

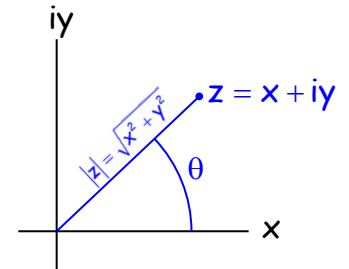
Essential Modern Physics Knowledge

COMPLEX NUMBERS

For $z = x + iy$, the complex conjugate is $z^* = x - iy$ and the absolute value is the distance on the complex plane from the origin to the point z .

$$|z|^2 = zz^* = (x + iy)(x - iy) = x^2 + y^2$$

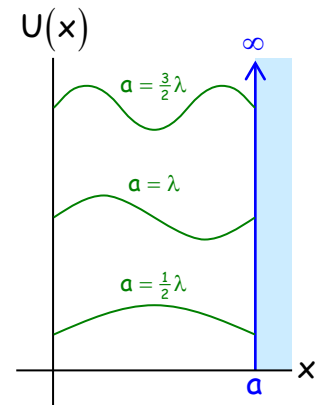
We also utilize Euler's formula stating that $e^{\pm i\theta} = \cos\theta \pm i\sin\theta$.



PARTICLE IN A BOX: ALLOWED ENERGY STATES

For a quantum particle of energy, E , in a potential box where $U(x) = 0$ for $0 < x < a$, it can only exist between $x = 0$ and $x = a$ (since $E = K + U$ and $U = \infty$ outside of $0 < x < a$). **A quantum particle is described by a wave function** that can exist in the box at only certain wavelengths (λ , first three shown) the wave function must be zero at the sides ($x = 0$ & $x = a$).

For a standing wave, $\psi(x) = A\sin(kx) + B\cos(kx)$, this requires that $ka = n\pi$ where $n = 1, 2, 3, \dots$ and $k = \frac{2\pi}{\lambda}$ is the wave number



*** Other than saying a quantum particle is described by a wave, this is just math! ***

The physics comes in with de Broglie:

$$p = \frac{h}{\lambda} = \hbar k \text{ for } k = \frac{2\pi}{\lambda} \text{ and } \hbar = \frac{h}{2\pi}$$

KNOW THESE RELATIONSHIPS!

Thus, the allowed momenta of the particle in the box are:

$$a = \frac{n}{2}\lambda = \frac{n\pi}{k} = \frac{n\pi\hbar}{p} \Rightarrow p = \frac{n\pi\hbar}{a}$$

BE ABLE TO FIGURE THESE OUT

Since the energy of the particle is purely kinetic ($U = 0$), $E = p^2/2m$ gives the allowed energies:

BE ABLE TO DERIVE THIS.

$$E = n^2 \frac{\pi^2 \hbar^2}{2ma^2}, \quad n = 1, 2, 3, \dots$$

TZDII (7.23)

PROBABILITY DENSITY, NORMALIZATION, & EXPECTATION VALUE

$$|\Psi(\vec{r}, t)|^2 = \text{probability (volume) density for finding particle at } \vec{r} \quad \text{TZDII (6.15)}$$

$$\text{Prob. of finding particle between } x_1 \text{ \& } x_2 = \int_{x_1}^{x_2} |\psi(x)|^2 dx \approx |\psi(x = x_1)|^2 \Delta x$$

UNDERSTAND WHY INTEGRAL IS APPROXIMATED BY A PRODUCT.

Normalization

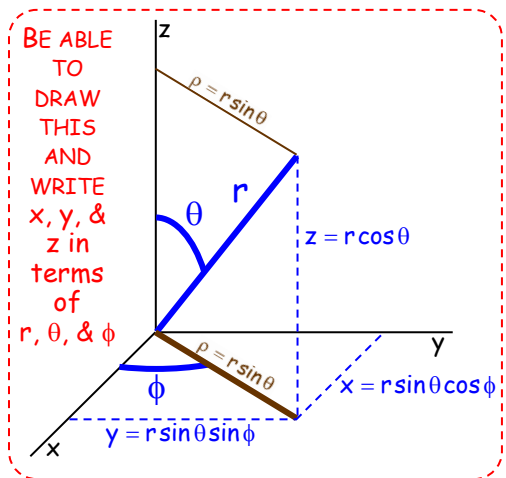
$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

TZDII (7.55)

