Physics 140A-Introduction to Solid State Physics

Winter, 2016

Final Examination, March 19, 2016

(4 problems, 100 points total)

Name:_____

Signature:_____

Student ID no.:_____

Some possibly useful constants and equations

$c = 3.00 \times 10^8$ m/s $e = 1.60 \times 10^{-19}$ C 1 eV = 1.60×10^{-19} J 1 Rydberg = 13.606 eV

1 Å = 10^{-10} m = 10^{-1} nm $h = 6.63 \times 10^{-34}$ J-s $\hbar = h/2\pi = 1.05 \times 10^{-34}$ J-s

$k_B = 1.38 \times 10^{-23}$ J-K^{-1} $m_e = 9.1094 \times 10^{-31}$ kg = 0.5110 MeV/c^2

$m_p = 1.6726 \times 10^{-27}$ kg = 938.27 MeV/c^2 $m_n = 1.6749 \times 10^{-27}$ kg = 939.57 MeV/c^2

$n\lambda = 2d\sin\theta$ $d_{hk\ell} = n/[h^2/a^2+k^2/b^2+\ell^2/c^2]^{1/2}$ $F_C = k_C q_1 q_2 / r^2$ $k_C \equiv 1/(4\pi\varepsilon_O) = 8.98 \times 10^9$ N-m^2-C^{-2}

$\lambda = h/p$ $p = \hbar k$ $\Delta x \Delta p_X \geq \hbar/2$ $\Delta E \Delta t \geq \hbar/2$

$$e^{\pm ix} = \cos x \pm i \sin x \quad \cos x = \frac{1}{2}\left[e^{ix} + e^{-ix}\right] \quad \sin x = \frac{1}{2i}\left[e^{ix} - e^{-ix}\right]$$

$\sin 2t = 2 \sin t \cos t$ $\cos 2t = \cos^2 t - \sin^2 t = 2\cos^2 t - 1 = 1 - 2\sin^2 t$

$$E_n = -\frac{Z^2 e^2}{8\pi\varepsilon_0 a_0 n^2} = -\frac{13.6 Z^2}{n^2}(eV) \quad r_n = \frac{4\pi\varepsilon_0\hbar^2}{m_e Z e^2} n^2 = a_0 \frac{n^2}{Z} \quad a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} = 0.529 \text{ Å}$$

$$x = r\sin\theta\cos\phi \quad y = r\sin\theta\sin\phi \quad z = r\cos\theta \quad dV = r^2 dr \sin\theta d\theta d\phi$$

$$\psi_{n\ell m_\ell}(r,\theta,\phi) = R_{n\ell}(r)\Theta_{\ell m_\ell}(\theta)\Phi_{m_\ell}(\phi) = R_{n\ell}(r)Y_{\ell m_\ell}(\theta,\phi) \quad P_{n\ell}(r) = r^2 R_{n\ell}^2(r) \quad \psi_{\vec{k}}(\vec{r}) = Ce^{i\vec{k}\bullet\vec{r}}$$

$$V = -\frac{C}{r^6} \quad V = q_0 \sum_{i=1}^{\infty} \frac{(+\text{or}-)n_i q_i}{4\pi\varepsilon_0 r_i} + \frac{A}{r_1^n} \quad F_{FD}(E) = \frac{1}{\exp[(E - E_F)/k_B T] + 1}$$

$$\omega = v_s q \quad v_S = \sqrt{\frac{Y}{\rho}} \quad \varepsilon = \hbar\omega \quad p = \hbar q \quad g(\omega) = \frac{V}{2\pi^2}\frac{\omega^2}{v_s^3} \quad \omega^2 = \alpha\left[\frac{1}{M_1} + \frac{1}{M_2}\right] \pm \alpha\sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4\sin^2(qa)}{M_1 M_2}}$$

$$\varphi_j^{MO}(\vec{r}) = \sum_{\substack{\text{Atoms } A \\ \text{Orbitals } i}}^{N} C_{Ai,j}\varphi_{Ai}^{AO}(\vec{r} - \vec{R}_A) \qquad \varphi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i\vec{k}\bullet\vec{r}} = \sum_{\substack{\text{Atoms } A \\ \text{Orbitals } i}}^{N} e^{i\vec{k}\bullet\vec{R}_A} C_{Ai,\vec{k}}\varphi_{Ai}^{AO}(\vec{r} - \vec{R}_A);\ u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r} + \vec{R}_\ell^{(c)})$$

