THE EFFECTIVE MASS THEORY

Gokhan Ozgur
Electrical Engineering
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Introduction

In this presentation, the effective mass theory (EMT) for the electron in the crystal lattice will be introduced. The dynamics of the electron in free space and in the lattice will be compared. The E-k diagram for direct band gap semiconductors will be studied and the hole concept will be introduced. Next, the EMT for single and degenerate bands will be presented. Finally, some application areas of the EMT will be mentioned.

What is the Effective Mass

An electron in crystal may behave as if it had a mass different from the free electron mass m_0. There are crystals in which the effective mass of the carriers is much larger or much smaller than m_0. The effective mass may be anisotropic, and it may even be negative. The important point is that the electron in a periodic potential is accelerated relative to the lattice in an applied electric or magnetic field as if its mass is equal to an effective mass.

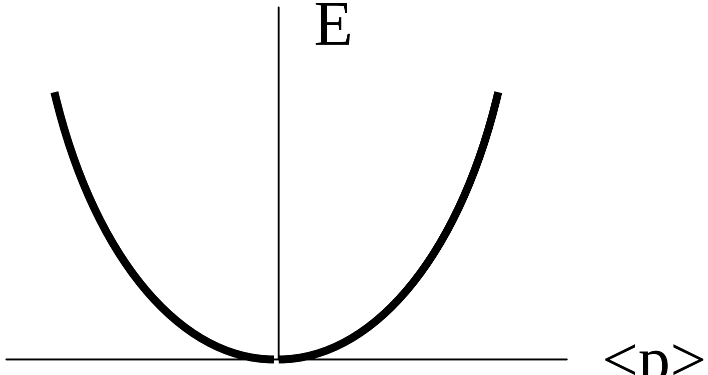
Free Electron Dynamics

If the electron is free then E represents the kinetic energy only. It is related to the wave vector k and momentum p by

(1) $$E = \frac{\hbar^2 k^2}{2m_0} = \frac{p^2}{2m_0}$$

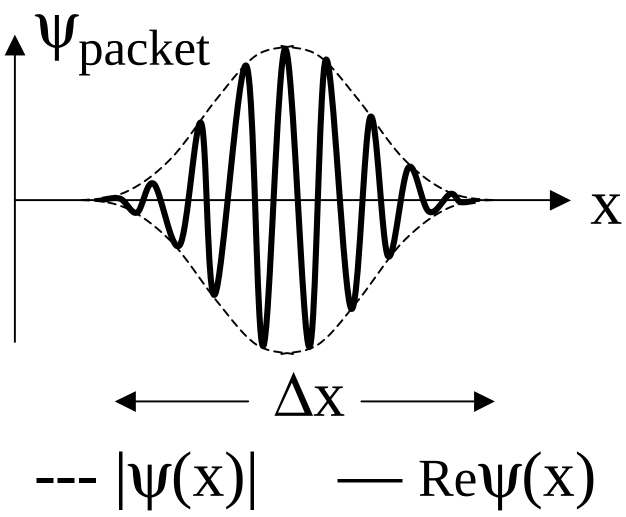
Therefore, the quantum mechanical and classical free particles exhibit precisely the same energy-momentum relationship, as shown below.

(2)



Group Velocity of a Wavepacket

The velocity of the real particle is the phase velocity of the wave packet envelope. It is called the group velocity and its relation to energy and momentum is obtained from (1)



(3) $$v_g = \frac{dE}{dp} = \frac{1}{\hbar}\frac{dE}{dk}$$

Here, E and k are interpreted as the center values of energy and crystal momentum, respectively.

Now, what happens when an “external” force F acts on the wavepacket? F could be any force other than the crystalline force associated with the periodic potential. The crystalline force is already taken into account in the wavefunction solution.

