Carriers in semiconductors – the semiclassical model

We care about the kinematics of electrons in semiconductors –
how electrons move (transport) driven by the electric field

For a classical particle (obeying Newton's laws), the total energy is the sum of kinetic and potential energies.

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

The potential energy is a function of position.

Side note

For some obvious reason, we love the energy unit eV.

Power $= I \, V$

$1 \, W = 1 \, A \cdot V$

Energy $= Q \, V$

$1 \, J = 1 \, C \cdot V$

SI units

How to convert eV to J ?

$1 \, eV = 1.6 \times 10^{-19} \, C \cdot V$

$= 1.6 \times 10^{-19} \, J$

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In a semiconductor, the term "(free) electron" often refers to an electron that somehow ends up in the conduction band. (We have heuristic explanations why valence electrons do not conduct. But do we really know why?)

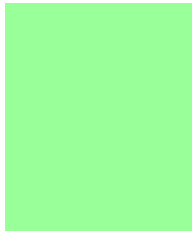Semiclassical e:

$$E = \frac{\hbar^2 k^2}{2m_e^*} + E_c$$

kinetic energy
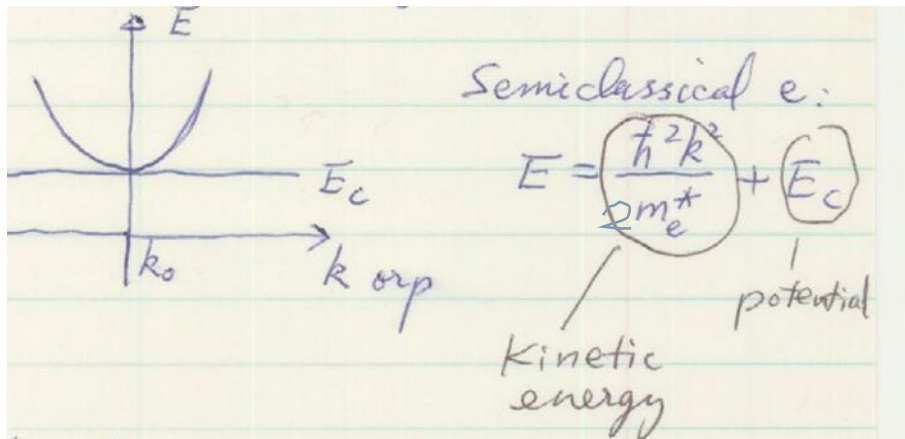
potential

Energy vs. momentum at one location

The "electron" behaves as if it were a classical particle with an effective mass m_e^* in a crystal, riding on a potential E_C, which is a function of location. Its (crystal) momentum is $\hbar k$, where k is the wavevector.

What does this model really mean? How's it justified?

Three types of "band diagrams"

E_C
E_F
E_V

Just levels at one location

Energy vs. momentum at one location

Potential profile like a topography map

What do we **really mean** by potential?

