Introduction to Quantum Properties of Solid State Devices

Please pay attention that these are only lectures notes prepared for using in the classroom by the instructor. For more detail refer to any textbook related to physics of solid state devices.
Principles of Quantum Mechanics

1) The principle of Energy Quanta:

Experiments which showed inconsistency between experimental results and classical theories:
Thermal Radiation

• Classical Physics: the frequency of the radiation of a heated cavity should increase monotonically as the thermal energy of the cavity increases.

• Observations: the frequency of the radiation of a heated cavity increases only up to a certain energy then decreases.
Principles of Quantum Mechanics

When a particle jumps from one discrete state to another, it either absorbs or emits energy quanta (most frequently it is a photon) which corresponds to a particular wavelength associated with the difference of the two states energy.

Max Planck’s postulate (1900): explains blackbody radiation

\[ E = h \nu \]

Typical light intensity vs its freq. when the object heated to a certain temperature, e.g. 6000 K
**Hydrogen Atoms:**

- **Classical Physics**: The atomic spectra should be continuous.
- **Observations**: The atomic spectra contain only some discrete lines.

**Photoelectric effect:**

- **Classical Physics**: The absorption of optical energy by the electrons in a metal is independent of light frequency.
- **Observations**: The absorption of optical energy by the electrons in a metal depends on optical frequency.
Principles of Quantum Mechanics

• Planck’s postulate in 1900 that radiation from a heated sample is emitted in discrete units of energy, called quanta.

\[ E = h\nu \]

\( h \) is the Planck’s constant, \( \nu \) is frequency of the radiation
Photoelectric effect:

- **Classical Physics**: The absorption of optical energy by the electrons in a metal is independent of light frequency.
- **Observations**: The absorption of optical energy by the electrons in a metal depends on optical frequency.

- Einstein in 1905 took a step further to interpret the photoelectric results by suggesting that the electromagnetic radiation exists in the form of packets of energy. This particle-like packet of energy is called photon.
2) **Wave-Particle Duality Principle**

The nature of light in the following observations:

- Photoelectric Effect (particle-like)
- Compton Effect (particle-like)
- Diffraction pattern by electrons (wave-like)
- Since waves behave as particles, then particles should be expected to show wave-like properties.

- Louis de Broglie hypothesized that the wavelength of a particle can be expressed as \( \lambda = h/\rho \)
- The momentum of a photon is then: \( \rho = h/\lambda = \hbar k \)
3) The Uncertainty Principle (Heisenberg)

- **First statement:**
  - It is impossible to simultaneously describe with absolute accuracy the position and momentum of a particle.
  - $\Delta x \Delta p \geq \hbar$
  - $\hbar$ is very small so this principle only applies to very small particles

- **Second statement:**
  - It is impossible to simultaneously describe with absolute accuracy the energy of a particle and the instant of time the particle has this energy.
  - $\Delta E \Delta t \geq \hbar$
A Particle in a Box
Classical Mechanics vs. Quantum Mechanics

- **CM:** The particle remains trapped inside the box and can acquire any energy available to it.

- **QM:** A particle trapped in such a box cannot have any energy, and will have only certain allowed energy.

- **CM:** If no other forces are in the system, then the particle should have Brownian motion and has an equal probability of being anywhere and everywhere in the box.

- **QM:** The particle has certain preferable points, where the probability of finding the particle is more than in other parts.

- **CM:** The exact position and momentum of the particle should be obtainable simultaneously for the particle in question.

- **QM:** We cannot measure the momentum and the position of the particle in the box simultaneously without some uncertainty.
A Particle in a Box
Classical Mechanics vs. Quantum Mechanics

- **CM**: At a particular moment, the exact energy of a particle should be measurable.

- **QM**: At any instant of time, the energy is not measurable above a certain extent.

- **CM**: The particle must be confined in the box and has no chance of escaping the box as long as its energy is lower than that of the box.

- **QM**: The particle has a finite chance of escaping the system even with energy lower than the box.

- **CM**: If by any chance the particle attains energy larger than that of the box, the particle will certainly leave the box.

- **QM**: If by any chance the particle attains energy larger than that of the box, there remains certain probability that particle might still be trapped inside.
Principle of Quantum Mechanics

Basic Postulates

– Late 1920’s Ervin Schrödinger developed wave mechanics based on Planck’s theory and de Broglie’s idea of the wave nature of matter.

– Warner Heisenberg formulated an alternative approach in terms of matrix algebra called Matrix Mechanics.
Dynamical Variables in Physics: position, momentum, energy

• In classical mechanics the state of a system with a number of particles at any time is defined by designating the particle and momentum coordinates of all particles.

