# "Complementi di Fisica" Lecture 19 

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## Course Outline - Reminder

- The physics of semiconductor devices: an introduction
- Quantum Mechanics: an introduction
- ...just a few more comments on:
- (3-d) Hydrogen atom, angular momentum, spin
- Systems with many particles: fermions and Pauli principle
- (slightly more) Advanced semiconductor fundamentals
- Energy bands, effective mass
- Equilibrium Carrier Statistics: density of states, Fermi function
- Non-equilibrium transport of charge carriers and the motion of electrons in real crystals
- Too late for...
- Simulations; revisiting Shockley; discussing a device as an example
- Measurements of semiconductor properties


## Lecture 19 - outline

- A very brief summary on:
- (3-d) Hydrogen atom, angular momentum, spin
- Systems with many particles: fermions and Pauli principle
- Multi-electron atoms, periodic table, and crystals
- Back to semiconductors: equilibrium carrier statistics
- Thermal equilibrium and detailed balancing
- Density of states
- Fermi probability distribution function
- consequences? ... see $1^{\text {st }}$ part of the course
- Boltzmann approximation
- Number of carriers at band edges
- Etc... (intrinsic, extrinsic semiconductors, ...)


## 3-d wave mechanics <br> (just a hint...)

Hydrogen atom
Angular momentum

## Spin

## Hydrogen atom

- "simple": time-independent Schrödinger equation for the electron:
- central "Coulomb" potential $V(r)=q^{2} /\left(4 \pi \varepsilon_{0} r\right)$
- spherical coordinates ( $r, \theta, \phi$ )
- Separation of variables (3)
- 3 integer quantum numbers identify each solution

$$
\psi_{\mathrm{n}, \mathrm{l}, \mathrm{~m}}(r, \theta, \phi)=R_{\mathrm{nl}}(\mathrm{r}) Y_{\mathrm{l}}^{\mathrm{m}}(\theta, \phi)
$$

```
n=1,2,3\cdots}\quad\ldots.\mathrm{ principal quantum number Energy (= Bohr!)
    l=0,1,2,\cdots n - 1 ... azimuthal quantum number
m = -l to l }\quad\ldots..\mathrm{ magnetic orbital quantum number
```

Angular momentum

$$
\hat{H} \psi_{n l m}=E_{n} \psi_{n l m} \quad \hat{L}^{2} \psi_{n l m}=\hbar^{2} l(l+1) \psi_{n l m} \quad \hat{L}_{z} \psi_{n l m}=\hbar m \psi_{n l m}
$$

## Radial pdf

## Radial

probability distribution function

$$
r^{2}\left[R_{n}(r)\right]^{2}
$$

Peaks occur at Bohr orbits radii


# Spherical harmonics 


(b1) $\ell=1, m= \pm 1$

Angular
Probability distribution functions

$$
\left|Y_{l m}\right|^{2}
$$


(c1) $\ell=2, m= \pm 2$

(c2) $\ell=2, m= \pm 1$
(b2) $\ell=1, m=0$


## Angular momentum

- Also angular momentum is quantized!
- One can only measure simultaneously the magnitude square and one component (the components don't commute !)
- Cartesian and spherical coordinates:

$$
\begin{aligned}
& \vec{L} \equiv \vec{r} \times \vec{p} \quad \hat{L}_{x}=y \hat{p}_{z}-z \hat{p}_{y} \quad \hat{L}_{y}=z \hat{p}_{x}-x \hat{p}_{z} \quad \hat{L}_{z}=x \hat{p}_{y}-y \hat{p}_{x} \\
& \hat{L}^{2} \equiv \hat{L}_{x}^{2}+\hat{L}_{y}^{2}+\hat{L}_{z}^{2}=-\hbar^{2}\left(\frac{\partial^{2}}{\partial \theta^{2}}+\cot \theta \frac{\partial}{\partial \theta}+\frac{1}{\sin ^{2} \theta} \frac{\partial^{2}}{\partial \phi^{2}}\right) \\
& \hat{L}_{z}=-i \hbar \frac{\partial}{\partial \phi}
\end{aligned}
$$

