**1. Crystal structure, etc**. (20 pts.)
Shown here are three views of the structure of $CeRhIn_5$. The Ce^{4+} (cerium) ions form an inert framework at the corners of the tetragonal cell, which has lattice constants $a=b=4.674$ Å, and $c=7.501(5)$ Å. The left view shows a single unit cell, and the right view shows two stacked cells. Below is shown a view with multiple cells. You can choose coordinates x,y,z to coincide with the a, b, c vectors which go from Ce ion to Ce ion.
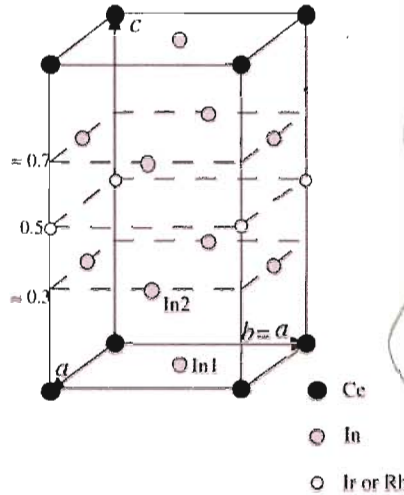
a. What are the primitive reciprocal lattice vectors?

$$\vec{A} = \frac{2\pi}{a}\hat{x} \qquad \vec{B} = \frac{2\pi}{a}\hat{y} \qquad \vec{C} = \frac{2\pi}{c}\hat{z}$$

b. In the left view, if you look carefully, you will see that one atom is labeled "In1" and another is labeled "In2". In is the element indium. A total of 10 In atoms are shown in the picture. How should they be labeled? Are the labels In1, In2 sufficient? You want to use as few sensible labels as possible and explain what that means.)

Every In atom is either type 1 (on $\hat{z}$-face of rectangular cell) or type 2 (on $\hat{x}$ or $\hat{y}$ face.) Every In_1 is equivalent to every other In_1 by translation. Every In_2 is equivalent to every other In_2 by translation and/or 90° rotation.
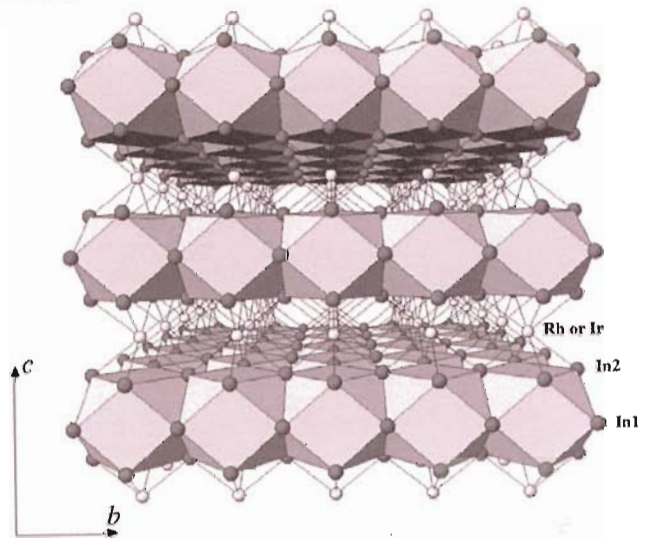
c. The Rh (rhodium) atoms lie halfway between the Ce ions on 4 edges of the unit cell. How many nearest-neighbor In atoms does each Rh atom have? How many near neighbor In atoms does each Ce ion have (these neighbors come in two varieties.)

Each Rh has 8 nn In atoms (all type 2)
Each Ce atom has 12 nn In atoms (8 of type 2, 4 of type 1)
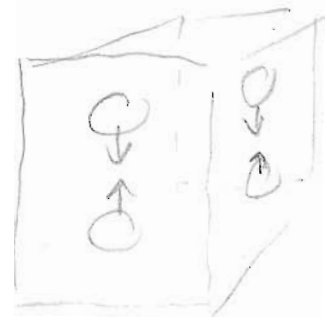
d. There is a vibrational eigenvector where only the In2 atoms move. They move in the z-direction, and the direction alternates $(+,-,+,-,\ldots)$ as you go up the z axis. The direction is the same for all In atoms with the same z coordinate. What quantum numbers or other descriptive labels would you give to such a mode? Try to make a convincing argument using symmetries that this is indeed an eigenmode (in harmonic approximation.)