• In quantum mechanics the state of a system is defined by a state function $\Psi$ that contains all the information we can obtain about the system.

• To approach quantum mechanics we consider several postulates that are assumed to be true.
Basic Postulates

• **Postulate I**: (in one-dimensional system)
  - There exists a state function $\Psi(x;t)$ which contains all the measurable information about each particle of a physical system. $\Psi(x;t)$ is also called wave function.

• **Postulate II**:
  - Every dynamical variable has a corresponding operator. This operator is operated on the state function to obtain measurable information about the system.
Principle of Quantum Mechanics

Basic Postulates

In a one-dimensional system

Dynamical Variables:

• Position $x$
• Momentum $p$
• Total Energy $E$
• Potential Energy $V(x)$
## Principle of Quantum Mechanics

### Basic Postulates

<table>
<thead>
<tr>
<th>Dynamical Variable</th>
<th>Quantum Mechanic Operator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position $x$</td>
<td>$\hat{X} \equiv X$</td>
</tr>
<tr>
<td>Momentum $p$</td>
<td>$\hat{P}_x \equiv \frac{\hbar}{i} \frac{\partial}{\partial X}$</td>
</tr>
<tr>
<td>Total Energy $E$</td>
<td>$\hat{E} \equiv -\frac{\hbar}{i} \frac{\partial}{\partial t}$</td>
</tr>
<tr>
<td>Potential Energy $V(x)$</td>
<td>$\hat{V}(x) \equiv V(x)$</td>
</tr>
</tbody>
</table>
Basic Postulates

• **Postulate III:**
  - The state function $\Psi(x; t)$ and its space derivative $\frac{\partial \Psi}{\partial x}$ must be continuous, finite and single-valued for all values of $x$.

• **Postulate IV**

The state function must be normalized i.e

$$\int_{-\infty}^{\infty} \Psi \Psi^* dx = 1$$

- $\Psi^*$ is the complex conjugate of $\Psi$. Obviously $\Psi \Psi^*$ is a positive and real number and is equal to $|\Psi|^2$. 
Basic Postulates

• Assume a single particle-like electron; then $\Psi \Psi^*$ is interpreted as the statistical probability that the particle is found in a distance element $dx$ at any instant of time. Thus $\Psi \Psi^*$ represents the probability density.
Principle of Quantum Mechanics

Basic Postulates

Postulate V.

- The average value $\langle Q \rangle$ of any variable corresponding to the state function $\Psi$ is given by expectation value:

$$\langle Q \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{Q} \Psi \, dx$$

- $\langle Q \rangle$ is the expected value of any observation.
- Once the state function corresponding to any particle is found, it is possible to calculate the average position, energy and momentum of the particle within the limit of the uncertainty principle.
Principle of Quantum Mechanics

**Schroedinger Equations**

**Assume:**

\[ E = \frac{p^2}{2m} + V(x, y, z) \]

*where*

\[ p^2 = p_x^2 + p_y^2 + p_z^2 \]

Recall the operators were defined in postulate II;

\[ \frac{p^2}{2m} \equiv - \frac{\hbar^2}{2m} \nabla^2 \quad V(x, y, z) \equiv \hat{V}(x, y, z) \quad E \equiv -\frac{\hbar}{i} \frac{\partial}{\partial t} \]
Schrodinger Equations:

\[ i\hbar \frac{\partial}{\partial t} \psi(r, t) = \left( -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right) \psi(r, t) \]

The potential energy term forms the necessary link between quantum mechanics and the real world. It contains all environmental factors that could influence the state of a particle.

Note than \( p(r) = \Psi \Psi^* = \psi \psi^* \) i.e. probability density is time-independent and define an stationary state
Time dependent Schrödinger’s Equation

single-particle 3D time-dependent Schrödinger equation

\[ i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t) + V(\mathbf{r})\psi(\mathbf{r}, t) \]

Let’s assume:

\[ \psi(\mathbf{r}, t) = \psi(\mathbf{r})f(t) \quad \Rightarrow \quad \psi(\mathbf{r})i\hbar \frac{df(t)}{dt} = f(t) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) \]

Or

\[ \frac{i\hbar}{f(t)} \frac{df}{dt} = \frac{1}{\psi(\mathbf{r})} \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) \]

\[ \frac{1}{f(t)} \frac{df(t)}{dt} = -\frac{iE}{\hbar} \]

\[ f(t) = e^{-iEt/\hbar} \]

And

\[ -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}) \]