- Eigenvalues and eigenfunctions

$$
\begin{array}{lrl}
\hat{L}^{2} Y_{l m}(\theta, \phi) & =\hbar^{2} l(l+1) Y_{l m}(\theta, \phi) & l=1,2,3, \ldots \\
\hat{L}_{z} Y_{l m}(\theta, \phi) & =\hbar m Y_{l m}(\theta, \phi) & -l \leq m \text { integer } \leq+l
\end{array}
$$

## Magnetic effects

- On dimensional grounds, for a charged particle with angular momentum we expect a magnetic moment and a contribution to potential energy when interacting with an external $B$ field:

$$
\vec{\mu}=g \frac{q}{2 m} \vec{L} \quad U=-\vec{\mu} \cdot \vec{B}
$$

- "Zeeman effect" (splitting of degenerate levels) and Stern-Gerlach experiment ("space quantization" bsplitting of an atomic beam)


10-12-2004


## Spin

- Elementary particles carry also an "intrinsic" angular momentum ("spin" S) besides the "orbital" angular momentum (L)
- The eigenstates are not the spherical harmonics: not functions of $\theta, \phi$ at all!
- The quantum numbers $s, m$ can be half-integer
- The magnitude $s$ is specific and fixed for each elementary particle, and is called "spin"
- Electrons have spin $\mathrm{s}=1 / 2$, with two possible eigenstates: "up" and "down"

$$
\begin{aligned}
& \hat{S}^{2}|s m\rangle=\hbar^{2} s(s+1)|s m\rangle \quad s=0, \frac{1}{2}, 1, \frac{3}{2}, \ldots ; \quad m=-s,-s+1, \ldots, s \\
& \hat{S}_{z}|s m\rangle=\hbar m|s m\rangle \\
& \text { electrons: eigenstates and eigenvalues: }
\end{aligned}
$$

$s=1 / 2 \quad \chi_{+}=\left|\frac{1}{2} \frac{1}{2}\right\rangle=\binom{1}{0}, \quad$ eigenvalue $+\frac{\hbar}{2}$

$$
\chi_{-}=\left|\frac{1}{2}\left(-\frac{1}{2}\right)\right\rangle=\binom{0}{1} \text {, eigenvalue }-\frac{\hbar}{2}
$$

## Spin: observable effects

- For example:
- "Anomalous Zeeman effect": further level splitting in strong B fields
- "Fine Structure" level splitting due to "spin-orbit coupling"

Anomalous Zeeman effect

Spin-orbit coupling


## This is not the end...

- Hydrogen has been a very interesting laboratory:
- Orders of magnitude of different effects, treated as "perturbations", in terms of the a-dimensional "fine structure constant" $\alpha$, expressing the strength of the electromagnetic coupling:

$$
\alpha \equiv \frac{e^{2}}{4 \pi \varepsilon_{0} \hbar c} \cong \frac{1}{137.036}
$$

Table 6.1: Hierarchy of corrections to the Bohr energies of hydrogen.

| Bohr energies: | of order | $\alpha^{2} m c^{2}$ |
| ---: | :--- | :--- |
| Fine structure: | of order | $\alpha^{4} m c^{2}$ |
| Lamb shift: |  |  |
| of order |  |  |
| of order | $\alpha^{5} m c^{2}$ | $\left(m / m_{p}\right) \alpha^{4} m c^{2}$ |
| Relativity, spin-orbit |  |  |
| Hyperfine splitting: | Coulomb field quantization |  |

