PHY 731 Fall 2006 Final Exam (closed book) Name Key

Friday 10/6/2006

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Score: Multiple Choice: _______ / 30 ; Multi-part Problems: _______ / 60: **Total Score** _______ / 90

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Part I. Multiple Choice questions (please circle the correct answer) (**3 pts each**)

1. The face-centered cubic lattice with conventional cubic cell of side a has as its reciprocal lattice ________________
   a. a face-centered cubic lattice with conventional cubic cell of side $2\pi/a$
   b. a body-centered cubic lattice with conventional cubic cell of side $2\pi/a$
   c. a face-centered cubic lattice with conventional cubic cell of side $4\pi/a$
   d. a body-centered cubic lattice with conventional cubic cell of side $4\pi/a$

2. The Miller indices of a plane in a lattice ___________
   a. are proportional to the intercepts of that plane with the crystal axes
   b. cannot be defined for hexagonal crystal lattices
   c. are the coordinates of the shortest reciprocal lattice vector normal to the plane
   d. do not depend on the particular choice of primitive vectors

3. The Bragg formulation of X-ray scattering is defined in terms of scattering from __________, whereas the Von Laue formulation is defined in terms of scattering from _________, respectively.
   a. planes of the lattice; points of the lattice
   b. points of the lattice; planes of the lattice
   c. planes of the lattice; points of the reciprocal lattice
   d. planes of the reciprocal lattice; points of the lattice

4. The geometrical structure factor ___________
   a. expresses the extent to which waves scattered from different types of ions within the basis interfere destructively
   b. expresses the extent to which waves scattered from different types of ions within the basis interfere constructively
   c. expresses the extent to which interference from waves scattered from identical ions within the basis affects the Bragg peak intensity
   d. has nothing to do with the Bragg peak intensity

5. Bloch's theorem __________
    a. cannot be proven conclusively.
    b. says that the eigenstates of the Hamiltonian in the case of a periodic potential can be written as a product of a plane wave and a function with the periodicity of the reciprocal lattice.
    c. says that the eigenstates of the Hamiltonian in the case of a periodic potential can be written as a product of a plane wave and a function with the periodicity of the Bravais lattice
    d. introduces a wave vector $\boldsymbol{k}$ which is proportional to the electronic momentum

6. Van Hove singularities __________
    a. lead to an infinite density of levels
    b. are not integrable in 3 dimensions
    c. occur when the real-space gradient of the energy vanishes
    d. occur when the k-space gradient of the energy vanishes

7. In the case of a weak periodic potential, __________
    a. the electronic eigen-energies are affected to first order in U in the case of non-degenerate energy levels, where U is the magnitude of the periodic potential
    b. the electronic eigen-energies are most strongly affected near Bragg planes
    c. the case of non-degenerate energy levels is the origin of band gaps
    d. the degenerate case leads to energy shifts of order U^2

8. Energy bands __________
    a. can only occur in the case of a weak periodic potential
    b. are a consequence of the periodicity of the Bravais lattice
    c. cannot be described in one dimension
    d. have nothing to do with electron transport in solids

9. The Fermi surface __________
    a. is always spherical.
    b. takes the shape of the surface of the first Brillouin zone
    c. takes the shapes of the intersections of the 'free electron-like' Fermi sphere with the different Brillouin zones
    d. has only components which are related to the first Brillouin zone
    e. only exists in the case of face-centered cubic lattices

10. In the tight binding method, __________
    a. the periodic wave-function solutions are *not* Bloch wave-functions
    b. energy bandwidth is *not* proportional to an overlap integral
    c. the eigen-energy solutions are independent of k
    d. the starting point for the periodic wave-function solutions are localized atomic orbital wave functions

Part II. Multi-Part Problems. (**20 pts each**)

Problem #1: X-ray diffraction from a body-centered cubic (bcc) lattice.

a. (4 pts) Consider a bcc lattice as simple cubic with lattice constant a and a basis of *two* atoms, one at $\mathbf{d}_1 = (0,0,0)$, the second at $\mathbf{d}_2 = a(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

