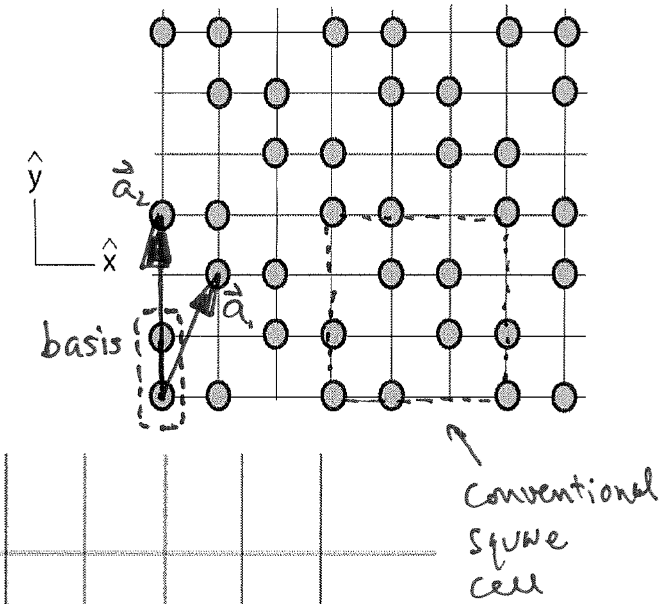
Solid State Physics Midterm Exam **In Class** Name Solutions

Consider the 2D arrangement of atoms shown. It's a small part of a very large crystal. The grid lines are at 2 Å separation.

a. Sketch **primitive** lattice vectors, and write them in terms of x and y. Circle the basis.



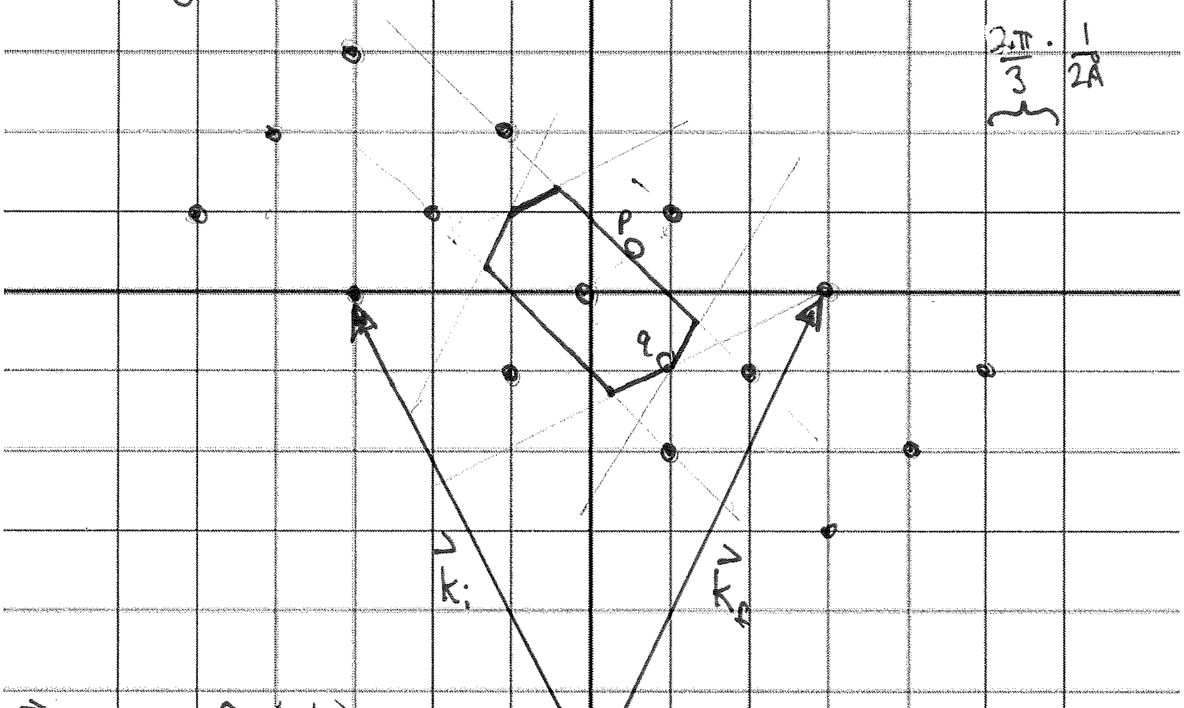
b. Write the reciprocal lattice vectors in terms of x, y. (Hint, which you may not need: you can add z as a third primitive lattice vector.)

