6.730 Physics for Solid State Applications

Lecture 24: Effective Mass

Outline

- A Closer Look at Valence Bands
- k.p and Effective Mass
- Heavy, light and split-off bands

April 5, 2004

Semiclassical Equations of Motion

$$\langle \mathbf{v_n(k)} \rangle = \frac{\langle \mathbf{p} \rangle}{\mathbf{m}} = \frac{\mathbf{1}}{\hbar}\nabla_{\mathbf{k}}\mathbf{E_n(k)}$$

$$\mathbf{F_{ext}} = \hbar\frac{\mathbf{dk}}{\mathbf{dt}}$$

Lets try to put these equations together....

$$a(t) = \frac{dv}{dt} = \frac{1}{\hbar}\frac{\partial}{\partial t}\frac{\partial E_N(k)}{\partial k} = \frac{1}{\hbar}\frac{\partial^2 E_N(k)}{\partial k^2}\frac{dk}{dt}$$

$$= \left[\frac{1}{\hbar^2}\frac{\partial^2 E_N(k)}{\partial k^2}\right] F_{\text{ext}}$$

Looks like Newton's Law if we define the mass as follows...

$$m^*(k) = \hbar^2\left(\frac{\partial^2 E_N(k)}{\partial k^2}\right)^{-1}$$

dynamical effective mass

→ mass changes with k...so it changes with time according to k

Dynamical Effective Mass (3D)

Extension to 3-D requires some care,

F and a don't necessarily point in the same direction

$$\mathbf{a} = \overline{\overline{\mathbf{M}}}^{-1}\mathbf{F}_{\text{ext}} \quad \text{where} \quad \overline{\overline{\mathbf{M}}}^{-1}_{i;j} = \frac{1}{\hbar^2}\frac{\partial^2 E_N}{\partial k_i \partial k_j}$$

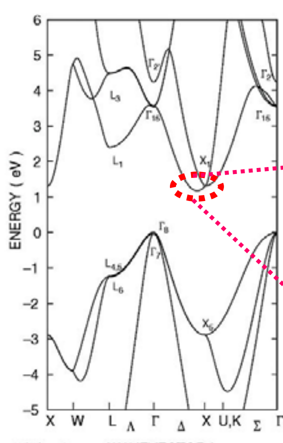
$$\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \frac{d}{dt}\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} \frac{1}{m_{xx}} & \frac{1}{m_{xy}} & \frac{1}{m_{xz}} \\ \frac{1}{m_{yx}} & \frac{1}{m_{yy}} & \frac{1}{m_{yz}} \\ \frac{1}{m_{zx}} & \frac{1}{m_{zy}} & \frac{1}{m_{zz}} \end{pmatrix}\begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix}$$

Dynamical Effective Mass (3D)

Ellipsoidal Energy Surfaces

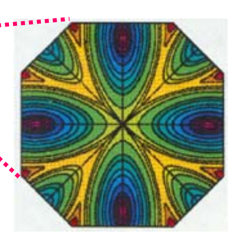
Fortunately, energy surfaces can often be approximate as…

$$E_N(k) = E_c + \frac{\hbar^2}{2}\left(\frac{(k_x - k_x^0)^2}{m_t} + \frac{(k_y - k_y^0)^2}{m_t} + \frac{(k_z - k_z^0)^2}{m_l}\right)$$



Why do we only care about engeries near the top of the valence band and bottom of the conduction band?

Silicon



$$\overline{\overline{\mathbf{M}}}^{-1} = \begin{pmatrix} \frac{1}{m_t} & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_l} \end{pmatrix}$$

$$\overline{\overline{\mathbf{M}}} = \begin{pmatrix} m_t & 0 & 0 \\ 0 & m_t & 0 \\ 0 & 0 & m_l \end{pmatrix}$$

