

MODERN PHYSICS FOR ENGINEERS PHY355

INDEX

3D infinite potential box	13	splitting	16, 17, 18	momentum operator	11	simple harmonic motion	12
allowed transitions		states	19	momentum-energy relation	5	spacelike	4
1-electron atoms.....	16	total	5	momentum-temperature		spacetime diagram	4
many-electron atoms	17	zero-point	12	relation	9	spacetime distance	3
Angstrom	21	energy distribution	18	Moseley's equation	9	spacetime interval	4
angular frequency.....	10	expectation value	11	most probable speed.....	18	spectral lines	9
appendix	21	radial	15	Newton's laws	2	spectroscopic symbols	16
atomic mass	2	Fermi energy	19	normalization	11	speed of light	3
average momentum	11	Fermi speed	19	normalization constant	14	spherical coordinates.....	22
Avogadro's number....	18, 21	Fermi temperature.....	19	normalizing functions.....	14	spin angular momentum..	16
binding energy	5	Fermi-Dirac distribution..	19	orbital angular momentum	15	spin-orbit splitting.....	17
binomial expansion	21	fermion	19	order of electron filling....	16	splitting due to spin.....	17
blackbody.....	6	frequency		particle in a box	12, 13	spring harmonics.....	12
Bohr magneton.....	21	angular	10	phase constant.....	10	statistical physics	18
Bohr model	8	fundamental forces.....	2	phase space	2, 19	Stefan-Boltzman law	6
Bohr radius	7	geometry	22	phase velocity	10	temperature	
Boltzmann constant.....	21	Greek alphabet.....	21	photoelectric effect	6	Fermi	19
Bose-Einstein distribution	19	group velocity	10	photon.....	6	temperature and momentum	9
boson	19	harmonic motion	12	momentum.....	4	thermodynamics	2
Bragg's law	9	Heisenberg limit	12	Planck's constant	21	time dilation	3
bremssstrahlung.....	6	Heisenberg uncertainty		Planck's radiation law.....	6	timelike	4
classical physics	1	principle	12	positron.....	6	total angular momentum..	16
classical wave equation ...	10	Hermite functions.....	12	potential barrier	13	total energy	5
Compton effect.....	7	impact parameter	7	probability	11	trig identities.....	22
conservation laws.....	1	infinite square well	12	radial	15	tunneling	13
constants.....	21	intensity of light	6	probability density		uncertainty of waves.....	10
coordinate systems	22	inverse photoelectric effect	6	radial	15	uncertainty principle	12
coordinate transformations	22	kinetic energy	2, 5, 9, 12, 13	probability of location	11	units	21
de Broglie wavelength.....	10	Landé factor	17	proper length	3	velocity addition	3
degenerate energy levels..	13	lattice planes	9	proper time	3	wave functions	10
density of energy states ...	19	laws of thermodynamics	2	quantum numbers	15	wave number	10, 11
density of occupied states	20	length contraction.....	3	radial acceleration	8	wave uncertainties	10
doppler effect.....	5	light wavefront	3	radial probability	15	wavelength	3, 10
Duane-Hunt rule	6	lightlike	4	radial probability density	15	spectrum	21
electron		line spectra	5	radial wave functions	14	waves	
acceleration.....	8	Lorentz force law	2	radiation power	6	envelope	10
angular momentum	7	Lorentz transformation	3	relativity	3	sum	10
filling.....	16	magnetic moment	16	rest energy	5	Wien's constant	6
orbit radius	8	Maxwell speed distribution		root mean square speed ...	18	work function	6
scattering	9	18	Rutherford scattering	8	x-ray	
velocity.....	8	Maxwell's equations	2	Rydberg constant	9, 21	L-alpha waves	9
energy		Maxwell-Boltzmann factor	18	scattering	7, 8	scattering	9
binding	5	mean speed	18	Schrödinger wave equation		Young's double slit	
density of states	19	Michelson-Morley		11, 12	experiment	5
Fermi	19	experiment	3	3D rectangular coord..	13	Zeeman splitting	16, 18
kinetic	5	minimum angle	17	3D spherical coord	14	zero-point energy	12
relation to momentum ..	5	molecular speeds	18				
relativistic kinetic	5	momentum	4				
rest	5	relativistic	4				

CLASSICAL PHYSICS

CLASSICAL CONSERVATION LAWS

Conservation of Energy: The total sum of energy (in all its forms) is conserved in all interactions.

