(1) For each of the following structures, indicate whether or not it is a Bravais lattice. If it is, give the three primitive vectors. If not, describe it as a Bravais lattice with the smallest possible basis.

(a) Base-centered cubic (simple cubic with additional points in the centers of the two horizontal faces).

(b) Side-centered cubic (simple cubic with additional points in the centers of the four vertical faces).

(c) Edge-centered cubic (simple cubic with additional points at the midpoints of all nearest-neighbor links).

Solution:

(a) This is a simple tetragonal lattice with elementary direct vectors

\[ a_1 = \frac{1}{2}a(\hat{x} - \hat{y}), \quad a_2 = \frac{1}{2}a(\hat{x} + \hat{y}), \quad a_3 = a\hat{z} \cdot \]

(b) Not a Bravais lattice! To see why, note that the side-centered sites at \( r_1 = \frac{1}{2}a(\hat{x} + \hat{z}) \) and \( r_2 = \frac{1}{2}a(\hat{y} + \hat{z}) \) differ by the vector \( \delta = r_2 - r_1 = \frac{1}{2}a(\hat{y} - \hat{x}) \). But while \( r_3 = 0 \) is a lattice site, \( r_3 + \delta \) is not a lattice site. Therefore the local environment of the side-centers is different from that of the simple cubic lattice sites.

(c) Not a Bravais lattice! The sites \( r_1 = 0 \) and \( r_2 = \frac{1}{2}a\hat{x} \) are separated by \( \delta = r_2 - r_1 = \frac{1}{2}a\hat{x} \). But while \( r_3 = \frac{1}{2}a\hat{y} \) is a lattice site, \( r_3 + \delta = \frac{1}{2}a(\hat{x} + \hat{y}) \) is a face center, and not an edge center, and hence is not in the lattice.

(2) Polycrystalline specimens of three different monatomic cubic crystals are analyzed with a Debye-Scherrer camera. It is known that one sample is fcc, one is bcc, and one has a diamond structure. The approximate angular position \( \phi \) of the first four diffraction rings are found to be

\[
\begin{align*}
\text{A} & : \ 42.2^\circ, 49.2^\circ, 72.0^\circ, 87.3^\circ \\
\text{B} & : \ 28.8^\circ, 41.0^\circ, 50.8^\circ, 59.6^\circ \\
\text{C} & : \ 42.8^\circ, 73.2^\circ, 89.0^\circ, 115^\circ
\end{align*}
\]

(a) Identify the crystal structures A, B, and C.

(b) If the wavelength of the incident X-ray is \( \lambda = 1.5\text{Å} \), what is the length of the side of the cubic cell in each case?

(c) If the (monatomic) diamond structure were replaced by a (binary) zincblende structure, at what angles would the first four rings be observed?
Solution:

(a) Crystallographic extinctions occur when $F(k) = 0$, where $F(k) = \sum_{\mathbf{r}} e^{i \mathbf{G} \cdot \mathbf{r}}$ is a sum over all unique lattice points within the fundamental $a \times a \times a$ cube and $\mathbf{G} = \frac{2\pi}{a} (h, k, l)$ is a reciprocal lattice vector. The locations $\mathbf{r}$ for the three structures are given by:

- **FCC**: $\mathbf{r}_1 = (0, 0, 0)$, $\mathbf{r}_2 = \left( \frac{1}{2}a, \frac{1}{2}a, 0 \right)$, $\mathbf{r}_3 = \left( \frac{1}{2}a, 0, \frac{1}{2}a \right)$, $\mathbf{r}_4 = (0, \frac{1}{2}a, \frac{1}{2}a)$
- **BCC**: $\mathbf{r}_1 = (0, 0, 0)$, $\mathbf{r}_2 = \left( \frac{1}{2}a, \frac{1}{2}a, \frac{1}{2}a \right)$, $\mathbf{r}_3 = \left( \frac{1}{2}a, 0, \frac{1}{2}a \right)$, $\mathbf{r}_4 = (0, \frac{1}{2}a, \frac{1}{2}a)$
- **DIA**: $\mathbf{r}_5 = \left( \frac{1}{4}a, \frac{1}{4}a, \frac{3}{4}a \right)$, $\mathbf{r}_6 = \left( \frac{1}{2}a, \frac{1}{4}a, \frac{3}{4}a \right)$, $\mathbf{r}_7 = \left( \frac{3}{4}a, \frac{3}{4}a, \frac{3}{4}a \right)$, $\mathbf{r}_8 = \left( \frac{3}{4}a, \frac{1}{4}a, \frac{1}{4}a \right)$

Thus,

\[
\begin{align*}
F_{\text{FCC}}(h, k, l) &= 1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(h+l)} \\
F_{\text{BCC}}(h, k, l) &= 1 + e^{i\pi(h+k+l)} \\
F_{\text{DIA}}(h, k, l) &= (1 + e^{i\pi(h+k+l)/2})(1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(h+l)})
\end{align*}
\]

The allowed values of $(h, k, l)$ are thus given by

- **FCC**: all $(h, k, l)$ even or odd
- **BCC**: only $h + k + l$ even
- **DIA**: all $(h, k, l)$ even and $h + k + l = 4n$, or $(h, k, l)$ all odd.