This is a completely symmetric mode (invariant under all translations/rotations.) It is the only completely symmetric distortion except for volume or uniaxial compression. Therefore it has to be an eigenmode. [Chemists use the label A_{1g}; Wigner would call it Γ_1; it has $\vec{k}=0$.]

2. **Surface vibrational mode.** (25 pts.) Consider a semi-infinite linear chain of atoms of mass M, coupled by nearest-neighbor springs K. The first atom, at $R_0 = 0$, has a different mass, m. All other atoms are at $R_n = na$, with n a positive integer. The true locations are of course $r_n = R_n + u_n$, where the displacement u_n is small compared with a. Bloch's theorem does not work, strictly speaking, because the system is not periodic. But no real solid is either. You have a right to expect that, not too close to the surface ($x=0$), the vibrational spectrum will be indistinguishable from the spectrum of a truly periodic (infinite) system. The main new thing that happens is a possible state localized near the surface. This state would have to be out of the frequency range of the eigenstates of the infinite sample, that is, at higher ω. Therefore, it should alternate in sign (u_{n+1} and u_n should have opposite signs.) Also it should decay exponentially. The simplest trial state is $u_n = \exp(-\kappa na - i\omega t)$. Show that there does there exist such a state when $m < M/2$. Find κ and ω in terms of the given parameters K and m/M.

(i) $\quad m\ddot{x}_0 = K(x_1 - x_0)$

(ii) $\quad M\ddot{x}_n = K(x_{n+1} + x_{n-1} - 2x_n) \qquad n > 0$

Let $x_n = (-1)^n e^{-n\kappa a} e^{-i\omega t}$

(i') $\quad -m\omega^2 = -K(e^{-\kappa a} + 1)$

(ii') $\quad -M\omega^2 = -K(e^{\kappa a} + e^{-\kappa a} + 2) = -K(e^{\kappa a} + 1)(e^{-\kappa a} + 1)$

Divide (ii') by (i')

$$\frac{M}{m} = e^{\kappa a} + 1$$

For κa real and positive, $M/m > 2$

$$K_a = \begin{cases} \frac{1}{a} \log\left(\frac{M}{m} - 1\right) & \text{if } \frac{M}{m} > 2, \; K > 0 \\ \text{no positive solution} & \text{if } \frac{M}{m} < 2 \end{cases}$$

$$\omega^2 = \frac{K}{m}\left(1 + \frac{1}{e^{Ka}}\right)$$

$$\to \frac{K}{m}\left(1 + \frac{1}{\frac{M}{m} - 1}\right) = \boxed{\frac{K}{m}\left(\frac{M}{M - m}\right) = \omega^2}$$
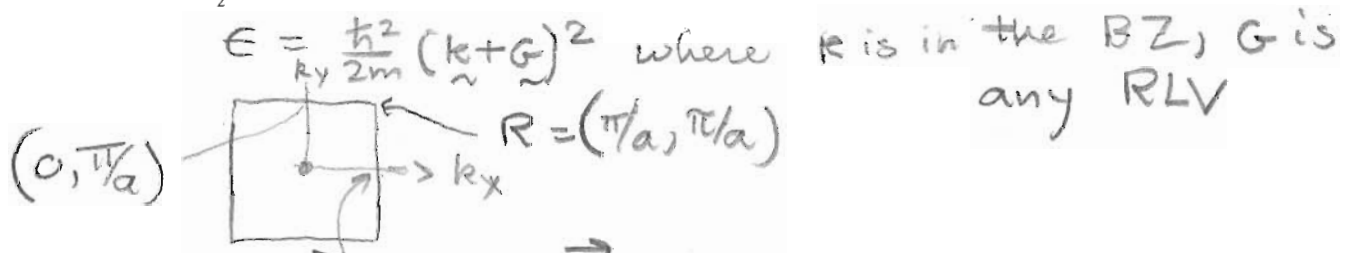
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3. Nearly free electrons in d=2. (25 pts.) Suppose electrons live on a two dimensional square lattice. Atoms are at positions $\vec{R}_{m,n} = m\vec{a} + n\vec{b}$, where $\vec{a} = a\hat{x}$ and $\vec{b} = a\hat{y}$. The crystal potential is periodic. It is weak, and is written as