Conservation of Linear Momentum: In the absence of external force, linear momentum is conserved in all interactions (vector relation). naustalgic

Conservation of Angular Momentum: In the absence of external torque, angular momentum is conserved in all interactions (vector relation).

Conservation of Charge: Electric charge is conserved in all interactions.

Conservation of Mass: (not valid)

FUNDAMENTAL FORCES

FORCE	RELATIVE STRENGTH	RANGE
Strong	1	Short, $\sim 10^{-15}$ m
Electroweak		
Electromagnetic	10^{-2}	Long, $1/r^2$
Weak	10^{-9}	Short, $\sim 10^{-15}$ m
Gravitational	10^{-39}	Long, $1/r^2$

ATOMIC MASS

The mass of an atom is its atomic number divided by the product of 1000 times Avogadro's number.

$$\frac{\text{atomic number}}{1000 \times N_a}$$

LORENTZ FORCE LAW

Lorentz force law: $\mathbf{F} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B}$

NEWTON'S LAWS

Newton's first law: Law of Inertia An object in motion with a constant velocity will continue in motion unless acted upon by some net external force.

Newton's second law: The acceleration a of a body is proportional to the net external force \mathbf{F} and inversely proportional to the mass m of the body. $\mathbf{F} = ma$

Newton's third law: law of action and reaction The force exerted by body 1 on body 2 is equal and opposite to the force that body 2 exerts on body 1.

LAWS OF THERMODYNAMICS

First law of thermodynamics: The change in the internal energy ΔU of a system is equal to the heat Q added to the system minus the work W done by the system.

Second law of thermodynamics: It is not possible to convert heat completely into work without some other change taking place.

Third law of thermodynamics: It is not possible to achieve an absolute zero temperature.

Zeroth law of thermodynamics: If two thermal systems are in thermodynamic equilibrium with a third system, they are in equilibrium with each other.

KINETIC ENERGY

The kinetic energy of a particle (ideal gas) in equilibrium with its surroundings is:

$$K = \frac{3kT}{2}$$

PHASE SPACE

A six-dimensional pseudospace populated by particles described by six position and velocity parameters:

position: (x, y, z) velocity: (v_x, v_y, v_z)

RELATIVITY

WAVELENGTH 1

$$c = \frac{1}{\sqrt{\mu_0 \epsilon_0}} = \lambda v$$

$$1\text{Å} = 10^{-10}\text{m}$$

c = speed of light 2.998×10^8 m/s
 λ = wavelength [m]
 v = (nu) radiation frequency [Hz]
 Å = (angstrom) unit of wavelength equal to 10^{-10} m
 m = (meters)

Michelson-Morley Experiment indicated that light was not influenced by the “flow of ether”.

LORENTZ TRANSFORMATION

Compares position and time in two coordinate systems moving with respect to each other along axis x.

$$x' = \frac{x - vt}{\sqrt{1 - v^2/c^2}}$$

$$t' = \frac{t - vx/c^2}{\sqrt{1 - v^2/c^2}}$$

v = velocity of (x',y',z') system along the x-axis. [m/s]

t = time [s]

c = speed of light 2.998×10^8 m/s

$$\text{or with } \beta = \frac{v}{c} \text{ and } \gamma = \frac{1}{\sqrt{1 - v^2/c^2}}$$

$$\text{so that } x' = \gamma(x - vt) \text{ and } t' = \gamma(t - \beta x/c)$$

LIGHT WAVEFRONT

Position of the wavefront of a light source located at the origin, also called the **spacetime distance**.

$$x^2 + y^2 + z^2 = c^2 t^2$$

Proper time T_0 The elapsed time between two events occurring at the same position in a system as recorded by a stationary clock in the system (shorter duration than other times). Objects moving at high speed age less.

Proper length L_0 a length that is not moving with respect to the observer. The proper length is longer than the length as observed outside the system. Objects moving at high speed become longer in the direction of motion.