CARTESIAN COORDINATES GO FROM $-\infty$ TO $+\infty$

The expectation value (value expected after many measurements) of $f(x)$ with a probability density $|\psi(x)|^2$ is

$$\int f(x) |\psi(x)|^2 dx = \int f(x) p(x) dx \quad \text{TZDII (7.69)}$$



3-D SCHRÖDINGER EQUATION

For the hydrogen, we assume a purely radial potential due to the charge of the proton (PE = force x distance).

$$U(r) = -\frac{ke^2}{r}$$

The electron's energy can only be multiples of the Rydberg Energy as shown in TZDII equations 5.22 and 5.23.

$$E = -\frac{m_e (ke^2)^2}{2\hbar^2} \frac{1}{n^2} = -\frac{E_R}{n^2} = -\frac{13.6}{n^2} \text{ eV} \quad \text{KNOW THIS.}$$

Separation of Variables

Assume that the wave function of the electron can be written as a product

$$\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$$

Substituting this into the Schrödinger equation and setting

$$\text{Function of } \phi = \text{Functions of } r \text{ and } \theta = -m^2$$

$$\text{Function of } \theta = \text{Function of } r = -k = -\ell(\ell + 1)$$

HAVE A CONCEPTUAL UNDERSTANDING OF THIS PROCESS.

Yields three differential equations, one in each variable that can be solved for various values of n , m and ℓ .

The ϕ and θ solutions depending on m and ℓ are the Spherical Harmonics with the θ solutions given in Table 8.1 as the Associated Legendre Functions.

The R solutions depending on n and ℓ are given in table 8.2. The normalization of these equations requires that the electron be found within a spherical volume, thus the differential volume element (supplied by the normalization of the θ and ϕ solutions in the full wave function) becomes $4\pi r^2 dr$, giving

$$\text{Prob. of finding } e^- \text{ in a spherical volume} = \int_{r_1}^{r_2} 4\pi r^2 |R(r)|^2 dr$$

Normalization

$$\int_0^\infty 4\pi r^2 |R(r)|^2 dr = 1$$

TZDII (8.84)

r IN SPHERICAL GOES FROM 0 TO ∞

Know how to demonstrate a function is a solution to a differential equation.

QUANTUM NUMBERS GIVE **PHYSICAL QUANTITIES** (THAT WE CAN MEASURE IN THE LAB!)

Principle Quantum Number, n gives the energy of a state:

$n = 1, 2, 3, \dots$

$$E_n = -\frac{1}{2} \frac{m_e (ke^2)^2}{n^2 \hbar^2} = \frac{-13.6 \text{ eV}}{n^2}$$

Angular Momentum Quantum Number, ℓ gives magnitude of the angular momentum:

$\ell = 0, 1, 2, 3, \dots, (n - 1)$

$$|\vec{L}| = \hbar \sqrt{\ell(\ell + 1)}$$

The orbitals are named for the ℓ values,

- s: $\ell = 0$ = sharp
- p: $\ell = 1$ = principle
- d: $\ell = 2$ = diffuse
- f: $\ell = 3$ = fundamental

} Named for spectral line classifications

Magnetic Quantum Number, m gives the z-component of the angular momentum:

$m = -\ell, \dots, 0, \dots, \ell$

$$L_z = m\hbar$$

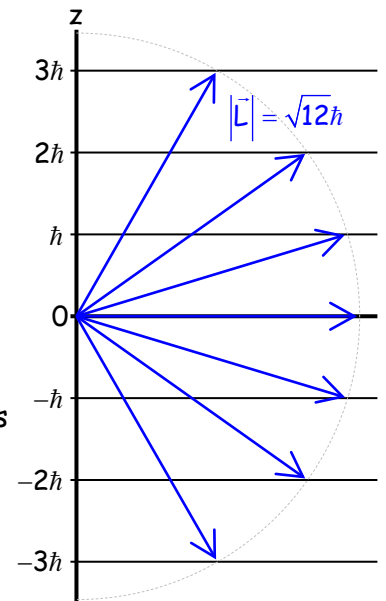
Spin Quantum Number, m_s gives the z-component of the spin angular momentum:

$m_s = \pm \frac{1}{2}$

$$S_z = m_s \hbar$$

Magnitude of the Spin Angular Momentum is given by S and s :

$$|\vec{S}| = \hbar \sqrt{s(s + 1)} = \frac{\sqrt{3}}{2} \hbar, \quad s = \frac{1}{2}$$

