Charge Carriers in Semiconductors

Electron in a band state moves at the group velocity.

In 1D, \( v_g = \frac{1}{\hbar} \frac{dE}{dk} \)

A full band does not conduct.

Due to symmetry, the net velocity of all states of a band is zero.

These concepts extended to 3D:

\[
v_g = \frac{1}{\hbar} \nabla_k E = \frac{1}{\hbar} \left( \hat{x} \frac{\partial E}{\partial k_x} + \hat{y} \frac{\partial E}{\partial k_y} + \hat{z} \frac{\partial E}{\partial k_z} \right)
\]

The 1\textsuperscript{st} BZ is always symmetric, therefore net velocity of all states of a band is zero.
Counting electrons

Examples:
Si (group IV element, diamond structure) & GaAs (octet compound, zincblende structure)

For a crystal of $N$ primitive unit cells,
there are $N$ band states each band, i.e., $N$ distinct $k$ in the 1st BZ.
The $N$ states in each band accommodate $2N$ electrons.

There are 4 bands originating from valence electron orbitals, together accommodating $4N \times 2 = 8N$ electrons.

For diamond & zincblende structures, each primitive unit cell contains 2 atoms.
Each primitive unit cell contributes $4 \times 2 = 8$ valence electrons.

$N$ primitive unit cells have $8N$ valence electrons.

Therefore the bands of valence electrons are full.
Near a band minimum, the $E$-$k$ dispersion can be written as (Taylor expansion):

$$E(k) = E(k_0) + \frac{1}{2} \frac{\partial^2 E}{\partial k^2} (k - k_0)^2$$

(good approx. near a minimum)

If we consider $E(k_0)$ as a potential energy $V$, and $\hbar (k - k_0)$ as a momentum $p$, then this becomes formally the same as a classical particle:

$$E = \frac{p^2}{2m} + V$$

The “effective mass” of the electron, $m_e^*$, can be found by:

$$\frac{1}{m_e^*} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2} \bigg|_{k=k_0}$$

We use a 1D heuristic for simple math. In 3D, the second derivative is a tensor (the effective mass is anisotropic), and $k_0 \leftarrow k_0$ may or may not be zero.
In this semiclassical model, \( \frac{\hbar}{d} \frac{dk}{dt} = \frac{\hbar}{d} (k - k_0) = F \)

The electron is pushed by the force to move in \( \mathbf{k} \)-space. At each \( \mathbf{k} \), the electron’s velocity is the group velocity:

\[
\mathbf{v}_g = \frac{1}{\hbar} \frac{dE}{dk} = \frac{1}{\hbar} \frac{dE}{d(k - k_0)}
\]

\[
\mathbf{v}_g = \frac{1}{\hbar} \mathbf{V}_k E = \frac{1}{\hbar} \left( \hat{x} \frac{\partial E}{\partial k_x} + \hat{y} \frac{\partial E}{\partial k_y} + \hat{z} \frac{\partial E}{\partial k_z} \right)
\]

Notice that \( \mathbf{v}_g = 0 \) at a minimum \( \mathbf{k} = \mathbf{k}_0 \).

**Question**: Describe the motion of a single electron added to a perfect, static \( (T = 0) \) semiconductor crystal in a constant electric field.

The **effective mass** of the electron, \( m_e^* \), is defined for the band minimum at \( \mathbf{k}_0 \):

\[
\frac{1}{m_e^*} = \left. \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2} \right|_{k=k_0}
\]

Near the band minimum, the \( E-k \) dispersion is well approximated by:

\[
E = \frac{\hbar^2}{2m_e^*} (k-k_0)^2 + E_c \quad \Leftrightarrow \quad E = \frac{p^2}{2m} + V
\]

\[
p = m_e^* v_g = \hbar (k - k_0)
\]

\( \mathbf{p} = \hbar (\mathbf{k} - \mathbf{k}_0) \) in 3D
We have learned:

A full band does not conduct.

The valence bands are full and conduction bands empty for perfect, pure semiconductors at $T = 0$. No conduction.

To conduct, need charge carriers, e.g., electrons near the conduction band minimum.

The semiclassical model works well in most circumstances, because mobile electrons are near the conduction band minimum/bottom (CBM):

- in equilibrium, these mobile electrons only occupy states near CBM with non-vanishing probabilities;
- when driven by a field, these electron can not go far from equilibrium, since each is “thermalized” by collision every time interval $\tau$.