TIME DILATION

Given two systems moving at great speed relative to each other; the time interval between two events occurring at the same location as measured within the same system is the **proper time** and is shorter than the time interval as measured outside the system.

$$T = \frac{T'_0}{\sqrt{1 - v^2/c^2}} \quad \text{or} \quad T' = \frac{T_0}{\sqrt{1 - v^2/c^2}} \quad \text{where:}$$

T'_0, T_0 = the proper time (shorter). [s]

T, T' = time measured in the other system [m]

v = velocity of (x',y',z') system along the x-axis. [m/s]

c = speed of light 2.998×10^8 m/s

LENGTH CONTRACTION

Given an object moving with great speed, the distance traveled as seen by a stationary observer is L_0 and the distance seen by the object is L' , which is contracted.

$$L_0 = \frac{L'}{\sqrt{1 - v^2/c^2}} \quad \text{where:}$$

L_0 = the **proper length** (longer). [m]

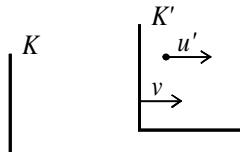
L' = contracted length [m]

v = velocity of (x',y',z') system along the x-axis. [m/s]

c = speed of light 2.998×10^8 m/s

RELATIVISTIC VELOCITY ADDITION

Where frame K' moves along the x-axis of K with velocity v , and an object moves along the x-axis with velocity u_x' with respect of K' , the velocity of the object with respect to K is u_x .



$$u_x = \frac{u'_x + v}{1 + (v/c^2)u'_x}$$

If there is u_y' or u_z' within the K' frame then

$$u_y = \frac{u'_y}{\gamma[1 - (v/c^2)u'_x]} \quad \text{and} \quad u_z = \frac{u'_z}{\gamma[1 - (v/c^2)u'_x]}$$

u_x = velocity of an object in the x direction [m/s]

v = velocity of (x',y',z') system along the x-axis. [m/s]

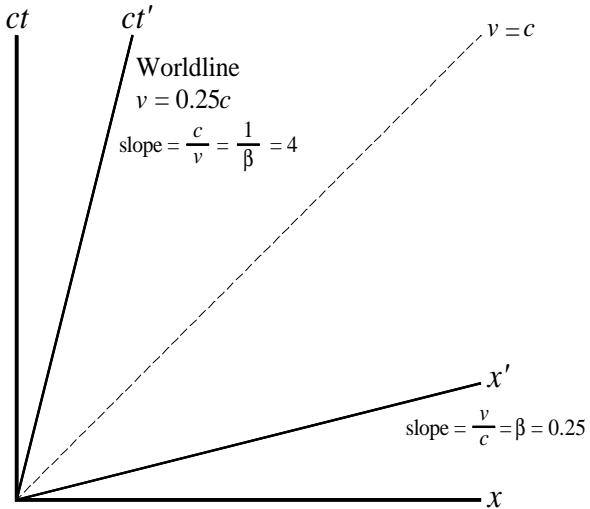
c = speed of light 2.998×10^8 m/s

$$\gamma = 1/\sqrt{1 - v^2/c^2}$$

For the situation where the velocity u with respect to the K frame is known, the relation may be rewritten exchanging the primes and changing the sign of v .

SPACETIME DIAGRAM

The diagram is a means of representing events in two systems. The horizontal x axis represents distance in the K system and the vertical ct axis represents time multiplied by the speed of light so that it is in units of distance as well. A point on the diagram represents an event in terms of its location in the x direction and the time it takes place. So points that are equidistant from the x axis represent simultaneous events.



A system K' traveling in the x direction at $\frac{1}{4}$ the speed of light is represented by the line ct' in this example, and is called a *worldline*. The line represents travel from one location to another over a period of time. The slope of the line is proportional to the velocity. A line with a slope of 1 (dashed line in illustration) indicates travel at the speed of light, so no worldline can have a slope less than 1. A straight line indicates zero acceleration. Simultaneous events occurring at $t = t' = 0$ in the K' system may be represented by points along the x' axis. Other simultaneous events in the K' system will be found on lines parallel to the x' axis.

SPACETIME INTERVAL Ds

The quantity Δs^2 is invariant between two frames of reference with relative movement along the x -axis.

$$s^2 = x^2 - (ct)^2 = x'^2 - (ct')^2$$

Two events occurring at different times and locations in the K -frame may be characterized by their Δs^2 quantity.

$$\Delta s^2 = \Delta x^2 - (c\Delta t)^2$$

lightlike - $Ds^2 = 0$: In this case, $\Delta x^2 = c^2\Delta t^2$, and the two events can only be connected by a light signal.

spacelike - $Ds^2 > 0$: In this case, $\Delta x^2 > c^2\Delta t^2$, and there exists a K' -frame in which the two events occur simultaneously but at different locations.

timelike - $Ds^2 < 0$: In this case, $\Delta x^2 < c^2\Delta t^2$, and there exists a K' -frame in which the two events occur at the same position but at different times. Events can be causally connected.

