Problem Set 5 Answers

[1] 4.1

Copper, $\rho_m = 8.95\ g/cm^3$ $\qquad \rho = 1.55\times10^{-8}\ \underline{ohm}\cdot m$ @ $T = 300K$

$m^* = m_0 = 9.1\times10^{-31}\ Kg$

a) concentration of counduction electron:

use (4.1) in OMAR

$$N = \underset{\text{VALENCE}}{Z_v}\ \frac{\rho_m \overset{\text{AVOGADRO's \#}}{N_A}}{\underset{\text{ATOMIC WEIGHT}}{M}}$$

for Cu → $Z_v = 1$, $M = 63.546\ g/mol$

$$\therefore\ N = \frac{8.95\ \cancel{g}/cm^3 \times 6.022\times10^{23}\ \cancel{mol^{-1}}}{63.546\ \cancel{g}\ \cancel{mol^{-1}}} \cong 8.48\times10^{22}\ cm^{-3}$$

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b) MEAN free TIME τ

USE (4.15) IN OMAR $\Rightarrow$ $\rho = \dfrac{m^*}{Ne^2}\dfrac{1}{\tau}$ $\Rightarrow$

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

<u>use</u> <u>MKS</u> UNITS ⇒

$$\tau = \frac{9.1\times10^{-31}}{8.48\times10^{28}\times(1.602)^2\times10^{-38}\,C^2\times1.55\times10^{-8}\ \Omega\cdot m} \cong 2.7\times10^{-14}\ s$$

c/ FERMI ENERGY E_F

USE (4.34) IN OMAR

$$E_F = \frac{\hbar^2}{2m}\left(3\pi^2 N\right)^{2/3} = \text{IN MKS UNITS} \Rightarrow$$

$$E_F = \frac{\left(\frac{6.63}{2\pi}\right)^2 \times 10^{-68}\ J^2 s^2 \times \left(3\pi^2 \times 8.48\times 10^{28}\ m^{-3}\right)^{2/3}}{2\times 9.1\times 10^{-31}\ kg} \cong 1.13\times 10^{-18}\ \text{Joule}$$

$$E_F \approx 1.13\times 10^{-18} \times \frac{1}{1,602}\times 10^{19}\ eV \approx 7\ eV$$

d/ FERMI VELOCITY → USE <u>4.33</u> IN OMAR

$$E_F = \frac{1}{2} m v_F^2 \Rightarrow$$

$$v_F = \left(\frac{2E_F}{m}\right)^{1/2} = \text{IN MKS} = \left(\frac{2\times 1.13\times 10^{-18}}{9,1\times 10^{-31}\ kg}\right)^{1/2} \cong 1.58\times 10^{6}\ m/s$$

e) MEAN FREE PATH @ FERMI LEVEL

USE 4.11 IN OMAR WITH $v_R = v_F$

$$l_F = v_F \cdot \tau = 1.58\times 10^{6}\ \frac{m}{s} \times 2.7\times 10^{-14}\ s \cong 4.266\times 10^{-8}\ m$$
$$\approx 426.6\ \mathring{A}$$

NOTICE HOW THESE VALUES ARE CLOSE TO THE ONES REPORTED IN TABLE 4.1 IN OMAR

✓

[2] 4.7, Cu only

ESTIMATE THE FRACTION of ELECTRONS EXCITED ABOVE F.L. @ ROOM TEMPERATURE

KT/E_F IS THE FRACTION of ELECTRON EXCITED ABOVE THE FERMI LEVEL (see p. 153 IN OMAR, ABOVE 4.31 for AN EXPLANATION)

YOU CAN EITHER CALCULATE E_F OR REFER TO TABLE 4.1

$\Rightarrow$ Cu $\Rightarrow E_F \cong 7$ eV
Na $\Rightarrow E_F \simeq 3.1$ eV

$$\therefore \text{ for Cu} \Rightarrow \frac{kT_R}{E_F} = \frac{8.617\times10^{-5}\ \cancel{eV}\,\cancel{K}^{-1} \times 300\,\cancel{K}}{7\ \cancel{eV}} \cong 0.35\%$$

$$\text{for Na} \Rightarrow \frac{KT_R}{E_F} = \frac{0{,}025}{3{,}1}\frac{\cancel{eV}}{\cancel{eV}} \cong 0{,}8\ \%$$

NOTE: USEFUL $k_B T$ @ ROOM $T = 0.025$ eV $= \frac{1}{40}$ eV

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[3] 8(a) only LOOKING AT p. 185 IN OMAR (FIG 5.7), IT IS NOT DIFFICULT TO REALIZE THAT THE FIRST BRILLOUIN ZONE IS THE WIGNER-SEITZ PRIMITIVE CELL of THE RECIPROCAL LATTICE, i.e,

THE SET of POINTS LYING CLOSER TO THE ORIGIN THAN TO ANY OTHER POINT IN THE RECIPROCAL LATTICE

RECALLING THAT for BCC (FCC) THE RECIPROCAL LATTICE IS FCC (BCC),

$\longrightarrow$

THESE FIGURES from ASHCROFT-MERMIN SHOULD CLARIFY THIS ISSUE, ONCE YOU COMPARE THESE TO FIG 5.8 IN OMAR

The Wigner-Seitz unit cell is illustrated for a two-dimensional Bravais lattice in Figure 4.14 and for the three-dimensional body-centered cubic and face-centered cubic Bravais lattices in Figures 4.15 and 4.16.