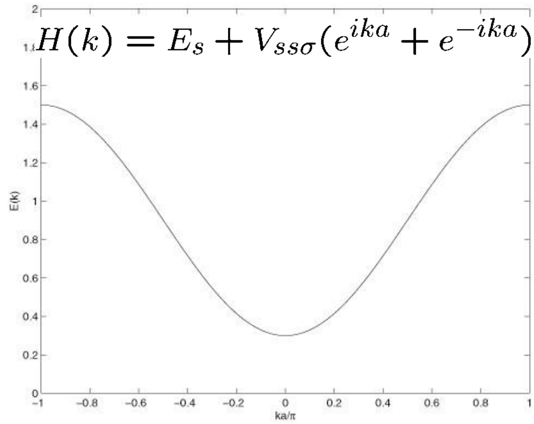
http://csmr.ca.sandia.gov/workshops/nacdm2002/viewgraphs/Conor_Rafferty_NACDM2002.pdf

Energy Band for 1-D Lattice

Single orbital, single atom basis

$$m^*(k) = \hbar^2 \left(\frac{\partial^2 E_N(k)}{\partial k^2}\right)^{-1} = \frac{\hbar^2}{2V_{ss\sigma}a^2}$$

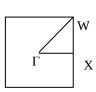
$$H(k) = E_s + V_{ss\sigma}(e^{ika} + e^{-ika})$$

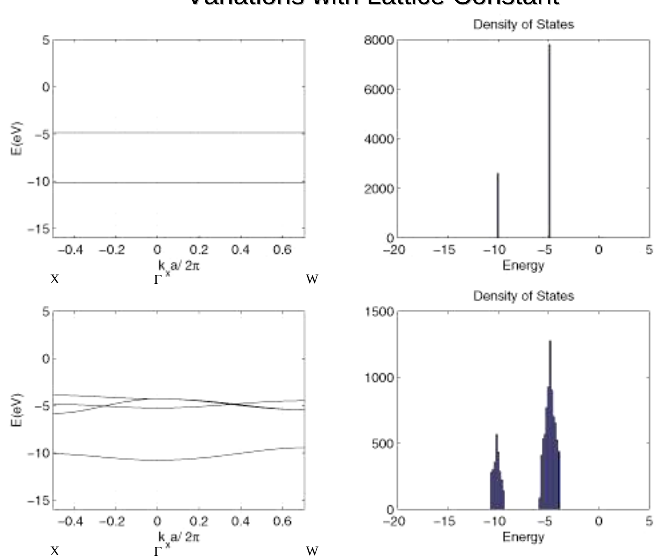


Increasing the orbital overlap, reduces the effective mass...

2D Monatomic Square Crystals

Variations with Lattice Constant





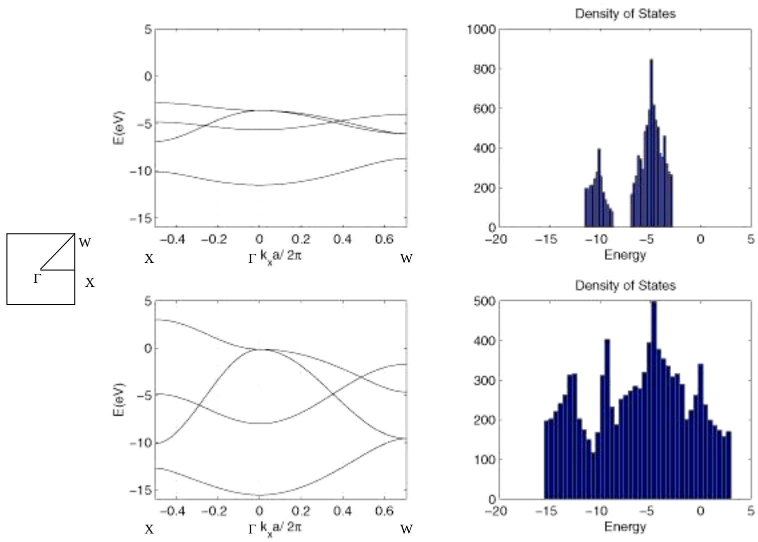
$a \rightarrow \infty$

a = 8.3 A

Increasing the orbital overlap, reduces the effective mass...