$$\vec{R}_\ell^{(c)} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \quad \vec{s} = \vec{k} - \vec{k}_0 = \vec{G} \quad f_a = \int_0^R 4\pi r^2 \rho(r)\frac{\sin(sr)}{sr}dr \quad F = \sum_j f_a e^{i\vec{s}\bullet\vec{\delta}_j} \quad S = \sum_\ell e^{i\vec{s}\bullet\vec{R}_\ell^{(c)}} \quad F_{Cryst} = F \bullet S$$

$$\vec{G}_{hk\ell} = h\vec{a}^* + k\vec{b}^* + \ell\vec{c}^* \quad \vec{a}^* = \frac{2\pi(\vec{b}\,x\,\vec{c})}{\vec{a}\bullet(\vec{b}\,x\,\vec{c})} \quad \vec{b}^* = \frac{2\pi(\vec{c}\,x\,\vec{a})}{\vec{a}\bullet(\vec{b}\,x\,\vec{c})} \quad \vec{c}^* = \frac{2\pi(\vec{a}\,x\,\vec{b})}{\vec{a}\bullet(\vec{b}\,x\,\vec{c})}$$

$$\vec{G}_{hk\ell}\bullet\vec{R}_\ell^{(c)} = 2\pi(n_1 h + n_2 k + n_3 \ell)$$

$$I_{hk\ell}(T) = I_{hk\ell}^{(0)} \exp[-\frac{1}{3} < u^2 > G_{hk\ell}^2] = I_{hk\ell}^{(0)} \exp[\frac{-k_B T G_{hk\ell}^2}{M\omega^2}]$$

$$C_V(T) = 9R\left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^4 dx}{(e^x - 1)^2};\ x = \frac{\hbar\omega}{k_B T} \quad C_V(T) = \frac{k_B^2\pi^2}{3}g(E_F)T \approx \frac{\pi^2}{2}RT\frac{k_B T}{E_F} \quad E_F = \frac{\hbar^2}{2m_e}(3\pi^2 N)^{2/3}$$