Electron Dynamics in the Lattice

The work done by the force on the wavepacket will then be

(4) $$dE = F dx = F v_g dt$$

From that we get the force expression using (3)

(5) $$F = \frac{1}{v_g}\frac{dE}{dt} = \frac{1}{v_g}\frac{dE}{dk}\frac{dk}{dt}$$

(6) $$F = \frac{d(\hbar k)}{dt}$$

The acceleration is found taking time derivative of (3)

(7) $$a = \frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left(\frac{dE}{dk}\right) = \frac{1}{\hbar^2}\left(\frac{d^2E}{dk^2}\right)\frac{d(\hbar k)}{dt}$$

Effective Mass Expression

Finally, we obtain the effective mass equation

(8) $$F = m^* \cdot \frac{dv_g}{dt}$$

(9) $$m^* = \frac{1}{\frac{1}{\hbar^2}\frac{d^2E}{dk^2}}$$

The equation (8) is identical to Newton’s second law of motion except that the actual particle mass is replaced by an *effective mass m**.

Effective Mass Tensor

In three dimensional crystals the electron acceleration will not be colinear. Thus, in general we have an effective mass tensor.

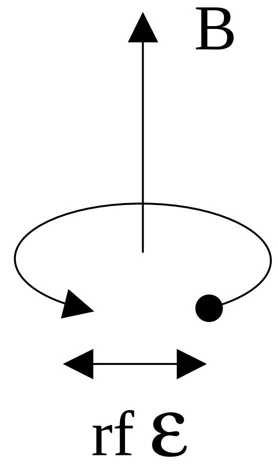
(10) $$\frac{dv_g}{dt} = m_{xx}^{-1} F_x \hat{x} + m_{yx}^{-1} F_x \hat{y} + m_{zx}^{-1} F_x \hat{z}$$

(11) $$\frac{1}{m*} = \begin{pmatrix} m_{xx}^{-1} & m_{xy}^{-1} & m_{xz}^{-1} \\ m_{yx}^{-1} & m_{yy}^{-1} & m_{yz}^{-1} \\ m_{zx}^{-1} & m_{zy}^{-1} & m_{zz}^{-1} \end{pmatrix}$$

The crystal and therefore the k-space can be aligned to the principal axis of the system centered at a band extrema. Since E-k relationship is parabolic at that point, all off-diagonal terms in the tensor will vanish. For GaAs, as an example, the conduction band effective mass becomes simply a scalar m_e* for parabolic approximation.

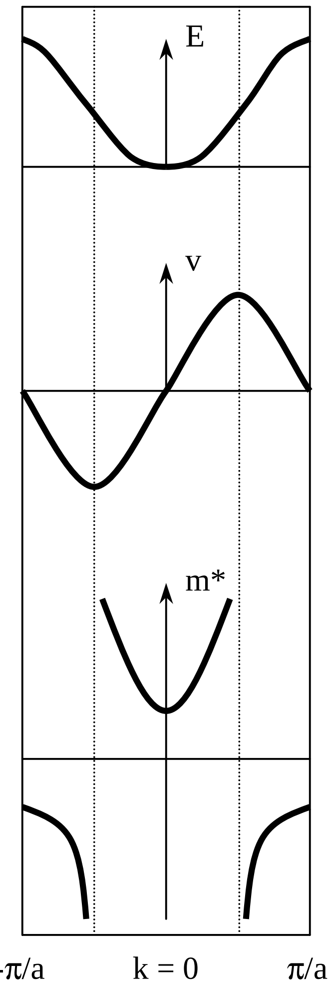
Measurement of Effective Mass

Effective mass is a directly measurable quantity, which can be obtained from cyclotron resonance experiment. The test material is placed in a microwave resonance cavity and cooled down to 4 °K. A static magnetic field B and rf electric field ε oriented normal to B are applied across the sample, as shown in the figure. The frequency of the orbit, called cyclotron frequency, is directly proportional to B and inversely dependent on the effective mass. When B field is adjusted such that cyclotron and rf frequencies are equal, then a resonance is observed. Then from B-field strength, direction and rf frequency, one can deduce the effective mass corresponding to the given experiment configuration. For different B-orientations the effective masses can be measured by this way.



E-k Diagram, Velocity and Effective Mass

The figure depicts the graphs for E, dE/dk, and d^2E/dk^2 for CB in the first BZ. At k=0, electron has a constant positive value and it rises rapidly as k value increases. After experiencing a singularity (infinite mass) the effective mass becomes negative up to the top of the first BZ.