2D Monatomic Square Crystals

Dispersion Relations



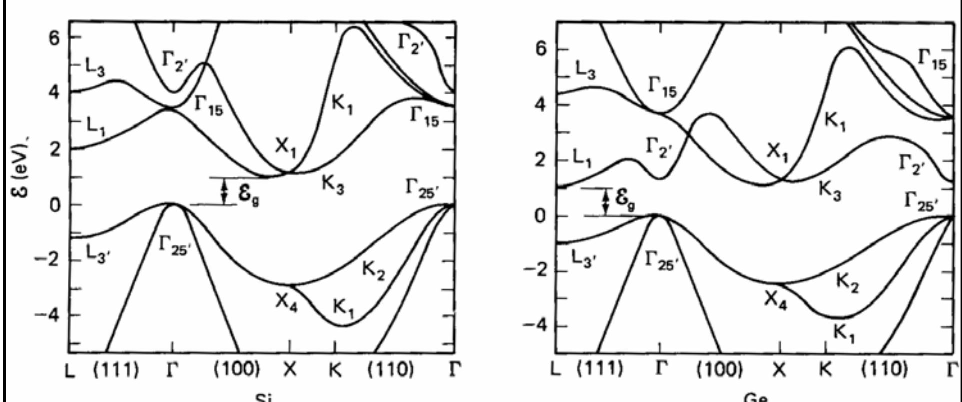
a = 5.5 A

a = 2.8 A

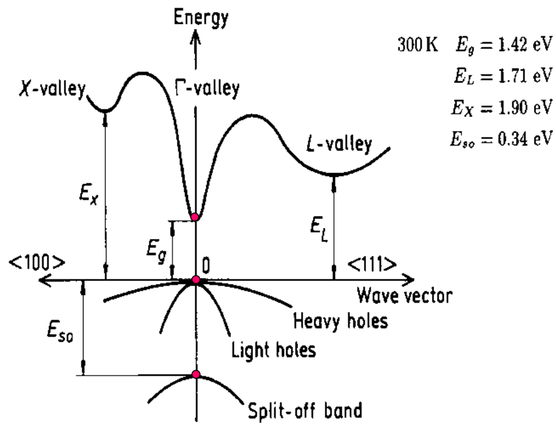
Increasing the orbital overlap, reduces the effective mass...

3D Band Structures

Dispersion Relations



Another Approach to Bandstructure: k.p



Often it is easier to know the energies at a particular point (ex. Bandgap) than it is to measure the effecitve mass

k.p is a way to relate your knowledge of energy levels at k to the effective mass...using perturbation theory

Momentum and Crystal Momentum

$$\hat{\mathrm{p}}\,\psi_{n,k} = \hbar k \psi_{n,k} + e^{ik\cdot r}\frac{\hbar}{i}\nabla \tilde{u}_{n,k}(r)$$

$$\hat{\mathrm{p}}\,\psi_{n,k} = e^{ik\cdot r}\hbar\left(k + \frac{1}{i}\nabla\right)\tilde{u}_{n,k}(r)$$

Leads us to, the action of the Hamiltonian on the Bloch amplitude....

$$e^{ik\cdot r}\left(\frac{\hbar^2}{2m}\left(\frac{1}{i}\nabla + k\right)^2 + V(r)\right)\tilde{u}_k(r) = E_k e^{ik\cdot r}\tilde{u}_k(r)$$

$$H_k\tilde{u}_k(r) \equiv \left(\frac{\hbar^2}{2m}\left(\frac{1}{i}\nabla + k\right)^2 + V(r)\right)\tilde{u}_k(r) = E_k\tilde{u}_k(r)$$

k.p Hamiltonian

(in our case q.p)

$$H_k \tilde{u}_k(r) = \left(\frac{\hbar^2}{2m}\left(\frac{1}{i}\nabla + k\right)^2 + V(r)\right)\tilde{u}_k(r)$$

If we know energies as k we can extend this to calculate energies at k+q for small q...

$$H_{k+q} = \frac{\hbar^2}{2m}\left(\frac{1}{i}\nabla + k + q\right)^2 + V(r)$$

$$H_{k+q} = H_k + \underbrace{\frac{\hbar^2}{m} q \cdot \left(\frac{1}{i}\nabla + k\right) + \frac{\hbar^2}{2m} q^2}_{\text{perturbation}}$$

k.p Effective Mass

$$H_{k+q} = H_k + \underbrace{\frac{\hbar^2}{m} q \cdot \left(\frac{1}{i}\nabla + k\right) + \frac{\hbar^2}{2m} q^2}_{\text{perturbation(V)}}$$

