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 $(x_j, y_j, z_j) = (0,0,0)$, $(0,\frac{a}{2},\frac{a}{2})$, $(\frac{a}{2},0,\frac{a}{2})$, $(\frac{a}{2},\frac{a}{2},0)$. 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 experimentaliats 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?

project:

MIDTERM EXAM P140A W2012

$\boxed{1}$ $V_c = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

$$\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \tfrac{1}{2}a & 0 & \tfrac{1}{2}a \\ \tfrac{1}{2}a & \tfrac{1}{2}a & 0 \end{vmatrix} = \hat{x}\left(-\tfrac{1}{4}a^2\right) + \hat{y}\left(\tfrac{1}{4}a^2\right) + \hat{z}\left(\tfrac{1}{4}a^2\right)$$

$$V_c = \tfrac{1}{2}a(\hat{y}+\hat{z}) \cdot \tfrac{1}{4}a^2(-\hat{x}+\hat{y}+\hat{z}) = \tfrac{1}{4}a^3$$

$$\vec{b}_1 = \frac{2\pi}{V_c}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{(1/4\,a^3)}\left(\tfrac{1}{4}a^2\right)(-\hat{x}+\hat{y}+\hat{z})$$

$$\vec{b}_1 = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z})$$

$$\vec{b}_2 = \frac{2\pi}{V_c}(\vec{a}_3 \times \vec{a}_1) = \frac{2\pi}{(1/4\,a^3)} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{vmatrix} \tfrac{1}{4}a^2$$

$$= \frac{2\pi}{a}(\hat{x} - \hat{y} + \hat{z})$$

Similarly $\vec{b}_3 = 2\pi/a\,(\hat{x}+\hat{y}-\hat{z})$

The $\vec{b}_i$ vectors form a <u>bcc</u> lattice. Its volume is

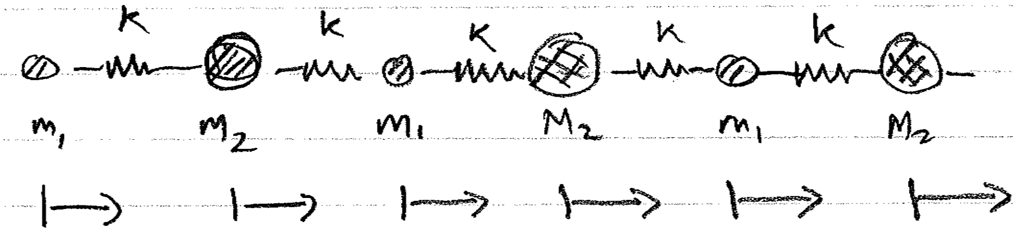
$$\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \left(\frac{2\pi}{a}\right)^3 (-\hat{x}+\hat{y}+\hat{z}) \cdot \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix}$$

$$= \left(\frac{2\pi}{a}\right)^3 (-\hat{x}+\hat{y}+\hat{z}) \cdot (0\hat{x} + 2\hat{y} + 2\hat{z}) = 4(2\pi/a)^3$$

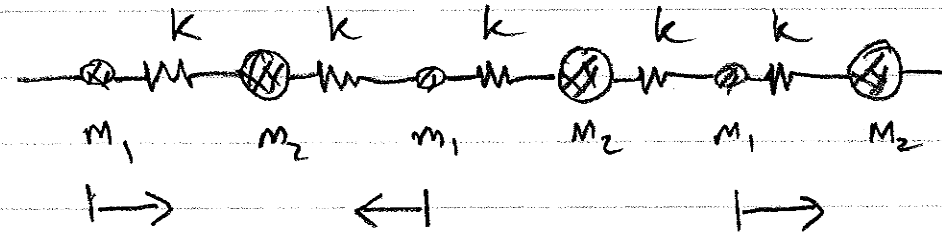
 This agrees with the general result $V_{BZ} = (2\pi)^3/V_c = \frac{4}{a^3}(2\pi)^3$

2

The lowest frequency normal mode is a uniform translation of all masses. No springs are stretched and $\omega = 0$



Two more normal modes are constructed by having only the m_1 masses move, or only the m_2 masses move. Also the masses which do move alternate in direction with equal amplitude



It is easy to see the 2 forces on each m_2 cancel, so they never move. The frequency of the m_1 masses is $\omega^2 = 2k/m_1$ since they are connected by 2 springs to motionless m_2 masses.