Time-independent Schrödinger equation
Consequences

1. The expectation value for any time-independent operator is also time-independent:

\[
|\psi(r, t)|^2 = \psi^*(r, t)\psi(r, t) = e^{iEt/\hbar}\psi^*(r)e^{-iEt/\hbar}\psi(r) = \psi^*(r)\psi(r)
\]

2. The general solution to equation will be a linear combination of these particular solutions:

\[
\psi(r, t) = \sum_i c_i e^{-iE_it/\hbar}\psi_i(r)
\]

\[
< A >= \int \psi^*(r, t)\hat{A}\psi(r, t) = \int \psi^*(r)\hat{A}\psi(r)
\]
if \( U(\vec{r}) = U_x(x) + U_y(y) + U_z(z) \)

\[
E_x X(x) = \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U_x(x) \right) X(x)
\]

\[
E_y Y(y) = \left( -\frac{\hbar^2}{2m} \frac{d^2}{dy^2} + U_y(y) \right) Y(y)
\]

\[
E_z Z(z) = \left( -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + U_z(z) \right) Z(z)
\]

separate the 3D equation into three sets of decoupled 1D equation and solve these three 1D equations independently

\[
\psi(\vec{r}) = X(x) + Y(y) + Z(z)
\]
If there is no force acting on the particle, then the potential function $V(r)$ will be constant and we must have $E>V(r)$.

Assume $V(r)=0$

\[
\psi(x) = A e^{\frac{ix\sqrt{2mE}}{\hbar}} + B e^{\frac{-ix\sqrt{2mE}}{\hbar}}
\]

\[
\psi(x,t) = Ae^{\left(\frac{i}{\hbar}(x\sqrt{2mE} - Et)\right)} + Be^{\left(\frac{-i}{\hbar}(x\sqrt{2mE} + Et)\right)}
\]

In +x direction

\[
\psi(x,t) = Ae^{i(kx - \omega t)}
\]
\[ k = \frac{2\pi}{\lambda} \quad \text{or} \quad \lambda = \frac{h}{\sqrt{2mE}} \]

\[ \lambda = \frac{h}{p} \]

\[ \psi(x,t)\psi^*(x,t) = AA^* \]

The probability density function \( \psi(x,t)\psi^*(x,t) = AA^* \) is a constant independent of position.

A free particle with a well-defined energy will also have a well-defined wavelength and momentum.

A free particle with a well-defined momentum can be found anywhere with equal probability.
Particle in a box

\[ E = \frac{p^2}{2m} + V(x) \]

\[ V(x) = 0 \text{ inside the box} \]

\[ \frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2} \psi(x) = 0 \]

\[ \psi(x) = A_1 \cos kx + A_2 \sin kx \]

\[ k = \sqrt{\frac{2mE}{\hbar^2}} \]

is the wave number.

A particular form of solution
Particle in a box…

First boundary condition, \( x=0, \psi(0)=0 \) then \( A_1=0 \) \[ \psi(x) = A_2 \sin kx \]

Second boundary condition \( x=a, \psi(a)=0 \) \[ \psi(a) = A_2 \sin ka = 0 \]

\( k = n\pi/a \)

From the normalization condition \[ \int_0^a (A_2^2 \sin^2 kx) \, dx = 1 \] \[ A_2 = \sqrt{\frac{2}{a}} \]

Final solution \[ \psi(x) = \sqrt{\frac{2}{a}} \sin \left( \frac{n\pi x}{a} \right) \]

\( p = \frac{h}{\lambda} = \hbar k \)

\[ \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2} \Rightarrow E = E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2} \]

Energy for this system is quantized.
Particle in an infinite potential well:

a) Four lowest discrete energy levels;

b) Corresponding wave functions

c) Corresponding probability functions
Reflection: Step potential

\[
\begin{align*}
\lambda_1 &= 2\pi / k_1 \\
\lambda_2 &= 2\pi / k_2
\end{align*}
\]

\[
\psi_1(x) = A_1 e^{jk_1x} + B_1 e^{-jk_1x} \quad (x \leq 0)
\]

\[
k_1 = \sqrt{\frac{2mE}{\hbar^2}}
\]

\(v_i\) and \(v_r\) are the magnitude of the incident and reflected wave velocity.
region II the Schrödinger equation \((E<V_o)\)

\[
\frac{\partial^2 \psi_2(x)}{\partial x^2} + \frac{2m}{\hbar^2} (V_0 - E) \psi_2(x) = 0
\]

\[
\psi_2(x) = A_2 e^{-k_2 x} + B_2 e^{k_2 x} (x \geq 0)
\]

\[
k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}
\]

\[B_2 = 0\] is zero due to fact that function must be finite everywhere and potential is a step function

boundary \(x=0\) \(\implies\) \(\psi_1(0) = \psi_2(0)\) \(\implies\) \(A_1 + B_1 = A_2\).

