MIDTERM EXAM

Physics 140A– WINTER 2013

Instructions: Do any six of the eight problems. (All are worth the same number of points.)

[**1.**] Numbers! Numbers! Numbers!
a) What is a typical spacing between atoms in a crystal (in meters)?
b) What is the wavelength of visible light (in meters)?
c) What are the energy levels of the Hydrogen atom in eV? In Joules?
d) What is the mass of the electron (in kg)?
e) What is the mass of the proton (in kg)?
f) What is Avogadro's Number?
g) What do you get when you multiply Avogadro's Number by the mass of a proton (in grams)? Why?

[**2.**] The primitive lattice vectors of a BCC lattice are

$$\begin{aligned}\vec{a}_1 &= \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z})\\ \vec{a}_2 &= \frac{a}{2}(+\hat{x}-\hat{y}+\hat{z})\\ \vec{a}_3 &= \frac{a}{2}(+\hat{x}+\hat{y}-\hat{z})\end{aligned}$$

a) Compute the volume of the unit cell.
b) Compute the reciprocal lattice vectors.
c) Compute the volume of the unit cell of the reciprocal lattice.

[**3.**] Given a crystal lattice defined by primitive lattice vectors $\vec{a}_i$ and reciprocal lattice vectors $\vec{b}_i$.
a) What must be true of the incoming and outgoing momenta $\vec{k}$ and $\vec{k}\,'$ to get a Bragg peak?
b) The "Ewald construction" begins by considering the incoming x-ray wave vector $\vec{k}$ with its tail at the origin and drawing a sphere centered at the tip of $\vec{k}$ and passing through the origin. Show that $\vec{G} = \vec{k}\,' - \vec{k}$ must lie on this sphere to get a Bragg peak. You can assume the scattering is elastic.

[**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? Prove your answer.

[**5.**] One way to describe a crystal lattice is via the families of parallel planes which contain infinite numbers of atoms. Show that, given such a family with separation d, there are always reciprocal lattice vectors perpendicular to these planes, and that the shortest one has length $2\pi/d$. For this second part, it is sufficient to do a couple of examples.

$q + k' =$

[6.] Consider a collection of eight masses m connected by springs of spring constant k with periodic boundary conditions.
a) What are the eight normal mode frequencies?
b) What are the eight normal mode vectors?
c) What is the physical interpretation of the mode (1 1 1 1 1 1 1 1)? How would you justify the fact the excitation energy is zero?
d) Some of the normal mode frequencies are degenerate. The normal modes that we wrote in class for those frequencies have entries which are complex numbers. Yet we expect the positions of the masses to be real. Is this a difficulty?

[7.] Words! Words! Words!
a) Why do we call the vibrations of a crystal lattice "phonons"?
b) What are the two branches of the phonons which arise when there are two different mass atoms in the unit cell called? What is the origin of the name of the branch which comes in to non-zero ω as $q \to 0$?
c) What is the difference between a transverse and a longitudinal wave?
d) What are "periodic boundary conditions" (pbcs)? Why are they useful? (If you like, answer this question about usefulness in terms of the consequence of the use of pbcs in our mass-spring problem.)
e) What are "Miller indices"?

[8.] Programming-related stuff!
a) Suppose the components of a vector are

$$v_n = A \exp\Big(- \frac{(n - N/2)^2}{\xi^2} \Big)$$

What would you get (roughly) if you computed the participation ratio?
b) What is the basic idea of root finding by the bisection method? If you start out with two bracket points separated by a spacing $\Delta x = 1$, to how many decimal places will you know the root after 20 iterations? (Hint: $2^{10} = 1024$.)
c) Consider a collection of random numbers r_i which are uniformly distributed $0 < r_i < 1$. What is the definition of the nth moment? What is its value?

1.

Physics 140A
MIDTERM EXAM – SOLUTIONS
WINTER 2013

$\boxed{1}$

(a) Typical interatomic distances in a crystal are $\sim 2-3\,\mathring{A}$ ($2-3\cdot 10^{-10}$ m). Compare this to the Bohr radius of the hydrogen atom $0.523\,\mathring{A}$.

(b) Wavelength of visible light $\sim 400-700$ nm $= 4-7\cdot 10^{-7}$ m

Notice this is 10^3 times larger than the interatomic spacing (a): Visible light is not the best probe of crystal structure

(c) $E_n = {-13.6\text{ eV}}/{n^2} \quad n=1,2,3,\ldots$

$1\text{ eV} = 1.6\cdot 10^{-19}$ J

(d) $m_e = 9.11\cdot 10^{-31}$ kg

(e) $m_p = 1.67\cdot 10^{-27}$ kg $= 1.67\cdot 10^{-24}$ g

(f) $N_A = 6\cdot 10^{23}$

(g) $N_A\, \underbrace{m_p}_{\text{in grams}} = 1$. This is because Avogadro's number is defined as the number of atoms in 1 gram of Hydrogen, and Hydrogen has a mass of one proton.