MOMENTUM p

$$\mathbf{p} = m\mathbf{v} \quad \text{for a photon: } \mathbf{p} = \frac{h\nu}{c}$$

\mathbf{p} = momentum [kg-m/s], convertible to [eV/c] by multiplying by c/q .

m = mass of the object in motion [kg]

\mathbf{v} = velocity of object [m/s]

n = (nu) the frequency of photon light [Hz]

c = speed of light 2.998×10^8 m/s

RELATIVISTIC MOMENTUM p

$$\mathbf{p} = \gamma m\mathbf{u} \quad \text{where:}$$

\mathbf{p} = relativistic momentum [kg-m/s], convertible to [eV/c] by multiplying by c/q .

$$\gamma = 1/\sqrt{1-u^2/c^2}$$

m = mass [kg]

\mathbf{u} = velocity of object [m/s]

DOPPLER EFFECT

Given two systems approaching each other at velocity v , light emitted by one system at frequency n_0 (nu, proper) will be perceived at the higher frequency of n (nu) in the other system.

$$v = \frac{\sqrt{1+\beta}}{\sqrt{1-\beta}} v_0$$

For two systems receding from each other, reverse the signs.

n = (nu) the frequency of emitted light as perceived in the other system [Hz]

n_0 = (nu) the **proper frequency** of the emitted light (lower for approaching systems) [Hz]. Frequency is related to wavelength by $c = \lambda v$.

$\beta = v/c$ where v is the closing velocity of the systems (Use a negative number for diverging systems.) and c is the speed of light 2.998×10^8 m/s

v = velocity of (x',y',z') system along the x-axis. [m/s]

RELATIVISTIC KINETIC ENERGY K

Relativistic kinetic energy is the total energy minus the rest energy. When the textbook speaks of a 50 Mev particle, it is talking about the particle's **kinetic energy**.

$$K = \gamma mc^2 - mc^2 \quad \text{where:}$$

K = relativistic kinetic energy [J], convertible to [eV] by dividing by q .

$$\gamma = 1/\sqrt{1-v^2/c^2}$$

m = mass [kg]

c = speed of light 2.998×10^8 m/s

REST ENERGY E_0

Rest energy is the energy an object has due to its mass.

$$E_0 = mc^2$$

TOTAL ENERGY E

Total energy is the kinetic energy plus the rest energy. When the textbook speaks of a 50 Mev particle, it is talking about the particle's **kinetic energy**.

$$E = K + E_0 \quad \text{or} \quad E = \gamma mc^2 \quad \text{where:}$$

E = total energy [J], convertible to [eV] by dividing by q .

K = kinetic energy [J], convertible to [eV] by dividing by q .

E_0 = rest energy [J], convertible to [eV] by dividing by q .

$$\gamma = 1/\sqrt{1-v^2/c^2}$$

m = mass [kg]

c = speed of light 2.998×10^8 m/s

MOMENTUM-ENERGY RELATION

$$(\text{energy})^2 = (\text{kinetic energy})^2 + (\text{rest energy})^2$$

$$E^2 = p^2 c^2 + m^2 c^4 \quad \text{where:}$$

E = total energy (Kinetic + Rest energies) [J]

p = momentum [kg-m/s]

m = mass [kg]

c = speed of light 2.998×10^8 m/s

BINDING ENERGY

- the potential energy associated with holding a system together, such as the coulomb force between a hydrogen proton and its electron
- the difference between the rest energies of the individual particles of a system and the rest energy of a the bound system
- the work required to pull particles out of a bound system into free particles at rest.

$$E_B = \sum_i m_i c^2 - M_{\text{bound system}} c^2$$

for hydrogen and single-electron ions, the binding energy of the electron in the ground state is

$$E_B = \frac{m Z^2 e^4}{2 \hbar^2 (4 \pi \epsilon_0)^2}$$

E_B = binding energy (can be negative or positive) [J]

m = mass [kg]

Z = atomic number of the element

$e = q$ = electron charge [c]

\hbar = Planck's constant divided by 2π [J-s]