We have $\lambda = 2d_{hkl} \sin(\phi/2)$ with $d_{hkl} = a/\sqrt{h^2 + k^2 + l^2}$, and so

\[
\sin^2(\frac{1}{2}\phi) = \frac{\lambda^2}{4d_{hkl}^2} = \frac{h^2 + k^2 + l^2}{4a^2} \frac{\lambda^2}{4a^2}.
\]

For FCC we have the first four values of $h^2 + k^2 + l^2$ are (1, 1, 1), (2, 0, 0), (2, 2, 0), and (3, 1, 1), corresponding to $d_{hkl}^2 = 3, 4, 8,$ and $11$, respectively. For BCC, we have (1, 1, 0), (2, 0, 0), (2, 1, 1), and (2, 2, 0), corresponding to $d_{hkl}^2 = 2, 4, 6,$ and $8$. Finally, for DIA, we have (1, 1, 1), (2, 2, 0), (3, 1, 1), and (4, 0, 0), corresponding to $d_{hkl}^2 = 3, 8, 11,$ and $16$. Comparing the ratios of these numbers, we find that crystal A is FCC, B is BCC, and C is DIA.

(b) Plugging into the formula $a = \frac{1}{2} \sqrt{h^2 + k^2 + l^2} \lambda$, we have $a_A = 3.61 \text{Å}, a_B = 4.26 \text{Å}$, and $a_C = 3.56 \text{Å}$.

(c) Distinguishing the two FCC sublattices of diamond results in an FCC structure, so with $\lambda/2a = 0.21$ we expect rings at $\phi = 42.8^\circ, 49.8^\circ, 73.2^\circ,$ and $89.0^\circ$.

(3) A monolayer of atoms is deposited on a surface. The atoms form a regular hexagonal lattice. This problem deals with the vibrations of these atoms.

(a) Suppose the surface is perfectly smooth. The atoms interact by a potential

\[
\Phi = \frac{1}{2} \sum_{\mathbf{R}, \mathbf{R}'} v(|\mathbf{R} + \mathbf{u}_\perp(\mathbf{R}) - \mathbf{R}' - \mathbf{u}_\perp(\mathbf{R}')|) + \frac{1}{2} K_z \sum_{\mathbf{R}} u_z^2(\mathbf{R})
\]
where \( \mathbf{u}_\perp = u_x \hat{x} + u_y \hat{y} \) is the displacement along the surface (perpendicular to the surface normal \( \hat{z} \)), \( \mathbf{R} \) and \( \mathbf{R}' \) denote sites of the hexagonal Bravais lattice, and the last term describes the binding of the atoms to the surface (\( u_z \) is the displacement along the surface normal). Show that the dynamical matrix for the lattice vibrations takes the form

\[
\hat{\Phi}(\mathbf{k}) = \begin{pmatrix}
\hat{\Phi}^{xx}(\mathbf{k}) & \hat{\Phi}^{xy}(\mathbf{k}) & 0 \\
\hat{\Phi}^{yx}(\mathbf{k}) & \hat{\Phi}^{yy}(\mathbf{k}) & 0 \\
0 & 0 & \hat{\Phi}^{zz}(\mathbf{k})
\end{pmatrix}
\]

where the upper left \( 2 \times 2 \) block is given by

\[
\Phi^{\alpha\beta}(\mathbf{k}) = 2 \sum_{\mathbf{R}} \sin^2\left(\frac{1}{2} \mathbf{k} \cdot \mathbf{R}\right) \left\{ (\delta^{\alpha\beta} - \hat{R}^\alpha \hat{R}^\beta) R^{-1} v'(\mathbf{R}) + \hat{R}^\alpha \hat{R}^\beta v''(\mathbf{R}) \right\}
\]

with \( \alpha, \beta = 1 \) or 2, and \( \hat{\Phi}^{zz}(\mathbf{k}) = K_z \) independent of \( \mathbf{k} \). You may find it useful to invoke Eqn. 3.54 of the lecture notes (you don’t have to derive it!).

(b) Assuming that the above sum for \( \Phi^{\alpha\beta}(\mathbf{k}) \) is dominated by the nearest neighbor terms, compute the phonon dispersions along the \((1,0)\) axis in reciprocal space. You should use \( M \) for the ionic mass, \( a \) for the lattice constant, and abbreviate \( A \equiv a^{-1} v'(a) \) and \( B \equiv v''(a) \).

(c) Find the general form of the dynamical matrix for arbitrary phonon wavevector \( \mathbf{k} \). For the acoustic modes, find the sound velocities \( c_\pm \) for \( k \approx 0 \).

**Solution:**

(a) The result for \( \Phi^{\alpha\beta}(\mathbf{k}) \) follows from Eqn. 3.54 of the lecture notes.