We will later discuss how these carriers distribute in the conduction band states.
The concept of the hole

Consider the topmost filled band (valence band), \[ \sum_k v(k) = 0 \]

Here \( v \) is short for \( v_g \), the velocity of each electron

(A full band of electrons do not conduct.)

Somehow one electron at \( k_e \) is removed.

\[ v_e(k_e) + \sum_{k \neq k_e} v(k) = 0 \]

\[ \Rightarrow v_e(k_e) = - \sum_{k \neq k_e} v(k) \]

The motion of all the electrons in this band can be described as the motion of this vacancy.

The effective mass of the empty state is

\[ \frac{1}{m^*} = \frac{1}{\hbar^2} \left. \frac{\partial^2 E}{\partial k^2} \right|_{k=k_0} \]

Wavevector of VBM
The effective mass of the empty state is
\[
\frac{1}{m_e^*} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2} \bigg|_{k=k_0}
\]
not the empty state

We define the hole energy \( E_h = -E \), then the hole effective mass is
\[
\frac{1}{m_h^*} = - \frac{1}{m_e^*} = - \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2} \bigg|_{k=k_0} = \frac{1}{\hbar^2} \frac{\partial^2 E_h}{\partial k^2} \bigg|_{k=k_0}
\]
So, it is positive.

In equilibrium, the hole is most likely to be at \( k = k_0 \).

A positive electric field \( \varepsilon \) will drive the entire band of electrons towards the negative, thus the empty state moves to \( k_e = k_0 + \Delta k \), where \( \Delta k = -q\varepsilon \tau / \hbar \). The corresponding momentum \( \hbar(k_e - k_0) \) and group velocity \( v_e \) are negative.

Convenient to define the hole charge to be \( +q \), thus moved towards the positive by the positive \( \varepsilon \). Therefore, \( k_h = k_0 - \Delta k \), so that momentum \( \hbar(k_h - k_0) \) and group velocity \( v_h \) are positive.


The hole carries charge \( +q \), and has a positive effective mass near VBM.
Carriers in semiconductors

Fermi-Dirac distribution of electrons: consequence of Pauli’s exclusion rule

Analogy: sand particles in a vessel

Fermi-Dirac distribution at $T = 0$: 
$f(E)$ is the probability of a state at energy $E$ being occupied.

$E_F$ depends on total amount of sand particles and available volume of the vessel per height (non-cylindrical vessel), or total number of electrons and number of available states per energy interval (per volume)

(Recall our calculation of in the Drude-Sommerfeld model)

For semiconductors, with a gap, $E_F$ is somewhat arbitrary.
The Fermi level $E_F(T)$ is a function of $T$.

Fermi level vs. chemical potential: difference in terminology in different fields. (See next slide)

Since $E_F$ depends on number of available states per energy interval (per volume), the way $E_F(T)$ varies with $T$ depends on it.

What is this called?
Digression:
Subtle difference in jargons used by EEs and physicists

We use the EE terminology, of course.

Fermi level \( E_F = E_F(T) \)

Same concept when \( T > 0 \)

Physicists:
Chemical potential \( \mu(T) \)
Fermi energy \( E_F = \mu(0) \)

We already used \( \mu \) for mobility.
Density of states (DOS) determines how $E_F(T)$ varies with $T$.

In this illustration, you may consider the electrons spinless or each small box a spin-Bloch state.

(a) 20 electrons at $T = 0$.

(b) $T > 0$, some electrons promoted to higher energies. If $E_F$ remained ~ the same, we would need 21 electrons.

(c) To keep the # of electrons unchanged, $E_F$ has to move down. The lower band is still full at low $T$.

(d) At higher $T$, $E_F$ moves further down and the distribution flattens more, so that some states in lower band vacate.

How to find density of states $D(E)$

1D case:
Each $k$ occupies $2\pi/L$ in $k$-space.

The take-home message is
$D(E) \propto [E - E(k_0)]^{-1/2}$

Here, $D(E) \propto L$ is the number of states per energy interval in the entire length $L$ of the 1D semiconductor.

In the interval $dk$, there are states.