Note that the Wigner-Seitz unit cell about a lattice point can be constructed by drawing lines connecting the point to all others[13] in the lattice, bisecting each line

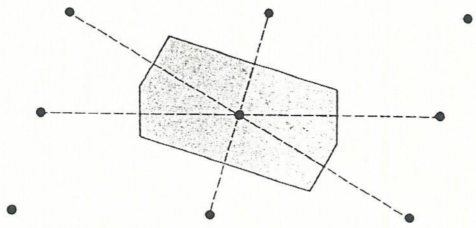
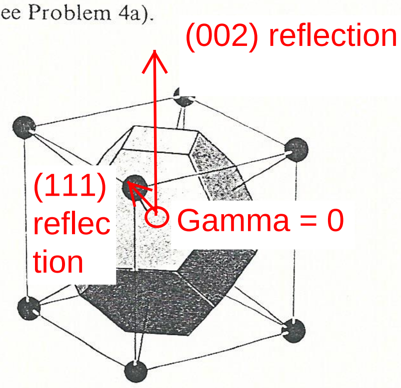


Figure 4.14
The Wigner-Seitz cell for a two-dimensional Bravais lattice. The six sides of the cell bisect the lines joining the central points to its six nearest neighboring points (shown as dashed lines). In two dimensions the Wigner-Seitz cell is always a hexagon unless the lattice is rectangular (see Problem 4a).

Figure 4.15
The Wigner-Seitz cell for the body-centered cubic Bravais lattice (a "truncated octahedron"). The surrounding cube is a conventional body-centered cubic cell with a lattice point at its center and on each vertex. The hexagonal faces bisect the lines joining the central point to the points on the vertices (drawn as solid lines). The square faces bisect the lines joining the central point to the central points in each of the six neighboring cubic cells (not drawn). The hexagons are regular (see Problem 4d).



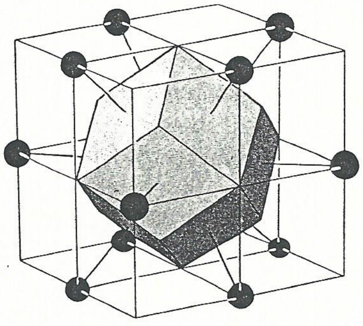


Figure 4.16
Wigner-Seitz cell for the face-centered cubic Bravais lattice (a "rhombic dodecahedron"). The surrounding cube is *not* the conventional cubic cell of Figure 4.12, but one in which lattice points are at the center of the cube and at the center of the 12 edges. Each of the 12 (congruent) faces is perpendicular to a line joining the central point to a point on the center of an edge.

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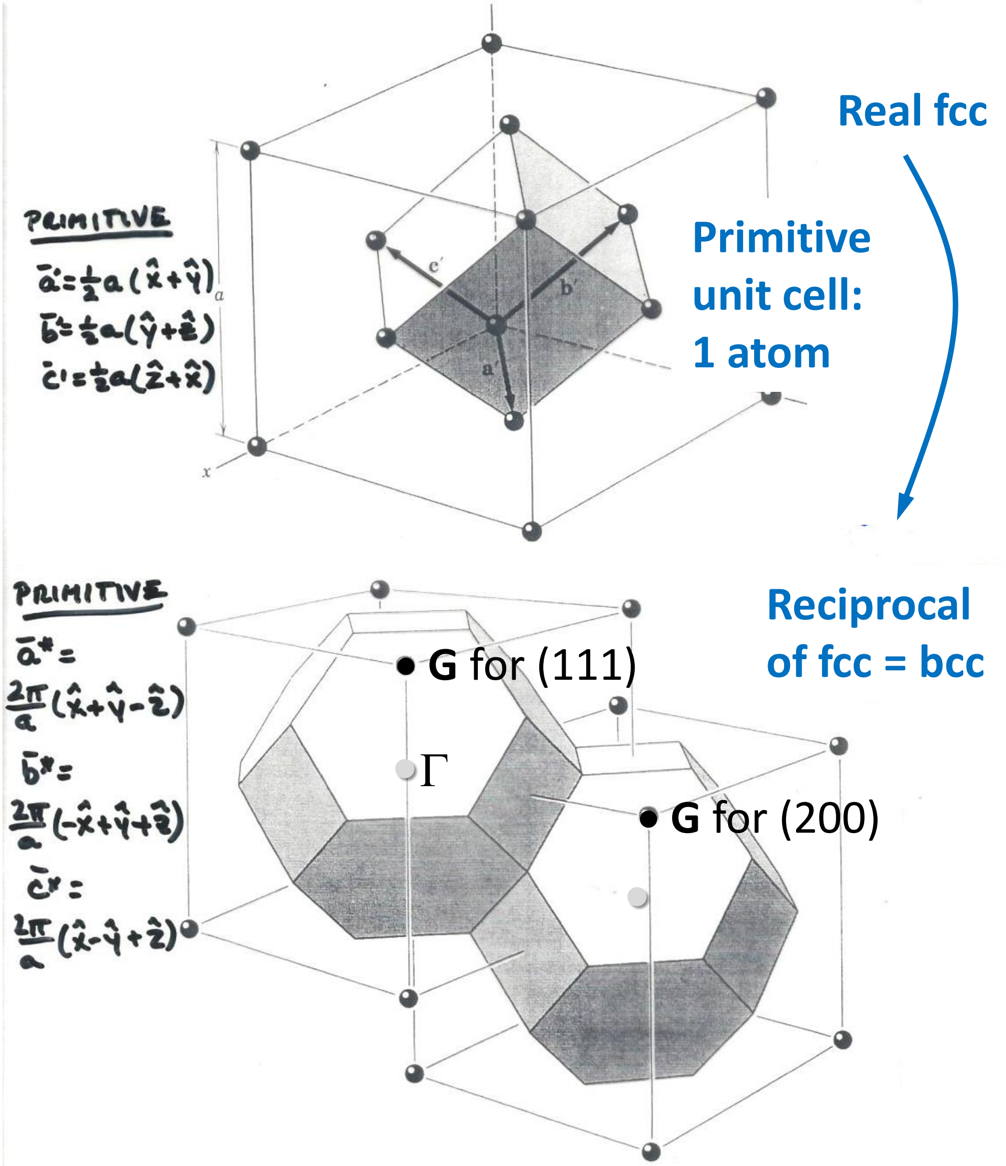
[12] A precise definition of "as symmetrical as" is given in Chapter 7.

