

Quantum Mechanics Review/Overview

Quantum mechanics is a new way of describing the world

- An amplitude for every “event”
- $|\text{the amplitude of an event}|^2 = \text{the probability of the event}$

In general, the amplitude is complex.

The amplitude is somewhat behind the scene. The probability is all that we can possibly know. This randomness is different from that in classic statistical mechanics.

Accept this as a basic assumption.

When the “event” is an object (electron) being at position \mathbf{r} at time t , the “amplitude” $\psi(\mathbf{r}, t)$ is the **wave function**.

$\psi(\mathbf{r}, t)$ can often be viewed as a superposition of plane waves $e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}$ (Fourier transform).

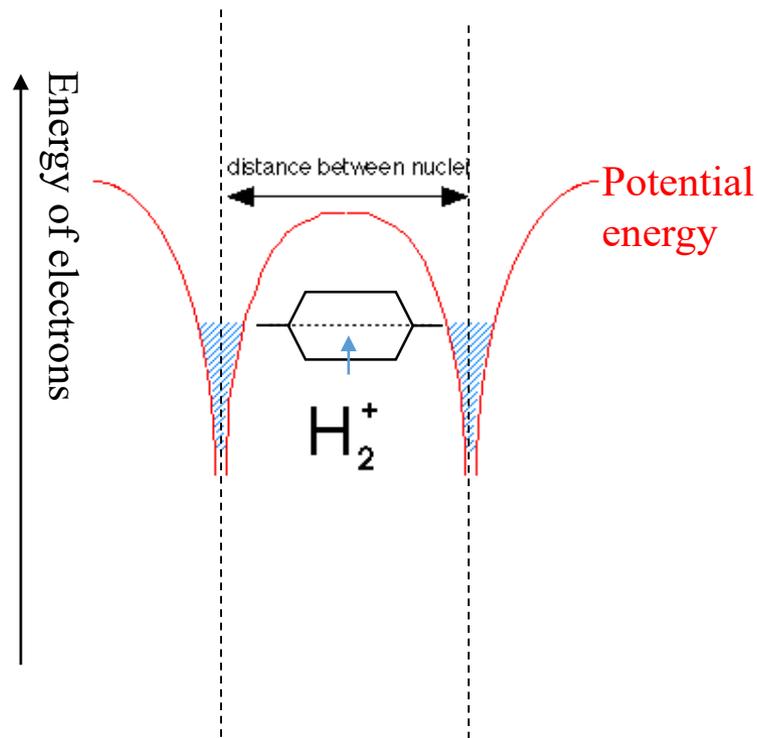
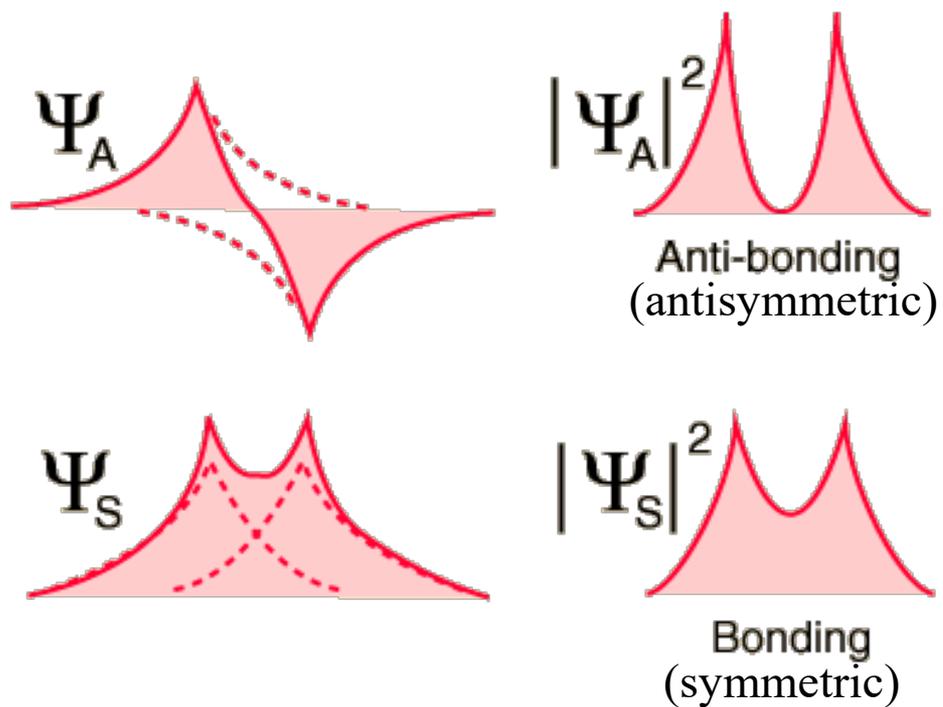
For the special case of plane waves,

$$\text{energy } E = \hbar\omega$$

$$\text{momentum } \mathbf{p} = \hbar\mathbf{k}$$

Example

H_2^+ molecular ion and H_2 molecule



Semiconductor Physics Review/Overview

Crystal structures

Mainstream semiconductors are crystalline

A crystal is a **periodic** structure.

Similar to a periodic signal as a function of time, but in 3D space.

As in the periodic signal, there is an internal structure in a period.

A period of the crystal structure is a **unit cell**.

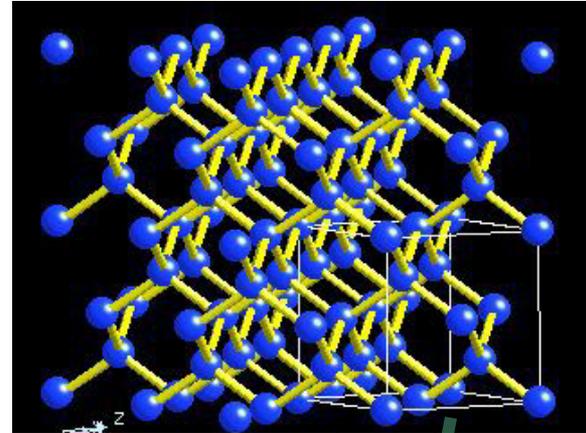
An integer multiple of a period is also a period.

The smallest possible period is called a **primitive unit cell**.

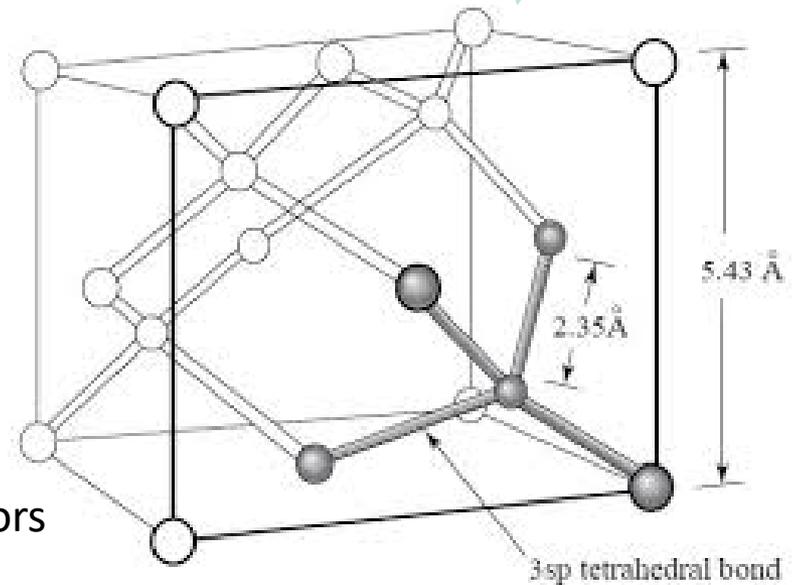
The situation in 3D space is more complicated than in 1D time.