(b) We take \( \mathbf{a}_1 = \frac{1}{2} a (\hat{x} - \sqrt{3} \hat{y}) \) and \( \mathbf{a}_2 = \frac{1}{2} a (\hat{x} + \sqrt{3} \hat{y}) \). The elementary reciprocal lattice vectors are then \( \mathbf{b}_1 = (2\pi/a\sqrt{3})(\sqrt{3} \hat{x} - \hat{y}) \) and \( \mathbf{b}_2 = (2\pi/a\sqrt{3})(\sqrt{3} \hat{x} + \hat{y}) \). The nearest neighbor separations are then the six vectors \( \pm \mathbf{a}_1, \pm \mathbf{a}_2, \) and \( \pm \mathbf{a}_3 \) where \( \mathbf{a}_3 \equiv -(\mathbf{a}_1 + \mathbf{a}_2) = -a\hat{x} \). With \( \mathbf{k} = (\frac{1}{2} a \theta_1) \mathbf{b}_1 + (\frac{1}{2} a \theta_2) \mathbf{b}_2 \) we have

\[
\Phi^{\alpha\beta}(\mathbf{k}) = 4 \sin^2\left(\frac{1}{2} \theta_1\right) \left( A \delta^{\alpha\beta} + (B - A) \hat{a}_1^\alpha \hat{a}_1^\beta \right) + 4 \sin^2\left(\frac{1}{2} \theta_2\right) \left( A \delta^{\alpha\beta} + (B - A) \hat{a}_2^\alpha \hat{a}_2^\beta \right) + 4 \sin^2\left(\frac{1}{2} \theta_3\right) \left( A \delta^{\alpha\beta} + (B - A) \hat{a}_3^\alpha \hat{a}_3^\beta \right)
\]

where \( \theta_3 \equiv - (\theta_1 + \theta_2) \), and

\[
\hat{a}_1^\alpha \hat{a}_1^\beta = \frac{1}{4} \begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & 3 \end{pmatrix}, \quad \hat{a}_2^\alpha \hat{a}_2^\beta = \frac{1}{4} \begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & 3 \end{pmatrix}, \quad \hat{a}_3^\alpha \hat{a}_3^\beta = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.
\]

Along \((1,0)\) we have \( \theta_2 = 0 \) and thus \( \theta_3 = -\theta_1 \). This yields

\[
\Phi^{\alpha\beta}(\mathbf{k}) = \sin^2\left(\frac{1}{2} \theta_1\right) \begin{pmatrix} 3A + 5B & \sqrt{3}(A - B) \\ \sqrt{3}(A - B) & 5A + 3B \end{pmatrix}.
\]

Thus the phonon dispersion is given by

\[
\omega_\pm(\theta_1, 0) = 2 \left| \sin\left(\frac{1}{2} \theta_1\right) \right| \sqrt{\frac{(A + B) \pm \frac{1}{2}|A - B|}{M}}.
\]
These are two of the three phonon branches. The third is a dispersionless Einstein phonon, \( \omega_3(k) = \sqrt{K_z/M} \).

(c) The general form of the dynamical matrix in the acoustic sector is

\[
\begin{align*}
\phi^{11}(k) &= (3A + B)[\sin^2(\frac{1}{2}\theta_1) + \sin^2(\frac{1}{2}\theta_2)] + 4B \sin^2(\frac{1}{2}\theta_3) \\
\phi^{22}(k) &= (A + 3B)[\sin^2(\frac{1}{2}\theta_1) + \sin^2(\frac{1}{2}\theta_2)] + 4A \sin^2(\frac{1}{2}\theta_3) \\
\phi^{12}(k) &= \sqrt{3}(A - B) \left[ \sin^2(\frac{1}{2}\theta_1) - \sin^2(\frac{1}{2}\theta_2) \right],
\end{align*}
\]

and

\[
M \omega^2_\pm(\theta_1, \theta_2) = \frac{1}{8}(\phi^{11}(k) + \phi^{22}(k)) + \frac{1}{4}(\phi^{11}(k) - \phi^{22}(k))^2 + |\phi^{12}(k)|^2
= 2(A + B)(s_1^2 + s_2^2 + s_3^2) \pm 2|A - B| \cdot (s_1^4 + s_2^4 + 2s_3^4 - 2s_1^2s_2^2 - 2s_1^2s_3^2 - 2s_2^2s_3^2),
\]

where \( s_j = \sin^2(\frac{1}{2}\theta_j) \). Note that setting \( \theta_1 = \theta_2 = \pi \) yields \( M \omega^2_+ = 8 \max(A, B) \) and \( M \omega^2_- = 8 \min(A, B) \) at an edge center of the BZ, whereas \( \theta_1 = \theta_2 = \frac{\pi}{3} \) yields \( M \omega^2_+ = 3(A + B) \) at the zone corners. In the long wavelength limit, we have

\[
\begin{align*}
\phi^{11}(k) &= \frac{1}{8}(3A + B)(k_x^2 + 3k_y^2)a^2 + Bk_y^2a^2 + \ldots \\
\phi^{22}(k) &= \frac{1}{8}(A + 3B)(k_x^2 + 3k_y^2)a^2 + Ak_y^2a^2 + \ldots \\
\phi^{12}(k) &= \frac{3}{4}(B - A)k_xk_ya^2 + \ldots
\end{align*}
\]