[13] In practice only a fairly small number of nearby points actually yield planes that bound the cell.

Additional drawings to illustrate Problem 8(a)



Real fcc

Primitive unit cell: 1 atom

Reciprocal of fcc = bcc

PRIMITIVE

$\bar{a}' = \frac{1}{2}a(\hat{x}+\hat{y})$

$\bar{b}' = \frac{1}{2}a(\hat{y}+\hat{z})$

$\bar{c}' = \frac{1}{2}a(\hat{z}+\hat{x})$

PRIMITIVE

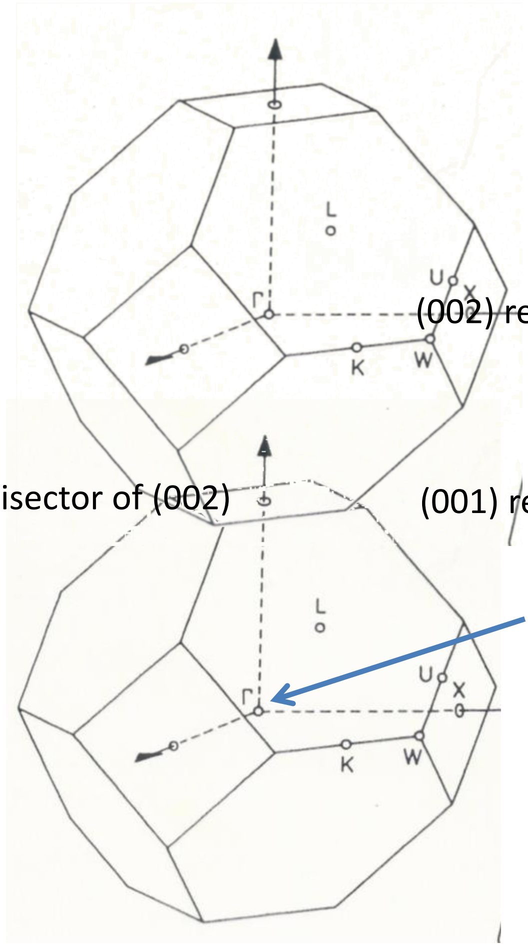
$\bar{a}^* = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})$

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

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

Figure 28 Brillouin zones of the face-centered cubic lattice. The cells are in reciprocal space, and the reciprocal lattice is body-centered, as drawn.

Additional drawings to illustrate Problem 8(a)



(002) reflection plane of atoms

Perpendicular bisector of (002)

(001) reflection plane of atoms

Primary ref. for Γ

Real

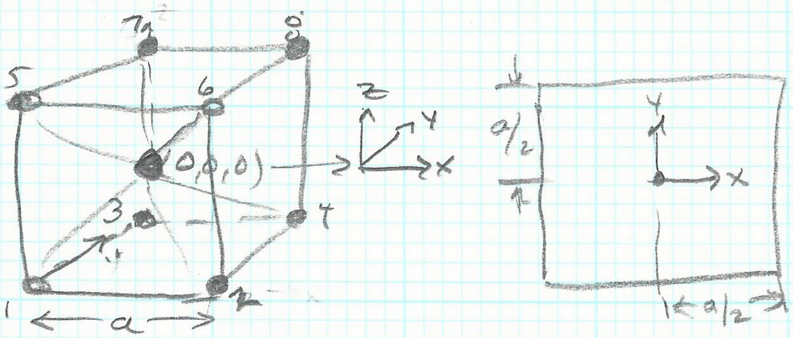
Reciprocal

FCC $\begin{cases} \vec{a}_1 = \tfrac{1}{2}a(\hat{x}+\hat{y}) \\ \vec{a}_2 = \tfrac{1}{2}a(\hat{y}+\hat{z}) \\ \vec{a}_3 = \tfrac{1}{2}a(\hat{z}+\hat{x}) \end{cases}$ $\begin{cases} \vec{b}_1 = \tfrac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z}) \\ \vec{b}_2 = \tfrac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z}) \\ \vec{b}_3 = \tfrac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z}) \end{cases}$ BCC $4(2\pi/a)^3$

In terms of actual reciprocal lattice points involved,
(002) is actually [011] = 0 + $\mathbf{b}_2$ + $\mathbf{b}_3$ above,
and
(111) = [111] = $\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3$

[4] 5.11(a) $E(\bar{k}) = E_\nu - \beta - \gamma \sum_j e^{i\bar{k}\cdot x_j}$

Use the simple cubic unit cell + basis: 8 nearest neighbors



Choose central atom as origin, then neighbors are at

$\bar{X}_1 = \frac{a}{2}\left[-\hat{x}-\hat{y}-\hat{z}\right]$ ✓

$\bar{X}_2 = \frac{a}{2}\left[\hat{x}-\hat{y}-\hat{z}\right]$ ✓

$\bar{X}_3 = \frac{a}{2}\left[-\hat{x}+\hat{y}-\hat{z}\right]$ ✓

$X_4 = \frac{a}{2}\left[+\hat{x}+\hat{y}-\hat{z}\right]$ ✓

$X_5 = \frac{a}{2}\left[-\hat{x}-\hat{y}+\hat{z}\right]$ ✓

$X_6 = \frac{a}{2}\left[+\hat{x}-\hat{y}+\hat{z}\right]$ ✓

$X_7 = \frac{a}{2}\left[-\hat{x}+\hat{y}+z\right]$ ✓

$X_8 = \frac{a}{2}\left[\hat{x}+\hat{y}+\hat{z}\right]$ ✓

Do sum of exponentials, evaluate dot products, use Euler relations to get finally:

$$E(k) = E_\nu - \beta - 8\gamma\left[\cos(k_x a/2)\cos(k_y a/2)\cos(k_z a/2)\right]$$