$$V(\vec{r}) = V_0 \sum_{i=1,2,3,4} \exp(i\vec{G}_i \cdot \vec{r}) + V_1 \sum_{i=5,6,7,8} \exp(i\vec{G}_i \cdot \vec{r})$$

where $\vec{G}_1 = (2\pi/a)\hat{x}$, $\vec{G}_2 = (-2\pi/a)\hat{x}$, $\vec{G}_3 = (2\pi/a)\hat{y}$, $\vec{G}_4 = (-2\pi/a)\hat{y}$, and
$\vec{G}_5 = (2\pi/a)(\hat{x} + \hat{y})$, $\vec{G}_6 = (2\pi/a)(-\hat{x} + \hat{y})$, $\vec{G}_7 = (2\pi/a)(\hat{x} - \hat{y})$, $\vec{G}_8 = (2\pi/a)(-\hat{x} - \hat{y})$.
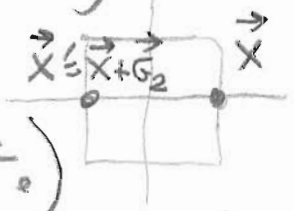
a. Suppose the potential is zero, i.e. $V_0 = V_1 = 0$. Explain why the lowest band at the "X" point is doubly degenerate ($\vec{X}$ denotes the wavevector $(\pi/a)\hat{x}$). Perhaps it is better to ask, "in what sense" is the lowest band at the X point doubly degenerate? After all, there are infinitely many examples of energies $\varepsilon_1(\vec{k}_1)$ and $\varepsilon_2(\vec{k}_2)$ which are equal. We do not refer to them as degenerate if the k-vector $\vec{k}_1$ is unrelated to the k-vector $\vec{k}_2$.
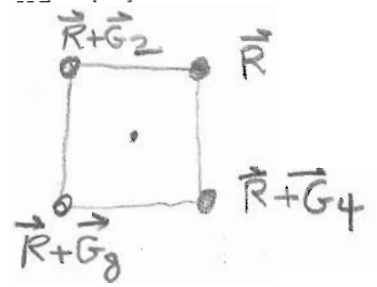
$E = \frac{\hbar^2}{2m}(\underset{\sim}{k} + \underset{\sim}{G})^2$ where $\underset{\sim}{k}$ is in the BZ, G is any RLV

$(0, \pi/a)$

$R = (\pi/a, \pi/a)$

$\vec{X} = (\pi/a, 0) = \vec{G}_1/2$

at the X point, $E(\vec{G}) = \frac{\hbar^2}{2m}(\vec{G}_1/2 + \vec{G})$

Note that $E(0) = E(-\vec{G}_1)$

(The 2 points labelled x, x'

$\vec{X} \leq \vec{X} + \vec{G}_2 \quad \vec{X}$

belong to the same $\vec{k}$-vector.)

This clarifies the "double degeneracy" of E at X_0.

b. What is the degeneracy of the "R" point ($\vec{R}$ denotes the wavevector $(\pi/a)(\hat{x}+\hat{y})$)?