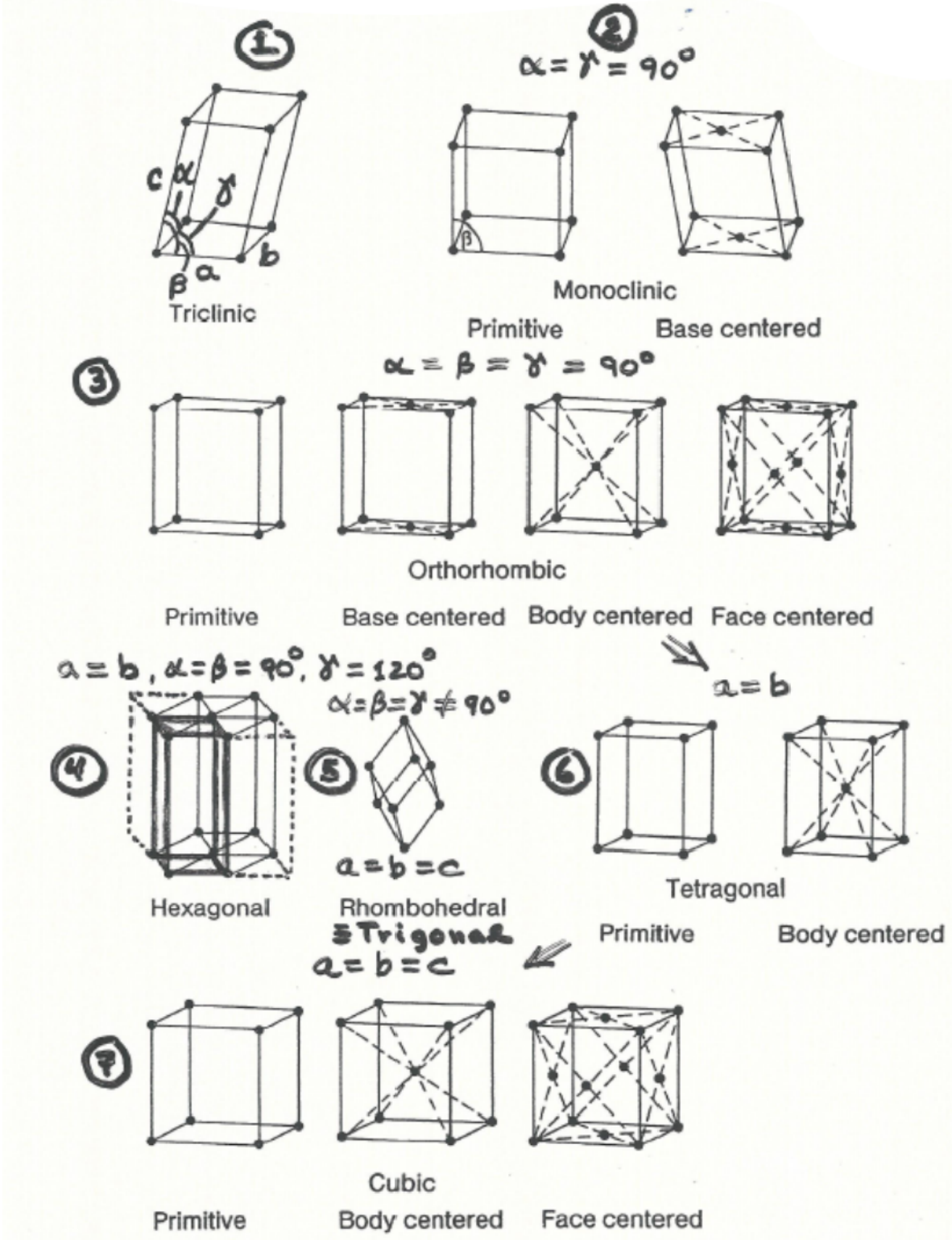
$$v_{ph} = \frac{\omega}{k};\ v_{gr} = \frac{d\omega}{dk} \quad g(E) = \frac{g(\omega)}{\hbar} = \left[\frac{L}{2\pi}\right]^3 \frac{4\pi k^2}{\hbar}\frac{d\omega}{dk} \quad E = \frac{\hbar^2 k^2}{2m_e} \quad \rho_{FE}(E) \propto E^{1/2}$$

$$K = \frac{1}{3}C_V \ell \quad \sigma = Ne^2\tau/m_e \quad V_{NFE}(\vec{r}) = \sum_{hk\ell} V_G e^{i\vec{G}_{hk\ell}\bullet\vec{r}} \quad E_{gap} = 2|V_{-G}| \quad V_{TB}(\vec{r}) = \sum_{R_\ell^{(c)},j} V_j(\vec{r} - R_\ell^{(c)}) \approx V'(x-a) + v(x) = V'(x+a)$$

$$E_{TB}(k) = E_v - \beta - 2\gamma\cos ka = E_0 + 4\gamma\sin^2\left[\frac{ka}{2}\right] \quad \beta = \langle\varphi_v(x)|V'(x)|\varphi_v(x)\rangle \quad \gamma = \langle\varphi_v(x)|V'(x-a)|\varphi_v(x-a)\rangle$$

$$E_{kin} = h\nu - E_{binding} - \varphi_{work} \quad \vec{k}^f = \vec{k}^i + \vec{g}$$

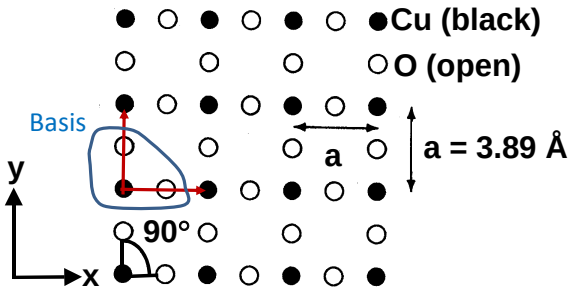
The seven 3D crystal systems and 14 Bravais Lattices



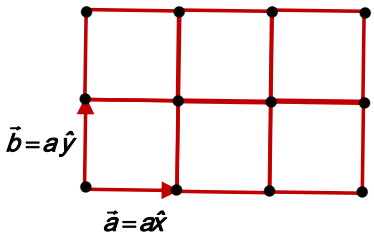
[1] [35 points] An important ingredient in the high-temperature cuprate superconductors is the two dimensional Cu-O planar structure shown below. Let us assume for simplicity that this is a strictly two-dimensional structure.