See details on next sheet

Prob. 5.11(a) continued

Here $\varepsilon = E_\nu - \beta$, and $t = \gamma$ in Omar

Example 3: Lithium

The metal lithium forms crystals with a body centered cubic Bravais lattice and one atom per primitive unit cell. The primitive lattice vectors for a bcc lattice with a lattice constant of a are,

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

Lithium has one valence electron in a 2s orbital, ϕ_{2s}. The tight binding wavefunction for lithium is,

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_{h,j,l} e^{i\left(h\vec{k}\cdot\vec{a}_1+j\vec{k}\cdot\vec{a}_2+l\vec{k}\cdot\vec{a}_3\right)}\phi_{2s}(\vec{r}-h\vec{a}_1-j\vec{a}_2-l\vec{a}_3).$$

Multiply the time independent Schrödinger equation from the left by $\phi^*_{2s}(\vec{r})$ and integrate over all space.

$$\langle\phi_{2s}(x)|\hat{H}|\psi_k(x)\rangle = E\langle\phi_{2s}(x)|\psi_k(x)\rangle.$$

In the tight binding approximation, only the on-site and nearest neighbor matrix elements are retained on the left side and only the on-site term is retained on the right side. It is assumed that all the other terms are small enough that they can be ignored. There are eight nearest neighbor matrix elements for a bcc lattice.

$$\epsilon - te^{i\vec{k}\cdot\vec{a}_1} - te^{i\vec{k}\cdot\vec{a}_2} - te^{i\vec{k}\cdot\vec{a}_3} - te^{-i\vec{k}\cdot\vec{a}_1} - te^{-i\vec{k}\cdot\vec{a}_2} - te^{-i\vec{k}\cdot\vec{a}_3} - te^{i\vec{k}\cdot\left(\vec{a}_1+\vec{a}_2+\vec{a}_3\right)} - te^{-i\vec{k}\cdot\left(\vec{a}_1+\vec{a}_2+\vec{a}_3\right)} + \text{small terms} = E + \text{small terms}.$$

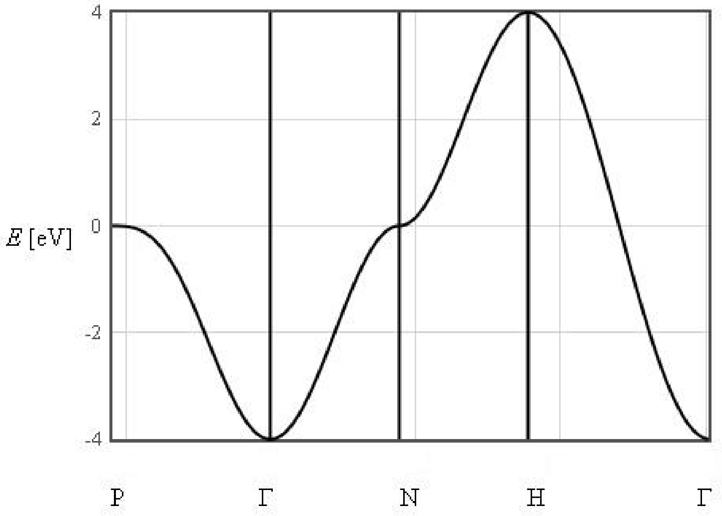
Where $\epsilon = \langle\phi_{2s}(\vec{r})|\hat{H}|\phi_{2s}(\vec{r})\rangle$ and $t = -\langle\phi_{2s}(\vec{r})|\hat{H}|\phi_{2s}(\vec{r}-\vec{a}_1)\rangle$. Due to symmetry, the matrix element t is the same for all nearest neighbors. Using the definition of the primitive lattice vectors, this can be rewritten as,

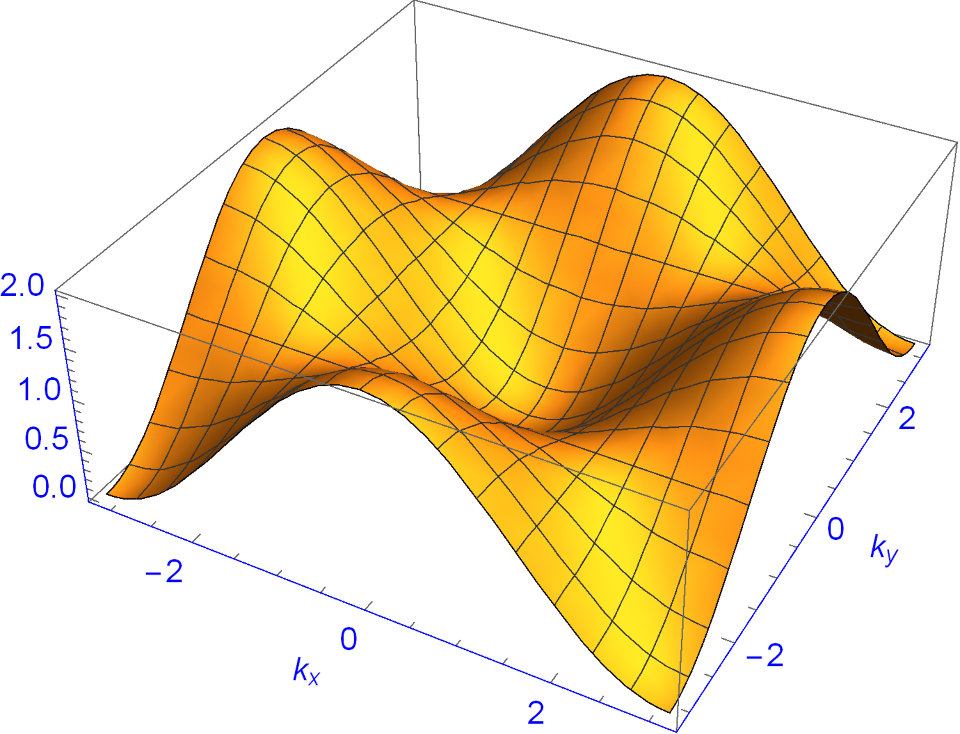
$$\begin{aligned}E = \epsilon &- te^{ik_xa/2}e^{ik_ya/2}e^{-ik_za/2} - te^{-ik_xa/2}e^{ik_ya/2}e^{ik_za/2} - te^{ik_xa/2}e^{-ik_ya/2}e^{ik_za/2} - te^{-ik_xa/2}e^{-ik_ya/2}e^{ik_za/2}\\ &- te^{ik_xa/2}e^{-ik_ya/2}e^{-ik_za/2} - te^{-ik_xa/2}e^{ik_ya/2}e^{-ik_za/2} - te^{ik_xa/2}e^{ik_ya/2}e^{ik_za/2} - te^{-ik_xa/2}e^{-ik_ya/2}e^{-ik_za/2}.\end{aligned}$$