Translate this $D(k)dk$ to $D(E)dE$ near a band extremum at $k_0$:

$E(k) = E(k_0) + \frac{\hbar^2(k - k_0)^2}{2m^*} \Rightarrow dE = \frac{\hbar^2}{2m^*} 2(k - k_0)dk$

And, $k - k_0 = \sqrt{2m^*[E - E(k_0)]}/\hbar$

$D(E) dE = \frac{L}{2\pi \hbar^2} \frac{m^*}{(k - k_0)} dE$

$= \frac{L}{2\pi \hbar} \sqrt{\frac{m^*}{2[E - E(k_0)]}} dE$
3D case:
Recall from Slide 9 of Lecture Note 4:

\[ k_x = \frac{2\pi}{L} n_x \quad k_y = \frac{2\pi}{L} n_y \quad k_z = \frac{2\pi}{L} n_z \]

Each state \(|k\) occupies a volume \((2\pi)^3 / V\) in the wavevector space.

We consider a simple case where \(E(k)\) is isotropic: \(E(k) = E(k_0) + \frac{\hbar^2 (k - k_0)^2}{2m^*}\)

The volume of a spherical shell with a thickness \(dq\) and radius \(q\) in \(k\)-space is \(4\pi q^2 dq\).

Here we just use \(q\) to represent \(|k - k_0|\) for the moment. We will continue to use it for the electron charge later.

\[
D(q)dq = \frac{4\pi q^2 dq}{(2\pi)^3 / V} = \frac{V}{2\pi^2} q^2 dq
\]

\[
\Rightarrow D(E)dE = \frac{V}{2\pi^2} \frac{m^*}{\hbar^2} q dE
\]

\[
q = \frac{\sqrt{2m^* (E - E(k_0))}}{\hbar}
\]

\[
\Rightarrow D(E)dE = \frac{V}{2\pi^2} \frac{\sqrt{2}(m^*)^{3/2}}{\hbar^3} \sqrt{E - E(k_0)}dE
\]
The take-home message is
\[ D(E) \propto [E - E(k_0)]^{1/2} \]

For the conduction band, \[ D(E) \propto (E - E_c)^{1/2} \]

For the valence band, \[ D(E) \propto (E_V - E)^{1/2} \]

Here, we take \( m^* \) as one parameter. Real world semiconductors are more complicated.
Homework 5: Problem 1

Assume isotropic quadratic dispersion: \( E(\mathbf{k}) = E(\mathbf{k}_0) + \frac{\hbar^2 (\mathbf{k} - \mathbf{k}_0)^2}{2m^*} \)

Find the density of states for a 2D semiconductor of area \( A \) (macroscopic).
Carrier distribution

\[ D(E) dE = \frac{V \sqrt{2} (m^*)^{3/2}}{2\pi^2 \hbar^3} \sqrt{E - E(k_0)} dE \]

For the conduction band, consider:

- Unit volume
- Spin (2 electrons each state)
- \( M_C \) equivalent minima (valleys), e.g., \( M_C = 6 \) for Si.
- Anisotropic \( E(k) \): some sort of averaged effective mass \( m_e \) in place of \( m^* \).

Anisotropic equienergy surfaces in \( k \)-space
For the conduction band, consider:

- Unit volume
- Spin (2 electrons each state)
- \( M_C \) equivalent minima (valleys), e.g., \( M_C = 6 \) for Si.
- Anisotropic \( E(k) \): some sort of averaged effective mass \( m_e \) in place of \( m^* \).

\[
\int_{E_C}^{E} \left[ M_C \frac{1}{\pi^2} \frac{\sqrt{2}(m_e)^{3/2}}{\hbar^3} \sqrt{E - E_C} \right] f(E) dE
\]

This integral (called a Fermi integral) cannot be solved analytically.

When \( E - E_F > 4k_B T \sim 0.1 \text{ eV} \), \( e^4 \approx 55 \gg 1 \) thus \( f(E) \) reduces to Boltzmann distribution.

The high-energy tail of the Fermi distribution, i.e. for \( E - E_F \gg kT \), can be approximated by the Boltzmann distribution:

\[
f_e(E) \approx \exp \left( -\frac{E - E_F}{kT} \right).
\]

Grundmann, *The Physics of Semiconductors*, p. 862
Digression: Physical justification of Boltzmann approximation to F-D distribution

F-D distribution is the consequence of Pauli’s exclusion rule. Since there are very few electrons at \( E - E_F > 4k_B T \), Pauli’s exclusion rule does not matter – electrons won’t run into each other anyway, just like molecules in an ideal gas.

\[
n = \int_{E_C}^{\infty} \left[ M_C \frac{1}{\pi^2} \frac{\sqrt{2}(m_e)^{3/2}}{\hbar^3} \sqrt{E - E_C} \right] f(E) dE
\]

With this approximation, the integral can be taken analytically, yielding

\[
n = N_C e^{-\frac{E_C - E_F}{k_B T}}
\]

as if all conduction band electrons are at \( E_C \), where there are \( N_C \) states per unit volume.