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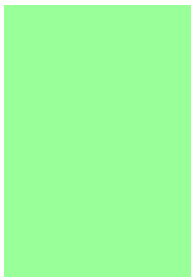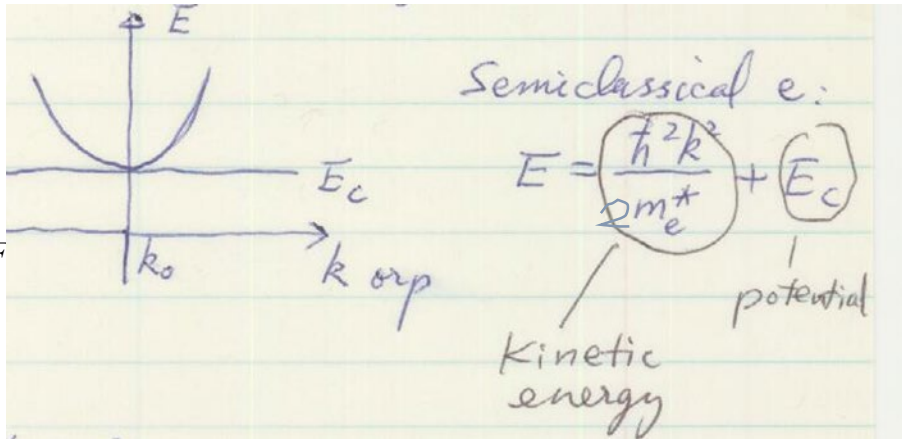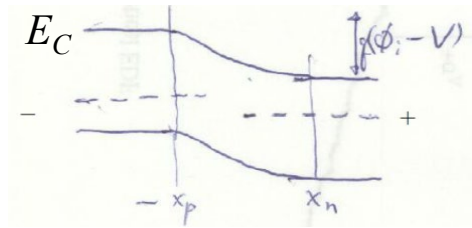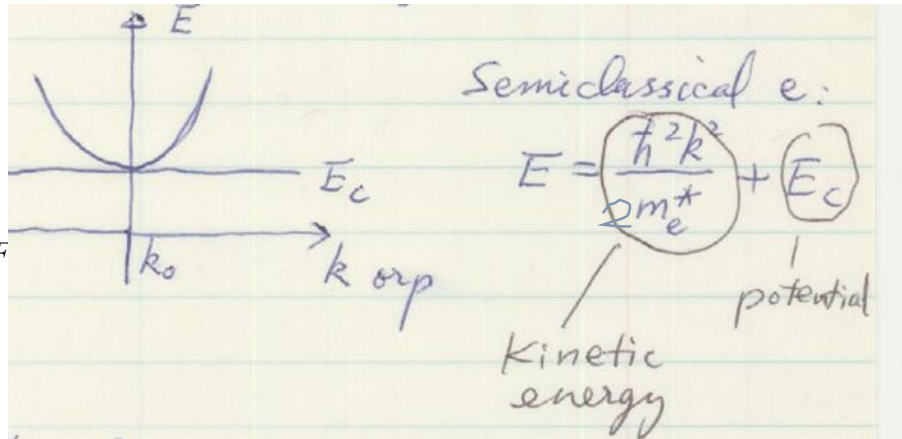
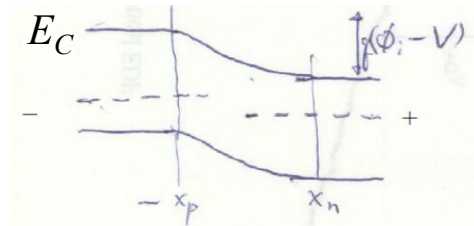What does this model really mean? How's it justified?

The "electron" behaves as if it were a classical particle with an **effective mass** m_e^* in a crystal, riding on a **potential** E_C, which is a function of location. Its **(crystal) momentum** is $\hbar k$, where k is the **wavevector**.

Energy vs. momentum at one location

Potential profile like a topography map

E_C
E_F
E_V

Just levels at one location

A "**hole**" refers to one fewer electron than a full valence band, which somehow loses it. (We have heuristic explanations why the hole is a positive charge carrier. But do we really know why?)

The hole is somewhat like an "anti-electron" (not really the positron, though). It has an **effective mass** m_h^*. You can **imagine flipping the electron E-k plot upside down**, with the parabola touching E_V. But, then you call the negative energy positive.

