Lecture 24: Effective Mass

Outline

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

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Semiclassical Equations of Motion

\[ \langle v_n(k) \rangle = \frac{\langle p \rangle}{m} = \frac{1}{\hbar} \nabla_k E_n(k) \]

\[ F_{\text{ext}} = \frac{\hbar}{m} \frac{dk}{dt} \]

Let's try to put these equations together...

\[
\alpha(t) = \frac{dv}{dt} = \frac{1}{\hbar} \frac{\partial E_N(k)}{\partial k} = \frac{1}{\hbar} \frac{\partial^2 E_N(k)}{\partial k^2} \frac{dk}{dt} \\
= \left[ \frac{1}{\hbar^2} \frac{\partial^2 E_N(k)}{\partial k^2} \right] F_{\text{ext}}
\]

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

$$a = \overline{M}^{-1} F_{ext} \quad \text{where} \quad \overline{M}^{-1}_{ij} = \frac{1}{\hbar^2} \partial^2 E_N / \partial k_i \partial k_j$$

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

Dynamical Effective Mass (3D)
Ellipsoidal Energy Surfaces

Fortunately, energy surfaces can often be approximate as...

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

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

Silicon

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

Energy Band for 1-D Lattice
Single orbital, single atom basis

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

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

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

2D Monatomic Square Crystals
Variations with Lattice Constant

Increasing the orbital overlap, reduces the effective mass...
2D Monatomic Square Crystals
Dispersion Relations

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 (e.g., Bandgap) than it is to measure the effective mass.

k.p is a way to relate your knowledge of energy levels at \( \mathbf{k} \) to the effective mass...using perturbation theory.

Momentum and Crystal Momentum

\[
\mathbf{p} \psi_{n,k} = \hbar \mathbf{k} \psi_{n,k} + e^{i \mathbf{k} \cdot \mathbf{r}} \frac{\hbar}{i} \nabla \tilde{u}_{n,k}(r)
\]

\[
\mathbf{p} \psi_{n,k} = e^{i \mathbf{k} \cdot \mathbf{r}} \frac{\hbar}{i} \left( \mathbf{k} + \frac{1}{i} \nabla \right) \tilde{u}_{n,k}(r)
\]

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

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

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

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

\[ H_{k+q} = H_k + \frac{\hbar^2}{m} q \cdot \left( \frac{1}{i} \nabla + k \right) + \frac{\hbar^2}{2m} q^2 \]

perturbation

k.p Effective Mass

\[ H_{k+q} = H_k + \frac{\hbar^2}{m} q \cdot \left( \frac{1}{i} \nabla + k \right) + \frac{\hbar^2}{2m} q^2 \]

Second-order perturbation theory...

\[ E_n^{(2)} \approx E_n^0 + V_{nn} + \sum_{\nu \neq n} \frac{|V_{n\nu}|^2}{E_n^0 - E_{\nu}^0} \quad \text{provided} \quad E_n^0 \neq E_{\nu}^0 \]

Taylor Series expansion of energies...

\[ E_n(k+q) = E_n(k) + \sum_i \frac{\partial E_n}{\partial k_i} q_i + \frac{1}{2} \sum_{ij} \frac{\partial^2 E_n}{\partial k_i \partial k_j} q_i q_j + O(q^3) \]

\[ \sum_{ij} \frac{1}{2} \frac{\partial^2 E_n}{\partial k_i \partial k_j} q_i q_j = \frac{\hbar^2}{2m} q^2 + \sum_{n' \neq n} \frac{|< \frac{\hbar^2}{2m} q \cdot \left( \frac{1}{i} \nabla + k \right> >|^2}{E_{nk} - E_{n'k}} \]
Let's only consider two bands (valence and conduction) and assume they are spherical...

\[
\frac{1}{m^*} = \frac{1}{m} + 2 \left( \frac{\hbar^2}{m^2} \right) \frac{\left| \langle \hat{p} \rangle >_{cv} \right|^2}{E_{cv0} - E_{v0}}
\]

\[
= \frac{1}{m} + 2 \left( \frac{\hbar^2}{m^2} \right) \frac{\left| \langle \hat{p} \rangle >_{cv} \right|^2}{E_q}
\]
k.p Effective Mass

Example

\[ \frac{1}{m^*} = \frac{1}{m} + 2 \left( \frac{\hbar^2}{m^2} \right) \frac{|\langle \hat{\mathbf{p}} \rangle_{cv}|^2}{E_g} \]

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

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

Effective Mass and Bandgap

\[ \frac{1}{m^*} = \frac{1}{m} + 2 \left( \frac{\hbar^2}{m^2} \right) \frac{|\langle \hat{\mathbf{p}} \rangle_{cv}|^2}{E_g} \]

Experimental Data

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

Energy

X-valley

\( E_g \)

\( E_x \)

L-valley

\( s \)-like orbital

\( p \)-like orbital

Wave vector

300 K

\( E_g = 1.42 \) eV

\( E_L = 1.71 \) eV

\( E_X = 1.90 \) eV

\( E_{so} = 0.34 \) eV

What is this split-off band?

Spin-orbit Coupling Wavefunctions

heavy hole charge distribution

light hole charge distribution
Angular momentum for quantum state with $l = 2$:

\[
L = \sqrt{l(l+1)\hbar} = \sqrt{6}\hbar = 2.45\hbar
\]

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

\[
L_z = 0, \pm \hbar, \pm 2\hbar
\]

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Spin-Orbit Coupling

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

\[
I = \frac{\Delta Q}{\Lambda t} = \frac{Ze\nu}{2\pi r^2}
\]

...generates an effective magnetic field...

\[
B = \frac{\mu_0 I}{2r} \quad B = \frac{\mu_0 Ze\nu}{4\pi r^2}
\]
Spin-Orbit Splitting

Spin up:
High Energy

Spin down:
Low Energy

Spin-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**

\[ j = l + s, |l - s| \]
\[ m_j = -j, -j + 1, \ldots, j - 1, j \]

*Example: l = 1, s = \frac{1}{2}*

\[
\begin{align*}
    j &= 1 + \frac{1}{2} = \frac{3}{2} \\
    m_j &= -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2} \\
    j &= |1 - \frac{1}{2}| = \frac{1}{2} \\
    m_j &= -\frac{1}{2}, \frac{1}{2}
\end{align*}
\]

### Spin-orbit Coupling Wavefunctions

- **Heavy hole charge distribution**
- **Light hole charge distribution**

- Heavy mass (along \( k_z \))
- Light mass (along \( k_z \))
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