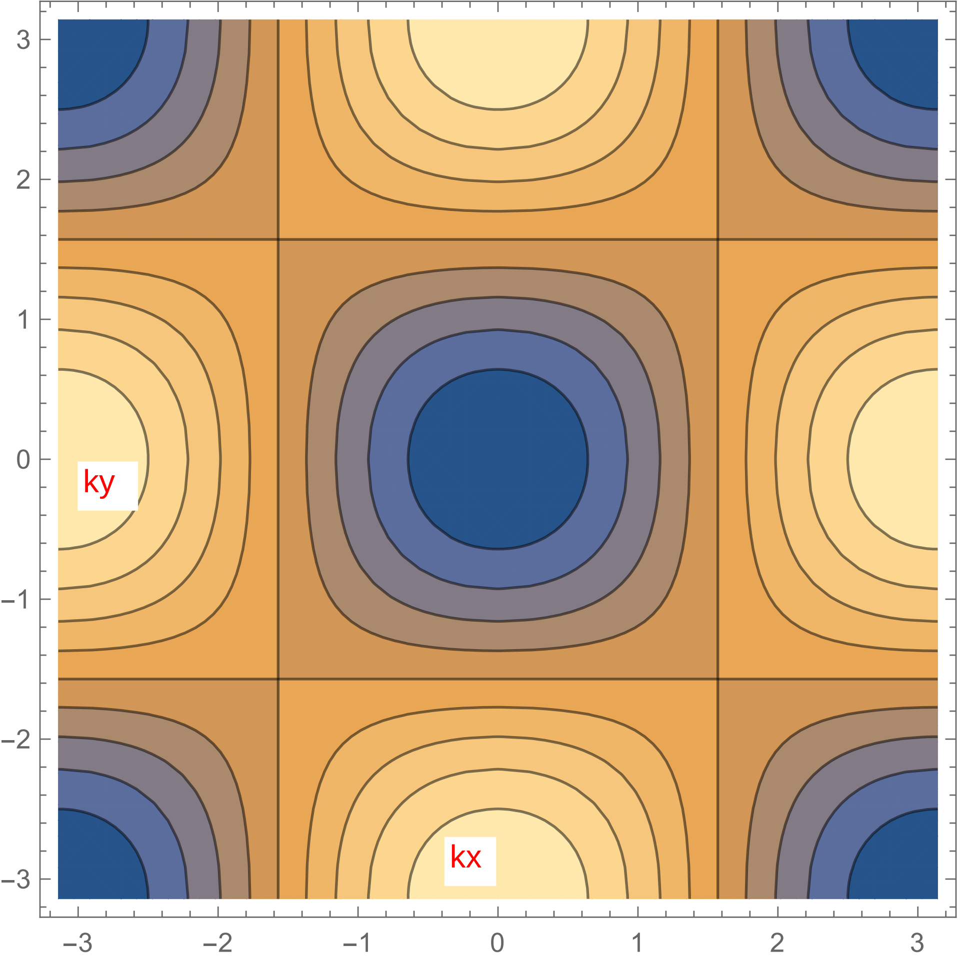
Using the definition of relation $2\cos x = e^{ix} + e^{-ix}$, this can be written as,

$$E = \epsilon - 8t\cos(k_xa/2)\cos(k_ya/2)\cos(k_za/2).$$

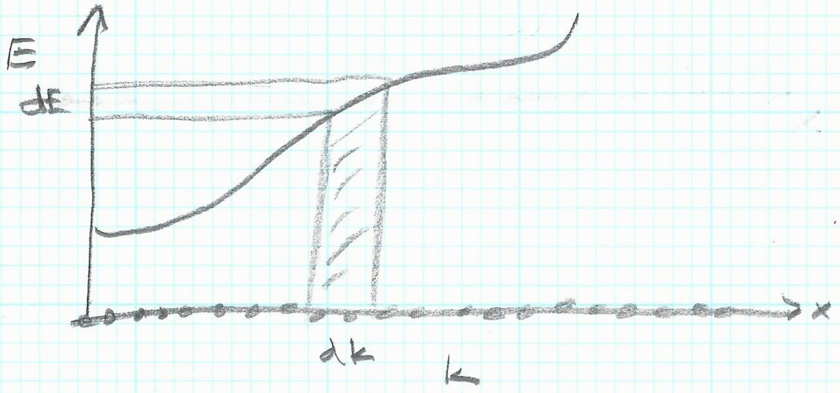
The dispersion relation for the 2s band for lithium in the tight binding approximatic




2.0
1.5
1.0
0.5
0.0
−2
0
k_x
2
2
0
k_y
−2


3
2
1
0
−1
−2
−3
ky
kx
−3
−2
−1
0
1
2
3

[5] 5.12(a) $k = n\left(\frac{2\pi}{L}\right)$, $n = 0, 1, 2, \ldots$, SO ADJACENT VALUES ARE SEPARATED BY $\frac{2\pi}{L}$ AND DENSITY $= \frac{L}{2\pi}$.