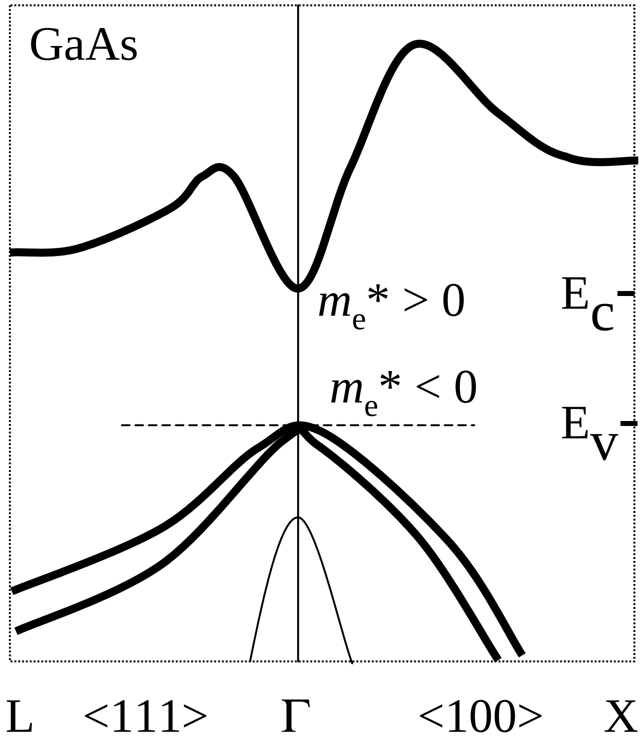


Therefore:

- *m** is positive near the bottoms of all bands,
- *m** is negative near the tops of all bands.

E-k Diagrams

The E-k curve is concave at the bottom of the CB, so m_e^* is positive. Whereas, it is convex at the top of the VB, thus m_e^* is negative. This means that a particle in that state will be accelerated by the field in the reverse direction expected for a negatively charged electron. That is, it behaves as if a positive charge and mass. This is the concept of the *hole*.

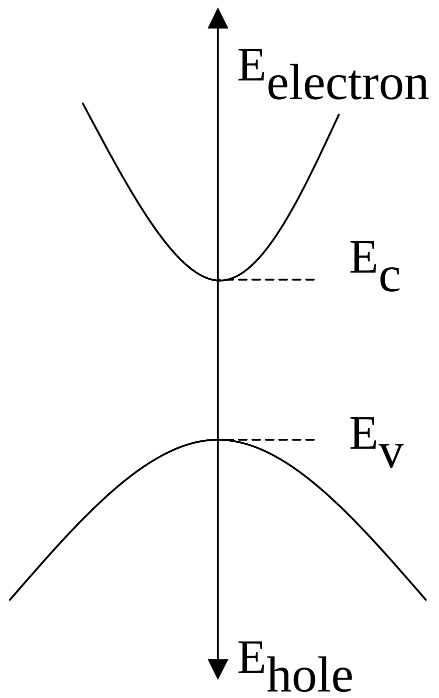


For valance band the degenerate band with smaller curvature around k=0 is called the heavy-hole band, and the one with larger curvature is the light-hole band.

Parabolic Approximations of Bands

Thus, for parabolic bands, the electron will move much like a free particle with *m**, which is related to the curvature of the band. For nonparabolic bands, *m** is not constant and the local slope and curvature of E–k relationship must be used to obtain the velocity and acceleration of the particle with energy E.

The shape of the bottom of the CB and the top of the VB can be approximated by parabolas, which results in constant effective masses.