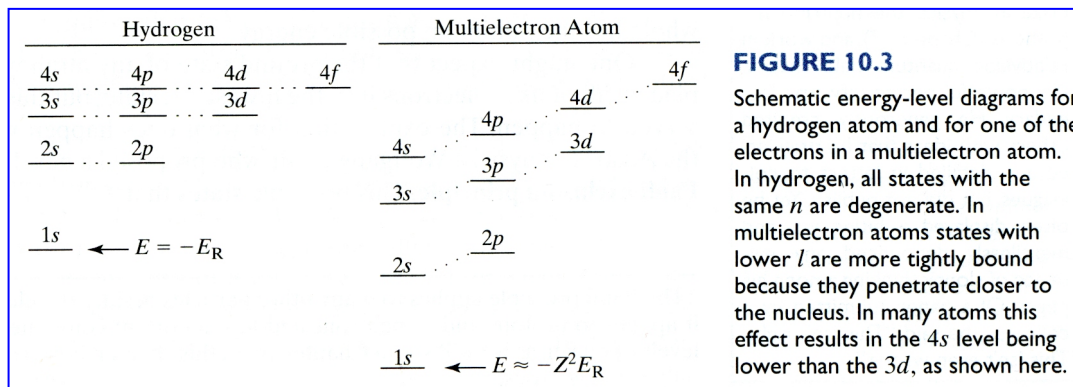


ATOMS AND MOLECULES

The independent particle approximation knits together the potentials of the innermost electron ($-Zke^2/r$) and the outermost ($-ke^2/r$) with Z_{eff} which accounts for electron shielding.

$$U_{\text{Multielectron}}(r) = -Z_{\text{eff}} \frac{ke^2}{r} \quad E_{\text{Multielectron}}(r) = -Z_{\text{eff}}^2 \frac{E_R}{n^2}$$

This makes the energy slightly different for the s, p, d, and f orbital levels.



ATOMS AND MOLECULES

As the number of protons increases in heavier nuclei, the electrons fill higher energy levels.

- The structure of the Periodic Table reflects the structure of electron energy levels

s: $2e^-$, p: $6e^-$, d: $10e^-$, f: $14e^-$

n	s-shell		d and f shells filling										p-shell filling					
1	H																	He
2	Li	Be																Ne
3	Na	Mg																Ar
4/3	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5/4	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6/5/4	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7/6/5	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og

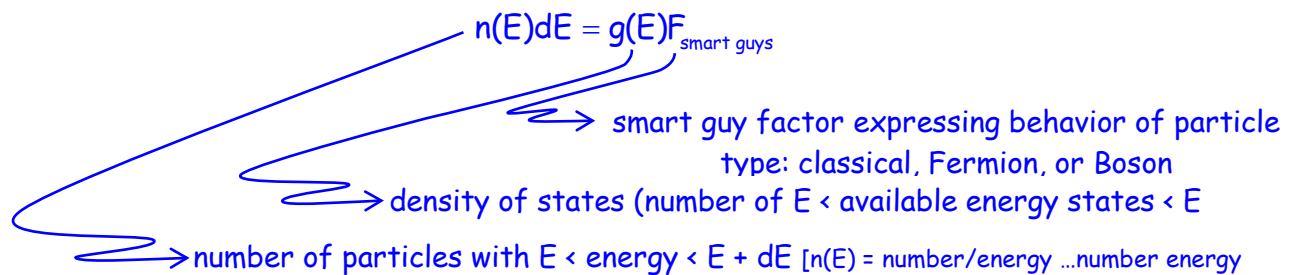
	f2	f3	f4	f5	f6	f7	f8	f9	f10	f11	f12	f13	f14	d1	
4	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Lanthanides: Rare Earths
5	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	Actinides

- electrons in inner shells shield nuclear charge from outer electrons ($\approx 1 e$ of charge)
- electrons in the same shell shield charge from each other ($\approx \frac{1}{2} e$ of charge)
- Elements with full shells (e.g. He, Ca, Zn, Kr) are the least chemically active in each row
- Elements one electron from full (Cl, Br) bind to fill that shell (high electron affinity)
- Elements with a single (or few) electrons in an outer shell (Na, Li) are easily ionized

STATISTICAL MECHANICS

Energy Distributions of Particles

To describe how the energy is distributed among particles in large collections (gases, liquids and solids), physicists developed different energy distributions based on the types of particles



Maxwell-Boltzmann Statistics: Classical Particles

Classical particles are distinguishable, only interact with each other through elastic collisions and are at a low enough density that the wave functions don't overlap.