Define the primitive lattice vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$. From these, determine the reciprocal lattice vectors $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$, using the expression

$$\mathbf{b}_i = \frac{2\pi\,(\mathbf{a}_j \times \mathbf{a}_k)}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)}$$

(with 3 permutations of i, j, and k)

b. (4 pts) Given the 2-point basis, consider the closest-spaced planes perpendicular to $\mathbf{a}_1$. What are the Miller indices of these planes?

c. (4 pts) Formulate a general reciprocal lattice vector $\mathbf{K}$ as a linear combination of the $\mathbf{b}_i$ with coefficients n_i. Calculate the structure factor $S_K = \sum \exp(i\,\mathbf{K}\cdot\mathbf{d}_j)$.

d. (4 pts) For what combinations of the n_i do you get finite values of S_K? For what combinations do you get $S_K = 0$?

e. (4 pts) For the close-spaced planes considered in part (b), do these planes give a Bragg peak? For next nearest-spaced planes, do these give a Bragg peak? If the conventional cube lattice constant is 4.5 Å, and the x-ray wave-length is 1.5 Å, at what angle θ will the 1st order Bragg peak appear?

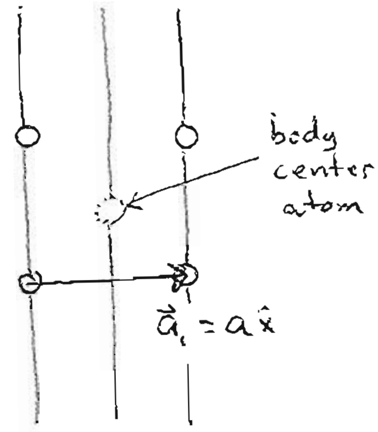
a) $\vec{a}_1 = a\,\hat{x} \qquad \vec{a}_2 = a\,\hat{y} \qquad \vec{a}_3 = a\,\hat{z}$

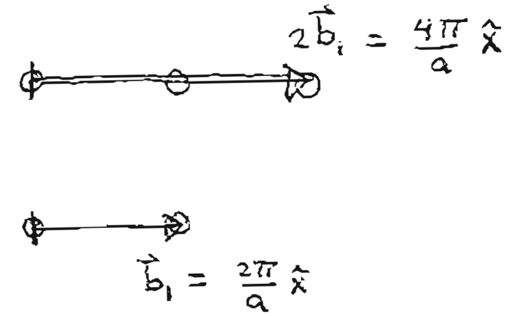
$$\vec{b}_1 = \frac{2\pi\;\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi\;a^2\,\hat{x}}{a^3} = \frac{2\pi}{a}\,\hat{x}$$

$$\vec{b}_2 = \frac{2\pi\;\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi\;a^2\,\hat{y}}{a^3} = \frac{2\pi}{a}\,\hat{y}$$

$$\vec{b}_3 = \frac{2\pi\;\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi\;a^2\,\hat{z}}{a^3} = \frac{2\pi}{a}\,\hat{z}$$

b)





$\vec{b}_1$ is reciprocal of $\vec{a}_1$

closest planar spacing in cubic system is $\frac{a}{2} \to \frac{\vec{a}_1}{2}$ $\Rightarrow$ reciprocal vector is $\underline{2\vec{b}_1}$

$\Rightarrow$ $\boxed{\text{Miller indices are } (2,0,0)}$

c)

$\vec{d}_1 = (0,0,0)$

$\vec{d}_2 = a\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$

$$\vec{K} = \sum_{i=1}^{3} n_i \vec{b}_i = \frac{2\pi}{a}\left(n_1\hat{x} + n_2\hat{y} + n_3\hat{z}\right)$$

$$S_{\vec{K}} = \sum_{j=1}^{2} e^{i\vec{K}\cdot\vec{d}_j} = 1 + e^{i\pi(n_1+n_2+n_3)}$$

d)

$$S_{\vec{K}} = 0 \qquad n_1+n_2+n_3 \text{ odd}$$

$$= 2 \qquad n_1+n_2+n_3 \text{ even}$$

e) nearest-spaced planes $\to$ $n_1 = 2,\ n_2 = n_3 = 0$ $\Rightarrow$ $n_1+n_2+n_3$ even