Second-order perturbation theory...

$$E_n^{(2)} \approx E_n^0 + V_{nn} + \sum_{p \neq n} \frac{|V_{np}|^2}{E_n^0 - E_p^0} \qquad \text{provided} \quad E_n^0 \neq E_p^0$$

Taylor Series expansion of energies...

$$E_n(k+q) = E_n(k) + \sum_i \frac{\partial E_n}{\partial k_i} q_i + \frac{1}{2}\sum_{ij} \underbrace{\frac{\partial^2 E_n}{\partial k_i \partial k_j}}_{\vec{\vec{M}}_{i,j}} q_i q_j + O(q^3)$$

$$\sum_{ij} \frac{1}{2}\frac{\partial^2 E_n}{\partial k_i \partial k_j} q_i q_j = \frac{\hbar^2}{2m} q^2 + \sum_{n' \neq n} \frac{|< \frac{\hbar^2}{2m} q \cdot \left(\frac{1}{i}\nabla + k\right) >|^2}{E_{nk} - E_{n'k}}$$

k.p Effective Mass

$$\sum_{ij} \frac{1}{2}\frac{\partial^2 E_n}{\partial k_i \partial k_j} q_i q_j = \frac{\hbar^2}{2m} q^2 + \sum_{n'\neq n} \frac{|< \frac{\hbar^2}{2m} q \cdot \left(\frac{1}{i}\nabla + k\right) > |^2}{E_{nk} - E_{n'k}}$$

$$= \frac{\hbar^2}{2m}q^2 + \sum_{n'\neq n} \frac{|\int dr\, \tilde{u}^*_{nk} \frac{\hbar^2}{2m} q\cdot\left(\frac{1}{i}\nabla+k\right)\tilde{u}_{n'k}|^2}{E_{nk}-E_{n'k}}$$

$$= \frac{\hbar^2}{2m}q^2 + \sum_{n'\neq n} \frac{|<\psi_{nk}|\frac{\hbar^2}{2m} q\cdot \frac{1}{i}\nabla|\psi_{n'k}>|^2}{E_{nk}-E_{n'k}}$$

$$= \frac{\hbar^2}{2m}q^2 + \left(\frac{\hbar^2}{m}\right)^2 \sum_{n'\neq n} \frac{|<q\cdot\hat{p}>_{nn'}|^2}{E_{nk}-E_{n'k}}$$

k.p Effective Mass

Example

$$\frac{\partial^2 E_n}{\partial k_i \partial k_j} = \frac{\hbar^2}{m}\delta_{i,j} + \left(\frac{\hbar^2}{m}\right)^2 \sum_{n'\neq n} \frac{<\hat{p}_i>_{nn'}<\hat{p}_j>_{n'n} + <\hat{p}_i>_{n'n}<\hat{p}_j>_{nn'}}{E_{nk}-E_{n'k}}$$

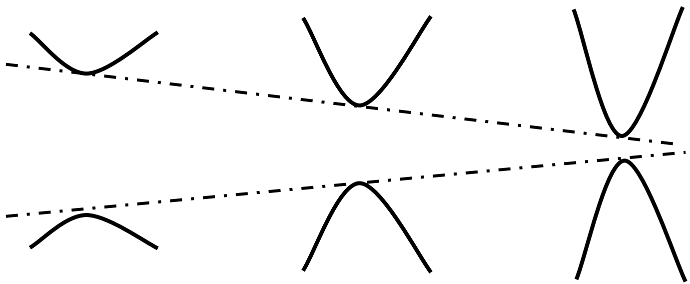
$$\overline{\overline{\mathbf{M}}}^{-1}_{i;j} = \frac{1}{\hbar^2}\frac{\partial^2 E_N}{\partial k_i \partial k_j}$$

Lets only consider two bands (valence and conduction) and assume they are spherical...