The mean square is the "average" physicists use since it relates to kinetic energy

$$\frac{1}{2}mv^2 = \frac{3}{2}kT$$

Classical vs. Quantum Statistics

Quantum statistics must be used if the particle wave functions overlap.

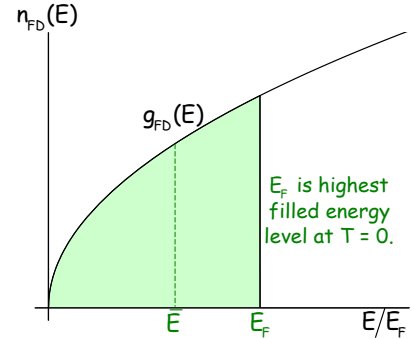
Fermi-Dirac Statistics: Fermion Quantum Particles

Fermions have $\frac{1}{2}$ -integer spins and obey the Pauli Exclusion Principal stating that only one can occupy any quantum state.

Fermi Energy, E_F is the highest occupied state at $T = 0$ and gives a Fermi energy and Fermi velocity

THIS WILL BE GIVEN. KNOW HOW TO GET T_F AND v_F .

$$E_F = \frac{h^2}{8m} \left(\frac{3N}{\pi L^3} \right)^{2/3} \quad T_F = \frac{E_F}{k} \quad v_F = \sqrt{\frac{2E_F}{m}}$$



Fermi-Dirac Factor

The probability that a given state will be occupied is given by F_{FD} that is equal to 1 for $E < E_F$ and zero for $E > E_F$.

$$F_{FD} = \frac{1}{e^{(E-E_F/kT)} + 1}$$

THIS WILL BE GIVEN. KNOW HOW TO GET ITS VALUES FOR $T = 0$.

Fermi-Dirac Electron Energies

The average energy of the conduction (valence) electrons (all the particles in the green area in the above plot)

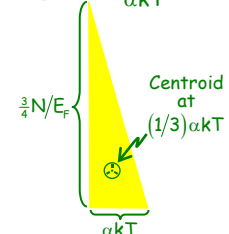
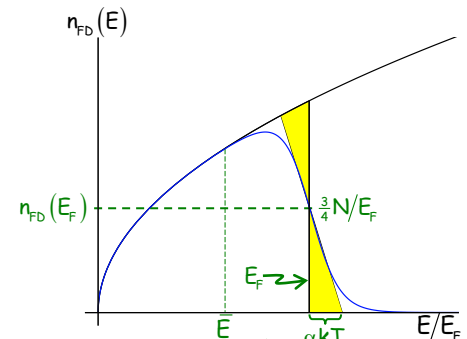
$$\bar{E}_{\text{Conduction } e^-} = \frac{3}{5} E_F$$

The number of particles at the Fermi Energy is ALWAYS

$$n_{FD}(E_F) = \frac{3N}{4E_F}$$

The energy of the particles excited above the Fermi Energy is

$$\bar{E}_{\text{excited}} = E_F + 2 \left(\frac{\pi}{3} kT \right)$$



Bose-Einstein Statistics: Boson Quantum Particles

Bosons have zero or integer spins and do not obey the Pauli Exclusion Principal, thus any number can occupy a given quantum state.

Wien Displacement Law: $\lambda_{\text{max}} T = 2.898 \times 10^{-3} \text{ mK}$

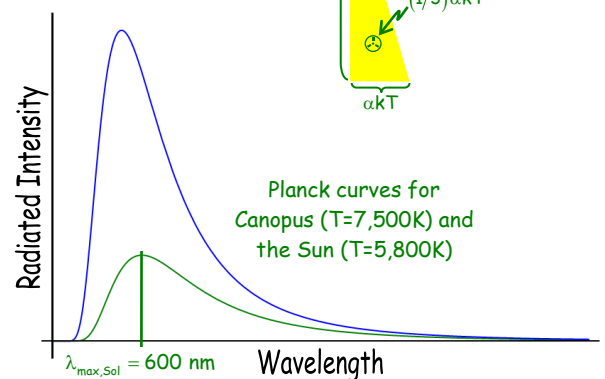
Stefan-Boltzmann Law: $R(T) = \epsilon \sigma T^4$

Where ϵ is the emissivity, the fraction of energy going into radiation, and the Stefan-Boltzmann constant is $\sigma = 5.67 \times 10^{-8} \text{ W}/(\text{m}^2\text{K}^4)$.