Each Si atom has 4 nearest neighbors

Si crystal structure



http://www.webelements.com/silicon/crystal_structure.html



<http://onlineheavytheory.net/silicon.html>

4.2 Types of solid: bond picture

This is about as far as we can go easily with a band model. But let us consider the semiconductors Si and Ge again. These have the 'diamond structure' which is like F.C.C. (see § 1.3) except that there

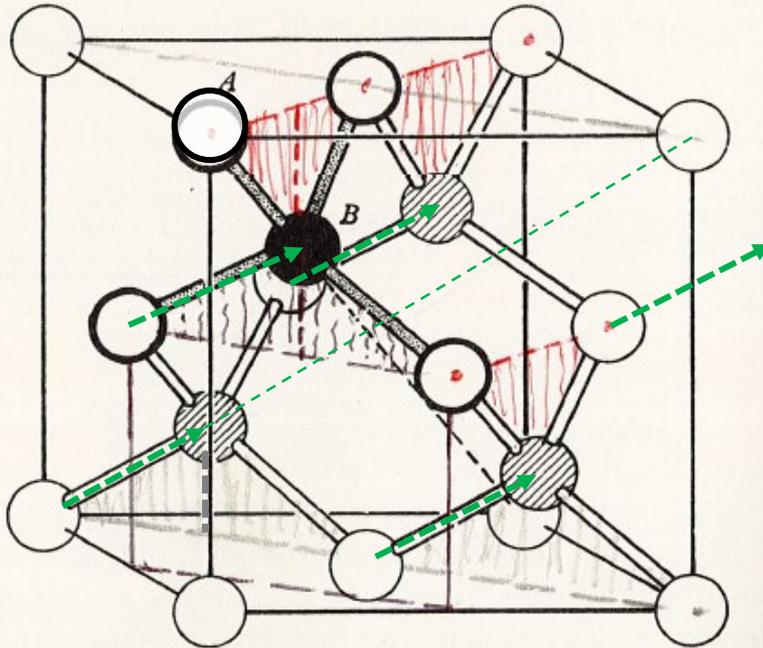


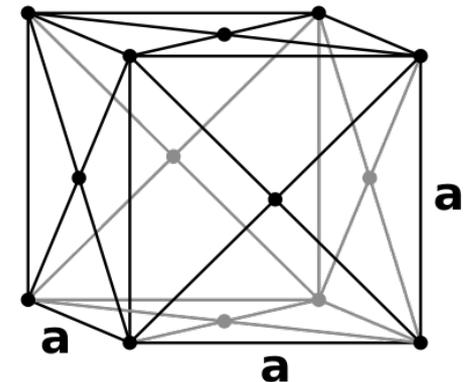
Fig. 72. Tetrahedral bonds in the diamond structure.

There are 2 **inequivalent** types of positions for atoms, A & B.

Each type forms a periodic lattice.

Each A position shifted by a **green arrow** is a B position.

For Si, the lattice formed by one type of positions is called **face-centered cubic (fcc)**.



From Ziman, Principles of the Theory of Solids

But this cube is **not** the smallest possible period, or **primitive unit cell**.

It is the **conventional unit cell** that we use when talking about Si.

It better visualized the features of the Si crystal structure.

$$a \approx 5.43 \text{ \AA}$$

Diamond has the same structure. So we say Si has the **diamond structure**.

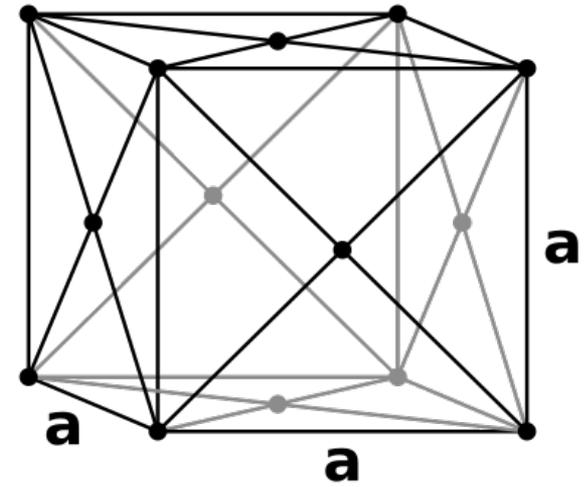
Ge also has the diamond structure.

In the **lattice** of one type of position (e.g. type A in Si), a **primitive unit cell** contains **one** atom.

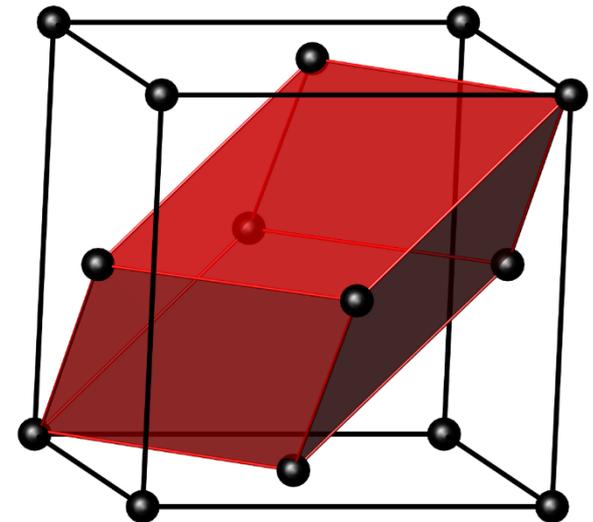
How many atoms each type (A or B) are in the **fcc conventional unit cell**?

The **lattice** of one type of position is called the **Bravais lattice**.

The underlying **Bravais lattice** of Si is fcc.



Conventional unit cell



<https://physics.stackexchange.com/questions/210963/primitive-unit-cell-of-fcc>

Primitive unit cell

4.2 Types of solid: bond picture

This is about as far as we can go easily with a band model. But let us consider the semiconductors Si and Ge again. These have the 'diamond structure' which is like F.C.C. (see § 1.3) except that there

Behind depicted primitive cell

In front of depicted primitive cell

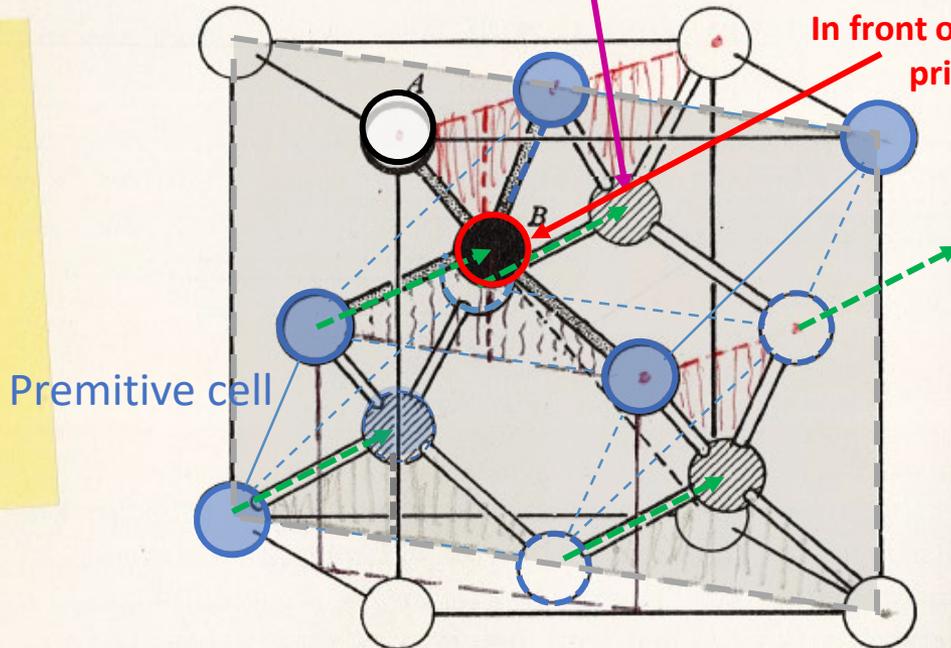
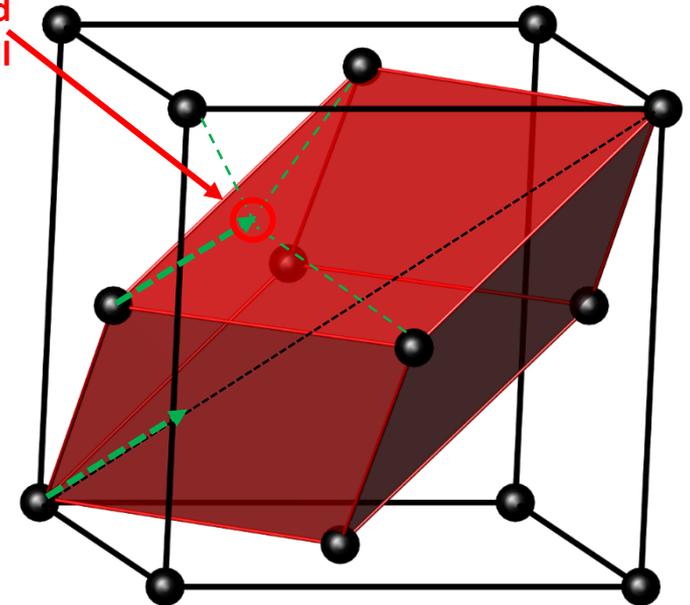


Fig. 72. Tetrahedral bonds in the diamond structure.



From Ziman, Principles of the Theory of Solids

For Si, each primitive unit cell contains 2 atoms, one at position A and one at B.

Exercise

How many Si atoms (both types A & B) are in the conventional unit cell?