2.

$\boxed{2}$ $V_c = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z}) \cdot \frac{a^2}{2}(\hat{y}+\hat{z}) = a^3/2.$

a)

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

b) $\vec{b}_1 = \frac{2\pi}{V_c}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{(a^3/2)} \frac{a^2}{2}(\hat{y}+\hat{z}) = \frac{2\pi}{a}(\hat{y}+\hat{z})$

Similarly $\vec{b}_2 = \frac{2\pi}{a}(\hat{x}+\hat{z})$

$\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y})$

c) General Thm $V_c V_{BZ} = (2\pi)^3$ so $V_{BZ} = \frac{(2\pi)^3}{a^3/2} = \frac{16\pi^3}{a^3}$

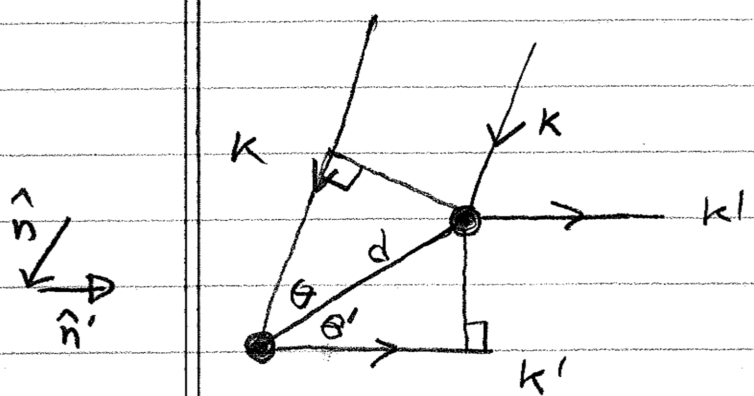
Explicit calculation: $\vec{b}_2 \times \vec{b}_3 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} \left(\frac{2\pi}{a}\right)^2 = \left(\frac{2\pi}{a}\right)^2 \left[-\hat{x}+\hat{y}+\hat{z}\right]$

$\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \left(\frac{2\pi}{a}\right)^3 \left[\hat{y}+\hat{z}\right] \cdot \left[-\hat{x}+\hat{y}+\hat{z}\right] = 2\left(\frac{2\pi}{a}\right)^3$ W

$\boxed{3.}$ a) Basic Principle of scattering is that $\vec{k}' - \vec{k} = \vec{G}$

where $\vec{G} = n_1 \vec{b}_1 + n_2 \vec{b}_2 + n_3 \vec{b}_3$ is a reciprocal lattice vector

The argument is due to von Laue:



For constructive interference

$$d\cos\theta + d\cos\theta' = n\lambda$$

$$\vec{d}\cdot\hat{n} - \vec{d}\cdot\hat{n}' = n\lambda$$

$$\frac{\vec{d}\cdot\vec{k}}{|\vec{k}|} - \frac{\vec{d}\cdot\vec{k}'}{|\vec{k}|} = n\lambda$$

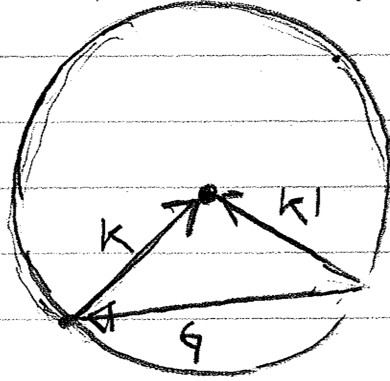
Elastic $|\vec{k}'| = |\vec{k}| = \frac{2\pi}{\lambda}$

$$\Rightarrow \quad \vec{d}\cdot(\vec{k} - \vec{k}') = 2\pi n$$

But the reciprocal lattice vectors $\vec{G}$ are defined by precisely the same condition $e^{i\vec{d}\cdot\vec{G}} = 1$

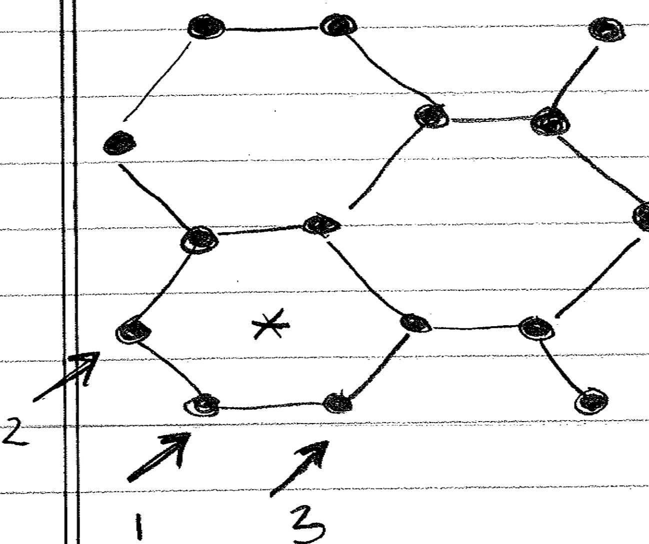
b) According to (a) we need $\vec{k}' - \vec{k} = \vec{G}$ and $|\vec{k}| = |\vec{k}'|$ for a Bragg peak