(a) [5 points] Show one possible set of primitive lattice vectors for this 2D structure, and draw the Bravais lattice associated with it.
(b) [5 points] What is one suitable unit cell, what is the atomic basis, and what is the "chemical formula" of this structure? Note that 2D atomic counting might be different from 3D.

See red vectors defining unit cell and outlined basis below. Formula for layer is CuO_2. The Bravais lattice is a simple square made up of multiples of the red vectors, as shown below also.



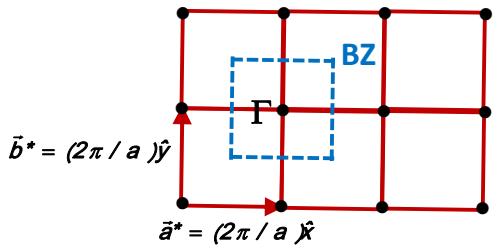
Bravais lattice:



(c) [8 Points] Calculate the reciprocal lattice vectors for this 2D crystal, sketch the reciprocal lattice, with correct magnitudes, and show also the Brillouin zone for this lattice. Note that, in 2D, the 3D formulas for $\vec{a}^*, \vec{b}^*$, and $\vec{c}^*$ (given to you) can still be used if you add a third unit vector $\hat{c}$ perpendicular to $\vec{a}$ and $\vec{b}$.

$$\vec{a}^* = \frac{2\pi(\vec{b}\times\vec{c})}{\vec{a}\bullet(\vec{b}\times\vec{c})} = \frac{2\pi(\vec{b}\times\hat{c})}{\vec{a}\bullet(\vec{b}\times\hat{c})}\hat{x} = \frac{2\pi a}{a^2}\hat{x} = \frac{2\pi}{a}\hat{x} \qquad \vec{b}^* = \frac{2\pi(\vec{c}\times\vec{a})}{\vec{a}\bullet(\vec{b}\times\vec{c})} = \frac{2\pi}{a}\hat{y}$$

Reciprocal lattice:



(d) [12 points] For an arbitrary (hkℓ) Bragg reflection, calculate the overall diffraction structure factor for this 2D crystal, including both the geometric (unit cell) structure factor and the lattice structure factor, and defining all quantities as precisely as you can.

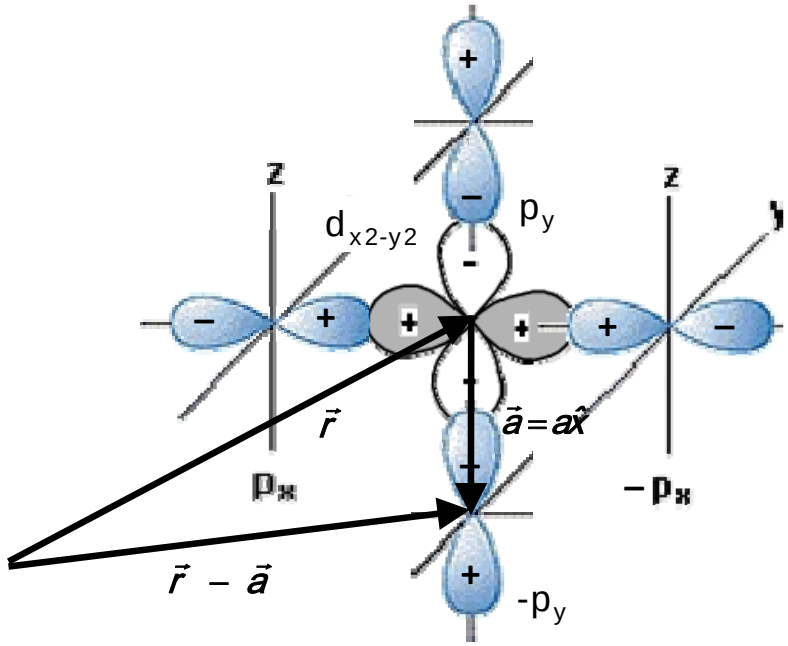
$$F_{Cryst} = F \bullet S = \sum_{j}^{Basis} f_a e^{i\vec{s}\bullet\vec{\delta}_j} \sum_{\ell}^{Lattice} e^{i\vec{s}\bullet\vec{R}_\ell^{(c)}}$$