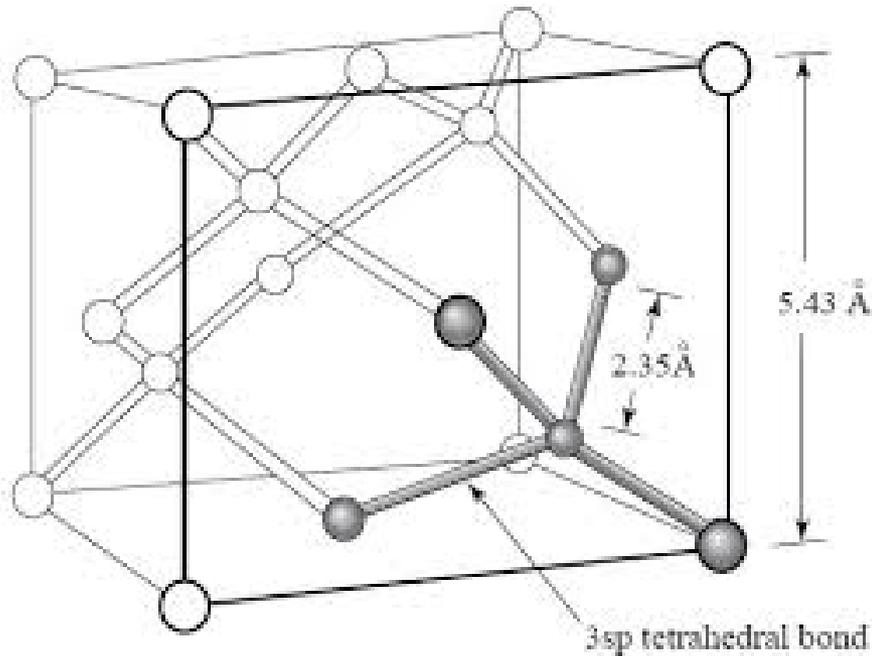
What is the atom density of Si (in atoms/cm³)?

Note: We mostly use the SI units, where the unit for length is m. In semiconductor device physics, however, we customarily use cm for length. **Make sure you get the units right.**

The underlying Bravais lattice of GaAs and many III-V semiconductors are also fcc, but the two types of positions are occupied by different elements.

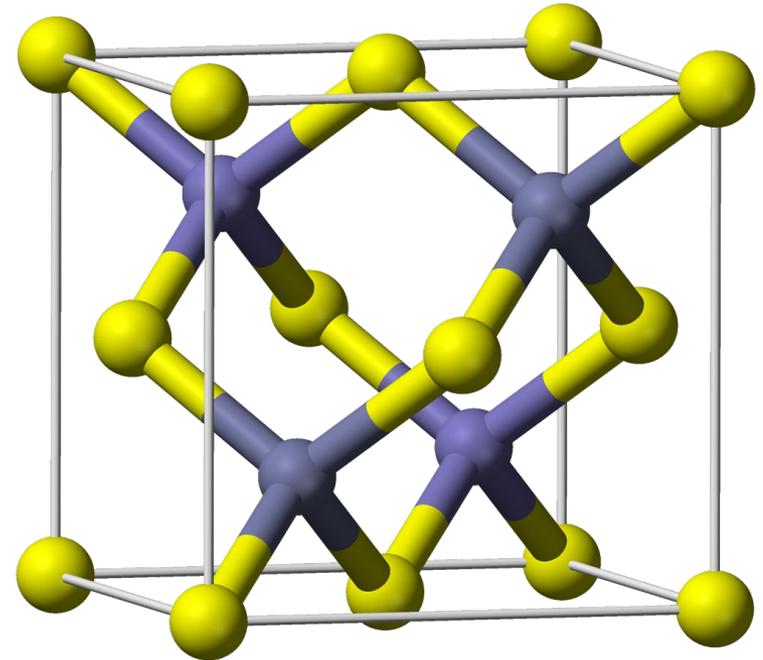
The crystal structure is called **zincblende**.

(Wide band gap nitrides, e.g. GaN, AlN, are of a different structure, to be discussed later.)



<http://onlineheavytheory.net/silicon.html>

Si: diamond



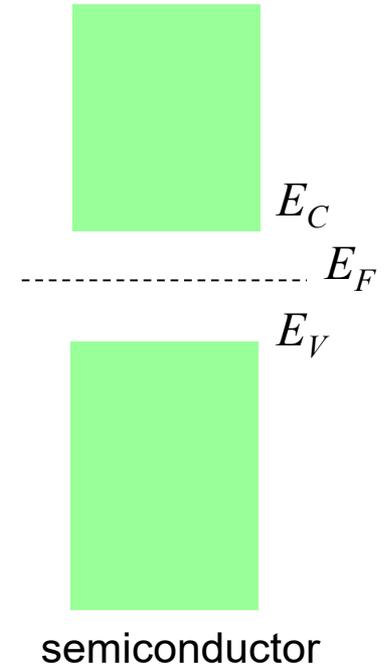
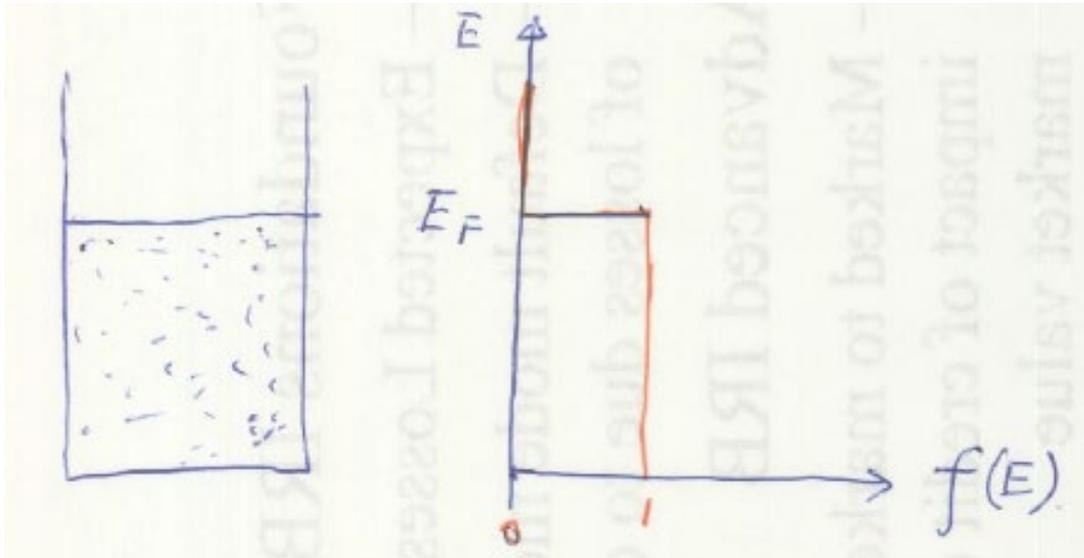
https://en.wikipedia.org/wiki/Cubic_crystal_system#Zincblende_structure

GaAs: zincblende

Carriers in semiconductors

Fermi-Dirac (F-D) distribution of electrons: consequence of Pauli's exclusion rule

Analogy: sand particles in a vessel



Fermi-Dirac distribution at $T = 0$:

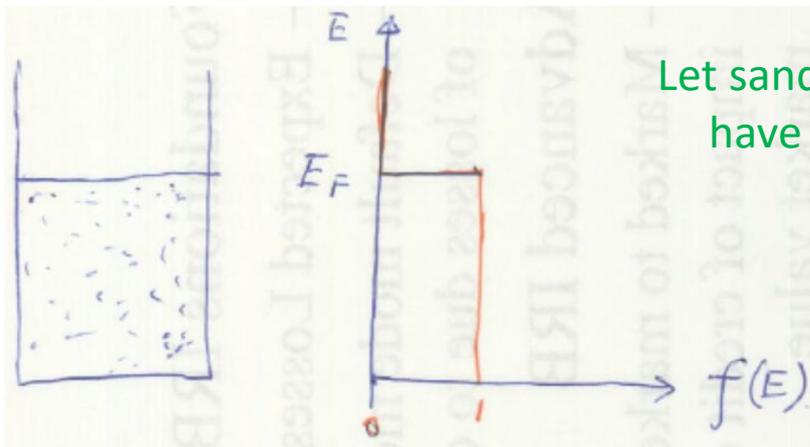
$f(E)$ is the probability of a state at energy E being occupied.

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

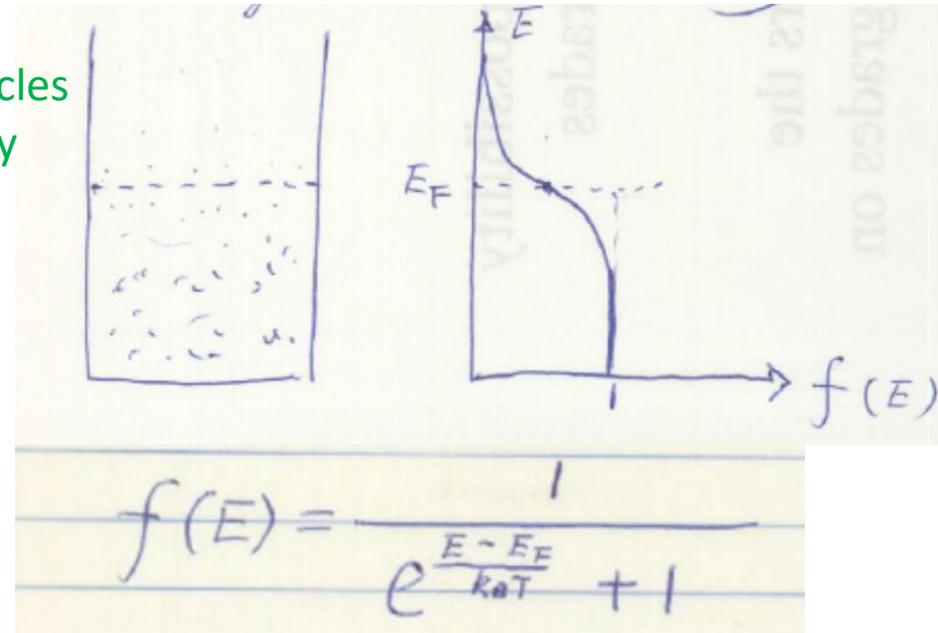
For semiconductors, with a gap, E_F is somewhat arbitrary at $T = 0$.