whence

\[
\frac{1}{4}(\phi^{11}(k) + \phi^{22}(k)) = \frac{3}{4}(A + B)(k_x^2 + k_y^2)a^2 + \ldots
\]
\[
\frac{1}{4}(\phi^{11}(k) - \phi^{22}(k)) = \frac{3}{4}(B - A)(k_x^2 + k_y^2)a^2 + \ldots
\]
\[
\frac{1}{4}(\phi^{11}(k) - \phi^{22}(k))^2 + |\phi^{12}(k)|^2 = \frac{3(3A - B)}{8M}(k_x^2 + k_y^2)^2a^4 + \ldots,
\]

and \( \omega_\pm(k) = c_\pm|k| \) with

\[
c_+ = \sqrt{\frac{3(3A + B)a^2}{8M}} \quad \text{and} \quad c_- = \sqrt{\frac{3(A + 3B)a^2}{8M}}.
\]

Again, there will be a third Einstein phonon with \( \omega_3(k) = \sqrt{K_z/M} \).

(4) Consider a one-dimensional chain of s-orbitals separated by a distance \( a_0 \), with

\[
H = \sum_n \left( \varepsilon_\text{A} |A_n \rangle \langle A_n| + \varepsilon_\text{B} |B_n \rangle \langle B_n| \right) - t \sum_n \left( |A_n \rangle \langle B_n| + |B_n \rangle \langle A_n+1| + |A_n \rangle \langle A_{n+1}| + |A_{n+1} \rangle \langle B_n| \right).
\]

(a) How many atoms are there per unit cell? What is the length of the Wigner-Seitz cell?
(b) Find the dispersions \( E_a(k) \) of the energy bands.
(c) Sketch the band structure over the one-dimensional Brillouin zone.

(d) Show that for \( \varepsilon_A = \varepsilon_B \) that you recover the correct energy band for the uniform one-dimensional nearest-neighbor chain.

**Solution:**

(a) There are two atoms per unit cell (one A and one B). The length of the Wigner-Seitz cell is \( a = 2a_0 \), where \( a_0 \) is the separation between neighboring A and B sites.

(b) From the Hamiltonian above, we read off the hopping matrix

\[
H_{aa'}(n - n') = \begin{pmatrix}
\varepsilon_A \delta_{n-n',0} & -t (\delta_{n-n',0} + \delta_{n-n',1}) \\
-t (\delta_{n-n',0} + \delta_{n-n',1}) & \varepsilon_B \delta_{n-n',0}
\end{pmatrix}
\]

Thus,

\[
\hat{H}_{aa'}(k) = \sum_j H_{aa'}(j) e^{-i k a} = \begin{pmatrix}
\varepsilon_A & -t (1 + e^{-i k a}) \\
-t (1 + e^{i k a}) & \varepsilon_B
\end{pmatrix}
\]

The energy eigenvalues are then

\[
E_{\pm}(k) = \frac{1}{2} (\varepsilon_A + \varepsilon_B) \pm \sqrt{\frac{1}{4} (\varepsilon_A - \varepsilon_B)^2 + 4t^2 \cos^2 \left(\frac{1}{2} k a\right)},
\]

where we’ve used \(|1 + e^{-i k a}|^2 = 2 + 2 \cos(ka) = 4 \cos^2 \left(\frac{1}{2} k a\right)\).

(c) See the plots in Fig. 1.

(d) Let \( \varepsilon_A = \varepsilon_B = \varepsilon_0 \). Then \( E_{\pm}(k) = \varepsilon_0 \pm 2t \cos \left(\frac{1}{2} k a\right) \). If we translate the section of the + band on the interval \( k \in \left[ -\frac{\pi}{a'}, 0 \right] \) by \( \frac{2\pi}{a'} \), and the section on the interval \( k \in \left[ 0, \frac{\pi}{a'} \right] \) by \( -\frac{2\pi}{a'} \), we obtain the dispersion \( E(k) = \varepsilon_0 - 2t \cos(ka') \) on the interval \( k \in \left[ -\frac{\pi}{a'}, \frac{\pi}{a'} \right] \), with \( a' = \frac{1}{2} a \).

(5) Hexagonal boron nitride, BN, has a honeycomb lattice structure, with boron atoms at A sites and nitrogen atoms at B sites. The tight binding Hamiltonian is

\[
H = \sum_R \left( \varepsilon_A \langle A_R | A_R \rangle + \varepsilon_B \langle B_R | B_R \rangle \right) - t \sum_R \left( |A_R \rangle \langle B_R | + |A_R \rangle \langle B_{R+a_1} | + |A_R \rangle \langle B_{R-a_2} | + H.c. \right).
\]

(a) Find the \( 2 \times 2 \) Hamiltonian matrix \( \hat{H}(k) \). You may find it convenient to write the wavevector as \( k = \frac{\theta_1}{2\pi} b_1 + \frac{\theta_2}{2\pi} b_2 \) and express your answer in terms of \( \theta_{1,2} \).

