MIDTERM EXAM

Physics 140A– WINTER 2012

Instructions: Do any six of the eight problems.

[**1.**] The primitive lattice vectors of an fcc lattice are

$$\vec{a}_1 = \frac{1}{2}\,a\,(\hat{y}+\hat{z}) \qquad \vec{a}_2 = \frac{1}{2}\,a\,(\hat{x}+\hat{z}) \qquad \vec{a}_3 = \frac{1}{2}\,a\,(\hat{x}+\hat{y})$$

What is the volume of the unit cell V_c? Compute the reciprocal lattice vectors $\vec{b}_1$, $\vec{b}_2$, $\vec{b}_3$. Do you recognize these as a particular lattice type? What is the volume of the unit cell of the reciprocal lattice (volume of the "first Brillouin zone")?

[**2.**] Consider a mass spring-system with all springs identical and two different, alternating, masses M_1 and M_2. Describe the normal mode with the lowest frequency ω. (Draw a picture of the motion of the masses.) What is the value of ω? Describe two more normal modes, again drawing pictures of how the masses move. What are the frequencies of these modes?

[**3.**] An alternative to regarding the fcc structure as having a single atom basis with the $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ in problem [**1**] is to consider it to have a cubic unit cell of sides a and a four atom basis, with atoms at $(x_j, y_j, z_j) = (0,0,0)$, $(0, \frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, 0, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}, 0)$. Then the structure factor S_G for a reciprocal lattice vector $\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3$ is given by,

$$S(v_1\,v_2\,v_3) = \sum_j f_j \exp\big(-2\pi i\,(v_1 x_j + v_2 y_j + v_3 z_j)\big)$$

Assume the atoms are identical so that $f_j = f$. Compute $S(v_1\,v_2\,v_3)$. What are the conditions on $v_1\,v_2\,v_3$ so that S does not vanish? (That is, what are the "allowed reflections"?)

[**4.**] What is graphene and what is its structure? Is it possible to describe the atomic positions without using a basis? That is, can you write the atomic positions as $\vec{R} = n_1\,\vec{a}_1 + n_2\,\vec{a}_2$ with n_1 and n_2 *any* integers and $\vec{a}_1, \vec{a}_2$ two primitive lattice vectors? Why or why not?

[**5.**] Show that the volume of the first Brillouin zone is $(2\pi)^3/V_c$ where V_c is the volume of the crystal primitive cell.

[**6.**] The hydrogen atom number density ground state is $n(r) = (\pi a_0^3)^{-1}\exp(-2r/a_0)$, where a_0 is the Bohr radius. Show that the form factor

$$f_G = 4\pi \int dr\, n(r)\, r^2\, \frac{\sin Gr}{Gr} = \frac{16}{(\,4 + G^2\,a_0^2\,)^2}$$

What are the limiting values of f_G at small and large G?

[**7.**] An x-ray scatters elastically off a crystal. What can you say about possible values of its change in momentum? Using your answer, prove that a Bragg peak can arise only if the incoming wave vector $\vec{k}$ lies on a plane bisecting one of the reciprocal lattice vectors $\vec{G}$. Since these planes are only a two dimensional subset of a three dimensional space, the chance of $\vec{k}$ satisfying this condition is incredibly small. How do experimentalists solve this problem?

[8.] The participation ratio for a normalized vector $\vec{v}$ with components v_n (where $n = 1, 2, 3, \cdots N$) is defined as,

$$\mathcal{P} = \left(\sum_{n=1}^{N} v_n^4 \right)^{-1}$$

Consider a vector $\vec{v}$ with only one nonzero component. What must the value of the component be for $\vec{v}$ to be normalized? Compute $\mathcal{P}$ for such a $\vec{v}$. Does it matter which component is the nonzero one?

Consider a vector $\vec{v}$ with all components equal. What must the value of the components be for $\vec{v}$ to be normalized? Compute $\mathcal{P}$ for such a $\vec{v}$.

Comment on your results. Does the name "participation ratio" make sense for these two extreme examples?