\[
\frac{\partial \psi_1}{\partial x} \bigg|_{x=0} = \frac{\partial \psi_2}{\partial x} \bigg|_{x=0}
\]

\[jk_1A_1 - jk_1B_1 = -k_2A_2\]
Continue

\[
\frac{B_1 \cdot B_1^*}{A_1 \cdot A_1^*} = \frac{\left(k_2^2 - k_1^2 + 2jk_1k_2\right)\left(k_2^2 - k_1^2 - 2jk_1k_2\right)}{\left(k_2^2 + k_1^2\right)^2}
\]

kinetic energy \[\rightarrow\] K.E. = \(mv^2/2\)

\[
k_1 = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{\frac{2m}{\hbar^2} \left(\frac{1}{2} mv^2\right)} = \sqrt{\frac{m^2 v^2}{\hbar^2}} = \frac{mv}{\hbar}
\]

\[
R = \frac{v_r \cdot B_1 \cdot B_1^*}{v_i \cdot A_1 \cdot A_1^*} = \frac{\left(k_2^2 - k_1^2\right)^2 + 4k_1^2k_2^2}{\left(k_2^2 + k_1^2\right)^2} = 1.0
\]
quantum particles can tunnel through the barrier and get out on the other side

\[ E < U_0 \]

\[ k_0 = p \sqrt{\frac{2mE}{\hbar}} \]
For wide barriers,

\[
T \approx 16 \frac{E}{U_0} \left( 1 - \frac{E}{U_0} \right) e^{-2L/\delta},
\]

\[
\delta = \frac{\hbar}{\sqrt{2m(U_0 - E)}}
\]

The tunneling rate is a very sensitive function of \(L\).
Energy States & Energy Bands

\[ E_n = \frac{-m \, q^4}{(4 \pi \varepsilon_0)^2 \, 2 \hbar^2 \, n^2} \]

\[ \psi_{100} = \frac{1}{\sqrt{\pi}} \left( \frac{1}{a_0} \right)^{3/2} q^{-r/a_0} \]
Pauli’s Exclusion Principle

Overlapping probability density functions of two adjacent hydrogen atoms.

The splitting of the n = 1 state
The potential experienced by an electron due to the coulomb interactions around an atom. 1s, 2s, 2p,… are the energy levels that the electron can occupy.

The potential wells due to the interactions between 2 atoms (in one molecule). Some electrons are shared between the atoms. Due to the interactions between electrons-electrons, nucleons-nucleons, and electrons-nucleons, the energy levels split, creating 1s, 2s, 2p,… doublets.

Larger molecules, larger splitting.

In Solid with n= 10e23 atoms, the sublevels are extremely close to each other. They coalesce and form an energy band. 1s, 2s, 2p… energy bands.
The splitting of an energy state into a band of allowed energies.
Schematic showing the splitting of three energy states into allowed bands of energies.
The splitting of the 3s and 3p states of silicon into the allowed and forbidden energy bands.
Classification of Solid Structures

**Amorphous:** Atoms (molecules) bond to form a very short-range (few atoms) periodic structure.

**Crystals:** Atoms (molecules) bond to form a long-range periodic structure. The constant bonds (coordination), bond distance and angles between bonds are the characteristics of a crystal structure.

**Polycrystalline:** made of pieces of crystalline structures (called grain) each oriented at different direction (intermediate-range-ordered)
An IDEAL CRYSTAL is constructed by the infinite repetition of identical structural units in space.
Crystalline Structures
Lattice Structures

- **A LATTICE** represents a set of points in space that form a periodic structure. Each point sees exactly the same environment. The lattice is by itself a mathematical abstraction.

- A building block of atoms called the **BASIS** is then attached to each lattice point yielding the crystal structure.

- \[ \text{LATTICE} + \text{BASIS} = \text{CRYSTAL STRUCTURE} \]

- The identical structure units that have small volume are called \text{UNIT CELL}. 

Crystal lattices

A 2-D lattice showing translation of a unit cell by $R = 4a + 2b$
Lattice Structures

Simple Cube (SC)

Body Centred Cube (BCC)

Face Centred Cube (FCC)

Lattice Constant

Side diagonal: $a\sqrt{2}$

Body diagonal: $a\sqrt{3}$
(a) The crystal structure of copper is face centered cubic (FCC). The atoms are positioned at well defined sites arranged periodically and there is a long range order in the crystal.

