Chapter 3
Solution Manual

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3.1:

The Born-von Karman periodic boundary condition requires:

$$e^{ikx} = e^{ik(x+L)} \tag{1}$$

This implies:

$$e^{ikL} = 1 = e^{in2\pi} \quad \text{where } n = 0, 1, 2 \ldots \tag{2}$$

The values of the wavevector are thus restricted to:

$$k = \frac{n2\pi}{L} \tag{3}$$

Each value of k thus occupies a volume in k-space of:

$$V_k = \left(\frac{2\pi}{L}\right)^3 \tag{4}$$

The density of k-states per sample volume is thus:

$$\rho_k = \frac{1}{V_k L^3} = \frac{1}{(2\pi)^3} \tag{5}$$

3.2:

The density of states is found by taking the derivative with respect to k of the number of k-states in a sphere of radius k:

$$\begin{aligned} g(k) &= \frac{dN}{dk} \\ &= \frac{d}{dk}\left[\frac{4}{3}\pi k^3 \frac{1}{(2\pi)^3}\right] \\ &= \frac{k^2}{2\pi^2} \end{aligned} \tag{6}$$

We have the dispersion relation for a parabolic band with effective mass m^*:

$$E(k) = \frac{\hbar^2 k^2}{2m^*} \rightarrow \frac{dE}{dk} = \frac{\hbar^2 k}{m^*} \tag{7}$$

or:

$$\begin{aligned}\frac{dk}{dE} &= \frac{m^*}{\hbar^2 k} \\ &= \frac{m^*}{\hbar^2}\sqrt{\frac{\hbar^2}{2m^*E}} \\ &= \sqrt{\frac{m^*}{2\hbar^2 E}}\end{aligned} \tag{8}$$

Noting that the density of states may be expressed as $g(k) = \frac{dN}{dk}$, we can write:

$$\begin{aligned}g(E) &= 2g(k)\frac{dk}{dE} \\ &= \frac{k^2}{\pi^2}\sqrt{\frac{m^*}{2\hbar^2 E}} \\ &= \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E}\end{aligned} \tag{9}$$

3.3:

(a) The parity operation refers to the transformation $\mathbf{r} \to -\mathbf{r}$. In spherical coordinates, this corresponds to $\theta \to \pi - \theta$ and $\phi \to \phi + \pi$. The polar part of the spherical harmonic is changed according to:

$$e^{im(\phi+\pi)} = (-1)^m e^{im\phi} \tag{10}$$

The polynomial functions $P_\ell^m(cos(\theta))$ (called the associated Legendre polynomials) are given by:

$$P_\ell^m(cos(\theta)) = (-1)^m(1-x^2)^{\frac{m}{2}}\frac{d^m}{dx^m}(P_\ell(cos(\theta))) \tag{11}$$

where $P_\ell(cos(\theta))$ are the Legendre polynomials given by:

$$P_1(cos(\theta)) = 1 \qquad P_2(cos(\theta)) = cos(\theta) \qquad P_3(cos(\theta)) = \frac{1}{2}\left[3cos^2(\theta) - 1\right] \quad \ldots \tag{12}$$

We know that the parity operation changes the polynomials by:

$$\begin{aligned}P_\ell^m(cos(\pi-\theta)) &= (-1)^m(1-cos^2(\pi-\theta))^{\frac{m}{2}}\frac{d^m}{dx^m}(P_\ell(cos(\pi-\theta))) \\ &= (-1)^m(-1)^m(-1)^\ell(1-cos^2(\theta))^{\frac{m}{2}}\frac{d^m}{dx^m}(P_\ell(cos(\theta)))\end{aligned} \tag{13}$$

The spherical harmonics thus transform as:

$$\begin{aligned}Y_{\ell m}(\pi-\theta,\phi+\pi) &= (-1)^m(-1)^m(-1)^m(-1)^\ell(1-cos^2(\theta))^{\frac{m}{2}}\frac{d^m}{dx^m}(P_\ell(cos(\theta)))e^{im\phi} \\ &= (-1)^\ell Y_{\ell m}(\theta,\phi)\end{aligned} \tag{14}$$

We thus see that the spherical harmonics are inversion symmetric for even values of ℓ and inversion anti-symmetric for odd values of ℓ.