The picture makes it clear that $\vec{G} = \vec{k}' - \vec{k}$ and also $|\vec{k}| = |\vec{k}'|$



4.

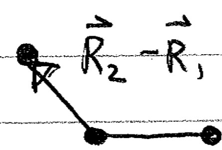
4 Graphene is a single layer/sheet of carbon atoms in a hexagonal arrangement:



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

$\vec{R}_1 = n_1 \vec{a}_1 + n_2 \vec{a}_2$

$\vec{R}_2 = n_1' \vec{a}_1 + n_2' \vec{a}_2$



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

Starting at $\vec{R}_3 = n_1'' \vec{a}_1 + n_2'' \vec{a}_2$ and adding $\vec{R}_2 - \vec{R}_1$

will get us to the center of the hexagon (marked $*$)

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

This is a linear combination of $\vec{a}_1$ and $\vec{a}_2$ with integer coefficients but we do not want it to be an allowed site. $\Rightarrow$ We must use a basis!

5.

$\boxed{5}$ Planes are defined by the eqn $\hat{n}\cdot\vec{r} = d$

where $\hat{n}$ is the normal and d is the distance

from the plane to the origin

The defining eqn of a reciprocal lattice vector $\vec{G}$

is $e^{i\vec{G}\cdot\vec{r}} = 1$. Consider the vectors

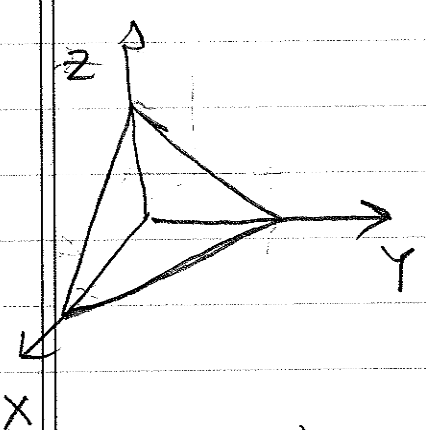
$$\vec{H} = \frac{2\pi}{d}\hat{n}\,(\text{integer})$$

These obey
$$\hat{H}\cdot\vec{r} = \frac{2\pi}{d}\hat{n}\cdot\vec{r}\,(\text{integer})$$
$$= 2\pi\,(\text{integer})$$

Hence $e^{i\vec{H}\cdot\vec{r}} = 1$ and $\vec{H}$ is a reciprocal lattice vector

Do a few examples to show $2\pi/d$ is the shortest length.

Ex 1 CUBIC LATTICE PLANES
$$x+y+z=a$$
$$x+y+z=2a$$
$$x+y+z=3a$$



Normal vector is $\frac{1}{\sqrt{3}}(\hat{x}+\hat{y}+\hat{z})$

$$\vec{G} = \frac{2\pi}{a}(\hat{x}+\hat{y}+\hat{z})(\text{integer})$$

Shortest is $|\vec{G}| = \frac{2\pi}{a}\sqrt{3}$

6.

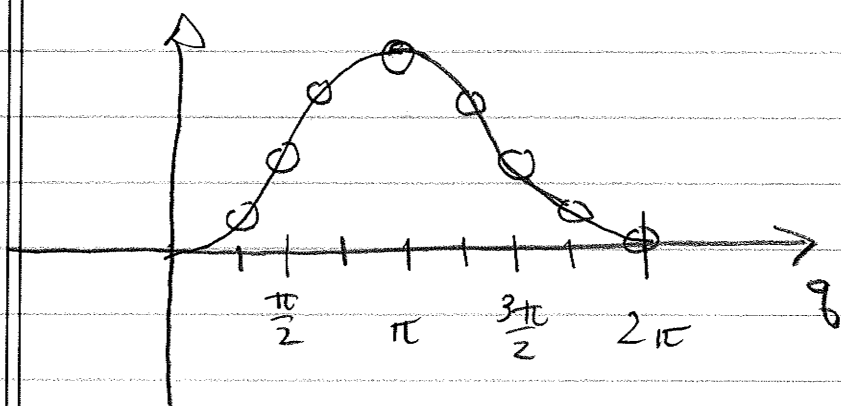
$\boxed{\text{5 cont'd}}$ Distance between planes is $a/\sqrt{3} = d$

$$\frac{2\pi}{d} = \frac{2\pi}{a/\sqrt{3}} = \frac{2\pi}{a}\sqrt{3} = \text{shortest } |\vec{G}| \checkmark$$

7.