ϵ_0 = permittivity of free space 8.85×10^{-12} F/m

c = speed of light 2.998×10^8 m/s

LINE SPECTRA

Light passing through a diffraction grating with thousands of ruling lines per centimeter is diffracted by an angle θ .

$$d \sin \theta = n\lambda$$

The equation also applies to **Young's double slit experiment**, where for every integer n , there is a lighting maxima. The off-center distance of the maxima is $y = l \tan \theta$

d = distance between rulings [m]

θ = angle of diffraction [degrees]

n = the order number (integer)

λ = wavelength [m]

l = distance from slits to screen [m]

WIEN'S CONSTANT

The product of the wavelength of peak intensity λ [m] and the temperature T [K] of a blackbody. A **blackbody** is an ideal device that absorbs all radiation falling on it.

$$\lambda_{\max} T = 2.898 \times 10^{-3} \text{ m} \cdot \text{K}$$

STEFAN-BOLTZMANN LAW

May be applied to a **blackbody** or any material for which the emissivity is known.

$$R(T) = \epsilon \sigma T^4 \quad \text{where:}$$

$R(T)$ = power per unit area radiated at temperature T [W/m²]

ϵ = emissivity ($\epsilon = 1$ for ideal **blackbody**)

σ = constant $5.6705 \times 10^{-8} \text{ W}/(\text{m}^2 \cdot \text{K}^4)$

T = temperature (K)

PLANCK'S RADIATION LAW

$$I(\lambda, T) = \frac{2\pi c^2 h}{\lambda^5} \frac{1}{e^{hc/\lambda kT} - 1}$$

where:

$I(\lambda, T)$ = light intensity [W/(m² · λ)]

λ = wavelength [m]

T = temperature [K]

c = speed of light $2.998 \times 10^8 \text{ m/s}$

h = Planck's constant $6.6260755 \times 10^{-34} \text{ J-s}$

k = Boltzmann's constant $1.380658 \times 10^{-23} \text{ J/K}$

positron – A particle having the same mass as an electron but with a positive charge

bremssstrahlung – from the German word for *braking radiation*, the process of an electron slowing down and giving up energy in photons as it passes through matter.

PHOTON

A photon is a massless particle that travels at the speed of light. A photon is generated when an electron moves to a lower energy state (orbit).

Photon energy: $E = h\nu = pc$ [Joules]

Momentum: $p = \frac{h\nu}{c}$ [kg-m/s], convertible to [eV/c] by multiplying by c/q .

Wavelength: $\lambda = \frac{c}{\nu}$ [meters]

h = Planck's constant $6.6260755 \times 10^{-34} \text{ J-s}$

ν = (nu) frequency of the electromagnetic wave associated with the light given off by the photon [Hz]

c = speed of light $2.998 \times 10^8 \text{ m/s}$

PHOTOELECTRIC EFFECT

This is the way the book shows the formula, but it is a units nightmare.

$$\frac{1}{2}mv_{\max}^2 = eV_0 = h\nu - \phi \quad \text{where:}$$

$\frac{1}{2}mv_{\max}^2$ = energy in Joules, but convert to eV for the formula by dividing by q .

eV_0 = potential required to stop electrons from leaving the metal [V]

$h\nu$ = Planck's constant [$6.6260755 \times 10^{-34} \text{ J-s}$] multiplied by the frequency of light [Hz]. This term will need to be divided by q to obtain eV.

ϕ = work function, minimum energy required to get an electron to leave the metal [eV]

INVERSE PHOTOELECTRIC EFFECT

$$eV_0 = h\nu_{\max} = \frac{hc}{\lambda_{\min}} \quad \text{where:}$$

eV_0 = the kinetic energy of an electron accelerated through a voltage V_0 [eV]

$h\nu$ = Planck's constant [$6.6260755 \times 10^{-34} \text{ J-s}$] multiplied by the frequency of light [Hz]. This term will need to be divided by q to obtain eV.