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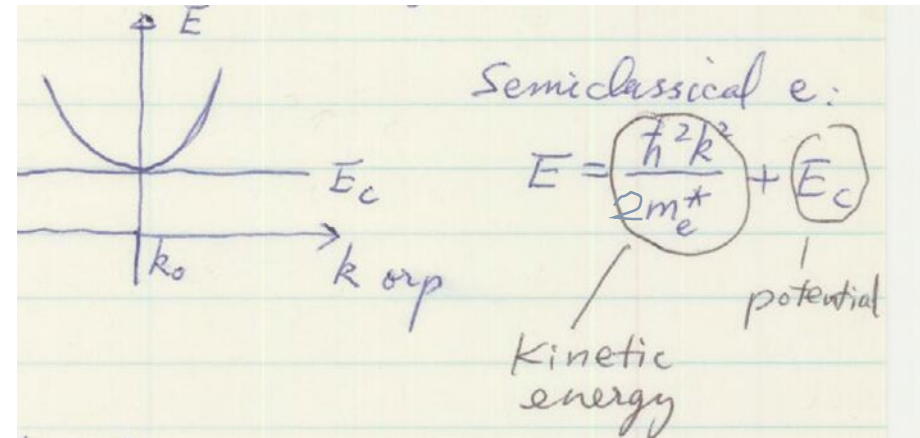
In general, the electron and hole E-k parabola vertices may not be at $k = 0$.

To be exact, for the electron,

$$E = \frac{\hbar^2 (k - k_0)^2}{2m_e^*} + E_c$$

Here, the electron (crystal) momentum is

$$\hbar (k - k_0)$$

Semiclassical e:

$$E = \left(\frac{\hbar^2 k^2}{2m_e^*}\right) + \left(E_c\right)$$

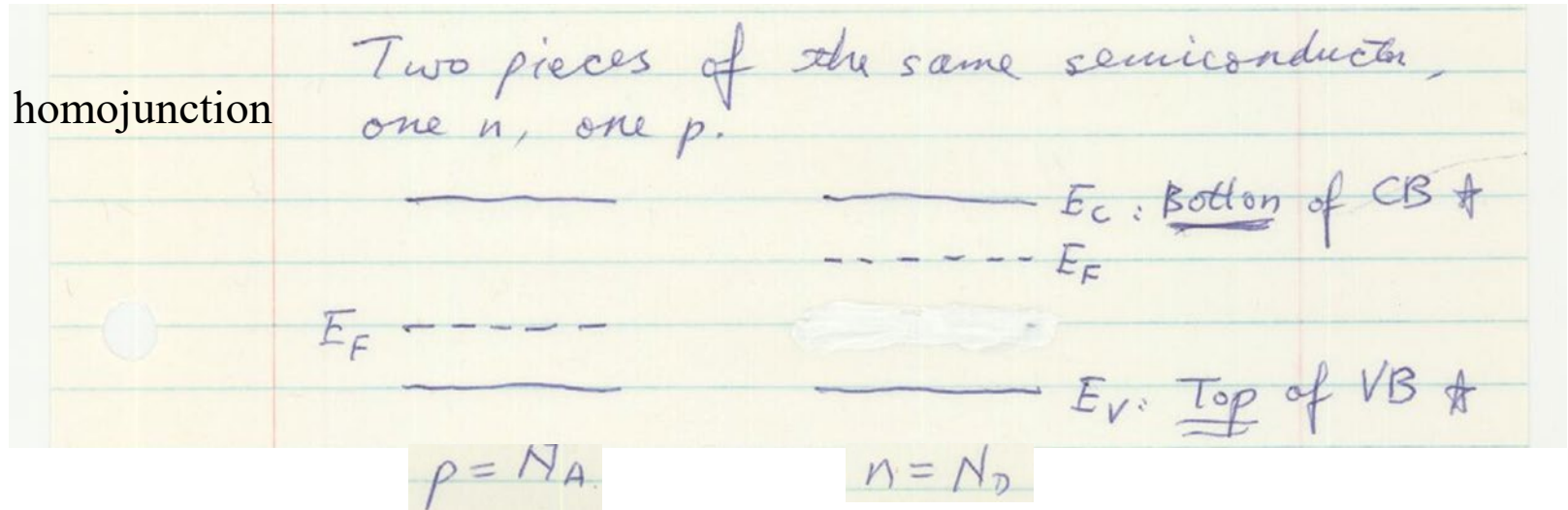$\quad$ Kinetic energy $\quad$ potential

The shifts k_0 for the electron and hole do not need to be the same.