(b) An FCC unit cell with closed packed spheres.

(c) Reduced sphere representation of the unit cell. Examples: Ag, Al, Au, Ca, Cu, Ni.

Number of atoms per unit cell
8 corners = 8 × (1/8) = 1
6 faces = 6 × (1/2) = 3
Some popular lattice planes
Parameters that characterize a unit cell:

- Lattice structure (e.g. cubic, tetragonal, etc.).
- Basis.
- Number of atoms in a unit cell.
- Crystal planes e.g. \{100\}, \{110\}, \{111\}, Miller Indices.
- Number of atoms in each plane.
- Chemical binding (e.g. metallic, covalent, …).
- Number of nearest (nn) and next nearest (nnn) atoms to each atom.
Example of (100)

(100)
Example of (110)
Example of (111)
Diamond Structure

- Top view of an extended (100) plane of the diamond lattice structure.
The unit cell of diamond (zinc blend) lattice structure. The position of each lattice point is shown with respect to the 000 lattice point.
Two Interpenetrating Face-Centered Cubic Lattices
Silicon – Diamond Structure

Common Planes
• \{100\} Plane
• \{110\} Plane
• \{111\} Plane

\(a\) – Lattice Constant
For Silicon
\(a = 5.34 \text{ Å}\)
Some Properties of Some Important Semiconductors

<table>
<thead>
<tr>
<th>Compound</th>
<th>$E_g$ Gap (eV)</th>
<th>Transition $\lambda$ (nm)</th>
<th>Bandgap</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diamond</td>
<td>5.4</td>
<td>230</td>
<td>indirect</td>
</tr>
<tr>
<td>ZnS</td>
<td>3.75</td>
<td>331</td>
<td>direct</td>
</tr>
<tr>
<td>ZnO</td>
<td>3.3</td>
<td>376</td>
<td>indirect</td>
</tr>
<tr>
<td>TiO$_2$</td>
<td>3</td>
<td>413</td>
<td>indirect</td>
</tr>
<tr>
<td>CdS</td>
<td>2.5</td>
<td>496</td>
<td>direct</td>
</tr>
<tr>
<td>CdSe</td>
<td>1.8</td>
<td>689</td>
<td>direct</td>
</tr>
<tr>
<td>CdTe</td>
<td>1.55</td>
<td>800</td>
<td>direct</td>
</tr>
<tr>
<td>GaAs</td>
<td>1.5</td>
<td>827</td>
<td>direct</td>
</tr>
<tr>
<td>InP</td>
<td>1.4</td>
<td>886</td>
<td>direct</td>
</tr>
<tr>
<td>Si</td>
<td>1.2</td>
<td>1033</td>
<td>indirect</td>
</tr>
<tr>
<td>AgCl</td>
<td>0.32</td>
<td>3875</td>
<td>indirect</td>
</tr>
<tr>
<td>PbS</td>
<td>0.3</td>
<td>4133</td>
<td>direct</td>
</tr>
<tr>
<td>AgI</td>
<td>0.28</td>
<td>4429</td>
<td>direct</td>
</tr>
<tr>
<td>PbTe</td>
<td>0.25</td>
<td>4960</td>
<td>indirect</td>
</tr>
</tbody>
</table>
Non-Periodical Potential

Periodical Potential

\[ \Psi(r) = u(r) \cdot e^{i k r} \]
The state function for electrons in a single crystal has a form of:

$$\Psi_k(r) = U_k(r)e^{jk \cdot r}$$

where

$$U_k(r) = U_k(r + R)$$

is the periodic potential in single crystals of semiconductors. $R = aX + bY + cZ$, $a$, $b$, and $c$ are integers.

$$\Psi_k(r + R) = U_k(r + R)e^{jk \cdot (r + R)} = U_k(r)e^{jk \cdot r}e^{jk \cdot R} = e^{jk \cdot R}\Psi_k(r)$$

Therefore:

$$\left|\Psi_k(r + R)\right|^2 = \left|\Psi_k(r)\right|^2$$

Which means that the probability of finding electrons is periodic.
Potential Function

Potential function of a single isolated atom
Overlapping potential functions of adjacent atoms.

Net potential function of a one-dimensional single crystal.

The one-dimensional periodic potential function of the Kronig-Penney model.
The $E$ versus $K$ diagram. The allowed energy bands and forbidden energy bandgaps are indicated.
The $E$ versus $k$ diagram in the reduced-zone representation.

Reduced $K$ space
Two-dimensional representation of the breaking of a covalent bond.