NO. STATES IN dk $= \frac{L}{2\pi} dk = g(k)$

UNIT LENGTH

NO. STATES IN dE $= g(E)dE = g(k)\frac{1}{\left(\frac{dE}{dk}\right)} = \frac{L}{2\pi}\Big/\left(\frac{dE}{dk}\right) = \underline{\underline{\frac{\overset{\|}{1}}{2\pi}\Big/\left(\frac{dE}{dk}\right)}}$

(b) $E(k) = E_0 + 4\gamma \sin^2\left(\frac{ka}{2}\right)$

$$\frac{dE}{dk} = 4 \cdot 2\gamma \sin\left(\frac{ka}{2}\right)\cos\left(\frac{ka}{2}\right)\frac{a}{2}$$

$$g(E) = \frac{1}{16\pi \sin\left(\frac{ka}{2}\right)\cos\left(\frac{ka}{2}\right)\frac{a}{2}}$$

Further derivation and plots on next pages

[5] (b) (CONT'D)

$$E = E_0 + 4\gamma \sin^2\left(\frac{ka}{2}\right)$$

Solving for k(E)

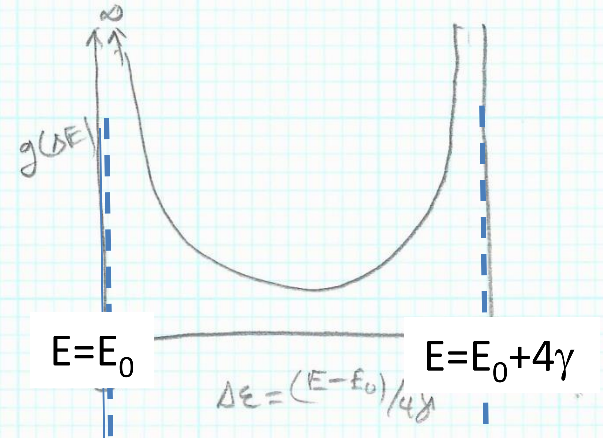
$$\sin\left(\frac{ka}{2}\right) = \frac{E-E_0}{4\gamma}$$

$$k = \frac{2}{a}\arcsin\left[\sqrt{\frac{E-E_0}{4\gamma}}\right] \qquad \left\{ d(\arcsin x) = \frac{1}{\sqrt{1-x^2}} = \frac{1}{\sqrt{1-\frac{E-E_0}{4\gamma}}}\, d\sqrt{\frac{E-E_0}{4\gamma}} = \frac{1}{\sqrt{1-\frac{E-E_0}{4\gamma}}}\cdot\frac{\frac{1}{4\gamma}}{\sqrt{\frac{E-E_0}{4\gamma}}} \right\}$$

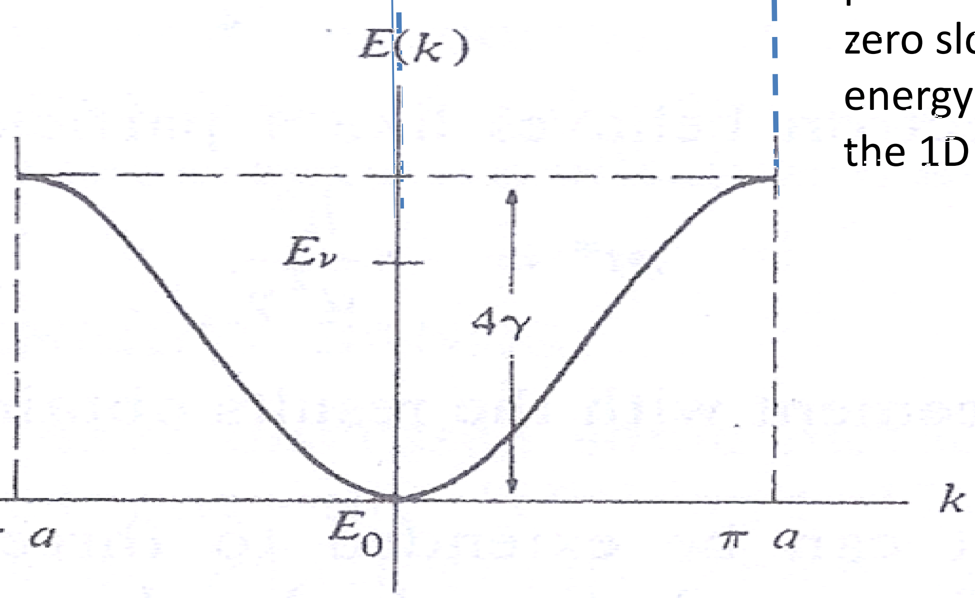
$$\therefore\ g(E) = \frac{1}{2\pi}\frac{dk}{dE} = \frac{1}{8\pi a\gamma}\cdot\frac{1}{\sqrt{1-\frac{E-E_0}{4\gamma}}\sqrt{\frac{E-E_0}{4\gamma}}}$$

OR, WITH $(E-E_0)/4\gamma \equiv \Delta E$, REQUIRED TO BE < 1

$$g(\Delta E) = \frac{1}{8\pi a\gamma}\ \frac{1}{\sqrt{1-\Delta\varepsilon}\sqrt{\Delta\varepsilon}}$$