(12a) $$E \cong E_c + \frac{\hbar^2 k^2}{2m_e^*}$$

(12b) $$E \cong E_v - \frac{\hbar^2 k^2}{2m_h^*}$$

Definition of Effective Mass, Using k·p theory, Slide no 4-5, by Jin Wang

The energy eigenvalues

$$E_m\left(\vec{k}\right) = E_m(0) + \frac{\hbar^2 k^2}{2m_o} + \left(\frac{\hbar}{m_o}\right)^2 \sum_{n\neq m} \frac{\left|\vec{k}\cdot\hat{p}_{nm}\right|^2}{E_m(0) - E_n(0)} \qquad (13a)$$

Or $$E_m\left(\vec{k}\right) = E_m(0) + \sum_{\alpha,\beta}\left[\frac{\hbar^2\delta_{\alpha\beta}}{2m_o} + \left(\frac{\hbar}{m_o}\right)^2 \sum_{n\neq m}\frac{p_{mn}^{(\alpha)}\,p_{nm}^{(\beta)}}{E_m(0) - E_n(0)}\right]k_\alpha k_\beta \qquad (13b)$$

The effective mass can be defined from

$$E_m\left(\vec{k}\right) - E_m(0) = \frac{\hbar^2}{2}\sum_{\alpha,\beta}\left(\frac{1}{m^*}\right)_{\alpha\beta} k_\alpha k_\beta \qquad (13c)$$

$$\Rightarrow \quad \left(\frac{1}{m^*}\right)_{\alpha\beta} = \left[\frac{\delta_{\alpha\beta}}{m_o} + \frac{2}{m_o^2}\sum_{n\neq m}\frac{p_{mn}^{(\alpha)}\,p_{nm}^{(\beta)}}{E_m(0) - E_n(0)}\right] \qquad (13d)$$

The EMT for a Single Band

If the energy dispersion relation for a single band n near k_0 (assuming 0) is given by

$$(14) \quad E_n(k) = E_n(0) + \sum_{\alpha,\beta} \frac{\hbar^2}{2} \left(\frac{1}{m^*} \right)_{\alpha\beta} k_\alpha k_\beta$$

for the Hamiltonian H_0 with a periodic potential $V(\mathbf{r})$

$$(15) \quad H_0 = \frac{p^2}{2m_0} + V(\mathbf{r}) \qquad (16) \quad H_0 \psi_{nk}(\mathbf{r}) = E_n(\mathbf{k}) \psi_{nk}(\mathbf{r})$$

then the solution for the Schrödinger equation with a perturbation $U(\mathbf{r})$ such as an impurity or quantum-well potential

$$(17) \quad [H_0 + U(\mathbf{r})]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

is obtainable by solving the following

The EMT for a Single Band (cont.)

(18)

$$\left[\sum_{\alpha,\beta}\frac{\hbar^2}{2}\left(\frac{1}{m^*}\right)_{\alpha\beta}\left(-i\frac{\partial}{\partial x_\alpha}\right)\left(-i\frac{\partial}{\partial x_\beta}\right)+U(\mathbf{r})\right]F(\mathbf{r})=\left[E-E_n(0)\right]F(\mathbf{r})$$

for the envelope function $F(\mathbf{r})$ and the energy E. The wave function is approximated by

(19) $$\psi(\mathbf{r})=F(\mathbf{r})u_{nk_0}(\mathbf{r})$$

The periodic potential determines the energy bands and the effective masses, $(1/m^*)_{\alpha\beta}$, and the EM equation (18) contains only the extra perturbation $U(\mathbf{r})$, since the effective masses already take into account the periodic potential. The perturbation potential $U(\mathbf{r})$ can also be a quantum-potential in a semiconductor heterostructure, such as GaAs/AlGaAs.

The EMT for Degenerate Bands

Following the discussion on **k·p** method for degenerate bands, like the heavy-hole, light-hole and split-off bands, the dispersion relation is given by

(20)

$$\sum_{j'=1}^{6} H_{jj'}^{LK} a_{j'}(\mathbf{k}) \equiv \sum_{j'=1}^{6} \left[E_j(0)\delta_{jj'} + \sum_{\alpha,\beta} D_{jj'}^{\alpha\beta} k_\alpha k_\beta \right] a_{j'}(\mathbf{k}) = E(\mathbf{k}) a_j(\mathbf{k})$$

which satisfies the following

(21) $H\psi_{nk}(\mathbf{r}) = E_n(\mathbf{k})\psi_{nk}(\mathbf{r})$ (22) $H = \dfrac{p^2}{2m_0} + V(\mathbf{r}) + H_{so}$