$$\frac{1}{m^*} = \frac{1}{m} + 2\left(\frac{\hbar^2}{m^2}\right)\frac{|<\hat{p}>_{cv}|^2}{E_{c0}-E_{v0}}$$

$$= \frac{1}{m} + 2\left(\frac{\hbar^2}{m^2}\right)\frac{|<\hat{p}>_{cv}|^2}{E_g}$$

k.p Effective Mass
Example



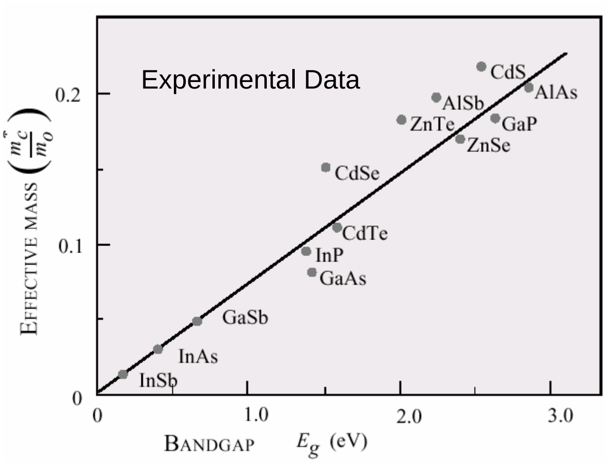
$$\frac{1}{m^*} = \frac{1}{m} + 2\left(\frac{\hbar^2}{m^2}\right)\frac{|<\hat{p}>_{cv}|^2}{E_g}$$

$$E_n^{(2)} \approx E_n^0 + V_{nn} + \sum_{p\neq n}\frac{|V_{np}|^2}{E_n^0 - E_p^0}$$

Level repulsion causes bands to curve as bandgap is reduceed...

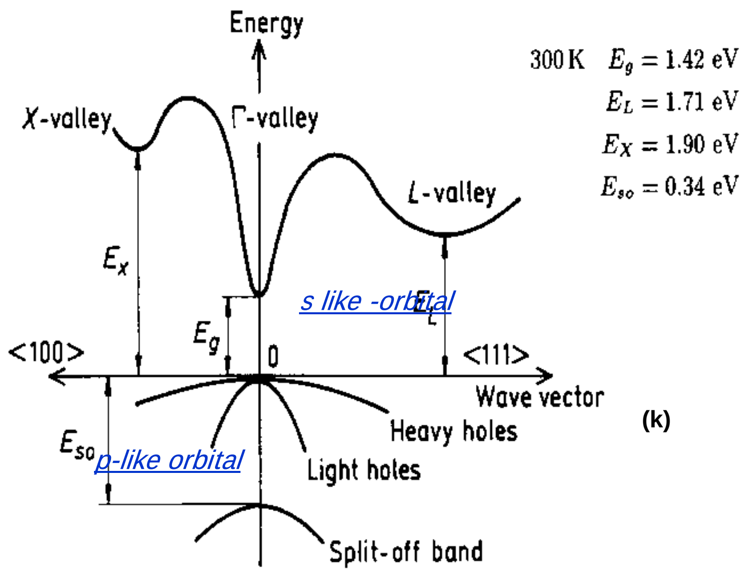
Effective Mass and Bandgap

$$\frac{1}{m^*} = \frac{1}{m} + 2\left(\frac{\hbar^2}{m^2}\right)\frac{|<\hat{p}>_{cv}|^2}{E_g}$$



http://www.eecs.umich.edu/~singh/bk7ch03.pdf

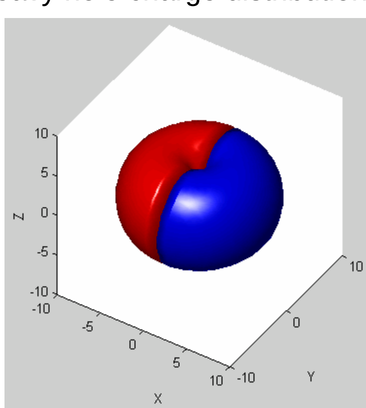
Bandstructure of GaAs



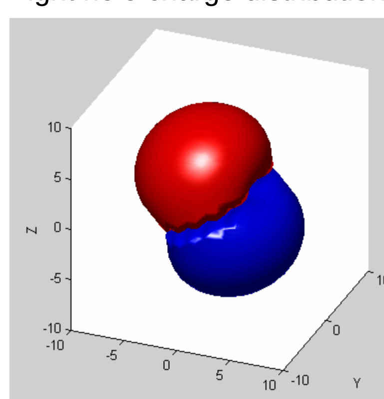
What is this split-off band ?