# Many-particle systems <br> (just a hint...) 

Identical particles
Bosons and fermions
Pauli Principle
Periodic table

## Identical particles

- Many-particle systems? Let's start with two:
- Wave function, probability distribution, hamiltonian; S.equation

$$
\begin{array}{ll}
\Psi\left(\vec{r}_{1}, \vec{r}_{2}, t\right) & \left|\Psi\left(\vec{r}_{1}, \vec{r}_{2}, t\right)\right|^{2} d \vec{r}_{1} d \vec{r}_{2} \\
i \hbar \frac{\partial \Psi}{\partial t}=\hat{H} \Psi & \hat{H}=-\frac{\hbar^{2}}{2 m_{1}} \nabla_{1}^{2}-\frac{\hbar^{2}}{2 m_{2}} \nabla_{2}^{2}+V\left(\vec{r}_{1}, \vec{r}_{2}, t\right)
\end{array}
$$

- For time-independent potentials: time-indep. S.eq. and stationary states

$$
\begin{aligned}
& \Psi\left(\vec{r}_{1}, \vec{r}_{2}, t\right)=\psi\left(\vec{r}_{1}, \vec{r}_{2}\right) e^{-i E t / \hbar} \\
& -\frac{\hbar^{2}}{2 m_{1}} \nabla_{1}^{2} \psi-\frac{\hbar^{2}}{2 m_{2}} \nabla_{2}^{2} \psi+V\left(\vec{r}_{1}, \vec{r}_{2}\right) \psi=E \psi
\end{aligned}
$$

## Bosons and fermions

- For distinguishable particles (for instance, an electron and a positron):
- particle 1 is in the (one-particle) state $\psi_{a}\left(r_{1}\right)$
- particle 2 in state $\psi_{b}\left(r_{2}\right)$

$$
\psi\left(\vec{r}_{1}, \vec{r}_{2}, t\right)=\psi_{a}\left(\vec{r}_{1}\right) \psi_{b}\left(\vec{r}_{2}\right)
$$

- But: identical particles (for instance, two electrons) are truly indistinguishable in quantum mechanics:
- There are two possible ways to construct the wave-function:
+ "symmetric": bosons

$$
\psi_{ \pm}\left(\vec{r}_{1}, \vec{r}_{2}\right)=A\left[\psi_{a}\left(\vec{r}_{1}\right) \psi_{b}\left(\vec{r}_{2}\right) \pm \psi_{b}\left(\vec{r}_{1}\right) \psi_{a}\left(\vec{r}_{2}\right)\right]
$$

- "anti-symmetric": fermions
- All particles with integer spin are bosons
- All particles with half-integer spin are fermions


## Fermions and Pauli principle

- Connection between spin and "statistics" (or wave-function exchange symmetry)
- can be proven in relativistic QM
- must be taken as an axiom in non-relativistic QM
- Pauli exclusion principle:
- Two fermions (anti-symmetric w.f.) cannot occupy the same state! Indeed:

$$
\psi_{a}=\psi_{b} \quad \Rightarrow \quad \psi_{-}\left(\vec{r}_{1}, \vec{r}_{2}\right)=A\left[\psi_{a}\left(\vec{r}_{1}\right) \psi_{a}\left(\vec{r}_{2}\right)-\psi_{a}\left(\vec{r}_{1}\right) \psi_{a}\left(\vec{r}_{2}\right)\right]=0
$$

- It can be shown that:
- The exchange operator P is a "compatible observable" commuting with $\mathrm{H} \Rightarrow$ one can find solutions that are either symmetric or antisymmetric
- For identical particles, the wave function is required to be symmetric (for bosons) or anti-symmetric (for fermions)


## Pauli Principle: consequences for electrons

- For electrons the total wave-function (including spin) must be anti-symmetric, and they cannot occupy the same state (two per level allowed, with opposite spin.
- The anti-symmetry requirement allows some wave-function configurations, prohibits others: equivalent to an "exchange force"
- Filling of available levels by electrons in a box (neglecting interactions among electrons!): Fermi level= highest energy level occupied at $\mathrm{T}=0 \mathrm{~K}$ (see exercises)
- "degeneracy pressure": even neglecting electric interactions between electrons, the Pauli principle implies that "the closest that two electrons can get to each other is roughly a half a DeBroglie wavelength corresponding to the Fermi energy (see exercises)