(b) We calculate the matrix element for the electric-dipole transition by breaking it up into two parts[1]:

$$
\begin{aligned}
M &= \left| -e \int_0^\infty \int_0^\pi \int_0^{2\pi} Y^*_{\ell' m'}(\theta,\phi)\mathbf{r}Y_{\ell m}(\theta,\phi) r^2 sin(\theta) d\phi d\theta dr \right| \\
&= e \left| \int_0^\infty r^2 \left[\int_0^\pi \int_0^\pi Y^*_{\ell' m'}(\theta,\phi)Y_{\ell m}(\theta,\phi)\mathbf{r} sin(\theta) d\phi d\theta + \int_0^\pi \int_\pi^{2\pi} Y^*_{\ell' m'}(\theta,\phi)Y_{\ell m}(\theta,\phi)\mathbf{r} sin(\theta) d\phi d\theta \right] dr \right| \\
&= e \left| \int_0^\infty r^2 \int_0^\pi \int_0^\pi \left[Y^*_{\ell' m'}(\theta,\phi)Y_{\ell m}(\theta,\phi) - Y^*_{\ell' m'}(\pi-\theta,\phi+\pi)Y_{\ell m}(\pi-\theta,\phi+\pi) \right] \mathbf{r} sin(\theta) d\phi d\theta dr \right| \\
&= e \left| \int_0^\infty r^2 \int_0^\pi \int_0^\pi \left[Y^*_{\ell' m'}(\theta,\phi)Y_{\ell m}(\theta,\phi) - (-1)^{\ell}(-1)^{\ell'} Y^*_{\ell' m'}(\theta,\phi)Y_{\ell m}(\theta,\phi) \right] \mathbf{r} sin(\theta) d\phi d\theta dr \right| \\
&= e \left| \int_0^\infty r^2 \int_0^\pi \int_0^\pi \left[Y^*_{\ell' m'}(\theta,\phi)Y_{\ell m}(\theta,\phi) - (-1)^{2\ell}(-1)^{\Delta\ell} Y^*_{\ell' m'}(\theta,\phi)Y_{\ell m}(\theta,\phi) \right] \mathbf{r} sin(\theta) d\phi d\theta dr \right| \\
&= e \left| \int_0^\infty r^2 \int_0^\pi \int_0^\pi Y^*_{\ell' m'}(\theta,\phi)Y_{\ell m}(\theta,\phi)\mathbf{r} sin(\theta) d\phi d\theta dr \left[1-(-1)^{\Delta\ell} \right] \right|
\end{aligned}
\tag{15}
$$

The matrix element is therefore non-zero only if $\Delta\ell = |\ell' - \ell|$ is odd.

(c) We first examine the matrix element for light polarized in the $\hat{\mathbf{z}}$ direction:

$$
\begin{aligned}
M_z &= \left| -eE_0 \int_0^\infty \int_0^\pi \int_0^{2\pi} Y^*_{\ell' m'}(\theta,\phi) r cos(\theta) Y_{\ell m}(\theta,\phi) r^2 sin(\theta) d\phi d\theta dr \right| \hat{\mathbf{z}} \\
&= \left| -eE_0 \left[\int_0^\infty r^3 dr \right] \left[\int_0^\pi P^{m'}_{\ell'}(cos\theta) P^m_\ell(cos\theta) cos(\theta) sin(\theta) d\theta \right] \left[\int_0^{2\pi} e^{-i\Delta m\phi} d\phi \right] \right|
\end{aligned}
\tag{16}
$$

We see that the last term in the brackets equals 2π if $\Delta m = m' - m = 0$ and 0 otherwise.

For light polarized in the $\hat{\mathbf{x}}$ direction:

$$
\begin{aligned}
M_x &= \left| -eE_0 \int_0^\infty \int_0^\pi \int_0^{2\pi} Y^*_{\ell' m'}(\theta,\phi) r cos(\theta) cos(\phi) Y_{\ell m}(\theta,\phi) r^2 sin(\theta) d\phi d\theta dr \right| \\
&= \left| -eE_0 \left[\int_0^\infty r^3 dr \right] \left[\int_0^\pi P^{m'}_{\ell'}(cos\theta) P^m_\ell(cos\theta) cos(\theta) sin(\theta) d\theta \right] \left[\int_0^{2\pi} e^{-i\Delta m\phi} cos(\phi) d\phi \right] \right| \\
&= \left| -\frac{eE_0}{2} \left[\int_0^\infty r^3 dr \right] \left[\int_0^\pi P^{m'}_{\ell'}(cos\theta) P^m_\ell(cos\theta) cos(\theta) sin(\theta) d\theta \right] \left[\int_0^{2\pi} \left(e^{-i(\Delta m-1)\phi} + e^{-i(\Delta m+1)\phi} \right) d\phi \right] \right|
\end{aligned}
\tag{17}
$$