$\vec{b}_1 \perp \vec{a}_2 \quad \vec{b}_2 \perp \vec{a}_1$

Sketch part of the reciprocal lattice nearest the origin, showing at least 9 reciprocal lattice points, using the graph paper below. You can choose whatever scale you want for the lines on the paper, so long as the reciprocal lattice is big enough to see.

$\vec{b}_1 = 2\pi \hat{x} \left(\frac{1}{2Å}\right) \quad (\vec{b}_1 \cdot \vec{a}_1 = 2\pi)$

$\vec{b}_2 = \frac{2\pi}{3} (-2\hat{x} + \hat{y}) \left(\frac{1}{2Å}\right)$



$\vec{G} = 2\pi \hat{x} \left(\frac{1}{2Å}\right)$

$S_G = f\left[1 + \exp\left(-i\left(2\pi \hat{x} \frac{1}{2Å} \cdot 2Å\, \hat{y}\right)\right)\right]$

$= 2f \quad$ so $\quad F_G = 2Nf.$

c. Add to your sketch the boundaries of the 1st Brillouin zone.

d. Add to your sketch **any pair** of initial and final k-vectors for an allowed, in-plane (elastic) x-ray diffraction.

e. Find the scattered amplitude for your choice in (d). Be sure to include the structure factor appropriate to your choice of basis in (a). Assume the crystal has N unit cells, and the atomic form factor is f.

f. Consider the continuum description of plane waves traveling at 45° to the x- and y-axes (up and to the right.) Take the spring constant for closely spaced atomic planes to be 3C and for widely spaced atomic planes to be C. Take the mass of a plane of atoms to be m. Write down the equations of motion for u_s and v_s. Then, substitute in a trial solution

$$\begin{pmatrix} u_s \\ v_s \end{pmatrix} = \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} e^{i(Ksa-\omega t)}$$

and find an equation for ω^2 (as a function of K). (a is the distance between identical planes, i.e. $3\sqrt{2}$ Å.) Find ω (or ω's, plural) at K=0 and K=π/a.

How many branches does the dispersion curve ω(K) have? Sketch *roughly. (No additional calculation required.)*

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g.In the continuum limit, acoustic wave speeds are related to the elastic constants, the matrix of C_{ij}. Finding a wave speed involves substituting a trial wave into "F=ma", given by eqns 55-57 in Kittel Chapter 3. (Eqns 57 are valid for cubic crystals, or for crystals in which C_{ij} has "cubic" form.)

Write down a trial longitudinal wave moving up and right (45° to the x and y axes), with wavevector K and frequency ω.
(In other words, write down the displacement of each atom in the x-direction = u, and the displacement in the y-direction, v. *Write down a wave that is guaranteed to be longitudinal, regardless of the choice of any variables you include in your expression.*)

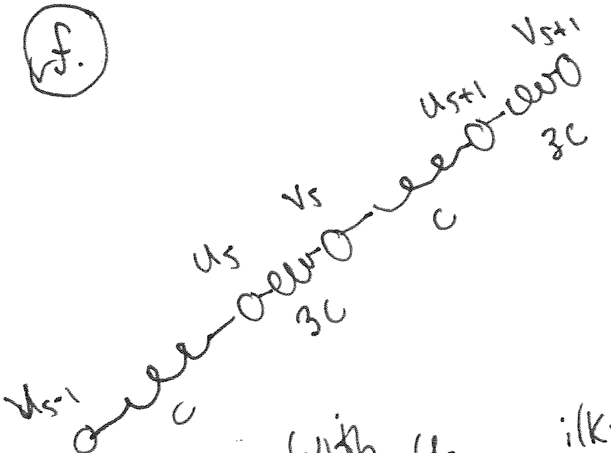
Extra credit: write down a trial in-plane shear wave moving in the same direction.

h. Suppose the 2D crystal above has a heat capacity that varies (at low temperature) like T^2. Do you expect it to be a conductor or an insulator?. Why? (No calculations necessary, just say which.)

Insulator. Conductors always have $C \propto T$, regardless of dimension.

i. In fact, each atom of the crystal can give up one electron to the electron sea. Find the Fermi energy, and the average kinetic energy of electrons at 0K.

f.