## Pauli principle: Periodic table of elements

- Multi-electron atoms are treated by approximate methods:
- wave functions are modified (and called "orbitals"), but:
- they are labeled by the same quantum numbers $\mathrm{n}, \mathrm{I}, \mathrm{m}$, and:
- Orbitals are filled by electrons following the Pauli exclusion principle: two electrons cannot have the same quantum numbers (state)
Table A. 3 Energy States and the Electronic Configuration in Elements 1-14. Atoms are assumed to be in the ground state.
Quantum
Numbers $\left(\begin{array}{c|c|c|c|c|c|c|c|c|c|c|c|c|c|c|c|c|c|c|}\hline \mathbf{n} & 1 & 1 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 3 & 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ \hline l & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ \hline \mathbf{m} & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 1 & 1 & 0 & 0 & -1 & -1 & 0 & 0 & 1 & 1 \\ \hline \mathbf{s} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \hline \hline \text { State } & 1 s & 1 s & 2 s & 2 s & 2 p & 2 p & 2 p & 2 p & 2 p & 2 p & 3 s & 3 s & 3 p & 3 p & 3 p & 3 p & 3 p & 3 p \\ \hline\end{array}\right.$


## Periodic table of the elements



## Back to semiconductors

Thermal equilibrium
Density of states
Fermi probability distribution function Carrier concentrations (Boltzmann approx.)

## Thermal equilibrium

- Thermal equilibrium = ?
- Between two bodies or systems in "thermal equilibrium" there can be no net transfer of any sort (law of detailed balancing).
- Thermal equilibrium: static, endless, useless... why do we care?
- Systems near thermal equilibrium tend to come to equilibrium in predictable ways
- The predictable behavior of systems not quite in equilibrium allows us to design and construct useful devices!
- From the statistical point of view:
- Thermal equilibrium represents the distribution of maximum probability, achieved when the detailed balancing between the possible processes is reached.


## Finding the maximum probability

- First part: specify all possible "states" (solutions to a wave equation) and a set of appropriate boundary conditions
- Possible eigenstates of the system (in our case E-k plot!)
- Total internal energy of the system
- Rules about filling states (in our case the Pauli principle)
- Rules about conservation of particles
- Second part: procedure to find the most likely distribution of particles among the states, that does not violate any of the rules
- Finding a maximum subject to constraints ("rules"): Lagrange's method of undetermined multipliers
- Let's start with the "density of states" (step 1)


## Step 1: density of states

## Density of states ...

- Density of states $g(E)$
- $g(E)=$ number of allowed states for electrons in the energy range ( $E, E+d E$ ), per unit volume of the crystal
- For a general solution (any $E$ ) we should use the full machinery of band theory... (possible, but complicated!)
- but we are mainly interested in the band edges, normally populated by carriers: much simpler! Shortcut:
- Equivalent problem: density of states for electrons in a 3-d box, provided we finally modify the solution, taking into account the "effective mass" m* and the band structure



## Electrons in a box

- Infinitely deep 3-d potential well:
Time-independent Schrödinger equation
$\frac{\partial^{2} \psi}{\partial x^{2}}+\frac{\partial^{2} \psi}{\partial y^{2}}+\frac{\partial^{2} \psi}{\partial z^{2}}+k^{2} \psi=0$
$k \equiv \sqrt{2 m E / \hbar^{2}} \quad$ or $: \quad E=\frac{\hbar^{2} k^{2}}{2 m}$