The last term in the brackets equals 2π if $\Delta m = \pm 1$, and 0 otherwise. Doing the same calculation for light polarized in the $\hat{\mathbf{y}}$ direction:

$$
\begin{aligned}
M_y &= \left| -eE_0 \int_0^\infty \int_0^\pi \int_0^{2\pi} Y^*_{\ell' m'}(\theta,\phi) r cos(\theta) sin(\phi) Y_{\ell m}(\theta,\phi) r^2 sin(\theta) d\phi d\theta dr \right| \\
&= \left| -eE_0 \left[\int_0^\infty r^3 dr \right] \left[\int_0^\pi P^{m'}_{\ell'}(cos\theta) P^m_\ell(cos\theta) cos(\theta) sin(\theta) d\theta \right] \left[\int_0^{2\pi} e^{-i\Delta m\phi} sin(\phi) d\phi \right] \right| \\
&= \left| i\frac{eE_0}{2} \left[\int_0^\infty r^3 dr \right] \left[\int_0^\pi P^{m'}_{\ell'}(cos\theta) P^m_\ell(cos\theta) cos(\theta) sin(\theta) d\theta \right] \left[\int_0^{2\pi} \left(e^{-i(\Delta m-1)\phi} - e^{-i(\Delta m+1)\phi} \right) d\phi \right] \right|
\end{aligned}
\tag{18}
$$

[1] Also recall that the transformation $\mathbf{r} \to -\mathbf{r}$ corresponds to $\theta \to \pi - \theta$ and $\phi \to \phi + \pi$.

where the same reasoning as that for $\hat{\mathbf{y}}$ polarized light applies.

(d) We can write the circularly polarized field vectors in the form:

$$\boldsymbol{\sigma}^+ = \frac{E_0}{\sqrt{2}}\left(\hat{\mathbf{x}} + i\hat{\mathbf{y}}\right) \qquad \boldsymbol{\sigma}^- = \frac{E_0}{\sqrt{2}}\left(\hat{\mathbf{x}} - i\hat{\mathbf{y}}\right) \tag{19}$$

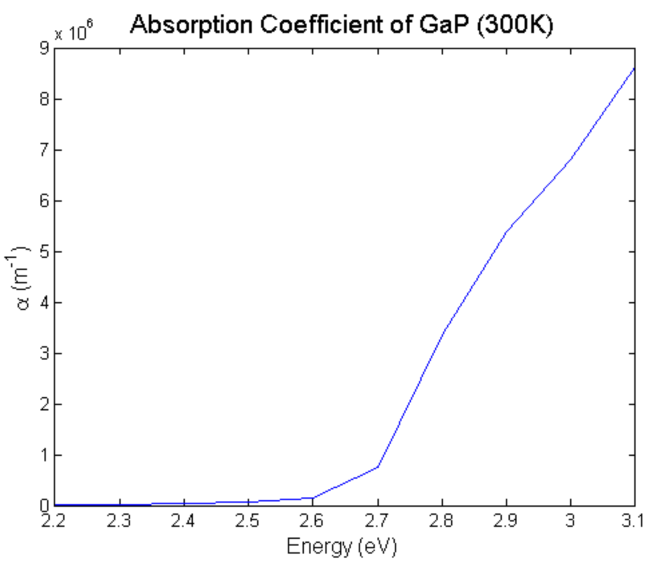
The matrix elements associated with each are given by:

$$\begin{aligned} M_{\sigma^+} &= \left|-\frac{eE_0}{\sqrt{2}}\int_0^\infty\int_0^\pi\int_0^{2\pi} Y^*_{\ell' m'}(\theta,\phi) r cos(\theta)\left[cos(\phi) + isin(\phi)\right] Y_{\ell m}(\theta,\phi) r^2 sin(\theta) d\phi d\theta dr\right| \\ &= \left|-\frac{eE_0}{\sqrt{2}}\left[\int_0^\infty r^3 dr\right]\left[\int_0^\pi P_{\ell'}^{m'}(cos\theta) P_\ell^m(cos\theta) cos(\theta) sin(\theta) d\theta\right]\left[\int_0^{2\pi} e^{-i(\Delta m - 1)\phi} d\phi\right]\right| \\ M_{\sigma^-} &= \left|-\frac{eE_0}{\sqrt{2}}\int_0^\infty\int_0^\pi\int_0^{2\pi} Y^*_{\ell' m'}(\theta,\phi) r cos(\theta)\left[cos(\phi) - isin(\phi)\right] Y_{\ell m}(\theta,\phi) r^2 sin(\theta) d\phi d\theta dr\right| \\ &= \left|-\frac{eE_0}{\sqrt{2}}\left[\int_0^\infty r^3 dr\right]\left[\int_0^\pi P_{\ell'}^{m'}(cos\theta) P_\ell^m(cos\theta) cos(\theta) sin(\theta) d\theta\right]\left[\int_0^{2\pi} e^{-i(\Delta m + 1)\phi} d\phi\right]\right| \end{aligned} \tag{20}$$

we see that the matrix elements are non-zero only if $\Delta m = +1$ and $\Delta m = -1$ for $\boldsymbol{\sigma}^+$ and $\boldsymbol{\sigma}^-$ polarized light respectively.

3.6:

We plot the data in Table 3.4 below:



From the absorption plot of GaP, we see a tail beginning at $\approx 3.7eV$. Since this data is taken at a high temperature, this tail is a clear indication of phonon-assisted absorption across an indirect gap, which tells us that GaP is an indirect semiconductor.

3.7:

We would like to estimate the absorption coefficient at $1200nm$ or $1.036eV$. We first note that $\alpha(.85eV) \approx 6 \times 10^5 m^{-1}$. From equation (3.25), we expect the ratio of the absorption coefficient at $1.036eV$ to that at $.85eV$ to be:

$$\frac{\alpha(1.036eV)}{\alpha(.85eV)} \approx \frac{\sqrt{1.036 - .8}}{\sqrt{.85 - .8}}$$
$$\rightarrow \alpha(1.036eV) \approx 1.304 \times 10^6 m^{-1} \tag{21}$$

3.8:

(a) The conduction and heavy hole bands energies are given by:

$$E_c = E_g + \frac{\hbar^2 k_e^2}{2m_e^*} \qquad E_{hh} = -\frac{\hbar^2 k_{hh}^2}{2m_{hh}^*} \tag{22}$$

We ignore the negligible photon momentum as usual, which gives $k_e = k_{hh} = k$. Energy conservation for the heavy hole absorption of a 1.6eV photon thus gives:

$$\begin{aligned} 1.6 &= E_c - E_{hh} \\ &= 1.424 + \frac{\hbar^2 k^2}{2}\left(\frac{1}{.067m_0} + \frac{1}{.5m_0}\right) \\ \rightarrow k &= 5.24 \times 10^8 m^{-1} \end{aligned} \tag{23}$$

For absorption from the light hole band, we find:

$$\begin{aligned} 1.6 &= 1.424 + \frac{\hbar^2 k^2}{2}\left(\frac{1}{.067m_0} + \frac{1}{.08m_0}\right) \\ \rightarrow k &= 4.12 \times 10^8 m^{-1} \end{aligned} \tag{24}$$

(b) The wavevector of a photon is given by:

$$k = \frac{nE}{\hbar c} = 3.01 \times 10^7 m^{-1} \tag{25}$$

This is an order of magnitude less than the electron/hole momenta, so it is reasonable to ignore it.