Corresponding line representation of the energy band and the generation of a negative and positive charge with the breaking of a covalent bond.
The $E$ versus $k$ diagram of the conduction and valence bands of a semiconductor at $T = 0 \, \text{K}$.

The $E$ versus $k$ diagram of the conduction and valence bands of a semiconductor at $T > 0 \, \text{K}$.

The asymmetric distribution of electrons in the $E$ versus $k$ diagram when an external force is applied.
Allowed energy bands showing:
(a) an almost empty band
(b) an almost full band
(c) the bandgap energy between the two allowed bands

Allowed energy bands showing:
(a) an almost empty band
(b) an almost full band
(c) the bandgap energy between the two allowed bands
Energy band structures of GaAs.
Energy band structures of Si.
The Concepts of:

1) Effective Mass

\[ \frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{1}{m^*} \]

2) Negative Mass

3) Positive charge

4) Holes
Density of states

**Pauli exclusion principle**, only one electron can occupy a given quantum state.

The number of carriers that can contribute to the conduction process is a function of the number of available energy or quantum states.

density of electronic quantum energy states are called density of states (DOS).
Bulk density of states

\[
\begin{cases}
V(x, y, z) = 0 & \text{for } 0 < x < a, 0 < y < a, 0 < z < a \\
V(x, y, z) = \infty & \text{elsewhere}
\end{cases}
\]

Schrödinger’s equation solution

\[
\frac{2mE}{\hbar^2} = k^2 = k_x^2 + k_y^2 + k_z^2 = (n_x^2 + n_y^2 + n_z^2)\left(\frac{\pi^2}{a^2}\right)
\]

the distance between two states in \( k \) space

\[
k_{x+1} - k_x = (n_x + 1)\left(\frac{\pi}{a}\right) - n_x\left(\frac{\pi}{a}\right) = \left(\frac{\pi}{a}\right)
\]

the differential density of quantum states in \( k \) space

\[
g_T(k) dk = 2\left(\frac{1}{8}\right)\frac{4\pi k^2 dk}{\left(\frac{\pi}{a}\right)^3} = \frac{k^2 dk}{\pi^2} a^3
\]
converting the states into energy space

\[
\begin{aligned}
  k^2 &= \frac{2mE}{\hbar^2} \implies k = \frac{\sqrt{2mE}}{\hbar} \\
dk &= \frac{1}{\hbar} \sqrt{\frac{m}{2E}} dE
\end{aligned}
\]

Density of states in K space

\[
g_T(E) dE = \frac{a^3}{\pi^2} \left( \frac{2mE}{\hbar^2} \right) \cdot \frac{1}{\hbar} \sqrt{\frac{m}{2E}} dE = \frac{4\pi a^3}{h^3} (2m)^{3/2} \cdot \sqrt{E} dE
\]

Density of states in energy space

\[
g(E) = \frac{4\pi (2m)^{3/2}}{h^3} \sqrt{E}
\]
Density of State.
Electrons Distribution.

\[ g_c(E) = \frac{4\pi (2m_n^*)^{3/2}}{h^3} \sqrt{E - E_c} \]

\[ g_v(E) = \frac{4\pi (2m_p^*)^{3/2}}{h^3} \sqrt{E_v - E} \]

The density of energy states in the conduction band and the density of the energy states in the valence band as a function of energy.
Density of states in thin films: 2D structures

\[ E = E_x + E_p \rightarrow E_p = E_y + E_z \]

if

\[ \frac{2mE}{h^2} = k^2 = k_y^2 + k_z^2 = \left( n_y^2 + n_z^2 \right) \left( \frac{\pi^2}{a^2} \right) \]

2D system to give a 2D plane of \( k \) values

\[ g_T(k)dk = 2\left( \frac{1}{4} \right) \frac{2\pi k dk}{\left( \frac{\pi}{a} \right)^2} = \frac{k dk}{\pi} a^2 \]

converting the \( k \) space into energy space

\[ g(E) = \frac{4\pi m}{h^2} \]

\[ g_T(E) dE = \frac{a^2}{\pi} \sqrt{\frac{2mE}{h^2}} \cdot \frac{1}{\hbar} \sqrt{\frac{m}{2E}} dE = \frac{4\pi ma^2}{h^2} dE \]
Density of state in Nanowire: 1D structure

Dispersion relation

\[ \frac{2mE}{\hbar^2} = k^2 = k_z^2 = \left( n_z^2 \right) \left( \frac{\pi^2}{a^2} \right) \]

Length associated with every quantum state \( L_k = \pi/a \)

\[ g_T(k)dk = 2\left( \frac{1}{2} \right) \left( \frac{dk}{\pi/a} \right) = \frac{dk}{\pi} a \]

Converting the \( k \) space to energy space

\[ g_T(E)dE = \frac{a}{\pi} \cdot \frac{1}{\hbar} \sqrt{\frac{m}{2E}} dE = \frac{a}{\hbar} \sqrt{\frac{2m}{E}} dE \]

\[ g(E) = \frac{1}{h} \sqrt{\frac{2m}{E}} \]
Density of states
Energy States vs Size of Structures.