What do we call the semiconductors when the two shifts are equal/not equal?

In general, **k** is a vector. It is called the wavevector after all.

The pn junction serves as a concrete example for us to review the commonly used concepts

homojunction

Two pieces of the same semiconductor, one n, one p.

E_C: Bottom of CB

- - - - - - E_F

E_F - - - - -

E_V: Top of VB

$p = N_A$ $n = N_D$

Donate electrons to or accept electrons from the host in this context
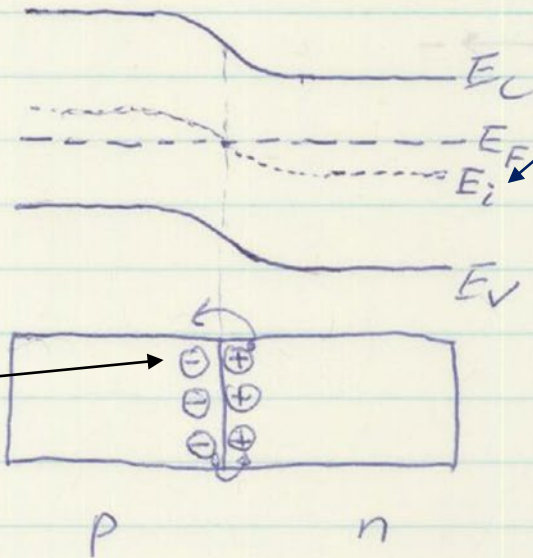
Fermi level
Carrier density
Units of these things

$$n = n_i\, e^{\frac{E_F - E_i}{k_B T}}$$

$$p = n_i\, e^{\frac{E_i - E_F}{k_B T}}$$

What happens when we put them in contact with each other?

What does this really mean?

The intrinsic level: the Fermi energy of the intrinsic semiconductor. For Si, it's about at the mid-gap.
We will discuss why.

E_C

E_F

E_i

E_V

Depletion region more or less intrinsic (depleted), but
cannot really be

p n

Diffusion : from high concentration to low concentration

electrostatic

Drift : from high potential to low potential

(Holes move uphill in this kind of diagrams.)

The two are against each other.
Equilibrium is reached eventually.

In the transition region, you don't have

$$n = N_D \quad \text{or} \quad p = N_A.$$

Field

Think about this eq. graphically (esp. with depletion approximation)

Remember Gauss's law.

$$\epsilon_0 \epsilon_r \frac{d\mathcal{E}}{dx} = \text{charge density}$$

$$= q(N_D - N_A + p - n)$$

electrostatic

Remember E_C is the potential energy?

So, $-\frac{E_C}{q}$ is the electric potential.

(electrostatic)

Work from definition

$$\Rightarrow \quad \mathcal{E} = -\frac{d}{dx}\left(-\frac{E_C}{q}\right) = \frac{1}{q}\frac{dE_C}{dx} \quad \checkmark$$

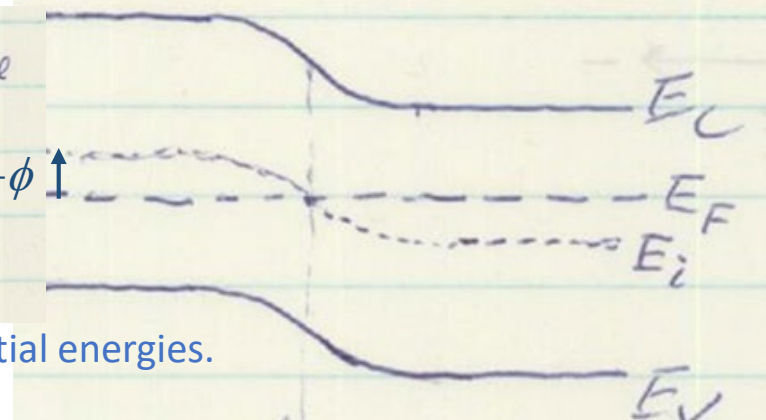$$\frac{d\mathcal{E}}{dx} = \frac{1}{q}\frac{d^2 E_C}{dx^2}$$