(c) We first define the reduced masses for the light hole and heavy hole transitions:

$$\mu_{lh} = \left(\frac{1}{m_e^*} + \frac{1}{m_{lh}^*}\right)^{-1} = .037m_0 \quad \text{and} \quad \mu_{hh} = \left(\frac{1}{m_e^*} + \frac{1}{m_{hh}^*}\right)^{-1} = .059m_0 \tag{26}$$

The ratio of the joint density of states for the heavy hole and light hole transitions is given by:

$$\frac{g_{hh}(\hbar\omega)}{g_{lh}(\hbar\omega)} = \left(\frac{\mu_{hh}}{\mu_{lh}}\right)^{\frac{3}{2}} = 2.02 \tag{27}$$

(d) The lowest possible energy photon that can excite an electron from the split-off band is:

$$E = \Delta + E_g = 1.764eV \tag{28}$$

which corresponds to a wavelength of:

$$\lambda = \frac{hc}{E} = 704.7nm \tag{29}$$

3.9:

The heavy hole states have the quantum numbers $J = \frac{3}{2}$ and $M_J = \pm\frac{3}{2}$, and the light hole states have the quantum numbers $J = \frac{3}{2}$ and $M_J = \pm\frac{1}{2}$. We calculate the matrix elements for circularly and linearly polarized light:

- $\boldsymbol{\sigma}^-$:

$$|M_{\boldsymbol{\sigma}^-}|^2 = \frac{1}{2}(J + M_J)(J + M_J - 1)C = \begin{cases} 3C & \text{(Heavy Hole)} \\ C & \text{(Light Hole)} \end{cases} \tag{30}$$

- $\boldsymbol{\sigma}^+$:

$$|M_{\boldsymbol{\sigma}^+}|^2 = \frac{1}{2}(J - M_J)(J - M_J - 1)C = \begin{cases} 3C & \text{(Heavy Hole)} \\ C & \text{(Light Hole)} \end{cases} \tag{31}$$

- $\hat{\mathbf{z}}$:

$$|M_{\hat{\mathbf{z}}}|^2 = (J^2 - M_J)^2 C = \begin{cases} \frac{225}{16}C, \frac{9}{16}C & \text{(Heavy Hole)} \\ \frac{121}{16}C, \frac{49}{16}C & \text{(Light Hole)} \end{cases} \tag{32}$$

3.10:

As found in problem (3.3), dipole transitions are only allowed if $\Delta m = 0$ for $\hat{\mathbf{z}}$ polarized light and $\Delta m = \pm 1$ or 0 for $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ polarized light. After accounting for spin, these same selection rules apply, except for ΔM_J instead. Since for linearly polarized light there is no preference between inducing spin down to spin up or spin up to spin down transitions. For circularly polarized light however, we found that for $\boldsymbol{\sigma}^+$ light only $\Delta M_J = +1$ transitions are allowed. This means only spin down electrons will transition to spin up states and not the other way around. The same reasoning applies to $\boldsymbol{\sigma}^-$ light.

3.15:

A classical particle in a magnetic field feels the lorentz force:

$$\mathbf{F} = e(\mathbf{v} \times \mathbf{B}) \tag{33}$$

which gives, according to Newton's second law, an acceleration normal to the particle's velocity given by:

$$a_n = \frac{evB}{m} \tag{34}$$

From basic classical mechanics, we also know the centripetal acceleration is given by:

$$a_n = \frac{v^2}{r} \tag{35}$$

where r is the radius of the particle's orbit. Setting the two expressions equal to each other:

$$v = \frac{erB}{m} \tag{36}$$

The angular frequency of the oscillation is given by:

$$\omega = 2\pi \frac{v}{2\pi r} = \frac{eB}{m} \tag{37}$$

3.16:

(a) As usual, we have the density of states:

$$g(E) = 2\frac{g(k)}{\frac{dE}{dk}} \tag{38}$$

In a one-dimensional material of length L, periodic boundary conditions give a spacing between k-values of $\frac{2\pi}{L}$. The number of k-states in a length L is thus:

$$N = \frac{L}{2\pi}k \tag{39}$$

which gives a k-space density of states:

$$g(k) = \frac{dN}{dk} = \frac{L}{2\pi} \tag{40}$$

For a parabolic band, we have $\frac{dE}{dk} = \frac{\hbar^2 k}{m^*} = \frac{\hbar\sqrt{2}}{\sqrt{m^*}}\sqrt{E}$. The density of states is thus:

$$g(E) = \frac{L\sqrt{m^*}}{\hbar\sqrt{2}\pi}\frac{1}{\sqrt{E}} \tag{41}$$