(b) Find expressions for the band energies at high symmetry points \( \Gamma, K, \) and \( M \).

(c) Find an expression for the band gap \( \Delta \). Is the gap direct or indirect?

**Solution:**
Figure 1: Energy bands $E_{\pm}(k)$ for problem 1. Top: $\varepsilon_A = 0.5$, $\varepsilon_B = 0.0$, $t = 1.0$. Bottom: $\varepsilon_A = \varepsilon_B = 0.5$, $t = 1.0$. The extended zone plot of the dispersion is shown for the latter case, in which the one-dimensional dispersion $E(k) = \varepsilon_0 - 2t \cos(ka')$ is recovered, with $a' = \frac{1}{2}a$ and $k \in \left[-\frac{\pi}{a'}, \frac{\pi}{a'}\right]$.

(a) The Hamiltonian matrix is
\[
\hat{H}(k) = \begin{pmatrix}
\varepsilon_A & -t \gamma(k) \\
-t \gamma^*(k) & \varepsilon_B
\end{pmatrix},
\]
where
\[
\gamma(k) = 1 + e^{ik \cdot a_1} + e^{-ik \cdot a_2} = 1 + e^{i\theta_1} + e^{-i\theta_2}.
\]

There are two bands:
\[
E_{\pm}(k) = \frac{1}{2} (\varepsilon_A + \varepsilon_B) \pm \sqrt{\frac{1}{4} (\varepsilon_A - \varepsilon_B)^2 + t^2 |\gamma(k)|^2}.
\]

(b) Recall $k_\Gamma = 0$, $k_K = \frac{1}{3} B_1 + \frac{1}{3} B_2$, and $k_M = \frac{1}{2} b_1$. Thus,
\[
\gamma(\Gamma) = 3 \quad , \quad \gamma(K) = 0 \quad , \quad \gamma(M) = 1.
\]
and

\[ E_{\pm}(\Gamma) = \frac{1}{2}(\varepsilon_A + \varepsilon_B) \pm \sqrt{\frac{1}{4}(\varepsilon_A - \varepsilon_B)^2 + 9t^2} \]
\[ E_{\pm}(K) = \varepsilon_A, \varepsilon_B \]
\[ E_{\pm}(M) = \frac{1}{2}(\varepsilon_A + \varepsilon_B) \pm \sqrt{\frac{1}{4}(\varepsilon_A - \varepsilon_B)^2 + t^2} . \]

(c) Since nitrogen has a greater nuclear charge, we expect \( \varepsilon_B < \varepsilon_A \). The maximum valence (-) band energy is then \( \varepsilon_B \), at K. The minimum conduction band energy is \( \varepsilon_A \), also at K. Thus, the gap is direct and equal to \( \Delta = \varepsilon_A - \varepsilon_B \). The direct gap at wavevector \( k \) is

\[ \Delta(k) \equiv E_+(k) - E_-(k) = \sqrt{(\varepsilon_A - \varepsilon_B)^2 + 4t^2|\gamma(k)|^2} . \]

(6) Consider a tight binding model of \( (p_x, p_y) \) orbitals on a triangular lattice. The hopping is restricted to nearest neighbor links. Recall that the hopping matrix elements are given by

\[ t_{\mu\nu}(\hat{\eta}) = t_w \delta_{\mu\nu} - (t_s + t_w) \hat{\eta}_\mu \hat{\eta}_\nu , \]

where the link direction is \( \hat{\eta} \).

(a) Find the matrix \( \hat{t}_{\mu\nu}(k) \). You may find it convenient to write \( k = \frac{\theta_1}{2\pi} b_1 + \frac{\theta_2}{2\pi} b_2 \) and express your answer in terms of \( \theta_{1,2} \).

(b) Find expressions for the band energies at the high symmetry points \( \Gamma, K, \) and \( M \).

(c) For \( t_s = 1 \) and \( t_w = \frac{1}{2} \), plot the dispersions \( E_{\pm}(k) \) along the path \( \Gamma M K \Gamma \).

<table>
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<th>( \hat{\eta} )</th>
<th>( \hat{\eta}_j^x \hat{\eta}_j^x )</th>
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Table 1: Values of \( \eta_j^\mu \eta_j^\nu \) for the six nearest neighbor vectors.

Solution:

(a) On the triangular lattice, there are six nearest neighbors. Defining the primitive direct lattice vectors \( a_1 = a \left( \frac{1}{2} \hat{x} - \frac{\sqrt{3}}{2} \hat{y} \right) \) and \( a_2 = a \left( \frac{1}{2} \hat{x} + \frac{\sqrt{3}}{2} \hat{y} \right) \), the six nearest neighbor vectors
Figure 2: Energy bands $E_{\pm}(k)$ along high symmetry directions for problem 3. Top: $t_s = 2.5$ and $t_w = 0.5$. Bottom: $t_s = 1.0$ and $t_w = 0.5$.