Notice the \( T \) dependence here!

\[
N_C = 2 \left( \frac{m_e kT}{2\pi \hbar^2} \right)^{3/2} M_C
\]
For the valence band, consider:

- Unit volume
- Spin (2 electrons each state)
- With spin-orbital coupling considered, for diamond and zincblende structures, usually two bands (heavy holes and light holes) are degenerate at $\Gamma$. Holes populate the top of these two bands.

**Question:** Which one is the heavy/light hole band?
\[
D(E)dE = \frac{V}{2\pi^2} \frac{\sqrt{2}(m^*)^{3/2}}{\hbar^3} \sqrt{E - E(k_0)}dE
\]

For the valence band, consider:

- Unit volume
- Spin (2 electrons each state)
- With spin-orbital coupling considered, for diamond and zincblende structures, usually two bands (heavy holes and light holes) are degenerate at \( \Gamma \). Holes populate the top of these two bands.
  
  Some sort of “total” effective mass \( m_h \) considering both light and heavy holes in place of \( m^* \).

\[
p = \int_{E_C}^{\infty} \left[ \frac{1}{\pi^2} \frac{\sqrt{2}(m_h)^{3/2}}{\hbar^3} \sqrt{E_V - E} \right] [1 - f(E)]dE
\]

Again, Boltzmann approximation yields analytical form:

\[
N_V = 2 \left( \frac{m_h kT}{2\pi \hbar^2} \right)^{3/2}
\]

\[
n\ p = N_V N_C \exp \left( -\frac{E_C - E_V}{kT} \right) = N_V N_C \exp \left( -\frac{E_g}{kT} \right)
\]

Grundmann, *The Physics of Semiconductors*, p. 184
How good the approximation is

Fig. 7.2 (a) $np$ for silicon at $T = 300$ K as a function of the position of the Fermi level. The valence-band edge $E_V$ is chosen as $E = 0$. $np$ is constant for the range of Fermi energies given by (7.13) $(4kT \approx 0.1$ eV). (b) $n$, $p$ and $\sqrt{np}$ as a function of the Fermi level

Grundmann, *The Physics of Semiconductors*, p. 207
Intrinsic carriers

Charge neutrality: \( n_i = p_i \). Therefore \( n_i = p_i = \sqrt{N_V N_C} \exp \left( \frac{-E_g}{2kT} \right) \)

\[
n p = n_i p_i = n_i^2 = p_i^2
\]

For Si \( (E_g = 1.12\text{eV}) \) at \( T = 300 \text{K} \),
\( kT = 25.9 \text{meV} \), \( E_g/kT = 43.2 \),
\( e^{21.6} = 2.45 \times 10^9 \).

Many text books list
\( N_C = 2.8 \times 10^{19}/\text{cm}^3 \), \( N_V = 1.04 \times 10^{19}/\text{cm}^3 \),
and \( n_i = 1.45 \times 10^{10}/\text{cm}^3 \), as if this \( n_i \) value
was calculated with the above equation.
Do your own calculation and see what you get.

Then, check out this document on the web:
https://ecee.colorado.edu/~bart/book/ex019.htm
Look for \( N_C, N_V, \) and \( n_i \) at 300 K. Find out how
consistent the \( n_i \) is with \( N_C \) and \( N_V \).
Examine how consistent the \( n_i \) value is with the \( N_C \) and \( N_V \) values here.

Read the online discussions here:
https://www.researchgate.net/post/Proper_calculation_of_intrinsic_carrier_concentration_in_silicon_at_300_K_with_erroneous_illustration_in_certain_frequently_followed_textbooks

What do you think? What’s the impact of any inaccuracy?
Do a literature search and try to find out why there has been this issue.
If you use or have access to simulators, try to find out what values are used.
For the intrinsic semiconductor,
\[ np = n_i \, p_i = n_i^2 = p_i^2 \]

\[ E_F = E_i = \frac{E_V + E_C}{2} + \frac{kT}{2} \ln \left( \frac{N_V}{N_C} \right) \]

This is the intrinsic Fermi level.