Which correlates perfectly with the zero slopes in the energy band for the 1D chain:



[6] 14(a) The 3D electron density of states is

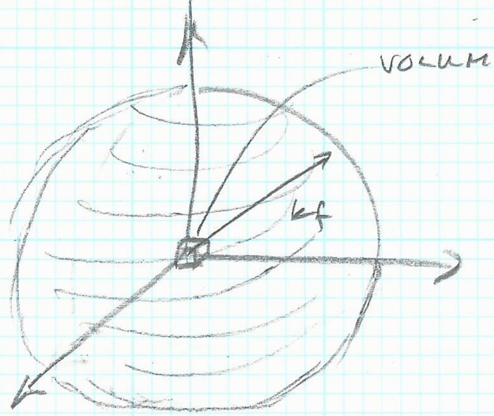
$$g(E) = \frac{(2m_e)^{3/2}}{2\pi^2\hbar^3}E^{1/2}$$

with $\int_0^{E_F} g(E)\,dE = n$ = electron density

But since nL^3 = no. electrons in the box, and sphere of radius k_f must contain $\cancel{2}\left(\frac{L^3}{\cancel{2}\pi^2}\right)\cdot\frac{4}{3}\pi k_f^2$, we can just equate

SPIN DENSITY

VOLUME OF 1 STATE = $\left(\frac{2\pi}{L}\right)^3$



The two

$$n\cancel{L^3} = \frac{\cancel{L^3}}{\pi^2}\frac{1}{3}k_f^2$$

$$3\pi^2 n = k_f^3$$

$$\underline{\underline{k_f = (3\pi^2 n)^{1/3}}}$$

]=

[7] Special problem: On the next page is shown a theoretical electronic band structure calculation for aluminum, together with the corresponding density of states. The energy is in Rydbergs = Ry = 13.605 eV. The electronic configuration of atomic aluminum is $1s^2 2s^2 2p^6 3s^2 3p^1$. It is fcc with lattice constant 4.05 Å.

(a) Which are the core electrons and which are the valence electrons in aluminum? $1s^2 2s^2 2p^6$ are core, and $3s^2 3p^1$ are valence.

(b) Show, by numerical check at five equally spaced points, that the band extending from Γ to X actually is very close to that expected for a totally free electron (what your text calls the empty lattice model). Note that you will need to use the correct magnitude for the wave vector along this direction.

See calculation on next page.

(c) Show, also by numerical check at five points, that the calculated density of states curve follows on average that expected for a free electron.

See calculation on next page.

(d) Do an approximate numerical integration of the density of states (given in states/eV) from the bottom of the bands to the Fermi level, and show that it yields an answer consistent with the number of valence electrons.

See calculation on following pages.

(e) What is the group velocity of an electron in a state just beyond L and going toward W?

Very small, essentially zero at the point where the bandgap is formed.

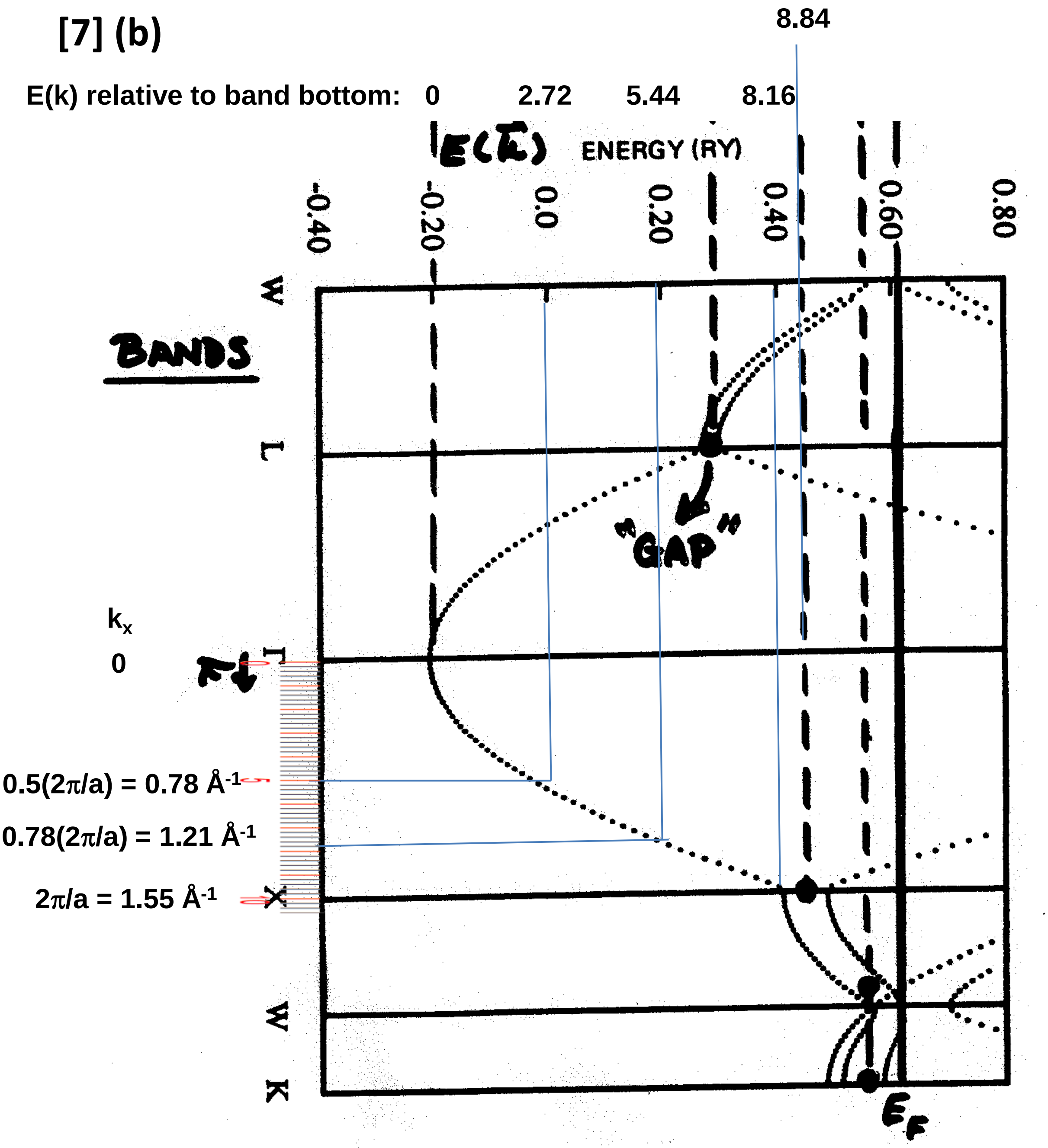
(f) Bragg reflection from which set of planes is responsible for the gap at X?