are $\pm a_1, \pm a_2$, and $\pm a_3$, where $a_3 \equiv -a_1 - a_2 = -a \hat{x}$. From the entries in Tab. 1, we have

$$
\tilde{t}_{xx}(k) = 2t_w(c_1 + c_2 + c_3) - (t_s + t_w)(\tfrac{1}{2}c_1 + \tfrac{1}{2}c_2 + 2c_3)
$$

$$
\tilde{t}_{yy}(k) = 2t_w(c_1 + c_2 + c_3) - (t_s + t_w)(\tfrac{3}{2}c_1 + \tfrac{1}{2}c_2)
$$

$$
\tilde{t}_{xy}(k) = \sqrt{3} \left( t_s + t_w)(c_1 - c_2) = \tilde{t}_{yx}(k) \right),
$$

where $\theta_3 \equiv -(\theta_1 + \theta_2)$ and where $c_j = \cos \theta_j$. Thus,

$$
\tilde{t}_{\mu\nu}(k) = \left( \begin{array}{c}
\tfrac{1}{2}(3t_w - t_s)(c_1 + c_2) - 2ts_3 & \sqrt{3} \left( t_s + t_w)(c_1 - c_2) \\
\sqrt{3} \left( t_s + t_w)(c_1 - c_2) & \tfrac{1}{2}(t_w - 3t_s)(c_1 + c_2) + 2twc_3
\end{array} \right)
\right)
$$

$$
= (t_w - t_s)(c_1 + c_2 + c_3) + \tfrac{1}{2}(t_w + t_s)(c_1 + c_2 - 2c_3) \sigma^z + \sqrt{3} \left( t_s + t_w)(c_1 - c_2) \sigma^x
$$

The eigenvalues of $\tilde{H}_{\mu\nu}(k) = \tilde{t}_{\mu\nu}(k)$ are then

$$
E_{\pm}(k) = (t_s - t_w)(c_1 + c_2 + c_3) \pm (t_s + t_w) \sqrt{c_1^2 + c_2^2 + c_3^2 - c_1c_2 - c_2c_3 - c_1c_3}.
$$

Note that under a $60^\circ$ rotation, $a_1 \rightarrow -a_3$, $a_2 \rightarrow -a_1$, and $a_3 \rightarrow -a_2$, so $(\theta_1, \theta_2, \theta_3) \rightarrow (-\theta_3, -\theta_1, -\theta_2)$. This symmetry is manifestly preserved by the above dispersions.
Table 2: Dispersion at high symmetry points.

<table>
<thead>
<tr>
<th>(k)</th>
<th>(\theta_1)</th>
<th>(\theta_2)</th>
<th>(\theta_3)</th>
<th>(c_1)</th>
<th>(c_2)</th>
<th>(c_3)</th>
<th>(E_+(k))</th>
<th>(E_-(k))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\Gamma)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>(3(t_s - t_w))</td>
<td>(3(t_s - t_w))</td>
</tr>
<tr>
<td>(K)</td>
<td>(\frac{2\pi}{3})</td>
<td>(\frac{2\pi}{3})</td>
<td>(-\frac{4\pi}{3})</td>
<td>(-\frac{1}{2})</td>
<td>(-\frac{1}{2})</td>
<td>(-\frac{1}{2})</td>
<td>(-\frac{3}{2}(t_s - t_w))</td>
<td>(-\frac{3}{2}(t_s - t_w))</td>
</tr>
<tr>
<td>(M)</td>
<td>(\pi)</td>
<td>0</td>
<td>(-\pi)</td>
<td>(-1)</td>
<td>1</td>
<td>(-1)</td>
<td>(3t_s + t_w)</td>
<td>(-t_w - 3t_s)</td>
</tr>
</tbody>
</table>

(b) See the results in Tab. 2. Note that the bands are degenerate at both \(\Gamma\) and \(K\).

(c) See the plot in Fig. 2.

(7) Make a sketch of the extended Brillouin zones like in Fig. 5.2.2 of the Lecture Notes, but for the triangular lattice. Then make plots the free electron Fermi surface for valences \(Z = 2\) and \(Z = 3\), such as in Fig. 2.3.

**Solution:**

See Fig. 3. For \(Z = 2\) the free electron Fermi sphere extends into the second Brillouin zone, and for \(Z = 3\) it extends into the third Brillouin zone!

![Figure 3](image)

Figure 3: Left: Brillouin zones for the triangular lattice structure. Right: The concentric circles correspond to electron fillings of \(Z = 1\), \(Z = 2\), and \(Z = 3\) per unit cell.