Insert the various \( N_C \) and \( N_V \) values you found. Think about the difference in results in the context of the questions in the last slide.
The temperature dependence is not simply exponential.

Recall the temperature dependence in $N_C$ and $N_V$.

\[ N_C = 2 \left( \frac{m_e kT}{2 \pi \hbar^2} \right)^{3/2} M_C \]

Some people use an $m_e$ value to account for $M_C$.

\[ N_V = 2 \left( \frac{m_h kT}{2 \pi \hbar^2} \right)^{3/2} \]

There is also temperature dependence in $E_g$.

This $n_i$ vs. $T$ chart is from a relatively recent paper (which may help you on the questions in the previous two slides).

Grundmann, *The Physics of Semiconductors*, p. 208
Doping

Carriers can be introduced by shallow defects.

Shallow donors: group V dopants in group IV semiconductor, e.g., P in Si.

The P substitution of a Si atom perturbs the Si lattice. The extra e wanders in the long-range Coulomb potential of the $P^+$ ion. This long-range potential determines the energy levels of the bound e. The H atom model approximates this situation.

Binding energy of shallow donor:

$$E_D^b = \frac{m_e^*}{m_0} \frac{1}{\varepsilon_r} \frac{m_0 e^4}{2 (4\pi\varepsilon_0 \hbar)^2}$$

- $m_e^*$: electron effective mass in semiconductor
- $m_0$: Free electron mass
- $e$: electron charge
- $\varepsilon_r$: dielectric constant of semiconductor
- $\hbar$: Planck's constant divided by $2\pi$

Bohr radius of shallow donor:

$$a_D = \frac{m_0}{m_e^* \varepsilon_r a_B}$$

- $a_B$: Bohr radius of H atom, 0.053 nm

Vacuum, $E = 0$

- 13.6 eV
- $E_1 = -13.6$ eV

H atom

- $E_C$
- $E_D$
- $E_D^b$

For Si, $m_e^*/m_0 \sim 0.3$, $\varepsilon_r = 11.9$.

- $E_D^b \sim 29$ meV
- $a_D \sim 2.1$ nm. Compare this to Si lattice parameter – shallow donor!
In contrast, deep defect potentials are short ranged,
⇒ the bound electron wave functions are highly localized.
⇒ The deep defects trap carriers
(The energy levels are often “deep” (close to midgap), but not always)

Impurity levels in Si

(Li is interstitial) Grundmann, *The Physics of Semiconductors*, p. 212

Binding energies of P, As, Sb agree reasonably well with the H model (29 meV).
The bound electron is not a mobile carrier. It is attracted to the P⁺.

The P⁺ with a bound e makes P⁰ – the neutral or un-ionized donor.

(Not union-ized)

The Bohr model approximates P⁰.

The bound e may gain enough energy ($\geq E_D^b$) to escape, and become a mobile e in CB.

The P⁺ left behind is an ionized (charged) donor.
Shallow acceptors: group III dopants in group IV semiconductor, e.g., B in Si.

Consider the valence band full, i.e., each of 4 bonds of B made of a *valence* electron pair.
(Full band does not conduct.)

- The valence band is filled with a borrowed valence electron.
  “Borrowed” from the entire system, which has a deficit of 1 valence electron.
- This deficit is accounted for by the **bound** hole.

The bound hole is **not** a mobile carrier. It is attracted to the $B^-$.  

- The $B^-$ with a bound hole makes $B^0$ – the **neutral** or **un-ionized** acceptor.
  (not union-ized)

The Bohr model provides a simple approximation, although not so well as for shallow donors, due to degeneracy of VBM (light, heavy holes).

- The bound hole may gain enough energy ($\geq E^b_A$) to escape, and become a **mobile hole** in VB.
- The $B^-$ left behind is an **ionized (charged)** acceptor.
n-type doping by shallow donors

\[ N_D : \text{donor concentration} \]
\[ N_{D^+} : \text{ionized donor concentration} \]
\[ N_{D^0} : \text{neutral donor concentration} \]

It is tempting to think that

\[ \frac{N_{D^+}}{N_{D^0}} = e^{-\frac{E_D^b}{kT}} \]

At RT, \( \frac{E_D^b}{kT} \sim 1.5 \) to 2 \( \Rightarrow \frac{N_{D^+}}{N_{D^0}} \sim 0.2 \)