The 4 corners all belong to the same $\vec{k}$-vector so degeneracy = 4.

c. What is the energy splitting of the lowest bands at the X point, in the case where both V_0 and V_1 are small compared with $E_0 = \hbar^2(\pi/a)^2/2m$? Give the answer to lowest order in the potential.

$$\Psi = c_1|k\rangle + c_2|k+G_2\rangle + \cdots$$

These 2 states become degenerate at X.

$$|\Psi\rangle = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \qquad H = \begin{pmatrix} \frac{\hbar^2}{2m}k^2 & V(G_2) \\ V(G_2) & \frac{\hbar^2}{2m}(k+G_2)^2 \end{pmatrix}$$

at X, $k^2 = \left(\frac{\pi}{a}\right)^2 = (k+G_2)^2$

$V(G_2) = V_0$

$$H = \begin{pmatrix} \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 & V_0 \\ V_0 & \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 \end{pmatrix}$$

Eigenvalues are $\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 \pm |V_0|$

Splitting is $2|V_0|$

d. What is the band mass m_{xx} of the lowest two bands at the X point? The definition is $\hbar^2/m_{xx} = \partial^2\varepsilon(\vec{k})/\partial k_x^2$, evaluated at the X point. Give the answer to lowest order in the potential parameters V_0 and V_1.

near X

$$E = \frac{1}{2}\left[\frac{\hbar^2 k^2}{2m} + \frac{\hbar^2(k+G_2)^2}{2m}\right] \pm \left\{\left(\frac{1}{2}\left[\frac{\hbar^2 k^2}{2m} - \frac{\hbar^2(k+G_2)^2}{2m}\right]\right)^2 + V_0^2\right\}^{1/2}$$

along $k = (1,0)$ direction let $k = \left(\frac{\pi}{a}+\delta\right)$

$(k+G_2) = \left(-\frac{\pi}{a}+\delta\right)$

$$\frac{1}{2}\left(\frac{\hbar^2 k^2}{2m} + \frac{\hbar^2(k+G_2)^2}{2m}\right) = \frac{\hbar^2}{2m}\left[\left(\frac{\pi}{a}\right)^2 + \delta^2\right]$$

$$\frac{1}{2}\left(\frac{\hbar^2 k^2}{2m} - \frac{\hbar^2(k+G_2)^2}{2m}\right) = \frac{\hbar^2}{2m}\left(2\frac{\pi}{a}\delta\right)$$

So for $\vec{k} = \left(\frac{\pi}{a} + \delta, 0\right)$

$$\epsilon = \frac{\hbar^2}{2m}\left(\left(\frac{\pi}{a}\right)^2 + \delta^2\right) \pm \sqrt{\left(\frac{\hbar^2}{m}\frac{\pi}{a}\delta\right)^2 + V_0^2}$$

$$\frac{\hbar^2}{m_{xx}} = \frac{\partial^2 \epsilon}{\partial \delta^2} = \frac{\hbar^2}{m} \pm \frac{d^2}{dE^2}\left(E^2 + V_0^2\right)^{1/2} \times \left(\frac{\partial E}{\partial \delta}\right)^2$$

where $E = \frac{\hbar^2}{m}\frac{\pi}{a}\delta$; $\frac{\delta E}{\delta \delta} = \left(\frac{\hbar^2}{m}\frac{\pi}{a}\right)$; $\frac{d^2}{dE^2}\left(E^2 + V_0^2\right)^{1/2} = \frac{V_0^2}{\left(E^2 + V_0^2\right)^{3/2}}$

at X, $E \to 0$,

$$\frac{\hbar^2}{m_{xx}} = \frac{\hbar^2}{m}\left[1 \pm \frac{1}{|V_0|}\frac{\hbar^2 \pi^2}{ma^2}\right]$$

$$\boxed{\frac{m_{xx}}{m} = \frac{1}{1 \pm \pi^2\hbar^2/ma^2|V_0|}}$$

e. **What is m_{yy} at this point?**

Note that near X we have $k = \left(\frac{\pi}{a}, \delta\right)$

where $\delta = k_y$ $\qquad (k + G_2) = \left(\frac{-\pi}{a}, \delta\right)$

So $\epsilon = \frac{\hbar^2\left((\pi/a)^2 + \delta^2\right)}{2m} \pm |V_0|$ and $\boxed{\frac{m_{yy}}{m} = 1}$

f. **Write the Hamiltonian matrix for the lowest degenerate manifold at the R point.**