In equation (20)

(22) $$D_{jj'}^{\alpha\beta} = \frac{\hbar^2}{2m_0}\left[\delta_{jj'}\delta_{\alpha\beta} + \sum_{\gamma}^{B} \frac{p_{j\gamma}^{\alpha}\, p_{\gamma j'}^{\beta} + p_{j\gamma}^{\beta}\, p_{\gamma j'}^{\alpha}}{m_0(E_0 - E_\gamma)} \right]$$

The EMT for Degenerate Bands (cont.)

Equation (22) is similar to (13b), the single band case where $j = j'$ = single band index n. It is generalized to include the degenerate bands.

Then, the solution $\psi(\mathbf{r})$ for the semiconductors in the presence of a perturbation potential $U(\mathbf{r})$ for the following

(23) $$[H + U(\mathbf{r})]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

is given by

(24) $$\psi(\mathbf{r}) = \sum_{j=1}^{6} F_j(\mathbf{r}) u_{jo}(\mathbf{r})$$

where F_j satisfies

The EMT for Degenerate Bands (cont.)

(25)

$$\sum_{j'=1}^{6}\left[E_j(0)\delta_{jj'}+\sum_{\alpha,\beta}D_{jj'}^{\alpha\beta}\left(-i\frac{\partial}{\partial x_\alpha}\right)\left(-i\frac{\partial}{\partial x_\beta}\right)+U(\mathbf{r})\delta_{jj'}\right]F_{j'}(\mathbf{r})=EF_j(\mathbf{r})$$

Recall that the wavefunction $\psi_{\mathrm{n}\mathbf{k}}(\mathbf{r})$ that satisfies (21) was

(26) $$\psi_{n\mathbf{k}}(\mathbf{r})=e^{i\mathrm{k}\cdot\mathrm{r}}u_{n\mathbf{k}}(\mathbf{r})$$

(27) $$u_{n\mathbf{k}}(\mathbf{r})=\sum_{j=1}^{6}a_j(\mathbf{k})u_{jo}(\mathbf{r})$$

Applications of EMT- Conductivity

Under the influence of electric field ε the acceleration of an electron in the lattice and the velocity gained by the electron in time τ is obtained by

(28) $$a = \frac{e\varepsilon}{m^*}$$

(29) $$v = \frac{e\varepsilon}{m^*} \cdot \tau$$

N being the number of conduction electrons per unit volume, the current density is found to be

(30) $$j = Nev$$

(31) $$j = \frac{Ne^2\tau}{m^*} \cdot \varepsilon$$

Following the Ohm's law, the conductivity is calculated as

(32) $$\sigma = \frac{Ne^2\tau}{m^*}$$

Applications of EMT – Density of States

The expressions for the conduction and valance band densities of states near the band edges in the semiconductor are

(33a) $$g_c(E) = \frac{m_n^* \sqrt{2m_n^*(E - E_c)}}{\pi^2 \hbar^3}$$

(33b) $$g_v(E) = \frac{m_p^* \sqrt{2m_p^*(E_v - E)}}{\pi^2 \hbar^3}$$

where m_n* and m_p* are the electron (n) and hole (p) density of states effective masses. As an example, for GaAs the conduction band effective mass becomes simply a scalar m_e* for parabolic approximation. Therefore, for GaAs it will be $m_n^* = m_e^*$. The density of states effective masses takes into account all band contributions in CB and VB.

Effective Mass Values for Some Materials

Here are the effective mass values for some materials:

Effective Mass	AlAs	GaAs	GaP	InP	InAs	InSb
m_e^* / m_0	0.124	0.067	0.5	0.079	0.024	0.014
m_{hh}^* / m_0	0.5	0.51	0.67	0.65	0.41	0.4
m_{lh}^* / m_0	0.26	0.082	0.17	0.12	0.025	0.016
m_{so}^* / m_0		0.154				
m_n^* / m_0		0.0655				
m_p^* / m_0		0.524				