In this kind of chart, lines just signifies energy levels, horizontal coordinate means nothing.

Fermi-Dirac distribution at $T = 0$: Imagine each sand particle is energetic



Let sand particles have energy



The Fermi level $E_F(T)$ is a function of T .

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.

(when the vessel is non-cylindrical)

Called density of states (DOS)

This slide was missing in the lecture presentation on Thu 8/26.

Digression:

Subtle difference in jargons used by EEs and physicists

We use the EE terminology, of course.

Fermi level

$$E_F = E_F(T)$$

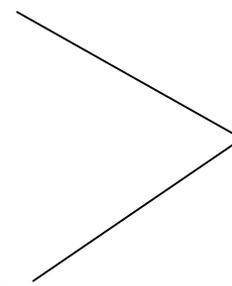
Physicists:

Chemical potential

$$\mu(T)$$

Fermi energy

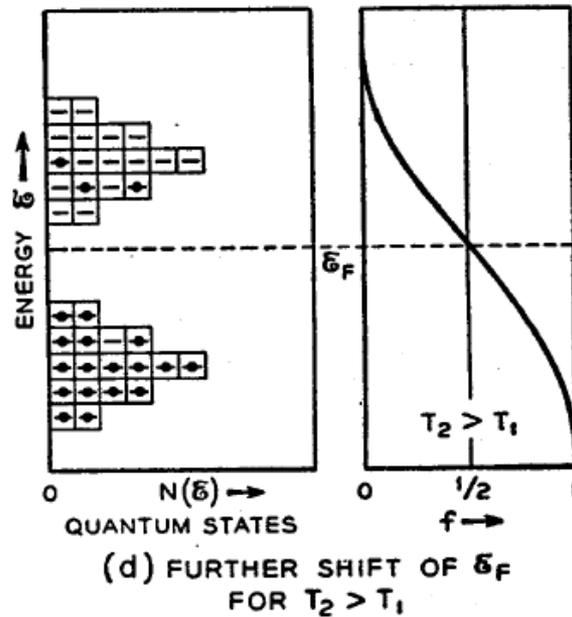
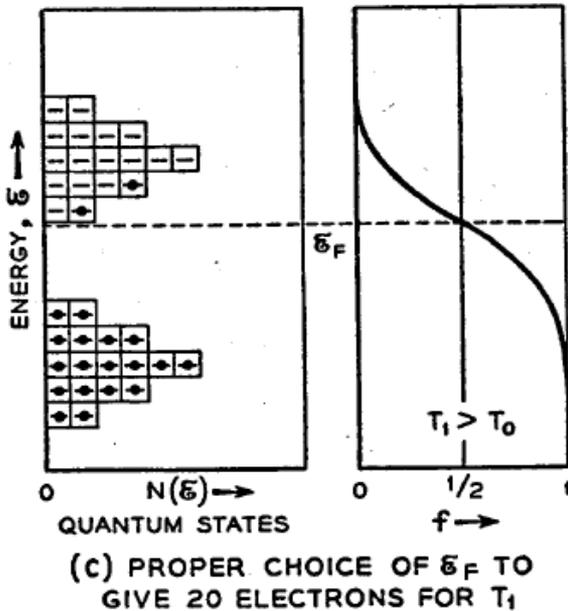
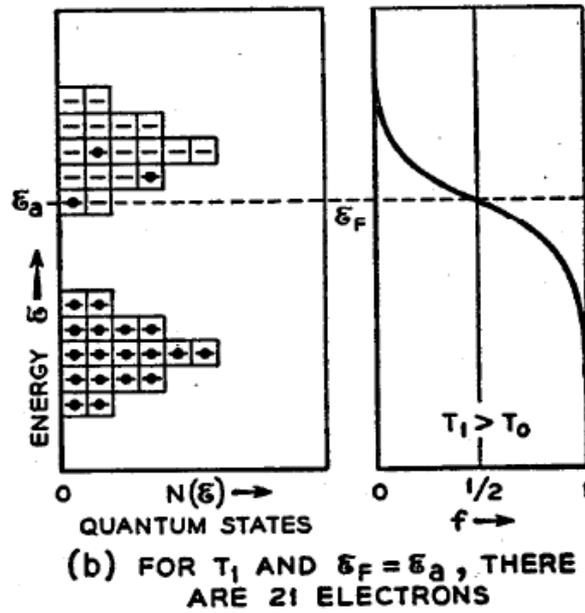
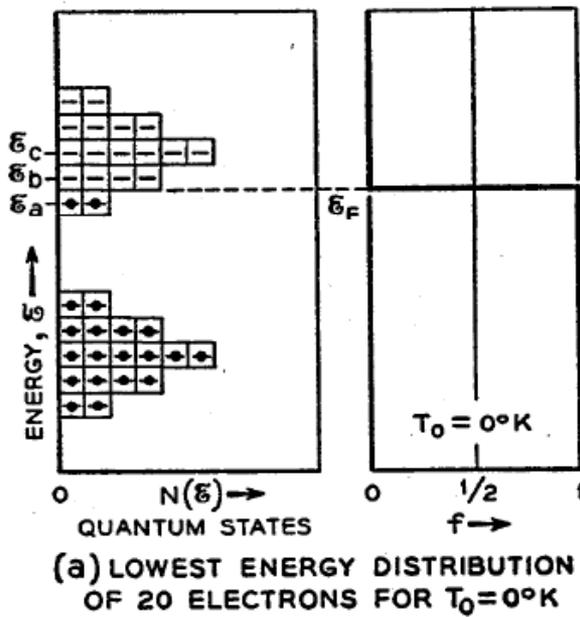
$$E_F = \mu(0)$$



Same concept when $T > 0$

We already used μ for mobility.

Density of states (DOS) determines how $E_F(T)$ varies with T .



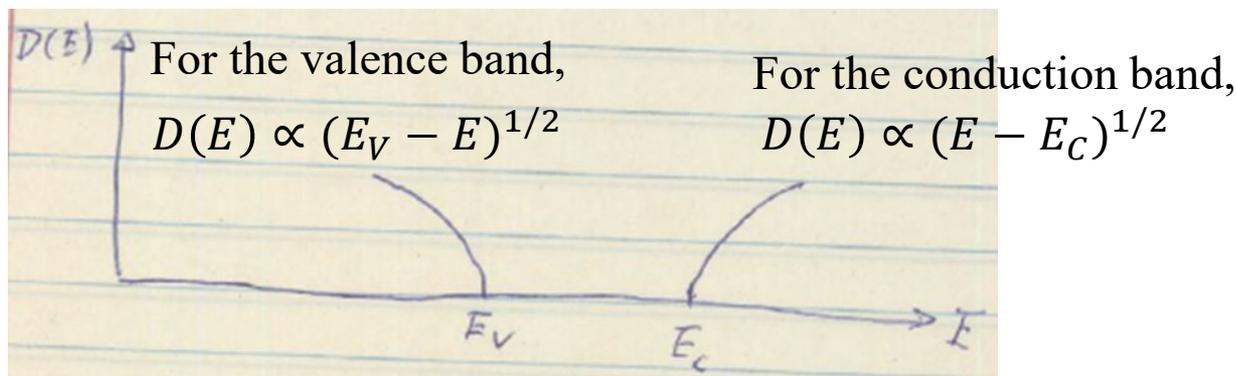
- (a) 20 electrons at $T = 0$.
- (b) $T > 0$, some electrons promoted to higher energies. If E_F remained \sim the same, we would need 21 electrons.
- (c) To keep the # of electrons unchanged, E_F has to move down. The lower band is still full at low T .
- (d) At higher T , E_F moves further down and the distribution flattens more, so that some states in lower band vacate.

From Shockley, *Electrons and Holes in Semiconductors*, 1976 (original ed.1950)

FIG. 10-3—Quantum State Distribution and Fermi-Dirac Distribution Combined to Give Equilibrium Distribution.

Density of states (DOS)

Expression is for $D(E)$ are discussed in the sister course ECE 634.