Separation of variables
For each of the three functions:
$\psi(x, y, z)=\psi_{x}(x) \psi_{y}(y) \psi_{x}(z)$
substituting and dividing by: $\psi=\psi_{x} \psi_{y} \psi_{x}$
$\frac{1}{\psi_{x}} \frac{\partial^{2} \psi_{x}}{\partial x^{2}}+\frac{1}{\psi_{y}} \frac{\partial^{2} \psi_{y}}{\partial y^{2}}+\frac{1}{\psi_{z}} \frac{\partial^{2} \psi_{z}}{\partial z^{2}}+k^{2}=0$

$$
\begin{aligned}
& \frac{1}{\psi_{x}} \frac{\partial^{2} \psi_{x}}{\partial x^{2}}=\text { constant }=-k_{x}^{2} \\
& \frac{\partial^{2} \psi_{x}}{\partial x^{2}}+k_{x}^{2} \psi_{x}=0 \quad 0<x<a
\end{aligned}
$$

(similar for the other two)

## Energy eigenstates and eigenvalues

Each solution is associated with a 3 -d $k$-space vector:

$$
\begin{array}{ll}
\psi_{E}(x, y, z)=A \sin \left(k_{x} x\right) \sin \left(k_{y} y\right) \sin \left(k_{z} z\right) & k_{x}=\frac{n_{x} \pi}{a}, k_{y}=\frac{n_{y} \pi}{b}, k_{z}=\frac{n_{z} \pi}{c} \\
E=\frac{\hbar^{2} k^{2}}{2 m} \quad k^{2}=k_{x}^{2}+k_{y}^{2}+k_{z}^{2} & n_{x}, n_{y}, n_{z}= \pm 1, \pm 2, \pm 3, \ldots
\end{array}
$$


(a)
 $\begin{array}{ll}k_{2} & \begin{array}{l}\text { One solution per "cell": } \\ \text { density per unit volume }\end{array}\end{array}$ of $k$-space:

$$
\frac{1}{\frac{\pi}{a} \frac{\pi}{b} \frac{\pi}{c}}=\frac{a b c}{\pi^{3}}
$$

(b)

## Counting the solutions in $E$ intervals

## Only the $1^{\text {st }}$ octant in k-space corresponds to independent solutions

## Each state can be occupied <br> by two electrons with opposite spin (Pauli principle)

$\left(\frac{\text { allowed energy states }}{\text { unit volume in } k \text {-space }}\right)=\frac{1}{8} \times 2 \times \frac{a b c}{\pi^{3}}=\frac{a b c}{4 \pi^{3}}$
$\binom{$ energy states with }{$k<k^{\prime}<k+d k}=\frac{a b c}{4 \pi^{3}} 4 \pi k^{2} d k$

$$
k^{2}=\frac{2 m E}{\hbar^{2}} \quad d k=\frac{\sqrt{2 m}}{\hbar} \frac{1}{2} \frac{d E}{\sqrt{E}}
$$

k-space volume between two spheres

Density of states
$\binom{$ energy states with }{$E<E^{\prime}<E+d E} \equiv \gamma(E) d E=a b c \frac{m \sqrt{2 m E}}{\pi^{2} \hbar^{3}} d E \Rightarrow g(E) \equiv \frac{\gamma(E)}{V}=\frac{m \sqrt{2 m E}}{\pi^{2} \hbar^{3}}$

Crystal volume V = abc

## ... density of states ...

- Density of states, simplified model (box with infinitely deep walls)

$$
g(E)=\frac{m \sqrt{2 m E}}{\pi^{2} \hbar^{3}}
$$

- But: bands? Interaction with the crystal periodic potential? No problem:
- the "average effective mass" m* and the "crystal wave number" $k$ describe the interactions with the crystal
- for $E$ close to $E_{C}$ :

$$
E-E_{C}=\frac{\hbar^{2} k^{2}}{2 m_{n}^{*}} \Rightarrow g_{C}(E)=\frac{m_{n}^{*} \sqrt{2 m_{n}^{*}\left(E-E_{C}\right)}}{\pi^{2} \hbar^{3}} \quad E \geq E_{C}
$$