For reflection with $G_{hk} = h\vec{a}^* + k\vec{b}^*, \vec{R}_\ell^{(c)} = n_1\vec{a} + n_2\vec{b}, \vec{G}_{hk\ell} \bullet \vec{R}_\ell^{(c)} = 2\pi(n_1 h + n_2 k + n_3 \ell)$, *and Cu at origin of unit cell, O at* $\vec{a}/2$ *and* $\vec{b}/2$, *we have*

$$F = \sum_{j}^{Basis} f_a e^{i\vec{s}\bullet\vec{\delta}_j} = f_{Cu} e^{i(h\vec{a}^*\bullet 0) + i(k\vec{b}^*\bullet 0)} + f_O\left[e^{i(h\vec{a}^*\bullet\vec{a}/2)} + e^{i(k\vec{b}^*\bullet\vec{a}/2)}\right] = f_{Cu} + f_O\left[e^{i(2\pi h/2a)} + e^{i(2\pi k/2a)}\right] = f_{Cu} + f_O\left[e^{i\pi h} + e^{i\pi k}\right]$$

$$S = \sum_{\ell}^{Lattice} e^{i\vec{s}\bullet\vec{R}_\ell^{(c)}} = \sum_{n_1,n_2}^{Lattice} e^{i(h\vec{a}^* + k\vec{b}^*)\bullet(n_1\vec{a} + n_2\vec{b})} = \sum_{n_1,n_2}^{Lattice} e^{i(2\pi h n_1 + 2\pi k n_2)} = \sum_{n_1,n_2}^{Lattice} e^{i2\pi(h n_1 + k n_2)} = \sum_{n_1,n_2}^{Lattice} 1 = N, \text{ the no. of cells}$$

(e) [5 points] Now, assuming covalent bonding, sketch one combination of atomic orbitals that would permit Cu (atomic configuration = core + $3d^{10}4s^1$) , using one of its 3d orbitals, to bond to all of its nearest neighbor O atoms (atomic configuration = core + $2s^2 2p^4$) in this 2D lattice. Describing this bonding in the tight-binding model, what integral involving potential would be involved between each Cu-O pair?



The integral will couple the O $2p_x$ *orbital on the nearest-neighbor O site with the Cu* $3d_{xy}$ *orbital through the potential on the O site with what Omar would write by analogy with the 1D integral* $\langle \varphi_v(x) | V'(x-a) | \varphi_w(x-a) \rangle$ *as* $\left\langle \varphi_{Cu\ 3d_{xy}}(\vec{r}) \middle| V_O(\vec{r} - a\hat{x}) \middle| \varphi_{O\ 2p_x}(\vec{r} - a\hat{x}) \right\rangle$. *See vectors on above diagram.*

(f) If bonding were ionic, with O having a charge of -2, write out the first few terms in the lattice energy, treating Cu as the center, and including nearest-neighbor and next-nearest-neighbor atoms.

Cu will be +4 due to stoichiometry. Then just use this general formula, including both Coulomb and short-distance repulsive terms for the four nearest neighbors only:

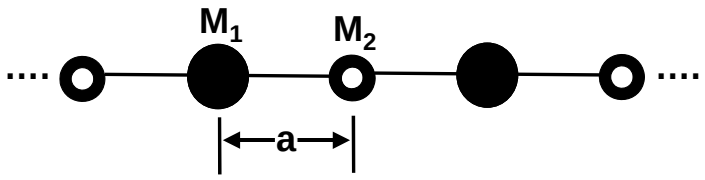
$$V = q_0 \sum_{i=1}^{\infty} \frac{(+\text{or}-)n_i q_i}{4\pi\varepsilon_0 r_i} + \frac{A}{r_1^n}$$

$$V = $$

$$= \frac{4(+4)(-2)}{4\pi\varepsilon_0 a} + \frac{4A}{a^n} + \frac{4(+4)(+4)}{4\pi\varepsilon_0 (2a)} = \frac{8}{\pi\varepsilon_0 a} + \frac{8}{\pi\varepsilon_0 a)} + \frac{4A}{a^n} = \frac{4A}{a^n}$$

and there is no net binding at the level of nearest and next-nearest neighbors!