$(2,0,0)$ $\Rightarrow$ Yes, a Bragg peak

next-nearest-spaced planes $\to$ $n_1 = 1,\ n_2 = n_3 = 0$ $\Rightarrow$ $n_1+n_2+n_3$ odd

$(1,0,0)$ $\Rightarrow$ No, not a Bragg peak

$$n\lambda = 2d\sin\theta$$

first-order $\rightarrow$ $n = 1$

$$\lambda = 2d\sin\theta$$

$$1.5\ \text{Å} = 2\left(\frac{4.5\ \text{Å}}{2}\right)\sin\theta$$

$$\Rightarrow \quad \sin\theta = \frac{1.5}{4.5}$$

$$\Rightarrow \quad \theta = \sin^{-1}\left(\frac{1.5}{4.5}\right) = \sin^{-1}\left(\frac{1}{3}\right) = \underline{19.47^\circ}$$

Problem#2: Determination of the band splitting using the central equation in the important case of 2 degenerate levels.

a. (5 pts) Write down a system of 2 equations for the band structure energy levels for a weak periodic potential in the special case that there are just 2 degenerate levels ε_{k-K1} and ε_{k-K2}, starting with the general central equation. The 2 equations should involve the eigen-energy ε, the c's, and the U's, appropriately subscripted by k-K1, k-K2, etc. Remember that $U_o = 0 = U_{K1-K1} = U_{K2-K2}$.

Central Equation

$$(\varepsilon - \varepsilon^{o}_{k-K_i}) c_{k-K_i} = \sum_{j=1}^{m} U_{K_j - K_i} c_{k-K_j}, \quad i = 1, \ldots m$$

b. (5 pts) Let q = k – K1, q-K = k – K2, and thus K = K2 – K1, to change subscripts to just q and K, i.e. c_q and c_{q-K}. What is the important meaning of this transformation interpreted in terms of Bragg planes?

c. (5 pts) Write your system of 2 equations involving q and q-K (as subscripts) in a matrix form. Solve for the eigenenergy. Show that there are two roots.

d. (5 pts) Finally, draw a picture of the ε vs. q relationship from q = 0 up to q = K/2. Indicate the band gap. What is it in terms of U_K?

a)

$$\boxed{\begin{aligned} (\varepsilon - \varepsilon^{o}_{k-K_1}) c_{k-K_1} &= U_{K_2-K_1} c_{k-K_2} \\ (\varepsilon - \varepsilon^{o}_{k-K_2}) c_{k-K_2} &= U_{K_1-K_2} c_{k-K_1} \end{aligned}}$$

b)

$$q = k - K_1, \quad q - K = k - K_2, \quad K = K_2 - K_1$$

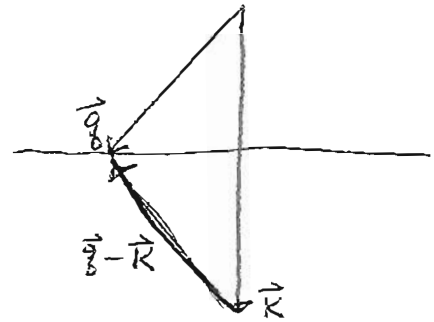
$$\Rightarrow \boxed{\begin{aligned} (\varepsilon - \varepsilon^{o}_{q}) c_{q} &= U_{K} c_{q-K} \\ (\varepsilon - \varepsilon^{o}_{q-K}) c_{q-K} &= U_{-K} c_{q} \end{aligned}}$$

important meaning:

$$\mathcal{E}^{\circ}_{k-K_1} \approx \mathcal{E}^{\circ}_{k-K_2} \longrightarrow \mathcal{E}^{\circ}_{q} \approx \mathcal{E}^{\circ}_{q-K}$$

$$\Rightarrow \quad |\vec{q}| = |\vec{q} - \vec{K}|$$

$\Rightarrow$ $\vec{q}$ must lie on a Bragg plane



c)

$$(\mathcal{E} - \mathcal{E}^{\circ}_{q}) c_q - U_K c_{q-K} = 0$$

$$-U_{-K} c_q + (\mathcal{E} - \mathcal{E}^{\circ}_{q-K}) c_{q-K} = 0$$

$$\Rightarrow \quad \begin{vmatrix} \mathcal{E} - \mathcal{E}^{\circ}_{q} & -U_K \\ -U_{-K} & \mathcal{E} - \mathcal{E}^{\circ}_{q-K} \end{vmatrix} = 0$$

$$\Rightarrow \quad (\mathcal{E} - \mathcal{E}^{\circ}_{q})(\mathcal{E} - \mathcal{E}^{\circ}_{q-K}) - U_K U_{-K} = 0$$