(8) Cyclotron resonance in Si and Ge – This problem is based on the following figures:

Both Si and Ge are indirect gap semiconductors with anisotropic conduction band minima and doubly degenerate valence band maxima. In Si, the conduction band minima occur along the \(\langle 100\rangle\) (\(\langle \Gamma X\rangle\)) directions, and are six-fold degenerate. The equal energy surfaces are cigar-shaped, and the effective mass along the \(\langle \Gamma X\rangle\) principal axes (the ‘longitudinal’
Figure 4: (a) Left: Constant energy surfaces near the conduction band minima in silicon. There are six symmetry-related ellipsoidal pockets whose long axes run along the \(\langle 100\rangle\) directions. Right: Cyclotron resonance data in Si (G. Dresselhaus et al., Phys. Rev, 98, 368 (1955).) The field lies in a \((110)\) plane and makes an angle of 30° with the \([001]\) axis. (b) Left: Constant energy surfaces near the conduction band minima in germanium. There are eight symmetry-related half-ellipsoids whose long axes run along the \(\langle 111\rangle\) directions, and are centered on the midpoints of the hexagonal zone faces. With a suitable choice of primitive cell in \(k\)-space, these can be represented as four ellipsoids, the half-ellipsoids on opposite faces being joined together by translations through suitable reciprocal lattice vectors. Right: Cyclotron resonance data in Ge (G. Dresselhaus et al., Phys. Rev, 98, 368 (1955).) The field lies in a \((110)\) plane and makes an angle of 60° with the \([001]\) axis.

The effective mass) is \(m^*_t \simeq 1.0 m_e\), while the effective mass in the plane perpendicular to this axis (the ‘transverse’ effective mass) is \(m^*_t \simeq 0.20 m_e\). The valence band maximum
occurs at the unique $\Gamma$ point, and there are two isotropic hole branches: a ‘heavy’ hole with $m_{hh}^* \simeq 0.49 m_e$, and a ‘light’ hole with $m_{lh}^* \simeq 0.16 m_e$.

In Ge, the conduction band minima occur at the fourfold degenerate L point (along the eight ⟨111⟩ directions) with effective masses $m_{l}^* \simeq 1.6 m_e$ and $m_{t}^* \simeq 0.08 m_e$. The valence band maximum again occurs at the $\Gamma$ point, where the hole masses are $m_{hh}^* \simeq 0.34 m_e$ and $m_{lh}^* \simeq 0.044 m_e$. Use the following figures to interpret the cyclotron resonance data shown below. Verify whether the data corroborate the quoted values of the effective masses in Si and Ge.

**Solution:**

We found that $\sigma_{\alpha\beta} = ne^2 \Gamma_{\alpha\beta}^{-1}$, with

$$\Gamma_{\alpha\beta} \equiv (\tau^{-1} - i\omega) m_{\alpha\beta} \pm \frac{e}{c} \epsilon_{\alpha\beta\gamma} B^\gamma$$

$$= \begin{pmatrix} (\tau^{-1} - i\omega)m_{x}^* & \pm eB_z/c & \mp eB_y/c \\ \mp eB_z/c & (\tau^{-1} - i\omega)m_{y}^* & \pm eB_x/c \\ \pm eB_y/c & \mp eB_x/c & (\tau^{-1} - i\omega)m_{z}^* \end{pmatrix}.$$

The valence band maxima are isotropic in both cases, with

$$m_{hh}^*(Si) \simeq 0.49 m_e \quad m_{hh}^*(Ge) \simeq 0.34 m_e$$

$$m_{lh}^*(Si) \simeq 0.16 m_e \quad m_{lh}^*(Ge) \simeq 0.044 m_e.$$

With isotropic bands, the absorption is peaked at $\omega = \omega_c = eB/m^* c$, assuming $\omega_c \tau \gg 1$. Writing $\omega = 2\pi f$, the resonance occurs at a field

$$B(f) = 2\pi f \cdot \frac{m^* c}{e}$$

$$= \frac{hc}{e} \cdot \frac{m^*}{m_e} \cdot \frac{1}{2\pi a_B^2} \cdot \frac{hf}{(e^2/a_B)}$$

$$= 3.58 \times 10^{-7} \text{ G} \cdot \frac{m^*}{m_e} \cdot f [\text{Hz}]$$

$$= 8590 \text{ G} \cdot \frac{m^*}{m_e},$$

where we have used

$$\frac{hc}{e} = 4.137 \times 10^{-7} \text{ G} \cdot \text{cm}^2$$

$$a_B = \frac{h^2}{m_e e^2} = 0.529 \text{ Å}$$

$$h = 4.136 \times 10^{-15} \text{ eV} \cdot \text{s}$$

$$\frac{e^2}{a_B} = 27.2 \text{ eV} = 2 \text{ Ry}$$

$$f = 2.40 \times 10^{10} \text{ Hz}.$$
Thus, we predict

\[
B_{hh}(Si) \simeq 4210 \, \text{G} \quad B_{hh}(Ge) \simeq 2920 \, \text{G} \\
B_{lh}(Si) \simeq 1370 \, \text{G} \quad B_{lh}(Ge) \simeq 378 \, \text{G}.
\]

All of these look pretty good.