Put into Gauss's law:

Poisson Eq.

$$\frac{1}{q}\frac{d^2 E_C}{dx^2} = \frac{q}{\epsilon_0 \epsilon_r}(N_D - N_A + p - n)$$

Let's define some reference for the electric potential.

$$\phi = -\frac{1}{q}(E_i - E_F)$$

$-\phi \updownarrow$

Pay attention to signs of electrostatic potentials and potential energies.

Side note: the unit of ϕ is V.

The electron (or hole) goes across 1 V. the energy gained or lost is 1 eV.

~ a convenient unit.

Power $= I\,V$

$1\,W = 1\,A \cdot V$

Energy $= Q\,V$

$1\,J = 1\,C \cdot V$

How to convert eV to J?

$1\,eV = 1.6 \times 10^{-19}\,C \cdot V$

$= 1.6 \times 10^{-19}\,J$

Now. we have the Poisson Eq as:

$$\frac{d^2\phi}{dx^2} = -\frac{q}{\varepsilon_0 \varepsilon_r}(N_D - N_A + p - n) \tag{1}$$

N_D & N_A are known.

$$n = n_i e^{\frac{E_F - E_i}{k_B T}} = n_i e^{+\frac{q\phi}{k_B T}} \tag{2}$$

$$p = n_i e^{\frac{E_i - E_F}{k_B T}} = n_i e^{-\frac{q\phi}{k_B T}} \tag{3}$$

3 Eq's, 3 unknowns. so we have

solutions.

$\searrow \phi, n, p$.

But no analytical solution!

We could solve them numerically, but we like analytical expressions since they provide physical insights.

The depletion approximation

n and p depend on ϕ exponentially.

$$n = n_i\, e^{\frac{E_F - E_i}{k_B T}} = n_i\, e^{+\frac{q\phi}{k_B T}}$$

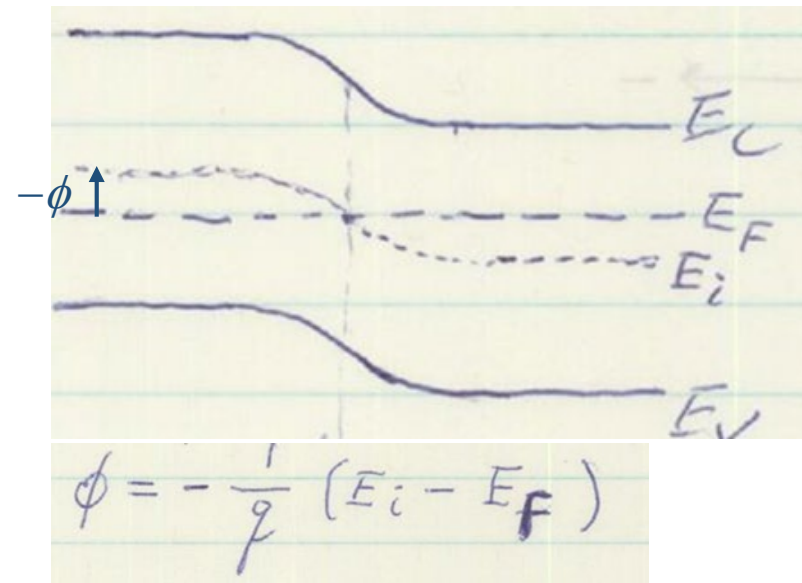$$p = n_i\, e^{\frac{E_i - E_F}{k_B T}} = n_i\, e^{-\frac{q\phi}{k_B T}}$$