- THREE
- TWO
- ONE
- ZERO

DENSITY OF STATES

ENERGY

200 Å
Discrete energy states and quantum states for a particular system for $T > 0K$.

Discrete energy states and quantum states for a particular system at $T = 0K$. 
Fermi-Dirac Distribution:

\[ f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)} \]

The Fermi probability function versus energy for \( T = 0 \)K.
The Fermi probability function versus energy for differential temperatures.

\[
f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}
\]

The corresponding line representation of the energy band and the generation of a negative and positive charge with the breaking of a covalent bond.
Density and Current operator

\[ \int \psi \psi^* d^3 r = 1 \quad \rightarrow \quad \text{probability } \propto |\psi|^2 = \psi \psi^* \]

many body system Fermi-Dirac distribution

\[ n(E_m) = |\psi_m|^2 \cdot f(E_m) \]

\[ n = \int_{-\infty}^{+\infty} n(E_m) dE = \sum_{m=1}^{\infty} |\psi_m|^2 \cdot f(E_m) \]

current conservation, more popularly known as the continuity equation

\[ \frac{\partial}{\partial t} \rho(r,t) = -\nabla \cdot J(r,t) \]
A particle of charge $e$

$$\rho = e|\psi|^2$$

$$\frac{\partial \rho}{\partial t} = e \frac{\partial |\psi|^2}{\partial t} = e \frac{\partial (\psi^* \psi)}{\partial t} = e \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right)$$

from Schrödinger’s equation

$$i\hbar \frac{\partial}{\partial t} \psi(r, t) = \left( -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right) \psi(r, t)$$

Multiplying both sides by $\psi^*(r, t) e^{i \hbar}$

$$e \psi^*(r, t) \frac{\partial}{\partial t} \psi(r, t) = e i \frac{\hbar}{2m} \psi^*(r, t) \nabla^2 \psi(r, t) - e \frac{i}{\hbar} \psi^*(r, t) V(r) \psi(r, t)$$

For the second term we take the complex conjugate and multiply both sides by $\psi(r, t)$

$$\frac{\partial \rho}{\partial t} = \psi^*(r, t) e^i \frac{\hbar}{2m} \nabla^2 \psi(r, t) - \psi(r, t) e^i \frac{\hbar}{2m} \nabla^2 \psi^*(r, t) + \frac{e \psi^* \psi}{i\hbar} (V(r) - V(r)) = e i \frac{\hbar}{2m} \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*) = -\nabla \cdot J$$

Finally

$$J = -e i \frac{\hbar}{2m} (\psi^* \nabla \psi - \psi \nabla \psi^*)$$
\[ n_0 = n_i \exp \left[ \frac{(E_F - E_{Fi})}{kT} \right] \]
\[ p_0 = n_i \exp \left[ -\frac{(E_F - E_{Fi})}{kT} \right] \]
Carrier Transport:

Current in Semiconductors: (Drift, Diffusion, Carriers Recommendation, Carriers Generation)

Drift Current:

\[ J_{drf} = q(\mu_n n + \mu_p p)E \]
Carrier drift velocity versus electric field for high-purity silicon, germanium, and gallium arsenide.
Diffusion Current

\[ J_{ndif} = qD_n \frac{dn}{dx} \]

\[ J_{pdif} = -qD_p \frac{dp}{dx} \]
Einstein Relation

\[ \frac{D_n}{\mu_n} = \frac{D_p}{\mu_p} = \frac{kT}{q} \]

\( kT/q \) at room temperature = 0.0259 V

\[ J_{total} = q(n\mu_n + p\mu_p)E + q(D_n \frac{dn}{dx} - D_p \frac{dp}{dx}) \]

Under Equilibrium Condition \( J(\text{total}) = 0 \).
Generation - Recombination

\[ R_n = R_p = \frac{\delta n(t)}{\tau_{no}} = \frac{\delta n(t)}{\tau_{po}} \]
Steady-state generation rate at $x=0$.

Steady-state electron and hole concentrations for the case when excess electrons and holes are generated at $x = 0$. 