Spin-orbit Coupling Wavefunctions

heavy hole charge distribution



light hole charge distribution



Orbital Angular Momentum

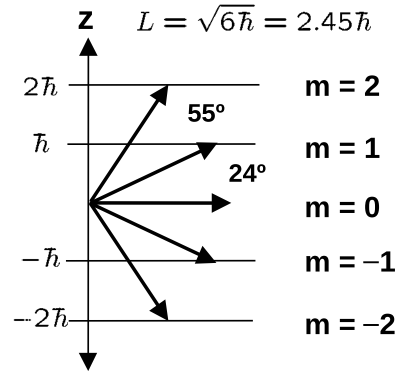
Angular momentum for quantum state with <u>*l* = 2</u>:

$l = 2$

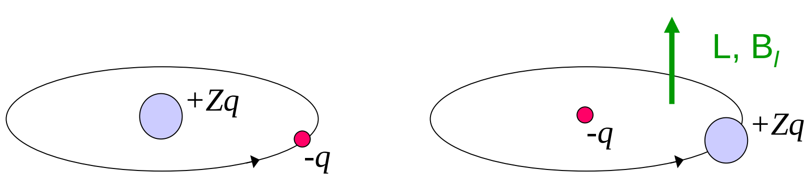
$$L = \sqrt{l(l+1}\hbar = \sqrt{6}\hbar = 2.45\hbar$$

$$m = -l \text{ to l} = 0, \pm 1, \pm 2$$

$$L_z = 0, \pm\hbar, \pm 2\hbar$$



Spin-Orbit Coupling



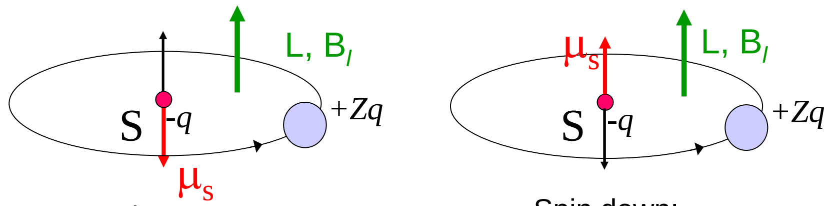
The effective current from the motion of a nucleus in a circular orbit...

$$I = \frac{\Delta Q}{\Delta t} = \frac{Zev}{2\pi r}$$

...generates an effective magnetic field...

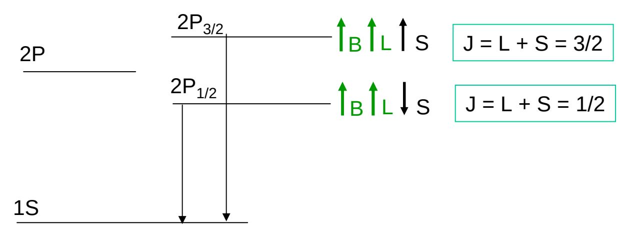
$$B = \frac{\mu_0 I}{2r} \Rightarrow B = \frac{\mu_0 Zev}{4\pi r^2}$$