Similarly there is a mode of $\omega^2 = 2k/m_2$

for which only m_2 masses move.

3

If we substitute in the given $(x_j\ y_j\ z_j)$ into S we get

$$S(v_1 v_2 v_3) = f\left[1 + e^{-\pi i(v_2+v_3)} + e^{-\pi i(v_1+v_3)} + e^{-\pi i(v_1+v_2)}\right]$$

We want to know for what tuples of integers $(v_1\ v_2\ v_3)$ S will be nonzero.

all v_i odd : $S(v_1 v_2 v_3) = 4f$

$$\left.\begin{array}{l} v_1+v_2 \\ v_1+v_3 \\ v_2+v_3 \end{array}\right\} \text{even}$$

all v_i even : $S(v_1 v_2 v_3) = 4f$

two v_i odd, 1 even

$\quad \overset{\uparrow}{v_1 v_2} \qquad \overset{\uparrow}{v_3}$ $\qquad S(v_1 v_2 v_3) = f\left[1+(-1)+(-1)+1\right] = 0$

v_1+v_2 even

v_1+v_3 odd

v_2+v_3 odd

two v_i even, 1 odd $\qquad S(v_1 v_2 v_3) = 0$ again

$\quad \overset{\uparrow}{v_1 v_2} \qquad \overset{\uparrow}{v_3}$

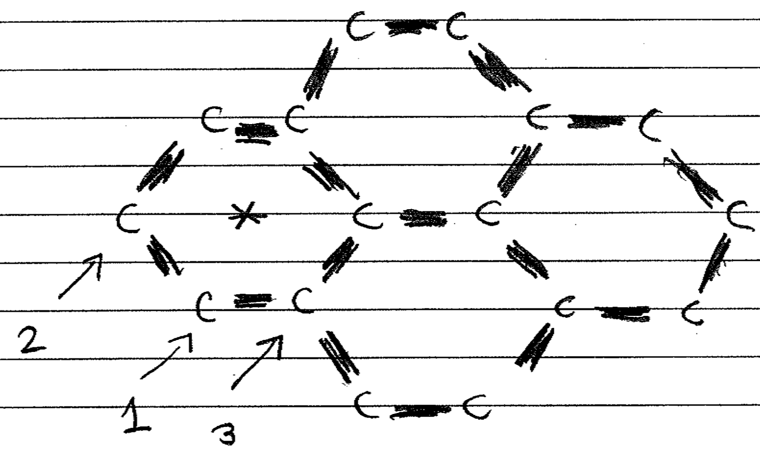
v_1+v_2 even

v_1+v_3 odd

v_2+v_3 odd

So all $v_1\ v_2\ v_3$ must be even or all odd.

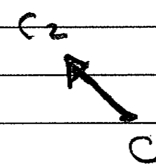
Graphene is a hexagonal array of carbon atoms, ie a single sheet of carbon with structure:



Suppose atoms 1, 2, 3 are all expressible as $n_1\vec{a}_1 + n_2\vec{a}_2$

1) $n_1\vec{a}_1 + n_2\vec{a}_2$

2) $n_1'\vec{a}_1 + n_2'\vec{a}_2$



$= (n_1'-n_1)\vec{a}_1 + (n_2'-n_2)\vec{a}_2$

Then starting at 3) $n_1''\vec{a}_1 + n_2''\vec{a}_2$

and adding $(n_1'-n_1)\vec{a}_1 + (n_2'-n_2)a_2$

will get us to the center of the hexagon marked *

$$*: (n_1''+n_1'-n_1)\vec{a}_1 + (n_2''+n_2'-n_2)\vec{a}_2$$

but this is not an atomic position of the hexagonal lattice.

So you must use a basis to describe graphene.

project:

$\boxed{5.}$

$$\vec{b}_1 = \frac{2\pi}{V_c}\,\vec{a}_2 \times \vec{a}_3 \qquad \vec{b}_2 = \frac{2\pi}{V_c}\,\vec{a}_1 \times \vec{a}_3 \qquad \vec{b}_3 = \frac{2\pi}{V_c}\,\vec{a}_1 \times \vec{a}_2$$

$$V_{BZ} = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)$$

$$= (2\pi/V_c)^3\,(\vec{a}_2 \times \vec{a}_3) \cdot \Big[\underbrace{(\vec{a}_1 \times \vec{a}_3)}_{\vec{A}} \times (\underbrace{\vec{a}_1}_{\vec{B}} \times \underbrace{\vec{a}_2}_{\vec{C}})\Big]$$

