of the j^{th} atom in the axis. Use this information to explain why the diffraction pattern of a bcc crystal will contain a (222) line but **not** a (111) line. [5]

Question 5 [14]

Consider the normal modes of a linear lattice with a primitive lattice constant a, having a basis of two identical atoms of mass *M* at equilibrium, separated by $\delta < 1/2\, a$. Both atoms of the basis are on a line. The force constant between the atoms of the basis is $C_1 = 10C$, that between one atom and the nearer of the two atoms belonging to the nearest basis is $C_2 = C$ (see figure). An example would be a crystal composed of diatomic molecules, for example H_2. Find the dispersion relation $\omega(K)$ at $K = 0$ and $K = \pi/a$. Sketch the dispersion relation qualitatively and discuss the sketch with special reference to the optical and acoustic modes. [14]



Question 6 [10]

In the Debye model for the density of states the thermal energy for each polarization is given by

$$U = \int_0^{\omega_D} d\omega D(\omega) \frac{\hbar\omega}{e^{\hbar\omega/\tau} - 1}.$$

Making use of periodic boundary conditions it can be shown that the density of states of the vibration modes is given by (DO NOT SHOW):

$$D(\omega) = \frac{VK^2}{2\pi^2}\left(\frac{dK}{d\omega}\right).$$

Make use of the Debye model to find the Debye heat capacity:

$$C_V = \frac{3V\hbar^2}{2\pi^2 v^3 k_B T^2} \int_0^{\omega_D} d\omega \frac{\omega^4 e^{\hbar\omega/\tau}}{\left(e^{\hbar\omega/\tau - 1}\right)^2}.$$

[10]

Question 7 [8]

Consider *N* free electrons at 0 K in a cube with side length *L*. Show that the kinetic energy of the gas is given by:

$$U_0 = \frac{3}{5} N \in_F.$$

Assume that the average electron energy is given by:

$$\langle \in \rangle = \frac{\int \in D(\in) f(\in) d\in}{\int D(\in) f(\in) d\in},$$

where $f(\in)$ represents the Fermi-Dirac distribution function. [8]

Question 8 [12]

Considering an electron moving in a linear periodic lattice, subjected to a periodic lattice potential *U*(*x*), the central equation can be derived as:

$$\left(\frac{\hbar^2 k^2}{2m} - \in\right) C(k) + \sum_G U_G C(k - G) = 0,$$

where $U(x) = \sum_G U_G e^{iGx}$. Here *C(k)* as well as *C(k-G)* are the Fourier coefficients.

Accept the information given and solve the central equation by only considering Fourier coefficients *C(½G)* and *C(-½G)* at the zone boundary $k = \frac{\pi}{a} = \frac{1}{2}G$, showing that an energy gap exists at the zone boundary. [12]

Given: $\psi_k(x) = \sum_G C(k - G) e^{i(k-G)x}$

Question 9 [8]

Show that the density of electrons in the conduction band is given by

$$n = 2\left(\frac{m_e k_B T}{2\pi\hbar^2}\right)^{3/2} \exp\left[(\mu - E_c)/k_B T\right].$$

All symbols have their normal meaning. State all assumptions clearly.

Given: $\int_0^\infty x^{1/2} e^{-x} dx = \frac{1}{2}\pi^{\frac{1}{2}}$ and the general equation for the density of states is given by

$D(\varepsilon) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{\frac{1}{2}}$. [8]

Question 10 [8]

The average number of magnons excited in the mode ω_k in thermal equilibrium is given by the Planck distribution function as: $\langle n_k \rangle = \left(e^{\hbar\omega/\tau} - 1\right)^{-1}$, where $\tau \equiv k_B T$.

The total number of magnons excited at a temperature T is given by: $\sum_k n_k = \int d\omega \ \ D\omega \ \langle n_k(\omega) \rangle$.

Show that for a three dimensional ferromagnet at low temperatures:

$$\frac{\Delta M}{M(0)} \propto T^{3/2},$$

where this result gives the Bloch $T^{3/2}$ law. [8]

Question 11 [8]

Consider a conductive electron gas at $T = 0$ K of which the concentrations of spin-up and spin-down electrons are respectively given by:

$$N^+ = \frac{1}{2} N(1 + \xi); \qquad N^- = \frac{1}{2} N(1 - \xi).$$

The effect of the exchange interaction between the conduction electrons is negligible. By using the minimizing of the total energy ($E_{Total} = E^+ + E^-$) and solving for ξ in the limit where $\xi << 1$, show that the Pauli spin susceptibility of the system is given by:

$$\chi = \frac{M}{B} = \frac{3N\mu^2}{2\in_F}; \quad \in_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}},$$

where M is the Pauli spin magnetism for the system. [8]

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