- Similarly for holes:

$$
g_{V}(E)=\frac{m_{p}^{*} \sqrt{2 m_{p}^{*}\left(E_{V}-E\right)}}{\pi^{2} \hbar^{3}}
$$

$$
E \leq E_{V}
$$

## ... with "average" effective masses

- The effective masses appearing in the density of states for some useful semiconductors (Si, Ge, GaAs) are averaged over crystal directions

Table 4.1 Density of States Effective Masses for $\mathrm{Ge}, \mathrm{Si}$, and GaAs

| Effective Mass |  | Ge | Si | GaAs |
| :--- | :--- | :---: | :---: | :--- |
| $m_{\mathrm{n}}^{*} / m_{0}$ | $\mathrm{~T}=4 \mathrm{~K}$ | 0.553 | 1.062 | 0.067 |
|  | $\mathrm{~T}=300 \mathrm{~K}$ | $\ldots$ | 1.182 | $0.0655^{\dagger}$ |
| $m_{\mathrm{p}}^{*} / m_{0}$ | $\mathrm{~T}=4 \mathrm{~K}$ | 0.357 | 0.590 | 0.532 |
|  | $\mathrm{~T}=300 \mathrm{~K}$ | $\ldots$ | 0.81 | 0.524 |

- only GaAs is approximately isotropic
- See R.F.Pierret, section 4.1.2, p.94, for details on Si and Ge


## Step 2: probability distribution function (Fermi-Dirac)

## F.-D. probability distribution function

- From thermodynamics:
- The most likely "macroscopic" state is the one corresponding to the largest number $W$ of equivalent "microscopic" states, compatible with a given total number $N$ of electrons and a fixed total energy $E_{\text {TOT }}$



## Maximization procedure

- Take the logarithm, use Stirling's approximation, and set the differential to zero ( $S_{i}$ are constant, $N_{i}$ variable):

$$
\begin{aligned}
\ln W & =\sum_{i}\left(\ln S_{i}!-\ln \left(S_{i}-N_{i}\right)!-\ln N_{i}!\right) \\
\ln x & \cong x \ln x-x \quad(x \operatorname{large}) \\
\ln W & \cong \sum_{i}\left[S_{i} \ln S_{i}-S_{i}-\left(S_{i}-N_{i}\right) \ln \left(S_{i}-N_{i}\right)+\left(S_{i}-N_{i}\right)-N_{i} \ln N_{i}+N_{i}\right] \\
& =\sum_{i}\left[S_{i} \ln S_{i}-\left(S_{i}-N_{i}\right) \ln \left(S_{i}-N_{i}\right)-N_{i} \ln N_{i}\right] \\
d(\ln W) & =\sum_{i} \frac{\partial(\ln W)}{\partial N_{i}} d N_{i} \\
& =\sum_{i}\left[\ln \left(S_{i}-N_{i}\right)+1-\ln N_{i}-1\right] d N_{i} \\
& =\sum_{i} \ln \left(S_{i} / N_{i}-1\right) d N_{i}=0
\end{aligned}
$$

## Constraints: Lagrange multipliers

$$
\begin{aligned}
d(\ln W)=0 . & \Rightarrow \sum_{i} \ln \left(S_{i} / N_{i}-1\right) d N_{i}=0 \\
\sum_{i} N_{i}=N . & \Rightarrow \sum_{i} d N_{i}=0 \\
\sum_{i} E_{i} N_{i}=E_{\text {TOT }} . & \Rightarrow \sum_{i} E_{i} d N_{i}=0
\end{aligned}
$$