(002), see earlier problem 8(a) for this answer.

(g) Qualitatively explain the little peaks and valleys in the density of states centered on the dashed lines.

The peaks are due to places where bandgaps form, involving standing-wave-like states with low group velocity $d\omega/dk$ and high $1/(dE/dk)$, the valleys are places where, just above a gap in k, the group velocity is higher than the free-electron value, and the density of states thus lower than the $E^{1/2}$ variation.

[7] (b)



$E = \hbar^2k^2/2m_e$

Plugging in the constants and converting to convenient units gives finally

$E(eV) = (k(Å^{-1})/0.512)^2$

So for the three k values at left, we get energies below, in reasonably good agreement with full band structure calculations

E(k) relative to E_F (eV): 0 2.32 5.58 9.16 (~in middle of bandgap at X)

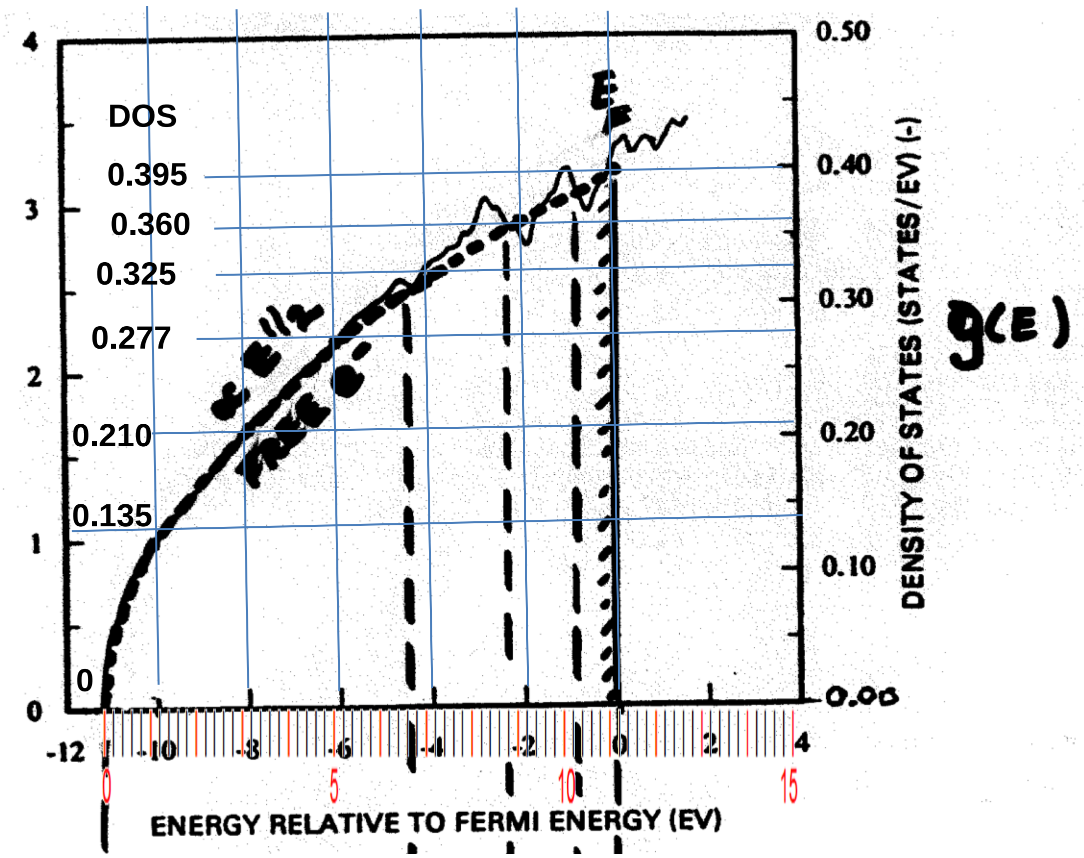
[7] (c)

E relative to band bottom: 1.1 3.1 5.1 7.1 9.1 11.1

DOS from $E^{1/2}$: $\times 0.395/(11.1)^{1/2} = 0.118$

0.124 0.207 0.266 0.314 0.355 0.393

Excellent agreement within a few %!



[7] (d) Estimated total density of state in electrons

= sum of each energy step x average DOS in step

= 1.1(0.135/2)+2.0[(0.210+0.135)/2]+2.0[(0.277+2.10)/2]

+2.0[(0.325+0.277]/2] +2.0[(0.360+0.325]/2]

+2.0[(0.395+0.360]/2]

= 0.135+0.210+0.135+0.277+0.210+0.325+0.277+0.360+0.325

0.395+0.360

= 3.009 Exactly the number of valence electrons in aluminum!