Let $E = (\hbar^2/2m)\left[(\pi/a)^2 + (\pi/a)^2\right]$ = Free electron energy at R.

$$H = \begin{pmatrix} E & V(G_2) & V(G_4) & V(G_8) \\ V(G_2) & E & V(G_2-G_4) & V(G_2-G_8) \\ V(G_4) & V(G_2G_4) & E & V(G_4-G_8) \\ V(G_8) & V(G_2-G_8) & V(G_4-G_8) & V \end{pmatrix} = \begin{pmatrix} E & V_0 & V_0 & V_1 \\ V_0 & E & V_1 & V_0 \\ V_0 & V_1 & E & V_0 \\ V_1 & V_0 & V_0 & E \end{pmatrix}$$

4. Numerical exercises. (30 pts.)

a. The resistivity of Cu metal at room temperature is $\rho = 1.4\ \mu\Omega$cm. Alternately, we could say that the conductivity is $\sigma = 0.71 \times 10^8\ (\Omega\mu)^{-1}$. What is the time τ between collisions (in sec.)? What is the lifetime broadening $\hbar/\tau$? You may use free electron approximation. The crystal structure is fcc, there is one valence electron per Cu atom, and the lattice constant a (side of the conventional cubic cell) is 3.6 Å.

$$1/\tau = \frac{ne^2}{m\sigma} \qquad n = \frac{4}{a^3} = 0.86 \times 10^{29}\ m^{-3}$$

$$= \frac{(0.86 \times 10^{29}\ m^{-3})(1.6 \times 10^{-19}\ C)^2}{(.911 \times 10^{-30}\ kg)}\left(1.4 \times 10^{-8}\ \frac{J}{C}\frac{S}{C}m\right)$$

$$= 3.4 \times 10^{13}\ s^{-1}$$

$$\boxed{\tau = 3.0 \times 10^{-14}\ s} \quad \boxed{\hbar/\tau = 22\ meV} \quad \left[\text{nearly } kT \text{ at RT}\right]$$

b. Suppose GaAs is n-doped, with $n = 3 \times 10^{17}\ cm^{-3}$. If the carriers go into the conduction band, and the temperature is low enough, find the Fermi energy (relative to the bottom of the conduction band which has effective mass $m*/m = 0.067$). How low a temperature is "low enough?"

$$k_F = (3\pi^2 n)^{1/3} = 2.1 \times 10^6\ cm^{-1} = 2.1 \times 10^8\ m^{-1}$$

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{(1.054 \times 10^{-34}\ Js)(2.1 \times 10^8\ m^{-1})}{2(.911 \times 10^{-30}\ kg)(m*/m)}\frac{1}{1.6 \times 10^{-19}\ J/eV}$$

$$\epsilon_F = 1.7 \times 10^{-3}\ eV \cdot \left(\frac{m}{m*}\right) = 25\ meV \approx 300K$$

"low enough" means $\ll 300K$ (30K, for example)

c. Silicon atoms have mass 28 amu. Neglecting quantum effects, what is the approximate specific heat of Si crystal, at 600K, in J/kgK? The Debye temperature is $\Theta = 520$K. By what factor is the specific heat altered from classical at $T = 10$K?

$$1\ kg = \frac{1000g}{28g/mole} = 36\ moles$$

$$C = 3nR = 3\left(36\ \frac{moles}{kg}\right)\left(8.314\ \frac{J}{mole\ k}\right)$$

$$= 890\ J/kgK$$

Neglecting all factors of π^4 etc, the reduction factor is $(T/\Theta_D)^3 = 7 \times 10^{-6}$