$$\vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}(\vec{A}\cdot\vec{C}) - \vec{C}(\vec{A}\cdot\vec{B})$$

$$= (2\pi/V_c)^3\,(\vec{a}_2 \times \vec{a}_3) \cdot \Big[\vec{a}_1\big(\underbrace{(\vec{a}_1 \times \vec{a}_3) \cdot \vec{a}_2}_{V_c}\big) - \vec{a}_2\,\big(\underbrace{(\vec{a}_1 \times \vec{a}_3) \cdot \vec{a}_1}_{\phi}\big)\Big]$$

$$= (2\pi/V_c)^3\,V_c\,\underbrace{(\vec{a}_2 \times \vec{a}_3) \cdot \vec{a}_1}_{V_c}$$

$$= (2\pi)^3/V_c$$

project:

$\boxed{6}$ $f_G = 4\pi \int dr\, n(r)\, r^2 \frac{\sin Gr}{r}$ $\quad n(r) = \frac{1}{\pi a_0^3} e^{-2r/a_0}$

$$= \frac{4\pi}{G} \int dr \frac{1}{\pi a_0^3} r \sin Gr\, e^{-2r/a_0}$$

$$= \frac{4}{a_0^3 G} \int dr\, r \frac{e^{iGr} - e^{-iGr}}{2i} e^{-2r/a_0}$$

$$= \frac{2}{i a_0^3 G} \int_0^\infty \left(r e^{(iG - 2/a_0)r} - r e^{(-iG - 2/a_0)r} \right) dr$$

$$\int_0^\infty \underbrace{x}_{u} \underbrace{e^{-bx} dx}_{dv} = \frac{x e^{-bx}}{-b} \Big|_0^\infty + \int_0^\infty \frac{e^{-bx}}{b} dx = \frac{1}{b} \int_0^\infty e^{-bx} dx = \frac{1}{b^2}$$

$$= \frac{2}{G i a_0^3} \left[\frac{1}{(iG - 2/a_0)^2} - \frac{1}{(-iG - 2/a_0)^2} \right]$$

$$= \frac{2}{G i a_0^3} (iG - 2/a_0)^{-2} (-iG - 2/a_0)^{-2} \left[(-iG - 2/a_0)^2 - (iG - 2/a_0)^2 \right]$$

$$= \frac{2}{G i a_0^3} (G^2 + 4/a_0^2)^{-2} \left[-G^2 + 4iG/a_0 + 4/a_0^2 + G^2 + \frac{4iG}{a_0} - \frac{4}{a_0^2} \right]$$

$$= \frac{2}{G a_0^3} \frac{1}{(G^2 + 4/a_0^2)^2} \frac{8iG}{a_0}$$

$$= 16 / (G^2 a_0^2 + 4)^2$$

For $G \to 0$ $\quad f_G \to 1$

For $G \to \infty$ $\quad f_G \to 16 / G^4 a_0^4$

project:

7

The charge in momentum must equal a reciprocal lattice vector

$$\vec{\Delta k} = \vec{k'} - \vec{k} = \vec{G}$$

If the scattering is elastic $|\vec{k'}| = |\vec{k}|$ and hence

$$\vec{k'} = \vec{k} + \vec{G}$$

$$\cancel{k'^2} = \cancel{k^2} + 2\vec{k}\cdot\vec{G} + G^2$$

$$\vec{k}\cdot\hat{G} = \tfrac{1}{2}|\vec{G}|$$

component of k along $\hat{G}$

$= \tfrac{1}{2}$ length of $\vec{G}$ $\Rightarrow$ $\vec{k}$ lies on plane bisecting $\vec{G}$

If x-ray source is nonmonochromatic so that $|\vec{k}|$ has a continuous range of values, or if crystal is rotated, experimentalists can guarantee the Bragg condition will be satisfied.

8 If only one $v_n \neq 0$ it must equal 1 by normalization.

Then $\sum v_n^4 = 1$ and $P = 1$.

If all v_n are equal they must be $v_n = 1/\sqrt{N}$ to normalize.

Then $\sum v_n^4 = \sum 1/N^2 = 1/N$ and $P = N$

The participation ratio makes sense here. In case 1 only a single component is nonzero. In ~~a~~ case 2 they all are.

DiVOGA