λ_{\min} = the minimum wavelength of light created when an electron gives up one **photon** of light energy [m]

DUANE-HUNT RULE

$$\lambda_{\min} = \frac{1.2398 \times 10^{-6}}{V_0}$$

ELECTRON ANGULAR MOMENTUM

from the Bohr model:

$$L = mvr = n\hbar \quad \text{where:}$$

L = angular momentum [kg-m²/s?]

m = mass [kg]

v = velocity [m/s]

r = radius [m]

n = principle quantum number

\hbar = Planck's constant divided by 2π [J-s]

a_0 BOHR RADIUS [m]

The Bohr radius is the radius of the orbit of the hydrogen electron in the ground state ($n=1$):

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} \quad \text{and for higher states } (n>1): \quad r_n = a_0 n^2$$

a_0 , r_n = Bohr radius 5.29177×10^{-11} m, quantized radius [m]

ϵ_0 = permittivity of free space 8.85×10^{-12} F/m

m_e = electron mass $9.1093897 \times 10^{-31}$ [kg]

$e = q$ = electron charge [c]

n = principle quantum number

\hbar = Planck's constant divided by 2π [J-s]

IMPACT PARAMETER b

The impact parameter b is the distance that a bombarding particle deviates from the direct-hit approach path, and is related to the angle θ at which it will be deflected by the target particle.

$$b = \frac{Z_1 Z_2 e^2}{8\pi\epsilon_0 K} \cot \frac{\theta}{2}$$

b = direct path deviation [m]

Z_1 = atomic number of the incident particle

Z_2 = atomic number of the target particle

$e = q$ = electron charge [c]

ϵ_0 = permittivity of free space 8.85×10^{-12} F/m

K = kinetic energy of the incident particle Z_1

θ = angle of particle Z_1 deflection or **scattering**

HEAD-ON SCATTERING

When a particle of kinetic energy K and atomic number Z_1 is fired directly at the nucleus, it approaches to r_{\min} before reversing direction. The entire kinetic energy is converted to Coulomb potential energy. Since r_{\min} is measured to the center of the particles, they will just touch when r_{\min} is the sum of their radii.

$$r_{\min} = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 K}$$

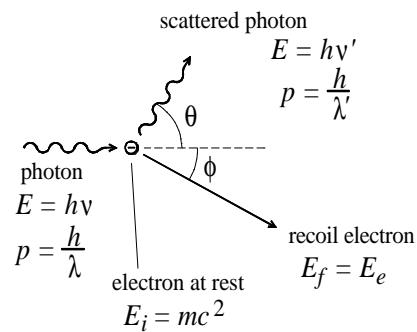
r_{\min} = particle separation (measured center to center) at the time that the bombarding particle reverses direction [m]

other variables are previously defined

COMPTON EFFECT

The scattering of a photon due to collision with a single electron results in a new wavelength λ' and a directional change of $\angle\theta$ and is described by the following relation:

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{mc} (1 - \cos\theta)$$



The ϕ relations come from the conservation of momentum:

$$p_x : \frac{h}{\lambda} = \frac{h}{\lambda'} \cos\theta + p_e \cos\phi$$

$$p_y : \frac{h}{\lambda} \sin\theta = p_e \sin\phi$$

RUTHERFORD SCATTERING

A particle of kinetic energy K and atomic number Z_1 when fired at a target film of thickness t and atomic number Z_2 , will be deflected by an angle θ .

$$N(\theta) = \frac{N_i nt}{16} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{Z_1^2 Z_2^2}{r^2 K^2 \sin^4(\theta/2)}$$

$N(\theta)$ = number of particles scattered per unit area [m^{-2}]

θ = angle of particle Z_1 deflection or **scattering**

N_i = total number of incident particles [kg]

n = number of atoms per unit volume [m^{-3}] $n = \frac{\rho N_A N_M}{M_g}$

where ρ is density [g/m^3], N_A is Avogadro's number, N_M is the number of atoms per molecule, and M_g is the gram-molecular weight [g/mole].

t = thickness of the target material [m]

$e = q$ = electron charge [c]

ϵ_0 = permittivity of free space $8.85 \times 10^{-12} \text{ F/m}$

Z_1 = atomic number of the incident particle

Z_2 = atomic number of the target particle

r = the radius at which the angle θ is measured [m]

K = kinetic energy of the incident particle Z_1

PROBABILITY OF A PARTICLE SCATTERING BY AN ANGLE GREATER THAN q

$$f = \pi n t \left(\frac{Z_1 Z_2 e^2}{8\pi\epsilon_0 K} \right)^2 \cot^2 \frac{\theta}{2}$$

f = the probability (a value between 0 and 1)

n = number of atoms per unit volume [m^{-3}] $n = \frac{\rho N_A N_M}{M_g}$

where ρ is density [g/m^3], N_A is Avogadro's number, N_M is the number of atoms per molecule, and M_g is the gram-molecular weight [g/mole].