But, we have always assumed that essentially all donors are ionized, \( n = N_{D^+} = N_D \)

**Why?**
The F-D distribution

\[ f(E) = \frac{1}{e^{\frac{E-E_F}{kT}} + 1} \]

The probability a donor state is neutral (D\(^0\)):

\[ f(E_D) = \frac{1}{E_D-E_F} \frac{e^{\frac{E_D-E_F}{kT}}}{e^{\frac{E_D-E_F}{kT}} + 1} \]

The probability a donor state is ionized (D\(^+\)):

\[ 1 - f(E_D) = \frac{E_D-E_F}{e^{\frac{E_D-E_F}{kT}} + 1} \]

Therefore,

\[ \frac{N_D^0}{N_D^+} = e^{-\left(\frac{E_D-E_F}{kT}\right)} = e^{\frac{E_F-E_D}{kT}} \]

(This is incorrect, but does not affect the big picture. Will correct soon)

Now we may say, \(\frac{E_F-E_D}{kT} \ll -1\), therefore \(\frac{N_D^0}{N_D^+} \sim 0\). But, saying so is self-fulfilling (and \(\frac{E_F-E_D}{kT} \gg -1\) is not necessarily true).
Charge neutrality:
\[ n = N_c e \]

\[
\frac{N_D^0}{N_D^+} = e^{-\left(\frac{E_V - E_F}{kT}\right)} = e^{\frac{E_F - E_D}{kT}} \Rightarrow
\]

\[
N_D^+ = \frac{N_D}{1 + e^{\frac{E_F - E_D}{kT}}} \quad \text{(to be corrected)}
\]

Charge neutrality:
\[ n = N_D^+ + p \]

\[ N_C \gg N_D \Rightarrow \]

Nearly all donors must ionize to satisfy

This holds up to \( N_D \sim 10^{18} \text{ cm}^{-3} \).

\( N_C \) is the effective DOS of CB. There are a lot more CB states near \( E_C \) than donor states at \( E_D \).
We did not consider the following:

- Each donor level is 2-fold degenerate when neutral, i.e., neutral donor DOS is $2N_D$.
- But, each donor atom can only have 1 bound electron. (There cannot be $D^-$.)
- Each donor level is nondegenerate when ionized, i.e., ionized donor DOS is $N_{D^+}$.

Consider the above and do the math (permutation and probability), then one can get

$$N_{D^+} = \frac{N_D}{1 + 2e^{-\frac{E_F-E_D}{kT}}}$$

The detailed math can be found in:


This is an old but really great book written by an electrical engineer AND physicist, providing unique, refreshing perspectives on many things.
Charge neutrality:

\[ n = N_c e \]

\[ \frac{N_D^0}{N_D^+} = e^{-\left(\frac{E_D - E_F}{kT}\right)} = e^{\frac{E_F - E_D}{kT}} \]

\[ N_D^+ = \frac{N_D}{1 + 2e^{\frac{E_F - E_D}{kT}}} \]

A factor of 2 does not make much difference.

Charge neutrality:

\[ n = N_D^+ + p \]

\[ N_C \gg N_D \implies \]

Nearly all donors must ionize to satisfy

This holds up to \( N_D \sim 10^{18} \) cm\(^{-3}\).

\( N_C \) is the effective DOS of CB. There are a lot more CB states near \( E_C \) than donor states at \( E_D \).

S. M. Sze (施敏), Physics of Semiconductor Devices.
Charge neutrality:

\[ \frac{N_D^0}{N_{D^+}} = e^{-\frac{(E_D-E_F)}{kT}} = e^{\frac{E_F-E_D}{kT}} \]

\[ N_{D^+} = \frac{N_D}{1 + 2e^{\frac{E_F-E_D}{kT}}} \]

A factor of 2 does not make much difference.

Charge neutrality:

\[ n = N_{D^+} + p \]

\[ N_C \gg N_D \quad \Rightarrow \]

Nearly all donors must ionize to satisfy

\[ n = N_C e \]

This holds up to \( N_D \sim 10^{18} \text{ cm}^{-3} \).

\( N_C \) is the effective DOS of CB.

There are a lot more CB states near \( E_C \) than donor states at \( E_D \).