[2] [20 points] The one-dimensional diatomic linear chain is shown below



and its allowed vibrational excitations have a dispersion relation of the form:

$$\omega^2 = \alpha\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm \alpha\left[\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4}{M_1 M_2}\sin^2\left(\frac{qa}{2}\right)\right]^{1/2}$$

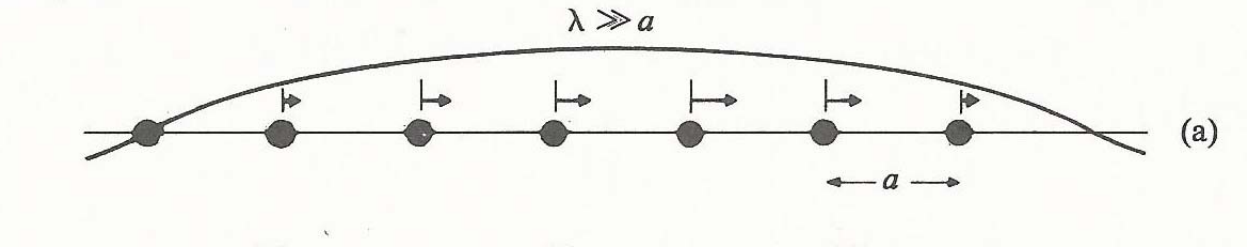
(a) [5 points] What is the meaning of α in the classical picture used to derive this?

α is the harmonic oscillator spring constant coupling the atoms, such that F(x) = -αx.

(b) [5 points] For which sign do we have the acoustic branch? Explain your answer briefly with a qualitative drawing of the type of relative motion of atoms 1 and 2 occurring in the acoustic branch for very small q values.

The negative sign, as the acoustic branch of levels has a lower energy than the optical branch.

The relative motion will look like that below:



(c) [10 points] Calculate the sound velocity for the acoustic branch for small q, making use of the simplifications that, in the limit that $q \to 0$, $\frac{\partial \omega}{\partial q} \to \frac{\omega}{q}$, $sin^2\left(\frac{qa}{2}\right) \to \left(\frac{qa}{2}\right)^2$ and in general $\sqrt{a+x} \to \sqrt{a}\left(1+\frac{x}{2a}\right)$ if x goes to zero.

$$\omega^2 = \alpha\left(\frac{1}{M_1}+\frac{1}{M_2}\right) - \alpha\left[\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4}{M_1 M_2} sin^2\left(\frac{qa}{2}\right)\right]^{1/2}$$

and with q very small,

$$= \alpha\left(\frac{1}{M_1}+\frac{1}{M_2}\right) - \alpha\left[\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4}{M_1 M_2}\left(\frac{qa}{2}\right)^2\right]^{1/2}$$

$$= \alpha\left(\frac{1}{M_1}+\frac{1}{M_2}\right) - \alpha\left(\frac{1}{M_1}+\frac{1}{M_2}\right)\left[1 - \frac{\frac{4}{M_1 M_2}\left(\frac{qa}{2}\right)^2}{2\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2}\right]$$

$$= \alpha\left(\frac{1}{M_1}+\frac{1}{M_2}\right) - \alpha\left(\frac{1}{M_1}+\frac{1}{M_2}\right) + \frac{\frac{4}{M_1 M_2}\left(\frac{q^2 a^2}{4}\right)}{2\left(\frac{1}{M_1}+\frac{1}{M_2}\right)}$$

$$= \frac{\frac{\alpha q^2 a^2}{M_1 M_2}}{2\left(\frac{M_2+M_1}{M_1 M_2}\right)} = \frac{\alpha q^2 a^2}{2\,(M_1+M_2)}$$

$$\omega = \sqrt{\frac{\alpha}{2\,(M_1+M_2)}}\,qa$$

$$v_s = \frac{\omega}{q} = \sqrt{\frac{\alpha}{2\,(M_1+M_2)}}\,a$$

[Not part of problem, but interesting, is that we also know that $v_s = \sqrt{\frac{Y}{\rho}}$ with 1D density ρ = M_1+M_2/a, so we can solve for *Y* to give

$$v_s = \sqrt{\frac{Y}{\rho}} = \sqrt{\frac{\alpha}{2\,(M_1+M_2)}}\,a$$

$$Y = \frac{\alpha}{2\,(M_1+M_2)}\,a^2\,\frac{(M_1+M_2)}{a} = \frac{\alpha}{2}\,a$$

which is just Eq. 3.48 in Omar, with a factor of 2 difference simply due to the definition of the unit cell in 1D as 2a versus a in Ibach and Luth.]