Electron (conduction band electron) density

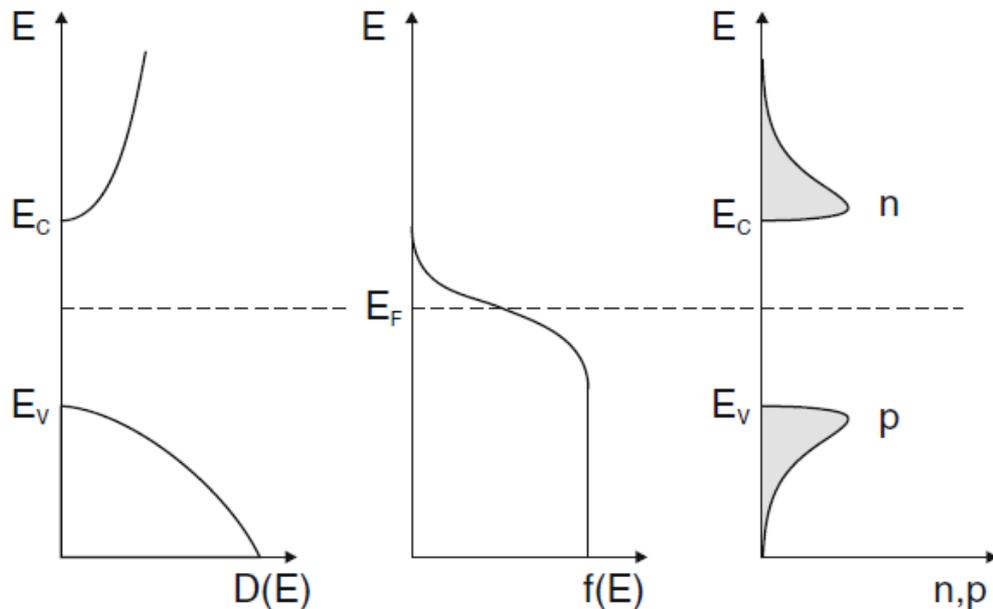
$$n = \int_{E_C}^{\infty} D(E) f(E) dE \propto \int_{E_C}^{\infty} \sqrt{E - E_C} f(E) dE$$

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.

$$f(E) = \frac{1}{e^{\frac{E-E_F}{k_B T}} + 1} \approx e^{-\frac{E-E_F}{k_B T}}$$

Then, $n = N_C e^{-\frac{E_C - E_F}{k_B T}}$



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

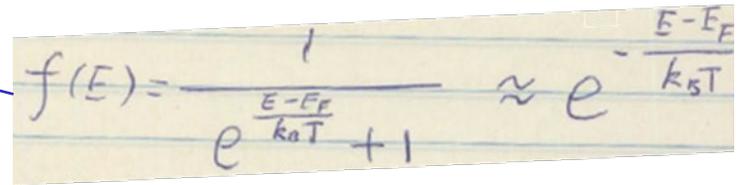
N_C is a proportional constant. Its expression is discussed in the sister course ECE 634.

Digression: Physical justification of Boltzmann approximation to F-D distribution

Fermi-Dirac (F-D) distribution is the consequence of Pauli's exclusion rule.

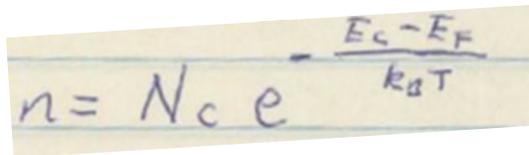
If there are very few electrons at $E - E_F > 4k_B T$, Pauli's exclusion rule does not matter – electrons won't run into each other anyway, just like molecules in an ideal gas.

$$n = \int_{E_C}^{\infty} D(E) f(E) dE \propto \int_{E_C}^{\infty} \sqrt{E - E_C} f(E) dE$$



A handwritten note on lined paper showing the Fermi-Dirac distribution function: $f(E) = \frac{1}{e^{\frac{E-E_F}{k_B T}} + 1} \approx e^{-\frac{E-E_F}{k_B T}}$. A blue arrow points from this note to the $f(E)$ term in the integral equation above.

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



A handwritten note on lined paper showing the carrier concentration: $n = N_C e^{-\frac{E_C - E_F}{k_B T}}$.

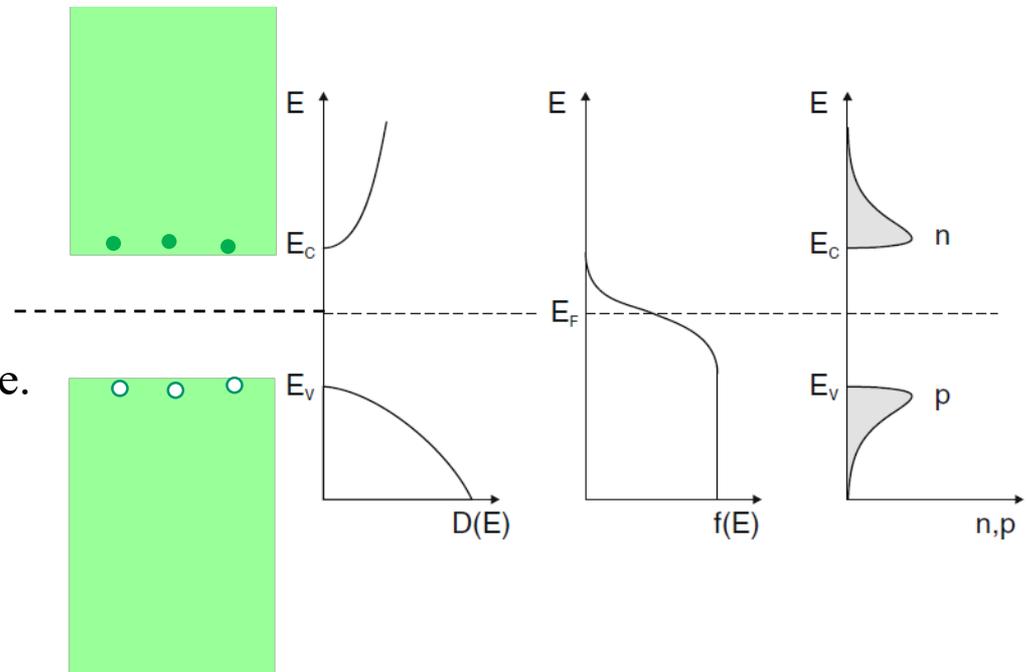
as if all conduction band electrons are at E_C , where there are N_C states per unit volume. Therefore, N_C is called the **effective** density of states (states/volume) of the conduction band.

A vacant valence band state is called hole.
The hole density

$$p = \int_{-\infty}^{E_V} D(E) [1 - f(E)] dE$$

Taking same approximation as done
for electrons yields

as if all holes are at E_V , where there are N_V states per unit volume.
Therefore, N_V is called the **effective** density of states (states/volume)
of the valence band.



$$\begin{aligned}
 n &= N_C e^{-\frac{E_C - E_F}{k_B T}} \\
 p &= N_V e^{-\frac{E_F - E_V}{k_B T}}
 \end{aligned}
 \Rightarrow np = N_V N_C \exp\left(-\frac{E_C - E_V}{kT}\right) = N_V N_C \exp\left(-\frac{E_g}{kT}\right)$$

Band gap

How good is the approximation (FD approximated by Boltzmann)?