$$\phi = -\frac{1}{q}(E_i - E_F)$$

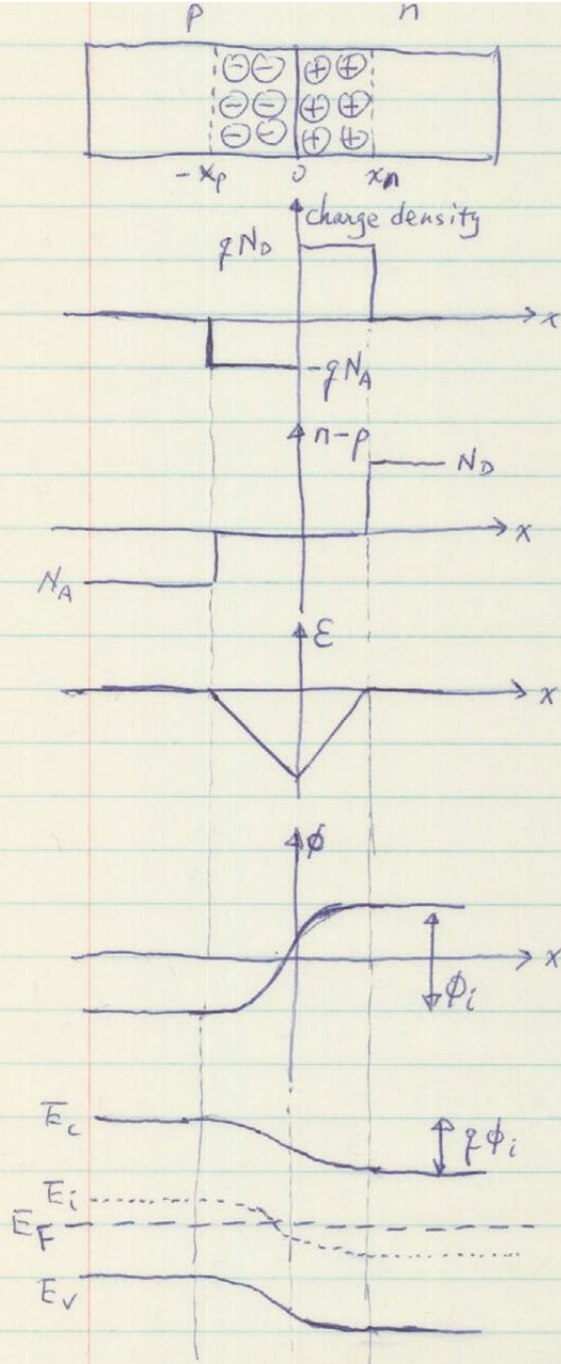When ϕ is not too much larger than $k_B T$,
$n \approx 0$ and $p \approx 0$.

$n_i = 1.45 \times 10^{10}/\mathrm{cm}^3$ for Si

$e \approx 2.718,\ e^2 \approx 7.4,\ e^4 \approx 55,\ e^5 \approx 148$

$n = 10^{12}\ /\mathrm{cm}^3 \approx 0$
???

depletion or neutral

On the n side of the depletion region.

$$\frac{d\mathcal{E}}{dx} = \frac{q}{\varepsilon_0 \varepsilon_r} N_D$$

The ionized donors are the only charge.

$$\frac{d\mathcal{E}}{dx} = \text{const} \quad \text{what should}$$

$\mathcal{E}(x)$ look like?