S. M. Sze (施敏), Physics of Semiconductor Devices.
Decrease $T \Rightarrow E_C > E_F > E_D$, similar to the intrinsic concentration:

$$n \approx \sqrt{\frac{N_D N_C}{\hat{g}_D}} \exp\left(-\frac{E_D^b}{2kT}\right)$$

The factor of 2 as in $N_{D^+} = \frac{N_D}{1 + 2e^{-\frac{E_F - E_D}{kT}}}$ for RT.

Grundmann, *The Physics of Semiconductors*, p. 216

S. M. Sze (施敏), *Physics of Semiconductor Devices*. What is this shallow slope?
p-type doping by shallow acceptors

\(N_A\) : acceptor concentration
\(N_{A^-}\) : ionized acceptor concentration
\(N_{A^0}\) : neutral acceptor concentration

At RT, essentially all acceptors are ionized, \(p = N_{A^-} = N_A\)

Grundmann, *The Physics of Semiconductors*, p. 209

p-type doping similar; flipped

Grundmann, *The Physics of Semiconductors*, p. 219
Charge transport

In the semiclassical model, \( \frac{\hbar}{\text{d}t} \frac{dk}{dt} = \hbar \frac{d}{dt}(k - k_0) = F \)

The electron is pushed by the force to move in \( k \)-space. At each \( k \), the electron’s velocity is the group velocity:

\[
v_g = \frac{1}{\hbar} \frac{dE}{dk} = \frac{1}{\hbar} \frac{dE}{d(k - k_0)}
\]

\[
v_g = \frac{1}{\hbar} \nabla_k E = \frac{1}{\hbar} \left( \hat{x} \frac{\partial E}{\partial k_x} + \hat{y} \frac{\partial E}{\partial k_y} + \hat{z} \frac{\partial E}{\partial k_z} \right)
\]

**Question:** Describe the motion of a single electron added to a perfect, static \((T = 0)\) semiconductor crystal in a constant electric field.

The static, perfect lattice does not scatter.

The expected oscillation (called Bloch oscillation) is prevented by scattering, therefore has not been observed.

Collisions thermalize carriers, which thus remain near band extrema.
Low-field transport

Collisions thermalize carriers, which thus remain near band extrema.

\[
\frac{\hbar}{i} \frac{dk}{dt} = \hbar \frac{d}{dt} (k - k_0) = F = -q\mathcal{E}
\]

Near a band extremum, the effective mass \(m^*\) can be defined.

For each carrier, \(m^* v = \hbar (k - k_0)\). \(\Rightarrow\) \(m^* \frac{dv}{dt} = F = -q\mathcal{E}\)

Here, \(v = v_g\), the group velocity.

In 3D, \(m^* v = \hbar (k - k_0)\). \(\Rightarrow\) \(m^* \frac{dv}{dt} = F = -q\mathcal{E}\)

Here, \(v = v_g\), the group velocity.

**Note:** In 3D, \((m^*)^{-1}\) is a tensor due to anisotropy. For simplicity, a single value \(m^*\), somehow averaged over all directions, is used here.

Recall that \((m^*)^{-1}\) as the curvature of the \(E(k)\) surface, is a factor in the DOS.

There, an averaged single value \(m^*\) is also used.

Different ways for averaging are used for the two purposes.

The \(m^*\) used for calculating DOS is called the density-of-states effective mass.

The \(m^*\) used for "Newton’s 2nd law" here is called the conductivity effective mass.

**Question:** An \(m^*\) is used in the H atom model for shallow impurities. Which \(m^*\) should be used there?
Difference between metals and semiconductors in charge transport

Metals:
- $E_F$ in partially occupied band.
- $f(E)$ at RT deviates little from that at $T = 0$ due to large DOS in the band.

Non-degenerate semiconductors:
- $E_F$ in gap.
- $f(E)$ at RT very different from that at $T = 0$.
- Very few electrons (compared to available states), thus Boltzmann distribution a good approximation to $f(E)$.
- Mathematically, the tail to $f(E)$ resembles Boltzmann distribution.
Metals

In equilibrium, all electrons are inside the Fermi surface at $T = 0$. (A few excited out of it at $T > 0$.)

If the Fermi surface is a sphere, what is the radius?

Electrons on the Fermi surface move at $v_F$.

In electric field $\mathcal{E}$, each electron is shifted by $\Delta k$.

Assuming energy-independent $\tau$, $\hbar \Delta k = q \mathcal{E} \tau$.

Only a small portion of the electrons contribute to the net momentum, which is averaged by the total electron density $n$.