$F = ma$

$$m\frac{d^2u_s}{dt^2} = -(u_s - v_{s-1})c + (v_s - u_s)\cdot 3c$$

$$m\frac{d^2v_s}{dt^2} = -(v_s - u_s)\cdot 3c + (u_{s+1} - v_s)\cdot c$$

with $\begin{matrix} u_s \\ v_s \end{matrix} \sim e^{i(ksa-\omega t)}$, we get

$$-\omega^2 u = -4cu + 3cv + cv e^{-ika}$$

$$-\omega^2 v = -4cv + 3cu + cu e^{+ika}$$

$m \to 1$.
Can add back later.

$$\begin{bmatrix} -4c+\omega^2 & c(3+e^{-ika}) \\ c(3+e^{+ika}) & -4c+\omega^2 \end{bmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = 0$$

Det $= 0$.

$$(\omega^2 - 4c)^2 - c^2(9 + 1 + 3(e^{ika} + e^{-ika})) = 0$$

$$\omega^4 - 8c\omega^2 + 16c^2 - c^2(10 + 6\cos ka) = 0$$

$$\omega^4 - 8c\omega^2 + 6c^2(1-\cos ka) = 0$$

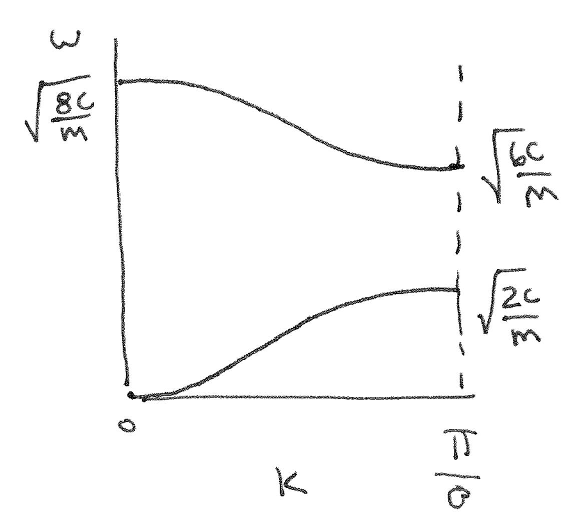
At $k=0$, $\cos ka = 1$

$\omega^2 = 0$ or $\omega^2 = 8c$.

At $ka = \pi$, $\cos ka = -1$

$$\omega^2 = \left(8c \pm \sqrt{64c^2 - 4\cdot 12c^2}\right)/2$$

$$= (8c \pm 4c)/2 \Rightarrow \omega^2 = 2c,\ 6c.$$



TWO BRANCHES

(g.) $u = u_0 e^{i(K_x x + K_y y - \omega t)}$

$v = v_0 e^{i(K_x x + K_y y - \omega t)}$

Longitudinal wave requires $u_0 = v_0$.

To move at 45°, $K_x = K_y = \frac{K}{\sqrt{2}}$.

Pure shear wave: $u_0 = -v_0$.

(i) Easiest: use a conventional square cell w. 6 e^-.

$$6N = \int_0^{k_f} 2\pi k\,dk \cdot \left(\frac{L}{2\pi}\right)^2 \cdot \underset{\downarrow\uparrow}{2}$$

$$= \frac{k_f^2}{2} \cdot \frac{1}{\pi} \cdot L^2 \qquad \text{Now } L^2 = Na^2 \text{ so}$$