[3] [25 points] The following multi-part problem relates to metallic sodium. For reference, atomic sodium has the electronic configuration $1s^2 2s^2 2p^6 3s^1$. The figures on the following page show the Brillouin zone for bcc sodium, the band structure as calculated by a very accurate quantum-mechanical method, the electronic density of states g(E), and the integrated density of states $\int_{-3.5\ eV}^{E} g(E')dE'$ expressed in electrons per primitive unit cell.

Based on this data, answer the following parts of this question.

(a) [5 points] How many valence electrons does sodium have and from which atomic orbital are they derived?

One, and it comes from the lone 3s electron outside of an inert gas configuration.

(b) (8 points) It is commonly stated that sodium is a "free-electron metal". How can you tell this from the density of states plot. Be as quantitative as you can.

The free-electron like parabolas are highlighted in red on the diagram. Even the ones in orange are very nearly also, but projected back into the first Brillouin zone by a higher G vector. See Fig. 7.3 in Ibach and Luth.

To be more quantitative, you could measure a couple of points along a line in k-space to see if the energy grows quadratically, as shown e.g. along Γ to N:

Distance from Γ	*Distance squared*	*Energy/0.29*
0	*0*	*0*
0.5	*0.25*	*0.06/0.29 = 0.206*
1.0	*1.00*	*0.29/0.29 = 1.00*

So scaling for comparison yields approximate agreement.

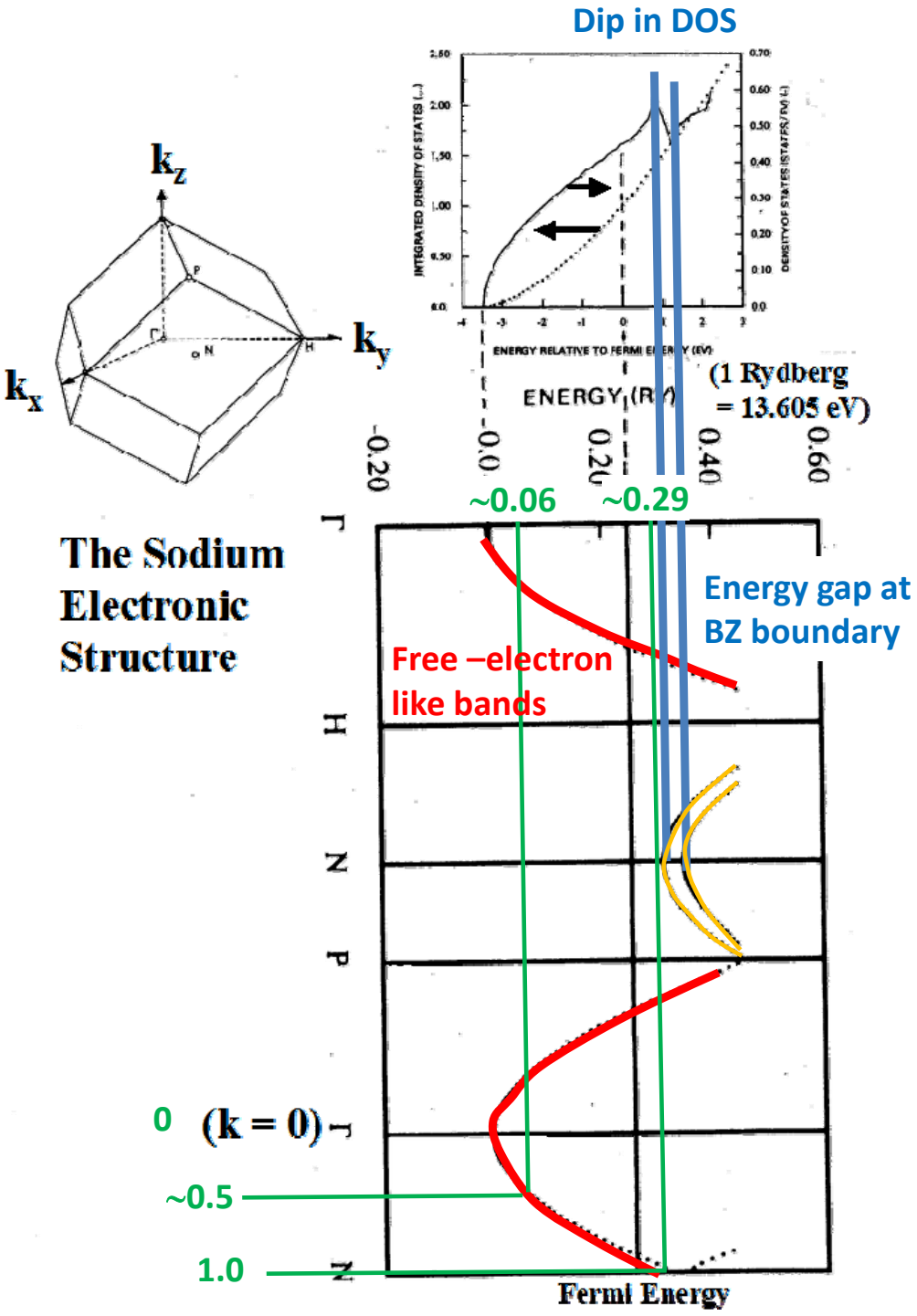
(c) (5 points) Why has the Fermi energy been located at the point at which the integrated density of states has a value of 1.0? Explain in terms of the electronic configuration of sodium.