$\boxed{6}$ $\omega_n^2 = \frac{2k}{m}(1-\cos q_n)$

a) $q_n = \frac{2\pi}{8}(1,2,3,4,5,6,7,8)$



degeneracy

$= \frac{2k}{m}\left(1-\frac{\sqrt{2}}{2}\right)$	2
$\frac{2k}{m}$	2
$\frac{2k}{m}\left(1+\frac{\sqrt{2}}{2}\right)$	2
$\frac{2k}{m}\,2$	1
0	1

b) Vectors $(V_n)_\ell = \frac{1}{\sqrt{8}} e^{iq_n \ell}$

eigenvector n ℓth component

c) Uniform translation

$\omega_{2\pi}^2 = \phi \iff$ no energy cost to move all masses identical amount since no springs stretch

d) No. All the modes with complex wavevectors have doubly degenerate eigenvalues. Can make linear combination with real wavevectors.

8.

$\boxed{7}$ a) $w^2 = \frac{2k}{m}(1-\cos q)$

Expand $\cos q = 1 - q^2/2$ small q

$w^2 = \frac{2k}{m} q^2/2$

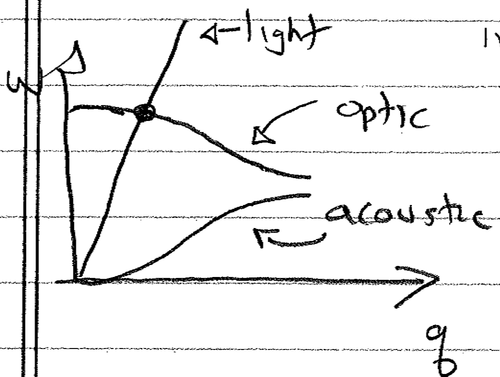
$w = \sqrt{\frac{k}{m}}\, q$

w is linear in q like photon $w = ck$

b) acoustic/optic

nonzero w as $q \to 0$

intersects photon dispersion $\Rightarrow$ interacts well with light



c) transverse: oscillation $\perp$ propagation direction

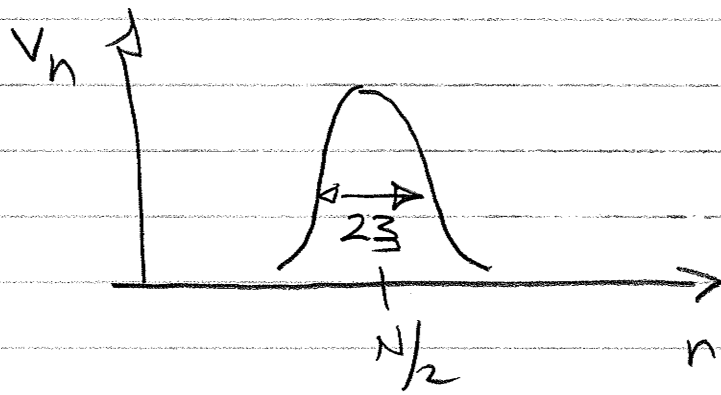
longitudinal: " $\parallel$ "

d) In mass spring problem we connected masses 1 and N.

This allowed a much simpler form for eigenvalues/vectors

(Restored translation invariance $\rightarrow$ momentum good quantum #)

$\boxed{8}$ a) $\gamma \approx 23$ because γ measures # of nonzero components and V_n looks like

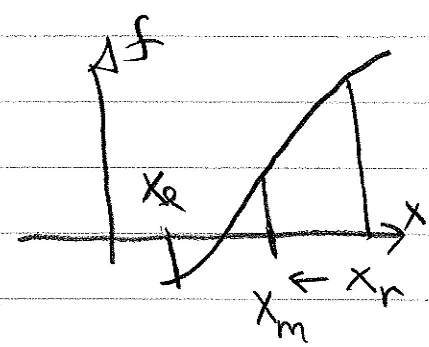


b) Make a guess for X_e and X_r that bracket root, i.e $f(x_e) < 0$ $f(x_r) > 0$.

Compute $f(x_m)$ $x_m = \frac{1}{2}(x_e + x_r)$

If $f(x_m) < 0$ $x_e = x_m$

$f(x_m) > 0$ $x_r = x_m$



Convergence $\sim 1/2^{\#its}$

If $\#its = 20$ $1/2^{20} = 10^{-6} \rightarrow$ 6 decimal places

c) $$\langle r^n \rangle = \frac{1}{N} \sum_{i=1}^{N} r_i^n$$

$$\langle r^n \rangle = 1/{n+1}$$