$$a^2 k_f^2 = 12\pi. \qquad \text{For conventional cell, } a = 6 Å.$$

$$k_f^2 = \frac{\pi}{3} \frac{1}{Å^2}.$$

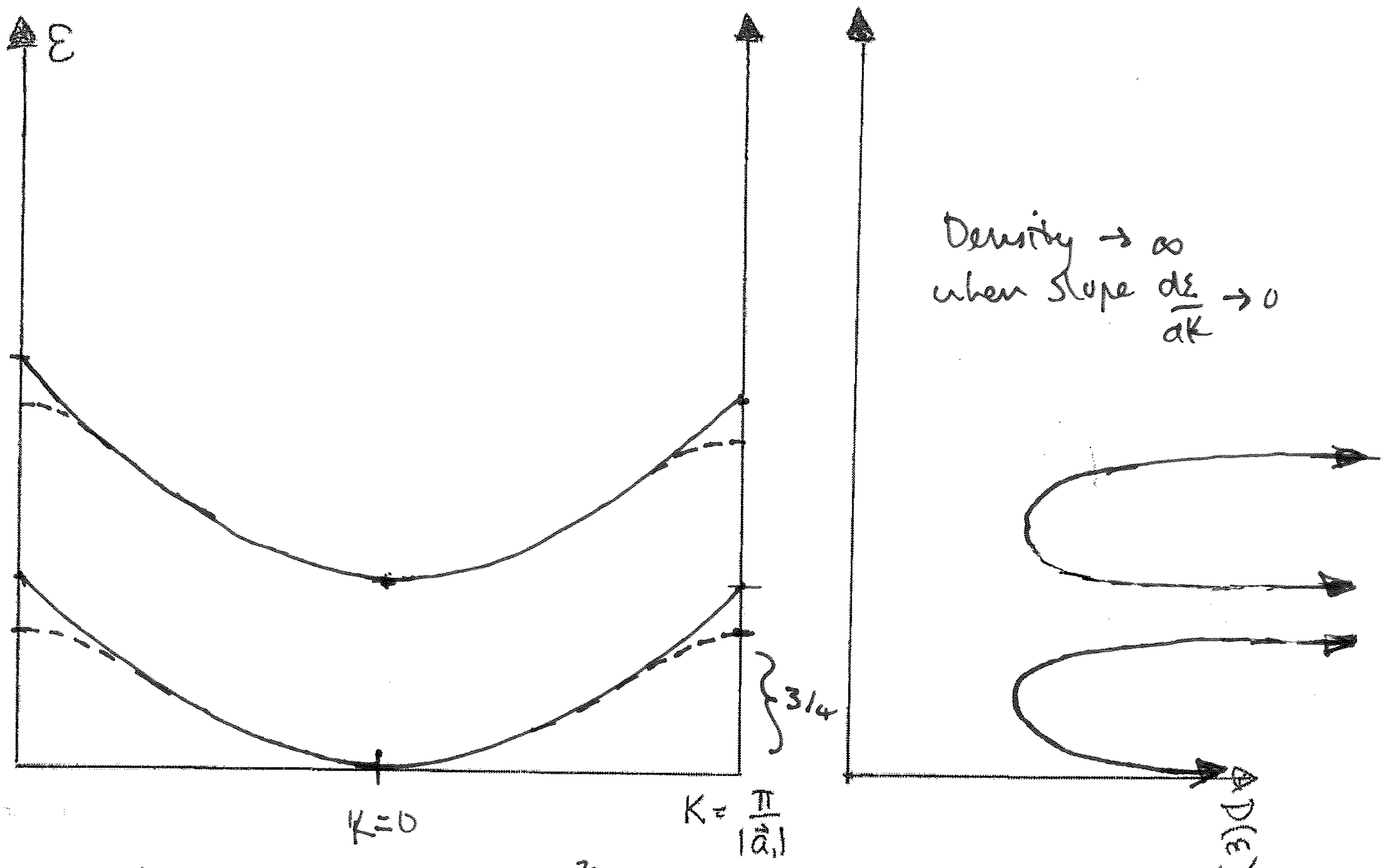
$$\mathcal{E}_f = \frac{\hbar^2 k_f^2}{2m} = \frac{\pi \hbar^2}{6m} \frac{1}{Å^2}.$$

$$\text{Avg } \mathcal{E} = \frac{\int_0^{k_f} \cancel{2}\pi k\,dk \cdot \frac{\hbar^2 k^2}{\cancel{2}m} \rightarrow \frac{k_f^4}{4} \cdot \frac{\pi \hbar^2}{m}}{\int_0^{k_f} 2\pi k\,dk \rightarrow \pi k_f^2} = \frac{\hbar^2 k_f^2}{4m} = \frac{\mathcal{E}_f}{2}.$$

j. Sketch two free electron bands in the "reduced zone scheme", along the longest direction of the 1st BZ. Sketch the lowest energy band, and the second lowest energy band (which you get from using the *smallest* G vector offset… not necessarily $\vec{b}_1$ or $\vec{b}_2$!)

k. Suppose the atomic potential is strong enough to distort the bands and make this a semi-metal. Draw the 2 bands in the presence of this potential on your sketch, using dashed lines. Need to make energy at p > energy at q.
With free e^-, it's half.

l. Very roughly sketch the density of electron states next to your bands.



Density → ∞ when slope $\frac{d\mathcal{E}}{dk} \to 0$

max k^2 in 1st BZ $= \left(\sqrt{2}\ \frac{2\pi}{3}\right)^2 \sim \mathcal{E}$

$\frac{8\pi^2}{9}$

With $G_{08} = \hat{x}+\hat{y}\ \left(\frac{2\pi}{3}\right)$

$k' = \alpha(\hat{x}-\hat{y})$ (long axis in 1st BZ) $\alpha: -\frac{2\pi}{3} \to +\frac{2\pi}{3}$