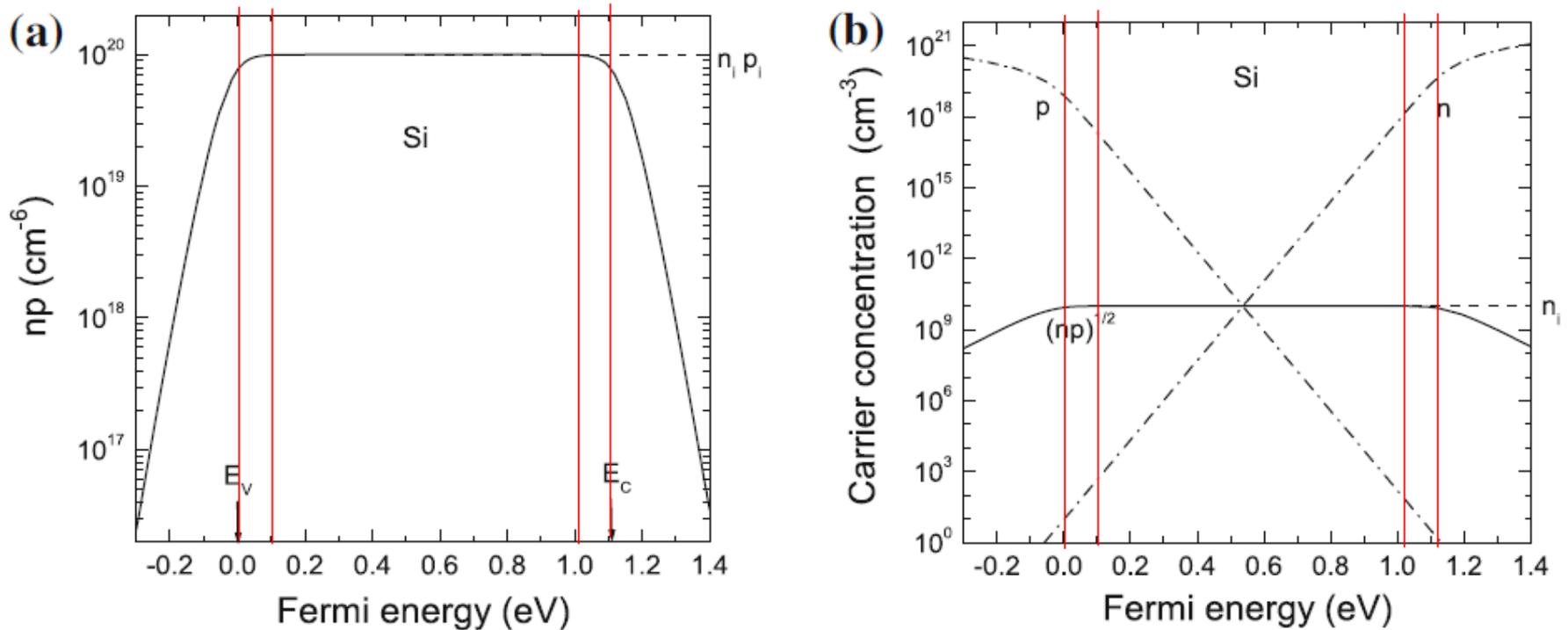
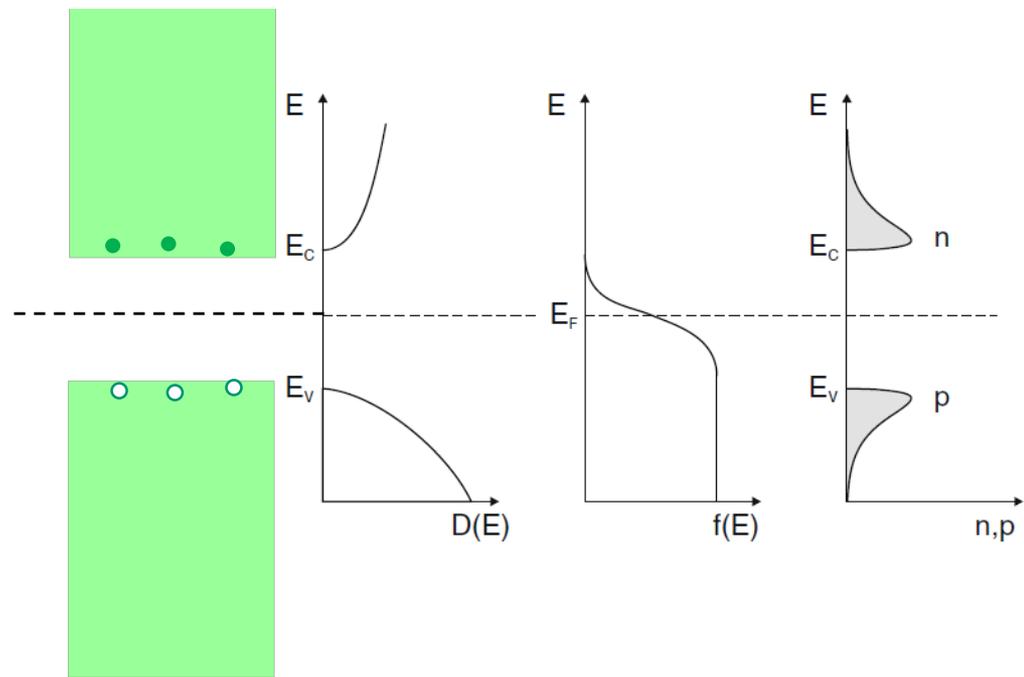


Fig. 7.2 (a) np for silicon at $T = 300$ K as a function of the position of the Fermi level. The valence-band edge E_V is chosen as $E = 0$. np is constant for the range of Fermi energies given by (7.13) ($4kT \approx 0.1$ eV). (b) n , p and \sqrt{np} as a function of the Fermi level

There are **very few** electrons at energy E such that $E - E_F > 4k_B T$.

For perfectly pure Si (called **intrinsic Si**), shouldn't we have $n = p$?

When $n = p$, where is E_F ?



$$n = N_c e^{-\frac{E_c - E_F}{k_B T}}$$

$$p = N_v e^{-\frac{E_F - E_v}{k_B T}}$$

For the intrinsic semiconductor, $n = p$ and

$$np = n_i p_i = n_i^2 = p_i^2$$

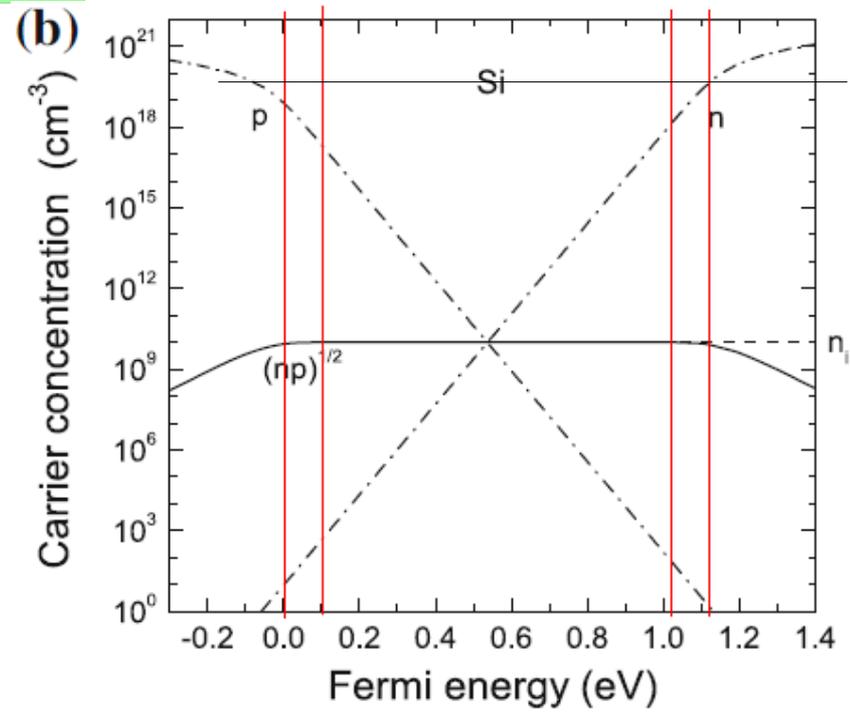
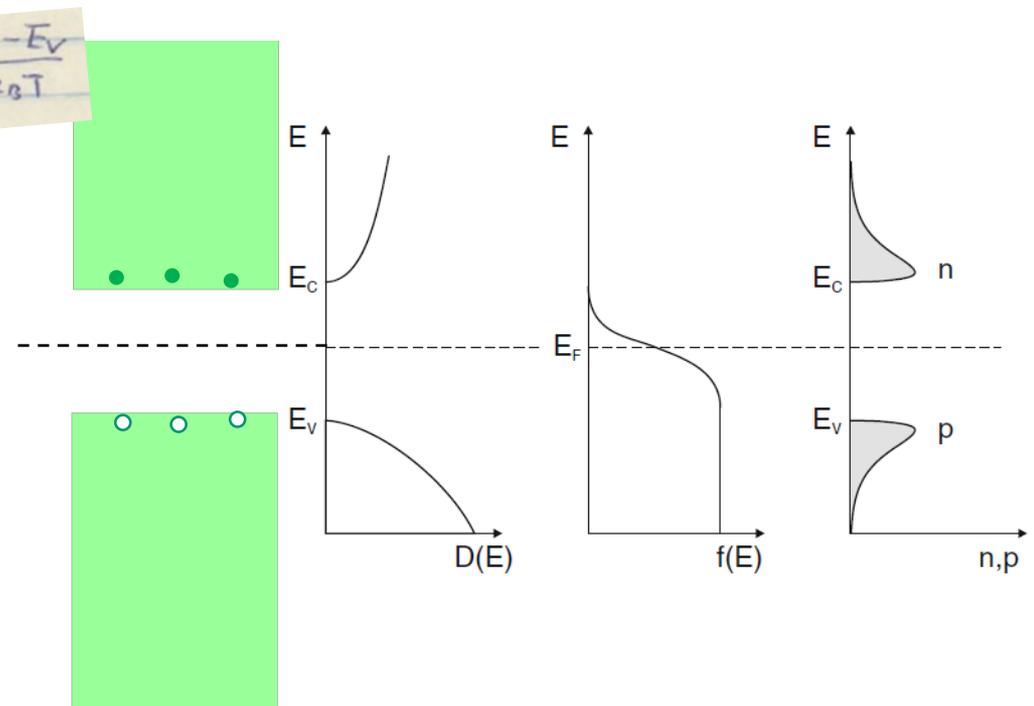
$$E_F = E_i = \frac{E_v + E_c}{2} + \frac{kT}{2} \ln\left(\frac{N_v}{N_c}\right)$$

Intrinsic Fermi level

$$n_i = p_i \approx 1.45 \times 10^{10} \text{ cm}^{-3} \text{ at RT.}$$

How can we say there are **very few** electrons?