Carrier concentration (log scale)

$p_0 + \delta n(0)$

$n_0 + \delta n(0)$

$x = 0$
Continuity Equations

\[ D_p \frac{\partial^2 p}{\partial x^2} - \mu_p (E \frac{\partial p}{\partial x} + p \frac{\partial E}{\partial x}) + g_p - \frac{p}{\tau_p} = \frac{\partial p}{\partial t} \]

\[ D_n \frac{\partial^2 n}{\partial x^2} + \mu_n (E \frac{\partial n}{\partial x} + n \frac{\partial E}{\partial x}) + g_n - \frac{n}{\tau_n} = \frac{\partial n}{\partial t} \]
Quantum Mechanics in nanostructures: some issues

1. Validity of effective mass approximation
2. Doping and effects in nanostructures
3. Surface Effects
4. Recombination
5. Hot Carrier Effects
6. Exciton
7. Density of States and Coulomb Blockade
Validity of effective mass approximation

Crystal can be thought to be effectively made of only periodic atoms applies Bloch’s theorem and uses Krönig-Penny model to treat the macroscopic potential due to applied bias or macroscopic space charge, and gets the band diagrams of the material.

lowest parts of the conduction band, is approximated parabolic.
an electron in an external electric field $E$

From the external electric field alone,

\[ \vec{F} = q \vec{E} \]

charge.

\[ a = \frac{1}{\hbar^2} \cdot \frac{d^2\varepsilon}{dk^2} qE \]

acceleration

reduced Planck's constant

\[ m^* = \hbar^2 \cdot \left[ \frac{d^2\varepsilon}{dk^2} \right]^{-1} \]

wave number

This concept of effective mass is valid for bulk materials where we can assume the dispersion relation to be periodic, but in nanostructures the periodicity is no longer there as dimensions get smaller. Hence the band diagram also fails for nanostructure and we can no longer use the effective mass approximation. Experiments have shown that below 5 nm, we can no longer use the effective mass approximation.
Doping and effects in nanostructures

In nanostructure, the semiconductor material could be small, specially in quantum dots, and a substitutional impurity should no longer be regarded as doping and a full quantum mechanical treatment is needed. But it has been experimentally found that still the concept of doping does remain somewhat valid in the range of QDs and p doped or n doped QD are readily available.
Surface Effects

In bulk material, surface pose only as the loss of continuity in otherwise perfectly periodic crystal, hence surface is considered a defect.

The unsatisfied bonding makes dangling bond at the surface.

In nanostructures, the ratio of surface to volume is very high and a considerable number of atoms may constitute the surface for a nanowire or a quantum dot. In these cases, surface plays a very important part in its physical, chemical and electronic property.

Some bulk indirect material becomes direct due to the surface recombination of electron holes, while some material conduct highly through the surface.

Some materials (eg Cs/p-type GaAs) can even be activated to negative electron affinity, and such materials form a potent source of electrons, which can also be spin-polarized as a result of the band structure.
The term 'hot carriers' refers to either holes or electrons (also referred to as 'hot electrons') that have gained very high kinetic energy after being accelerated by a strong electric field in areas of high field intensities within a semiconductor (especially MOS) device.

The term 'hot carrier effects', refers to device degradation or instability caused by hot carrier injection.

four commonly encountered hot carrier injection mechanisms:

1) the drain avalanche hot carrier injection;

2) the channel hot electron injection;

3) the substrate hot electron injection;

4) the secondary generated hot electron injection.

The drain avalanche hot carrier (DAHC) injection is said to produce the worst device degradation under normal operating temperature range under non-saturated conditions ($V_D > V_G$) → high voltage applied at the drain.
Other Implications

- Effective resistance
  (ballistic & effects of splitting energy level)
  
  Effective resistance may rise dramatically as current approaches saturation level

- Conductance is quantized and has a maximum value for a channel with one level

\[ G = \frac{2q^2}{h} \frac{2\lambda}{L} \]

- Familiar voltage divider and current divider rule may not be valid on submicron scales
Conclusions
Quantum Confinement

- Transport properties are function of confinement length in quantum structures because of the change in the Density of States
- Relative strength of each scattering is different from bulk materials
- Electrons tend to stay away from the interface as wave function vanishes near the interface
Conclusions
High-Field Driven Transport

• Electric field puts an order into otherwise completely random motion

• Higher mobility may not necessary lead to higher saturation velocity
Conclusions
Failure of Ohm’s Law

• Effective resistance may rise dramatically as current approaches saturation level

• Familiar voltage divider and current divider rule may not be valid on submicron scales