Solid State Physics 240A: MidTerm Exam #1.

Name: SOLUTIONS

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$\hbar$=1.05×10^{-27} erg-s; m=9.11×10^{-28} gm; e=1.60×10^{-19} coulomb; 1 Ha = e^2/a_o.

You will have to introduce symbols; be specific about what the symbols are, or mean.

1. The electronic charge density $n(\vec{r})$ in a crystal is cell-periodic, that is, every cell is the same.

(a) Give the expression for its Fourier expansion.

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$$n(r) = \sum_K n_K e^{iK\cdot r}, \quad K \text{ are recip. lattice vectors}$$

(b) $n(\vec{r})$ is (always) real, and suppose the crystal has inversion symmetry. Say as much as possible about the Fourier coefficients of the expansion.

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Real: $n^*(r) = \sum_K n_K^* e^{-iK\cdot r} = n(r) = \sum_K n_K e^{iK\cdot r} \Rightarrow n_{-K} = n_K^*$

Inv: $n(-r) = \sum_K n_K e^{-iK\cdot r} = n(r) = \sum_K n_K e^{iK\cdot r} \rightarrow n_{-K} = n_K$

So: $n_K = n_{-K} = n_K^*$: real and $n_K = n_{-K}$. $\left[n(r) = n_0 + 2\sum_{\text{"}K>0\text{"}} \cos(K\cdot r) \right]$ ← just for fun.

2. Given $\vec{a}_1 = (2, 3, 1)$, $\vec{a}_2 = (5, 0, 7)$, $\vec{a}_3 = (-1, -1, -1)$ in Angstroms, calculate (only) the first reciprocal lattice vector $\vec{b}_1$ from the conventional expression.

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$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot a_2 \times a_3} \qquad a_2 \times a_3 = \begin{vmatrix} i & j & k \\ 5 & 0 & 7 \\ -1 & -1 & -1 \end{vmatrix} = \hat{i}(7) + \hat{j}(-7+5) + \hat{k}(-5) = (7,-2,-5)$$

$$\boxed{b_1 = \frac{2\pi}{3}(7,-2,-5)\,\mathring{A}^{-1}}$$

$$a_1 \cdot (a_2 \times a_3) = 14 - 6 - 5 = 3$$

3. 3D homogeneous electron gas of constant density n.

(a) What are (i) the electron gas parameter r_s, and (ii) the Fermi wavevector (magnitude, to be precise) k_F, in terms of n?

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$$N = 2\left(\frac{4\pi k_F^3}{3}\right)\left(\frac{V}{(2\pi)^3}\right) \Rightarrow \boxed{n = \frac{k_F^3}{3\pi^2}}. \qquad \frac{4\pi r_s^3}{3} = \frac{1}{n} \Rightarrow \boxed{r_s = \left(\frac{3}{4\pi n}\right)^{1/3}}$$

vol. in k-space; density of k-pts.

$$\boxed{k_F = (3\pi^2 n)^{1/3}}$$

(b) If n = 1 electron/$\mathring{A}^3$, what is the value of the Fermi energy in eV?

$E_F = \frac{\hbar^2 k_F^2}{2m}$. Use above.

Atomic units: $n \approx \frac{1}{8} / a_0^3$

$\hbar = 1$, $m = 1$. $E_F = \frac{1}{2}(3\pi^2 n)^{2/3} \approx \frac{1}{2}\left(3^3/2^3\right)^{2/3} = \frac{1}{2}\frac{3^2}{2^2} = \frac{9}{8}$ Hartree

≈ 30 eV.

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4. How many Bravais lattices are there in 3D? Name five (only) of them.

14. {Grader: see list.}

2
2
1
1
1

5. State the *types* of symmetries that a general crystal can have. What is wanted here is classes, **not** names such as hexagonal, etc. This question has a brief answer – a short list.

8

translations
rigid rotations (incl. improper)
non-symmorphic translations

10

6. Give the direct lattice vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$ that define a body-centered tetragonal Bravais lattice, describing why they do so. The answer is not unique, any correct answer will suffice.

$\underset{\sim}{a}_1 = (a, 0, 0)$ & $\underset{\sim}{a}_2 = (0, a, 0)$ connect all points in plane.

$\underset{\sim}{a}_3 = \left(\frac{a}{2}, \frac{a}{2}, \frac{c}{2}\right)$ connects to nearest plane $\Rightarrow$ all lattice sites.

7. Give three of Ashcroft & Mermin's four assumptions underlying the classical Drude model of an electronic system.

4
3
3
3.

3 of these.

No interactions except for collisions.
Collisions are instantaneous.
Scattering time τ.
Scattering thermalizes electrons.

Mermin page 5 & 6

8. Scattering from a 2D crystal.

A 2D square lattice with lattice constant a has a basis of two identical atoms at $\pm(\frac{a}{4}, \frac{a}{4})$. Calculate the structure factor $S_{\vec{K}}$ for general $\vec{K} = n_1\vec{b}_1 + n_2\vec{b}_2$. What are the possible values of $S_{\vec{K}}$?

$$S_K = \sum_j^{\text{cell}} f_j e^{i K \cdot r_j} \leftarrow \text{positions in cell}$$

5.

$(\frac{a}{4}, \frac{a}{4})$: $K \cdot r_j = (n_1 b_1 + n_2 b_2) \cdot \frac{1}{4}(a_1, a_2) = \frac{2\pi}{4} n_1 + \frac{2\pi}{4} n_2$

$(-\frac{a}{4}, -\frac{a}{4})$: $-\frac{2\pi}{4}(n_1+n_2)$.

$f_1 = f_2$ (identical)

5. $$S_K = f\, 2\cos\left[\frac{\pi}{2}(n_1+n_2)\right]$$

integer

2.5 each

for $n_1+n_2 = 4M$, $S_K = 2f$

" " $= 4M+1$, $S_K = 0$

" " $= 4M+2$, $S_K = -2f$

" " $= 4M+3$, $S_K = 0$

3 distinct value, one is zero!

1. 15
2. 10
3. 20
4. 7
5. 8
6. 10
7. 10 = 3+3+4
8. 20