Electrons and holes are always generated in pairs.
How can we have $n \neq p$?



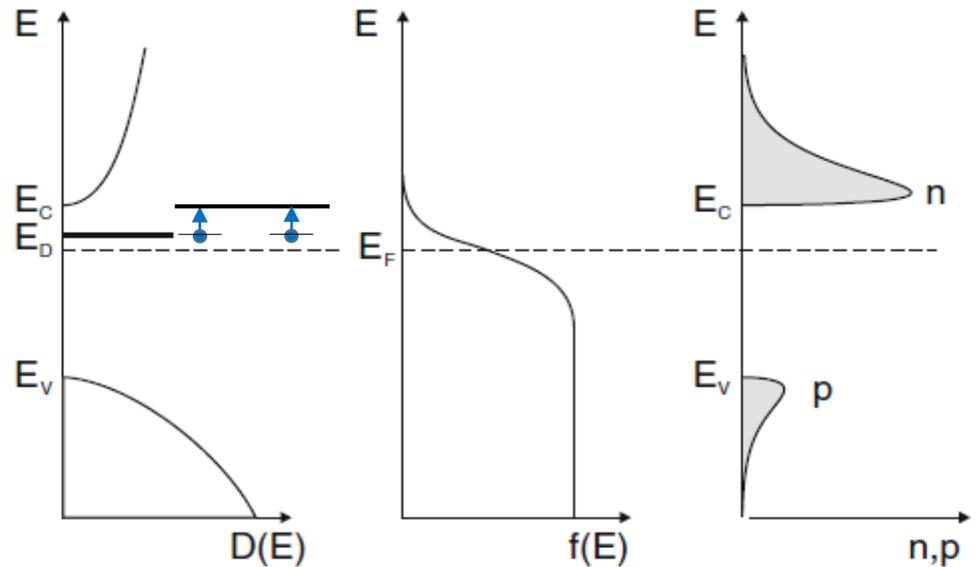
n-type doping by shallow donors

Usually sufficient to assume that, at room temperature (RT), all donors contribute to electron density, $n = N_D$, i.e., they are **fully ionized**.

N_D : donor concentration

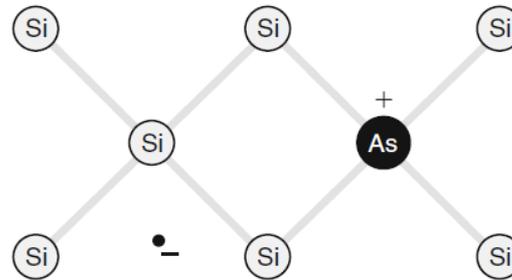
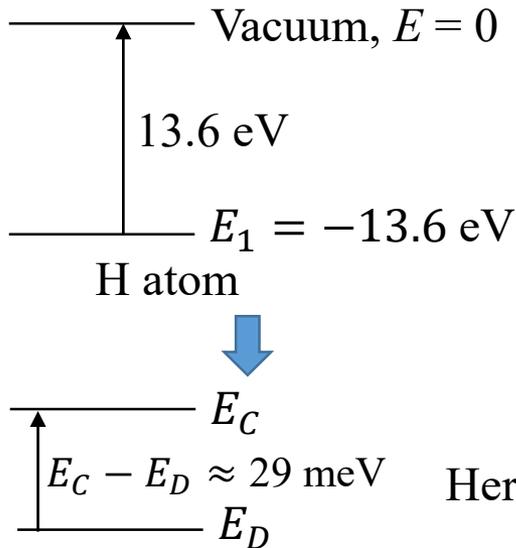
We stopped here on Thu 8/26/2021 before moving on to the pn junction.

My presentation omitted Slides 10 and 11 in this ppt, which I shall quickly go over on Tue 8/31.

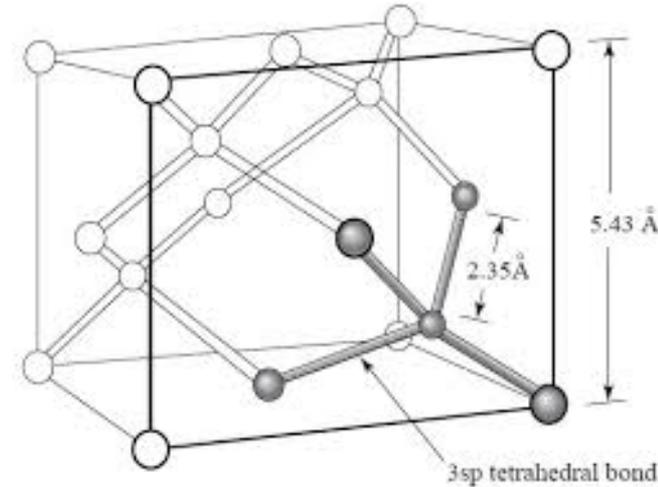


Grundmann, *The Physics of Semiconductors*, p. 209

A very rough approximation: the hydrogen-atom model



Grundmann, *The Physics of Semiconductors*, p. 212

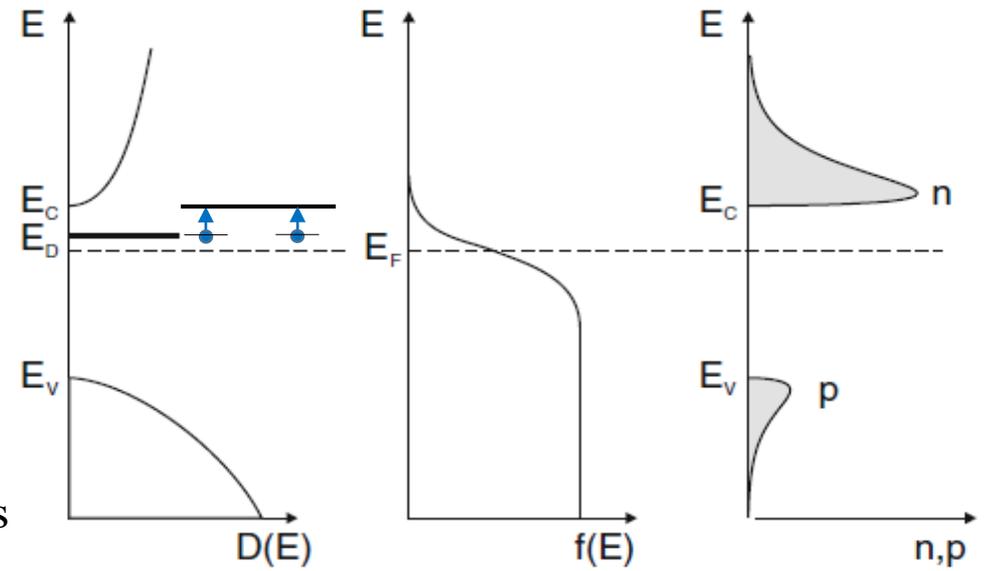
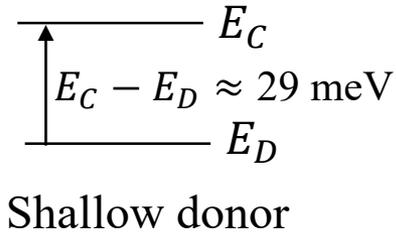


Here donor $D = \text{As}$, ionized donor $D^+ = \text{As}^+$, un-ionized donor $D^0 = \text{As}^0$. (not union-ized)

Shallow donor

We say: at RT ($k_B T \sim 25 \text{ meV}$), donors are **fully ionized**. *Why??!*

We say: at RT ($k_B T \sim 25$ meV), donors are **fully ionized**. *Why??!*



The **short answer** is:
There are a lot more conduction band states near E_C than there are donors.

It is tempting to think that $\frac{N_{D^+}}{N_{D^0}} = e^{-\left(\frac{E_D^b}{kT}\right)}$

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

Less than 20% ionized?!

What's missing here?

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

For Si, $N_C \approx 2.8 \times 10^{19} \text{ cm}^{-3}$, light to moderate doping 10^{13} to 10^{18} cm^{-3} .