In some metals, the nearly-free-electron model works well thus an $m^*$ (same as at the band bottom) can be defined for the electrons near $E_F$. Thus,

$$m^* v_d = \hbar \Delta k$$

**Question:** When $\mathcal{E}$ is very small, what is the average speed of those electrons contributing to the net momentum?
In some metals, the nearly-free-electron model works well thus an \(m^*\) (same as at the band bottom) can be defined for the electrons near \(E_F\). Thus,
\[
m^*v_d = \hbar \Delta k
\]
In these metals, \(m^* \sim m_0\), the free electron mass.

Therefore, the Drude model works well:
\[
\frac{1}{\rho} = \sigma = \frac{q^2 n \tau}{m}
\]
With correction that the mean-free path is \(v_F \tau\) (Drude-Sommerfeld model), it is a sufficient model for many metals.
Semiconductors

A carrier behaves as a classical particle of mass $m^*$. Carriers follow Boltzmann distribution. Therefore, classical statistical mechanics works.

The semiclassical model of semiconductors is similar to the Drude model:

$$m^* \frac{dv}{dt} = F = -q\mathcal{E}$$

In equilibrium or under low field, the average speed of carriers is the thermal velocity:

$$\frac{1}{2}m^* v_{th}^2 = \frac{3}{2}k_B T$$

At RT, $v_{th} \sim 10^7$ cm/s.

If $\tau \sim 10^{-14}$ s, similar to those of metals, the mean free path $v_{th} \tau \sim 10^{-7}$ cm = $10^0$ nm.

Compare with metals: $v_F \sim 10^8$ cm/s, thus mean free path $v_F \tau \sim 10^{-6}$ cm $\sim 10^1$ nm.

**Question**: Given similar $\tau$, is a long mean free path good or bad for metals used as interconnects in modern ICs? (Hint: conductivity $\propto \tau$.)
Electrons near Fermi surface move at speed $v_F$ in all directions. They travel longer between collisions if $v_F$ is larger.

Interconnects need to be thin and narrow. Collisions with surfaces lowers $\tau$ from the bulk value.

Grundmann, *The Physics of Semiconductors*, p. 824

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**Fig. 24.32** Resistivity of copper at room temperature for various film thickness (solid circles), and for a 100 nm-film as a function of line width $w$ (empty circles). *Solid lines* are theoretical dependence according to (24.80). The *dashed lines* indicate the limits for bulk material ($t \to \infty$) and for large line thickness ($d = 100 \text{ nm}$, $w \to \infty$).
Low-field transport in semiconductor

Collisions thermalize carriers, which thus remain near band extrema.

\[\hbar \frac{dk}{dt} = \hbar \frac{d}{dt} (k - k_0) = F = -q\varepsilon\]

Near a band extremum, the effective mass \(m^*\) can be defined.

For each carrier, \(m^*v = \hbar(k - k_0). \implies m^* \frac{dv}{dt} = F = -q\varepsilon\)

Here, \(v = v_g\), the group velocity.

In 3D, \(m^*v = \hbar(k - k_0). \implies m^* \frac{dv}{dt} = F = -q\varepsilon\)

Here, \(v = v_g\), the group velocity.

Define mobility \(\mu = \frac{q\tau}{m^*}\) \implies \(v_d = -q\mu\varepsilon\)

\[J = -nqv_d = \frac{q^2n\tau}{m^*}\varepsilon \implies \frac{1}{\rho} = \sigma = \frac{q^2n\tau}{m^*} = qn\mu\]

Consider both electrons and holes: \(\sigma = qn\mu_e + qp\mu_h\)
Scattering processes/mechanisms

Carrier may collide with, or be scattered by, multiple scatters.

Each scattering has its own signature dependence on temperature and carrier density.

\[ \mu = \frac{q\tau}{m^*} \]

The more frequently carriers are scattered, the lower the mobility.

Different scattering processes have different contributions to the total scattering rate:

\[ \frac{1}{\tau} = \sum_i \frac{1}{\tau_i} \]  \text{The scattering rate or frequency due to the } i\text{th process/mechanism}

We can then assign \[ \mu_i = \frac{q\tau_i}{m^*} \]

Thus,

\[ \frac{1}{\mu} = \sum_i \frac{1}{\mu_i} \]

By measuring the dependence of \( \mu \) on \( T, n \) or \( p \), and parameters related to the scattering processes, we can find which processes are the dominating ones.