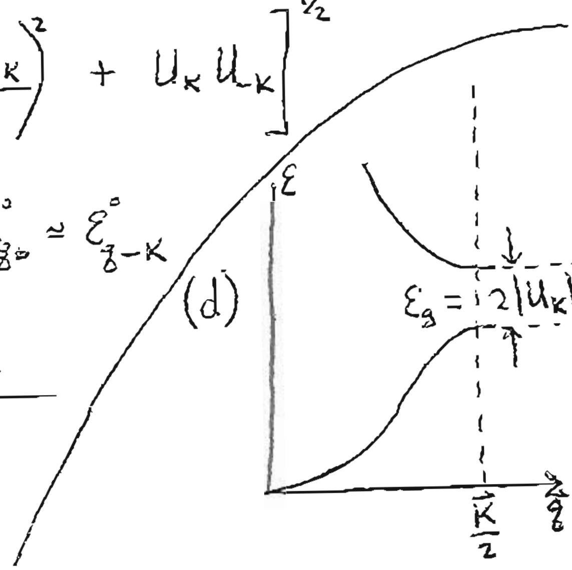
$$\Rightarrow \quad \mathcal{E}^2 + (-\mathcal{E}^{\circ}_{q} - \mathcal{E}^{\circ}_{q-K})\mathcal{E} + (\mathcal{E}^{\circ}_{q}\mathcal{E}^{\circ}_{q-K} - U_K U_{-K}) = 0$$

$$\Rightarrow \quad \mathcal{E} = \frac{\mathcal{E}^{\circ}_{q} + \mathcal{E}^{\circ}_{q-K}}{2} \pm \left[\frac{(\mathcal{E}^{\circ}_{q})^2 + 2\mathcal{E}^{\circ}_{q}\mathcal{E}^{\circ}_{q-K} + (\mathcal{E}^{\circ}_{q-K})^2 - 4\mathcal{E}^{\circ}_{q}\mathcal{E}^{\circ}_{q-K} + 4U_K U_{-K}}{4} \right]^{1/2}$$

$$\mathcal{E} = \frac{\mathcal{E}^{\circ}_{q} + \mathcal{E}^{\circ}_{q-K}}{2} \pm \left[\left(\frac{\mathcal{E}^{\circ}_{q} - \mathcal{E}^{\circ}_{q-K}}{2} \right)^2 + U_K U_{-K} \right]^{1/2}$$

$U_K U_{-K} = |U_K|^2$ and at $\vec{q} = \vec{q} - \vec{K}$, $\mathcal{E}^{\circ}_{q_0} \approx \mathcal{E}^{\circ}_{q-K}$

$$\Rightarrow \underline{\text{at } \vec{q} = \vec{q} - \vec{K}, \quad \mathcal{E} = \mathcal{E}^{\circ}_{q} \pm |U_K|}$$



Problem#3: Two-dimensional Fermi Surface and Brillouin Zones.