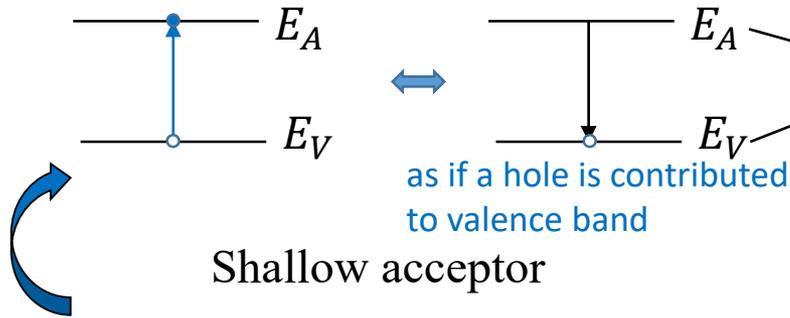
Up to $N_D \sim 10^{18} \text{ cm}^{-3}$, we can assume donors are **fully ionized** at RT. (What about low T?)

p-type doping by shallow acceptors

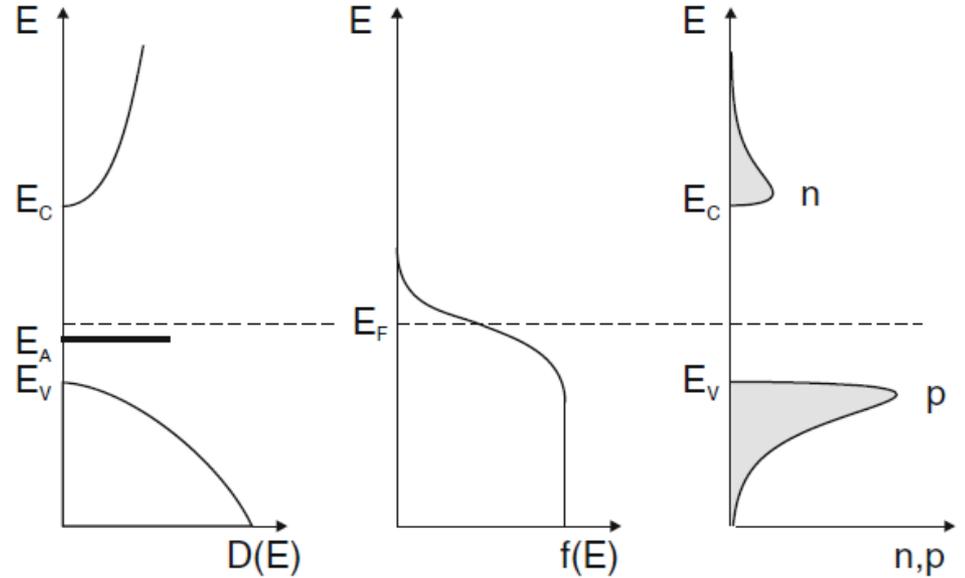
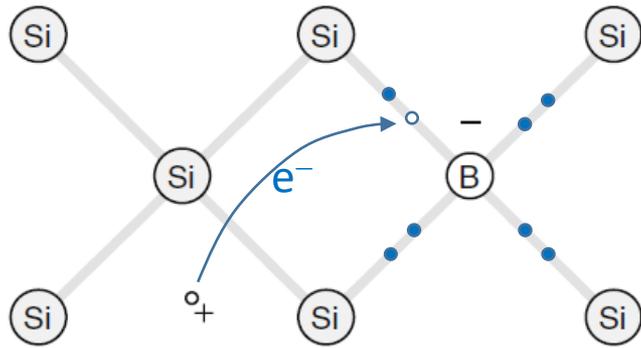
N_A : acceptor concentration

N_{A^-} : ionized acceptor concentration

N_{A^0} : neutral acceptor concentration



e^- from valence band fill vacancy in Si-B bond
 → ionized acceptor B^- , leaving behind hole in valence band

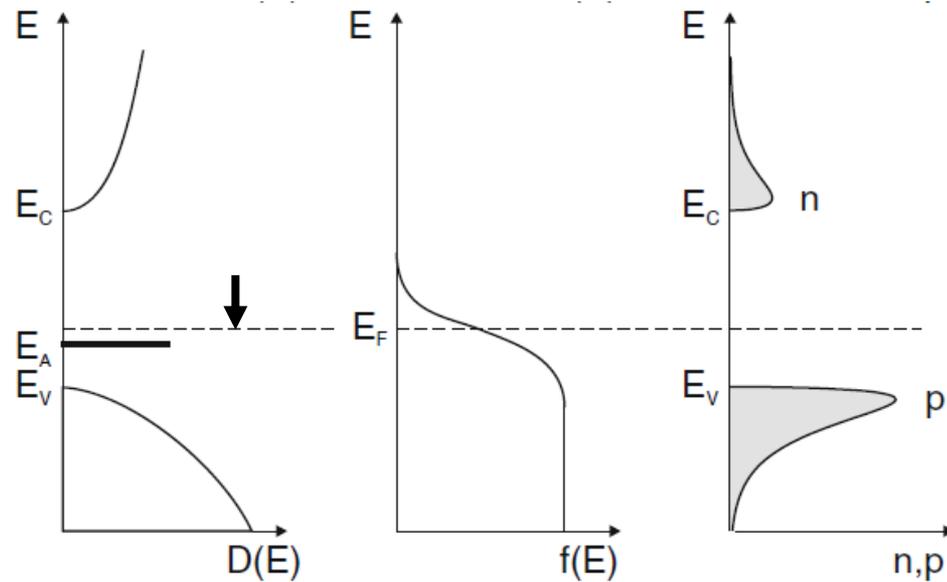
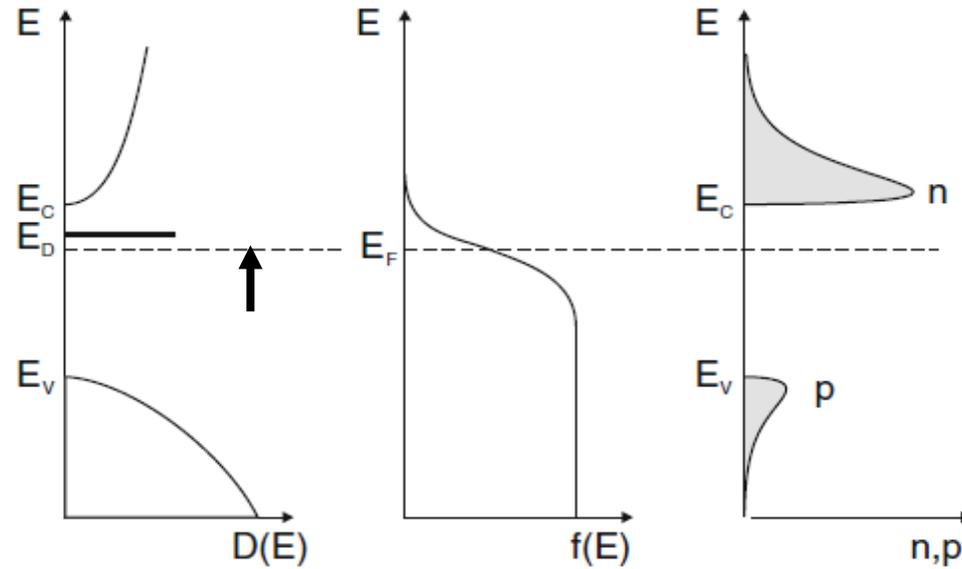


Grundmann, *The Physics of Semiconductors*, p. 209

At RT, essentially all acceptors are **fully** ionized, $p = N_A$. Why?

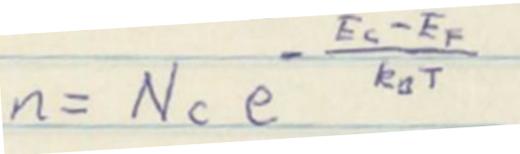
Although **the acceptor state** is higher in energy than E_V and $E_A - E_V$ is comparable to $k_B T$, it **is in a sea of valence band electrons** therefore is almost certain to be filled by an electron from valence band.

Fermi level shifts upon doping.



Homework 2

Why is the intrinsic carrier density $\sim 1.45 \times 10^{10} \text{ cm}^{-3}$ considered small?

Assume 

Plot $E_F - E_C$ vs. n . What is the range of $E_F - E_C$ for n from 10^{15} to 10^{17} cm^{-3} ? (What scales make sense? What should be the ranges of the quantities to plot?)

You may simply make a sketch and label several important data points.

Above approximately what value of n (corresponding to what range of $E_F - E_C$) will this approximation become inaccurate? In what way would the actual curve deviate from the approximate equation?

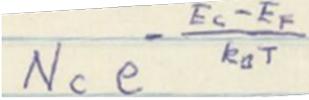
At this point you don't need to consider how the electrons are obtained.

You may find out by reasoning.

You may want to be more thorough: Find from somewhere how to do (or just the result of)

$$n = \int_{E_C}^{\infty} D(E) f(E) dE$$

Then use some tool to plot the curve. But at the end, you need to give explanations.

Now, plot $E_F - E_C$ vs. N_D . Above what N_D will $n = N_D =$  become inaccurate?

Again, you may simply make a sketch and label several important data points.

Homework 2: How we do it?

We will have someone (or a 2-member team) present the answers in class on Tue 9/7 (after Labor Day). You may use the (physical) whiteboard or a ppt.

The criterion for a good job is whether your classmates can learn something.

If you (or your team) would like to present, volunteer now or email me **by 9 pm on Wed 9/1**.

The earliest responder will present.

If you took ECE 634, please volunteer later, not this time.

If you volunteered to present HW1, you may still volunteer, but will be selected to present only in case there are no other vols.

Class canceled on Thu 9/2.