Boundary condition known.

$$\mathcal{E}(x_n) = 0$$

$$\therefore \mathcal{E}(x) = -\frac{q N_D}{\varepsilon_r \varepsilon_0}(x - x_d)$$

Similarly, on the p side.

$$\mathcal{E}(x) = -\frac{q N_A}{\varepsilon_0 \varepsilon_r}(x + x_p)$$

On the n side,

$$\phi(x) = \phi(x_n)$$

$$- \int_{x_n}^{x} \mathcal{E}(x)\, dx$$

$$= \phi_n - \frac{q N_D}{2 \varepsilon_0 \varepsilon_r}(x - x_n)^2$$

Similarly, on the p side.

$$\phi(x) = \phi_p + \frac{qN_A}{2\varepsilon_s\varepsilon_0}(x + x_p)^2$$

Define $\quad \phi_n = \phi(x_n) = -\frac{1}{q}\left[E_{i(x_n)} - E_F\right]$

In the n side neutral region

$$N_D = n = n_i e^{\frac{E_F - E_i}{kT}}$$

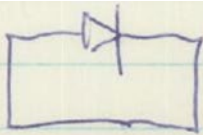$$\therefore \phi_n = \frac{kT}{q}\ln\frac{N_D}{n_i}$$

Similarly, on the p side,

$$\phi_p = -\frac{kT}{q}\ln\frac{N_A}{n_i}$$

The built-in potential

$$\phi_i = \phi_n - \phi_p = \frac{kT}{q}\ln\frac{N_D N_A}{n_i}$$

Can you short out ϕ_i ?

at $x=0$, where the n joins the p.

$$\phi(0) = \phi_n - \frac{q N_D}{2 \varepsilon_0 \varepsilon_r} x_n^2$$

and

$$\phi(0) = \phi_p + \frac{q N_A}{2 \varepsilon_0 \varepsilon_r} x_p^2$$

$$\therefore \quad \phi_n - \phi_p \equiv \phi_i = \frac{q}{2 \varepsilon_0 \varepsilon_r} \left(N_D x_n^2 + N_A x_p^2 \right) \Bigg\} \Rightarrow$$

Why?

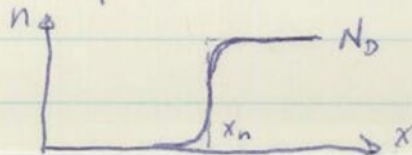Recall that $N_D x_n = N_A x_p$

$$x_n + x_p = \sqrt{2 \frac{\varepsilon_0 \varepsilon_r}{q} \phi_i \left(\frac{1}{N_D} + \frac{1}{N_A} \right)}$$

It's easy for you to write the expressions for x_n & x_p.

So far so good? But this is not even self-consistent! For example for $0 < x < x_n$,

$$n = n_i\, e^{-\frac{E_i(x) - E_F}{kT}} = n_i\, e^{\frac{q \phi}{kT}} \neq 0$$

Especially for $x \to x_n$, $\quad n(x) \to N_D$

Concepts Reviewed

Semiclassical model: The electron and the hole are treated as if they were classical particles. The kinetic energy-momentum dependence is given by Newton's laws. The total energy is the sum of kinetic and electrostatic potential energies. The E_C, E_V, and E_i profiles follows the electrostatic potential energy profile.

> Read three types of band diagrams: energy levels in homogeneous material (or at one location), energy-momentum (E-k) dependence (dispersion), energy level profiles (band diagram).

Carrier statistics: Fermi distribution (probability of a state being occupied), density of states (number of states per energy interval per volume), carrier density (numbers of carriers per volume).

> Be familiar with units of physical quantities and orders of magnitude of frequently encountered parameters. **Unit system of the trade**: SI except length (m replaced with cm).

Impurity doping: H atom model: $E_C - E_D$ is analogous to that 13.6 eV ionization energy of the H atom, and this simplest model gives the right order of magnitude of values for the shallow-level dopants (commonly used for intentional doping). Under usual conditions (moderate doping, room temperature), almost all dopant atoms are ionized, therefore carrier density = dopant density.

The pn junction: By solving a set of three equations (Poisson, electron & hole densities), you know everything. But, they cannot be solved analytically, even in the simplest case of abrupt junction between two semi-infinite homogeneous chunks of semiconductors. The depletion approximation make things easy.