Very simple, the integrated density of states has to equal the number of valence electrons, which is one!

(d) (7 points) Discuss the origin of the peak and dip seen in the density of states above E_F in terms of the "nearly-free-electron" band structure of sodium and the Brillouin zone, making reference to the fundamental integral used to calculate the density of states and relating specific points in the Brillouin zone to these features. Draw on the plots to illustrate your answer as appropriate.

The peak is due to the flattening of the upper and lower bands when a Brillouin zone-boundary bandgap is formed in the nearly-free electron model, with magnitude of $|-V_G|$,

and the dip to the formation of the bandgap over some region of the zone, as indicated by the blue lines in the drawing.



[4] [15 points] Answer the following questions on different topics briefly.

(a) [5 points] Indicate briefly the basic assumptions of the Einstein and Debye models of heat capacity, including an explanation of why there must be a cutoff in q in the Debye model.

Einstein: Quantized independent harmonic oscillators with energies $\varepsilon = n\hbar\omega$ and obeying Maxwell-Boltzmann statistics, with $3N_A$ of them per mole to allow for motion in 3 dimensions.

Debye: Quantized oscillators filling the whole space, like Planck assumed in describing Blackbody Radiation, with $\omega = v_s q$ like simple sound, energy ε equal to $\hbar\omega_D$, and with a density of states $g(\omega)$ integrated up to a value ω_D that yields $3N_A$ modes. This in turn yields a Debye temperature $\theta_D = \hbar\omega_D/k_B$.

(b) [5 points] Discuss briefly the meaning of the individual factors in the electrical conductivity of an ideal metal, with formula given by

$$\sigma = \frac{Ne^2\tau}{m^*}$$

σ = electrical conductivity, N = no. electrons per unit volume, e is the electron charge, τ is the relaxation time or time between electron collisions with phonons, and m is an effective mass as the electron moves through the material, acting sort of as a viscous liquid, due to the phonon collisions. m* is usually very close to m_e.*

(c) [5 points] Consider an electronic wave function $\psi(\vec{r},\vec{k})$ in a solid as given by Bloch's Theorem, and show that the probability density (or equivalently the electron charge density) associated with this wave function has the full translational periodicity of the crystal.

The Bloch function must satisfy
$\psi(r,k) = u(k,r)\exp(ikr)$, with $u(k,r) = u(k,r+\text{lattice vector})$

So probability density will be given by
$\psi^*(r,k)\psi(r,k) = u^*(k,r)\exp(-ikr)u(k,r)\exp(ikr) = |u(k,r)^2|$

But $|u(k,r)^2| = |u(k,r+\text{lattice vector})^2|$, so probability density will be translationally periodic in the lattice.

----------END OF EXAMINATION----------