Bose-Einstein Factor

No normalization constant because particles can be ephemeral.

$$F_{BE} = \frac{1}{e^{E/kT} - 1}$$



Electrical Conductivity

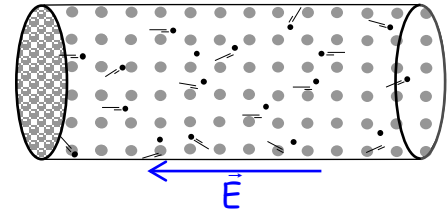
Ohm's Law, in terms of current density (C/m^2), electric field and electrical conductivity.

$$\vec{J} = \sigma \vec{E}$$

Drude model:

$$v_{rms,MB} = \sqrt{\frac{3kT}{m_e}} \quad v_{drift} = a_E \tau = \left(\frac{eE}{m_e}\right) \left(\frac{l}{v_{MB}}\right)$$

$$j_{Drude} = nev_{drift} = ne(a_E \tau) = \left(\frac{ne^2 l}{\sqrt{3m_e k}} T^{-1/2}\right) E$$



10 times too small and $\propto T$

Einstein model:

$$v_{Fermi} = \sqrt{\frac{2E_F}{m_e}} \quad l_{mean\ free\ path} = 100 \frac{l_{interatomic}}{T}$$

10 times too small and $\propto T^{-1}$

Heat Capacity

Energy sorts itself into all the available bins (equipartition). Maxwell-Boltzmann, Fermi-Dirac, and Bose-Einstein statistics were all needed to explain the bins into which energy is sorted as it absorbs energy. This allows us to explain how the temperature rises in a solid.

Region I: MB Statistics

Each quadratic energy term absorbs $\frac{1}{2}kT$ of energy. Ions vibrate in 3-D as if on springs: $3 \times (\frac{1}{2}kx^2 + \frac{1}{2}mv^2)$

$$C_{V,MB} = 3R$$

Region II: BE Statistics

Quantum phonons (bosons) vibrate at an energy, $E_{ph} = \hbar\omega_{ph}$ with $T_E = \hbar\omega_{ph}/k$

$$C_{V,BE} = 3R \left(\frac{T_E}{T}\right)^2 \frac{e^{T_E/T}}{(e^{T_E/T} - 1)^2}$$

Region III: BE Statistics + Debye

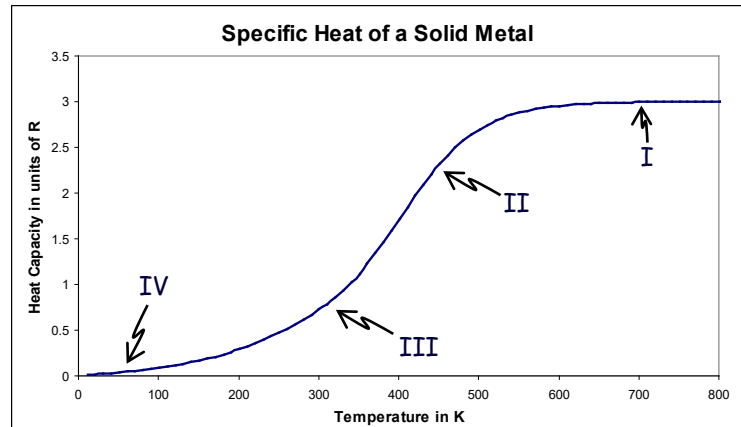
Quantum phonons (bosons) vibrate at a range of energies from zero to a maximum expressed by the Debye temperature, $T_D = \hbar f_D/k$

$$C_{V,D} = \frac{12\pi^4}{5} R \left(\frac{T}{T_D}\right)^3$$

Region IV: FD Statistics

Conduction electrons absorb energy to "leak" above the Fermi Energy expressed by T_F

$$C_{V,FD} = \frac{\pi^2}{2} R \frac{T}{T_F}$$



YOU DON'T NEED TO MEMORIZE ANY OF THE EQUATIONS, BUT BE ABLE TO IDENTIFY WHICH STATISTICS THEY ARE DERIVED FROM, WHY THOSE STATISTICS ARE USED, WHAT EACH EQUATION EXPLAINS AND WHAT ITS LIMITATIONS ARE.