Spin-Orbit Splitting

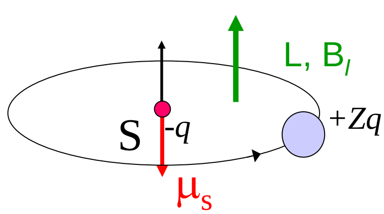


Spin up:
High Energy

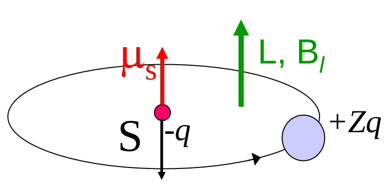
Spin down:
Low Energy



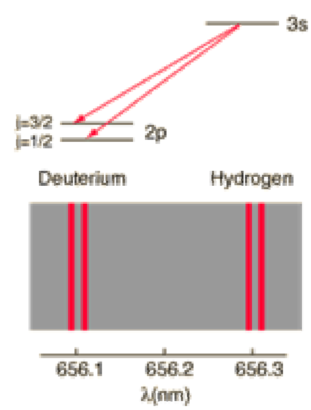
Spin-Orbit Splitting in Hydrogen



Spin up:
High Energy



Spin down:
Low Energy



Angular Momentum Addition Rules

Vectors

$$J = L + S$$

$$|J| = \sqrt{j(j+1)}\hbar$$

Quantum Numbers

$$j = l + s, |l - s|$$

$$m_j = -j, -j+1, ...j-1, j$$

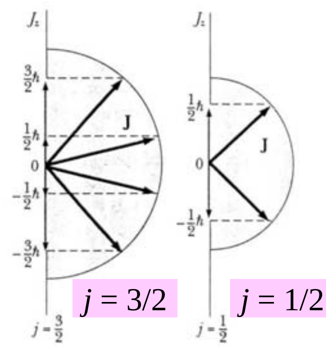
Example: $l = 1, s = ½$

$$j = 1 + \frac{1}{2} = \frac{3}{2}$$

$$m_j = -\frac{3}{2}, -\frac{1}{2}, +\frac{1}{2}, +\frac{3}{2}$$

$$j = |1 - \frac{1}{2}| = \frac{1}{2}$$

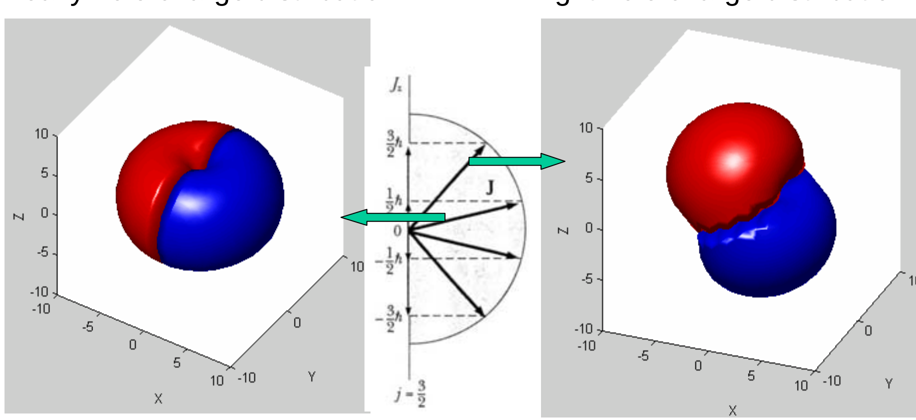
$$m_j = -\frac{1}{2}, +\frac{1}{2}$$



Spin-orbit Coupling Wavefunctions

heavy hole charge distribution

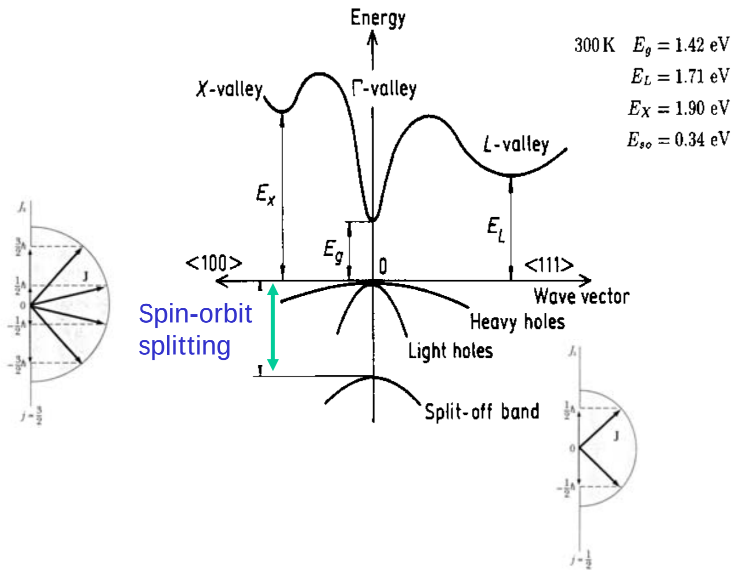
light hole charge distribution



heavy mass (along k_z)

light mass (along k_z)

Bandstructure of GaAs



Summary

- k-p method explains why the effective mass increases as the bandgap increases
- Spin-orbit interaction is necessary to explain the origin of
  – Heavy and Light Holes
  – The Split-Off Band