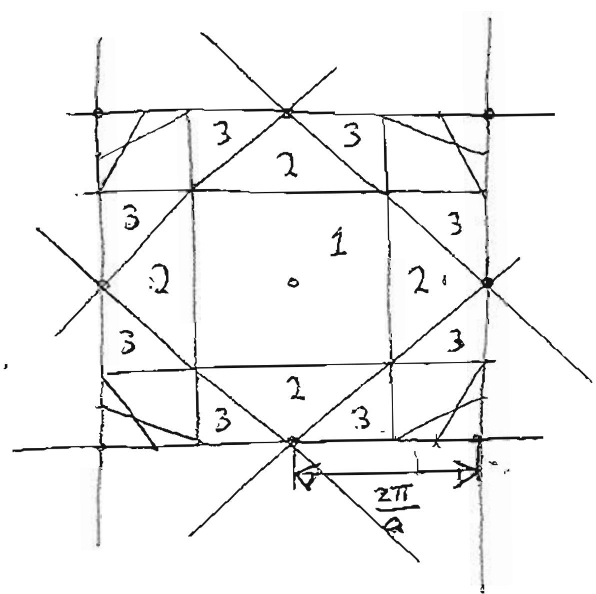
a. (5 pts) Consider a 2-dimensional square lattice with lattice constant a. Determine its reciprocal lattice and the spacing of k-points in the reciprocal lattice in terms of a. Draw a picture of the 2-D reciprocal lattice. On this picture, draw and label the 1st, 2nd, and 3rd Brillouin zones.

b. (5 pts) Next, draw a Fermi "sphere" having a radius $k_F = 0.75(2\pi/a)$ superimposed on the picture of the reciprocal lattice and centered on a reciprocal lattice point. Which of the 3 Brillouin zones does the Fermi sphere cut through?

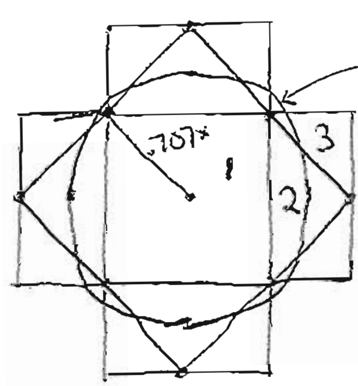
c. (5 pts) Next, determine the Fermi surface by translating appropriate pieces of this picture by a reciprocal lattice vector. Show the 1st, 2nd, and 3rd zone Fermi surfaces in the reduced zone picture. Label which of them is "hole-like" and which of them is "electron-like".

d. (5 pts) Finally, redraw the Fermi surfaces for 1st zone, 2nd zone, and 3rd zone in the repeated zone scheme, and indicate effects of a weak periodic potential on the shape of these surfaces.

a)



b)



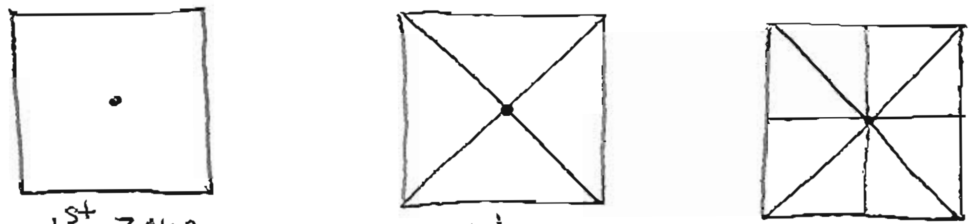
sphere radius is $.75\left(\frac{2\pi}{a}\right)$

$> .707\left(\frac{2\pi}{a}\right)$

$\Rightarrow$ cuts through zones 2 and 3

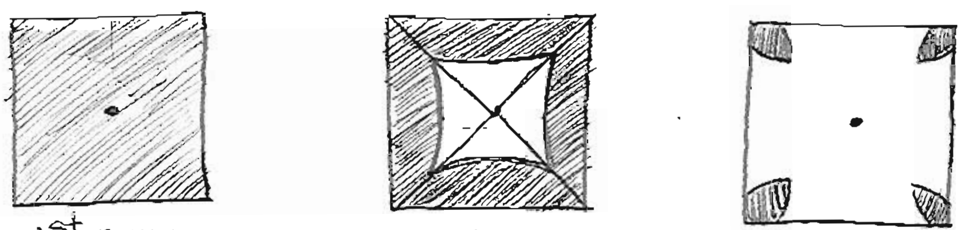
but encloses all of zone 1

c)



1st zone 2nd zone 3rd zone

reduced zone scheme



1st zone completely occupied	2nd zone Fermi surface (hole-like)	3rd zone Fermi surface (electron-like)

d) repeated zone scheme

1st zone completely occupied → when translated (repeated) fills all of k-space

2nd zone Fermi Surface

3rd zone Fermi Surface