Now let us review the situation with electrons near the conduction band minima:

Si: 6-fold degenerate minima along \( \langle 100 \rangle \)

Ge: 4-fold degenerate minima along \( \langle 111 \rangle \) (at L point)

\[
m^*_t(Si) \simeq 1.0 \, m_e \quad m^*_t(\text{Ge}) \simeq 1.6 \, m_e \\
m^*_l(Si) \simeq 0.20 \, m_e \quad m^*_l(\text{Ge}) \simeq 0.08 \, m_e.
\]

The resonance condition is that \( \sigma_{\alpha\beta} = \infty \), which for \( \tau > 0 \) occurs only at complex frequencies, i.e. for real frequencies there are no true divergences, only resonances. The location of the resonance is determined by \( \det \Gamma = 0 \). Taking the determinant, one finds

\[
\det \Gamma = (\tau^{-1} - i\omega) m_t^* \cdot \left\{ (\tau^{-1} - i\omega)^2 m_t^{*2} + \frac{e^2}{c^2} B_z^2 + \frac{m_t^*}{m_l^*} \frac{e^2}{c^2} \left( B_x^2 + B_y^2 \right) \right\}.
\]

Assuming \( \omega\tau \gg 1 \), the location of the resonance is given by

\[
\omega^2 = \left( \frac{eB_\|}{m_t^* c} \right)^2 + \frac{m_t^*}{m_l^*} \left( \frac{eB_\perp}{m_t^* c} \right)^2,
\]

where \( B_\| \equiv B_z \) and \( B_\perp \equiv B_x \hat{x} + B_y \hat{y} \). Let the polar angle of \( B \) be \( \theta \), so \( B_\| = B \cos \theta \) and \( B_\perp = B \sin \theta \). We then have

\[
\omega^2 = \left( \frac{eB}{m_t^* c} \right)^2 \left\{ \cos^2 \theta + \frac{m_t^*}{m_l^*} \sin^2 \theta \right\}
\]

\[
B(f) = 8600 \, \text{G} \cdot \left( \frac{m_t^*}{m_e} \right) / \sqrt{\cos^2 \theta + \frac{m_t^*}{m_l^*} \sin^2 \theta},
\]

where again we take \( f = \omega/2\pi = 2.4 \times 10^{10} \, \text{Hz} \).

According to the diagrams, the field lies in the (110) plane, which means we can write

\[
\hat{B} = \sqrt{\frac{1}{2}} \sin \chi \hat{e}_1 - \sqrt{\frac{1}{2}} \sin \chi \hat{e}_2 + \cos \chi \hat{e}_3,
\]

where \( \chi \) is the angle \( \hat{B} \) makes with \( \hat{e}_3 = [001] \).

**Ge**

We have

\[
\frac{m_t^*}{m_e} = 0.082 \quad \frac{m_l^*}{m_t^*} = 0.051.
\]
and we are told $\chi = 60^\circ$, so

$$\hat{B} = \sqrt{\frac{3}{8}} \hat{e}_1 - \sqrt{\frac{3}{8}} \hat{e}_2 + \frac{1}{2} \hat{e}_3.$$  

The conduction band minima lie along (111), which denotes a set of directions in real space:

- $\pm [111]: \hat{n} = \pm \frac{1}{\sqrt{3}} (\hat{e}_1 + \hat{e}_2 + \hat{e}_3) \Rightarrow \cos^2 \theta = (\hat{B} \cdot \hat{n})^2 = \frac{1}{12} \Rightarrow B = 1950 \text{ G}$
- $\pm [111]: \hat{n} = \pm \frac{1}{\sqrt{3}} (\hat{e}_1 + \hat{e}_2 - \hat{e}_3) \Rightarrow \cos^2 \theta = (\hat{B} \cdot \hat{n})^2 = \frac{1}{12} \Rightarrow B = 1950 \text{ G}$
- $\pm [111]: \hat{n} = \pm \frac{1}{\sqrt{3}} (-\hat{e}_1 + \hat{e}_2 + \hat{e}_3) \Rightarrow \cos^2 \theta = (\hat{B} \cdot \hat{n})^2 = \frac{7 - 2\sqrt{6}}{12} \Rightarrow B = 1510 \text{ G}$
- $\pm [111]: \hat{n} = \pm \frac{1}{\sqrt{3}} (\hat{e}_1 - \hat{e}_2 + \hat{e}_3) \Rightarrow \cos^2 \theta = (\hat{B} \cdot \hat{n})^2 = \frac{7 + 2\sqrt{6}}{12} \Rightarrow B = 710 \text{ G}$.

All OK!

**Si:**

Again, $B$ lies in the (110) plane, this time with $\chi = 30^\circ$, so

$$\hat{B} = \sqrt{\frac{3}{8}} \hat{e}_1 - \sqrt{\frac{3}{8}} \hat{e}_2 + \sqrt{\frac{1}{8}} \hat{e}_3.$$  

The conduction band minima lie along (100), so

- $\pm [001]: \hat{n} = \pm \hat{e}_3 \Rightarrow \cos^2 \theta = (\hat{B} \cdot \hat{n})^2 = \frac{3}{4} \Rightarrow B = 1820 \text{ G}$
- $\pm [010]: \hat{n} = \pm \hat{e}_2 \Rightarrow \cos^2 \theta = (\hat{B} \cdot \hat{n})^2 = \frac{1}{8} \Rightarrow B = 2980 \text{ G}$
- $\pm [100]: \hat{n} = \pm \hat{e}_1 \Rightarrow \cos^2 \theta = (\hat{B} \cdot \hat{n})^2 = \frac{1}{8} \Rightarrow B = 2980 \text{ G}$.

These also look pretty good.