Introducing the undetermined Lagrange multipliers $-\alpha$ and $-\beta$ :

$$
\begin{gathered}
\sum_{i}\left[\ln \left(S_{i} / N_{i}-1\right)-\alpha-\beta E_{i}\right] d N_{i}=0 \\
\ln \left(S_{i} / N_{i}-1\right)-\alpha-\beta E_{i}=0 \\
S_{i} / N_{i}-1=e^{\alpha+\beta E_{i}} \\
f\left(E_{i}\right)=\frac{1}{1+e^{\alpha+\beta E_{i}}} \rightarrow f(E)=\frac{1}{1+e^{\alpha+\beta E}}
\end{gathered}
$$

For closely spaced levels, $E_{i} \rightarrow E$

## Physical meaning of $\alpha$ and $\beta$

- $\alpha$ and $\beta$ : from thermo-dynamical arguments $\Rightarrow$ for fermions, Fermi distribution:

$$
\begin{aligned}
& \beta=\frac{1}{k_{B} T} \\
& \alpha=-\frac{E_{F}}{k_{B} T} \\
& f(E)=\frac{1}{1+e^{\left(E-E_{F}\right) / k_{B} T}}
\end{aligned}
$$

$$
k_{B}=8.617 \times 10^{-5} \mathrm{eV} / \mathrm{K}
$$

$$
T=\text { absolute temperature }
$$

$E_{F}$ "electrochemical potential" or "Fermi energy"


## Fermions, bosons and classical limit

- Fermions: Fermi-Dirac distribution (at most one fermion per state):

$$
f_{F D}(E)=\frac{1}{e^{\left(E-E_{F}\right) / k_{B} T}+1}
$$

- Bosons: Bose-Einstein distribution (any number of bosons per state)

$$
f_{B E}(E)=\frac{1}{e^{\left(E-E_{B}\right) / k_{B} T}-1}
$$

- Classical: Maxwell-Boltzmann (good limit of quantum statistics when: few particles / high temperature, small filling probability per state)

$$
f_{M B}(E)=\frac{1}{e^{E / k_{B} T}}
$$

## Number of carriers at band edges (Boltzmann approximation)

- From here:
- We have now "understood" all the ingredients used in Lecture_3 to obtain carrier concentrations in intrinsic and extrinsic semiconductors at equilibrium
- allowed and forbidden energy bands
- density of available states
- Fermi probability density function
- In particular, remember that the "Boltzmann approximation" to the Fermi function near band edges for "non-degenerate semiconductors" allowed us to compute concentrations explicitly!
- Go back to Lecture 3 and appreciate the consequences...


## Lecture 19 - summary

- We had a quick look at 3-d wave mechanics, including angular momentum and spin.
- Many-particle systems brought us to consider also identical particles and their wave-functions, that must have a definite exchange (anti)-symmetry.
- Electrons are fermions and are described by anti-symmetric (overall, including spin) wave functions, with interesting consequences ("exchange forces", "degeneracy pressure", "Fermi energy").
- Back to semiconductors, we considered equilibrium statistics and obtained both the density of states and the Fermi-Dirac probability distribution functions, essential ingredients to predict equilibrium carrier concentrations.
- Next step: re-consider non-equilibrium transport of charge carriers (drift, diffusion; generation/recombination) and its explanation.


## Lecture 19 - exercises

- Exercise 19.1: Consider a simplified model of a conductor with non-interacting conduction electrons in a 3 -d infinite well. Find the Fermi energy and the average inter-electron spacing. Apply the results to the case of aluminum ( $A=27$ ), assuming: density $\rho=2.7 \times 10^{3} \mathrm{~kg} / \mathrm{m}^{3}$, and three free atoms per electron (hint: see Bernstein, par.10-5 and example 10-5).
- Exercise 19.2: Write down the results of this lecture on the density of states for the conduction and valence bands and on the Fermi probability density function. Compare them with those used in previous lectures to compute the concentration of carriers in semiconductors at a given temperature. OK? Explain the reason for introducing the effective mass in the density of states as obtained from the "infinite well" box model.