t = thickness of the target material [m]

Z_1 = atomic number of the incident particle

Z_2 = atomic number of the target particle

$e = q$ = electron charge [c]

ϵ_0 = permittivity of free space $8.85 \times 10^{-12} \text{ F/m}$

K = kinetic energy of the incident particle Z_1

θ = angle of particle Z_1 deflection or **scattering**

Alpha particle: $Z=2$

Proton: $Z=1$

ELECTRON VELOCITY

This comes from the **Bohr model** and only applies to atoms and ions having a single electron.

$$v_n = \frac{1}{n} \frac{Ze^2}{4\pi\epsilon_0\hbar} = \frac{e\sqrt{Z}}{2\sqrt{\pi\epsilon_0 m_e r}}$$

v = electron velocity [m/s]

Z = atomic number or number of protons in the nucleus

$e = q$ = electron charge [c]

n = the electron orbit or shell

ϵ_0 = permittivity of free space $8.85 \times 10^{-12} \text{ F/m}$

m_e = mass of an electron $9.1093897 \times 10^{-31} \text{ kg}$

\hbar = Planck's constant divided by 2π [J-s]

r = the radius of the electron's orbit [m]

ELECTRON ORBIT RADIUS

This comes from the **Bohr model** and only applies to atoms and ions having a single electron.

$$r_n = \frac{4\pi\epsilon_0 n^2 \hbar^2}{m_e Ze^2}$$

r_n = electron orbit radius in the n shell [m]

other variables are previously defined

a_r RADIAL ACCELERATION

a_r = the radial acceleration of an orbiting electron [m/s^2]

v = tangential velocity of the electron [m/s]

$$a_r = \frac{v^2}{r}$$

r = electron orbit radius [m]

R_Y RYDBERG CONSTANT

R_{∞} is used in the **Bohr model** and is a close approximation assuming an infinite nuclear mass. R is the adjusted value. These values are appropriate for hydrogen and single-electron ions.

$$R = \frac{\mu_e Z^2 e^4}{4\pi c \hbar^3 (4\pi\epsilon_0)^2} \quad \text{where } \mu_e = \frac{m_e M}{m_e + M}$$

R_{∞} = Rydberg constant $1.09678 \times 10^7 \text{ m}^{-1}$ ($1.096776 \times 10^7 \text{ m}^{-1}$ for hydrogen)

μ_e = adjusted electron mass

Z = atomic number, or number of protons in the nucleus

ϵ_0 = permittivity of free space $8.85 \times 10^{-12} \text{ F/m}$

c = speed of light $2.998 \times 10^8 \text{ m/s}$

\hbar = Planck's constant divided by 2π [J-s]

m_e = mass of an electron $9.1093897 \times 10^{-31} \text{ kg}$

M = mass of the nucleus (essentially the same as the mass of the atom \Rightarrow atomic number $\times 1.6605 \times 10^{-27}$) [kg]

L_a MOSELEY'S EQUATION

British physicist, Henry Moseley determined this equation experimentally for the frequency of L_a x-rays. L_a waves are produced by an electron decaying from the n=3 orbit to the n=2 or L orbit.

$$v_{L_a} = \frac{5}{36} c R (Z - 7.4)$$

n = (nu) frequency [Hz]

c = speed of light $2.998 \times 10^8 \text{ m/s}$

R = Adjusted Rydberg constant (see above) [m^{-1}]

Z = atomic number or number of protons in the nucleus

SPECTRAL LINES

This formula gives the wavelength of light emitted when an electron in a single-electron atom or ion decays from orbit n_u to n_l .

$$\frac{1}{\lambda} = Z^2 R \left(\frac{1}{n_l^2} - \frac{1}{n_u^2} \right)$$

λ = wavelength [m]

Z = atomic number or number of protons in the nucleus

R = Rydberg constant ($1.096776 \times 10^7 \text{ m}^{-1}$ for hydrogen)

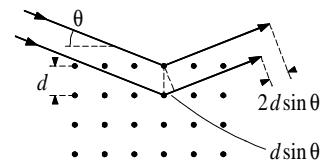
n_l = the lower electron orbit number

n_u = the upper electron orbit number

BRAGG'S LAW

X-ray Scattering - X-rays reflected from a crystal experience interference effects since rays reflecting from the interior of the material take a longer path than those reflecting from the surface. Compare to ELECTRON SCATTERING below.

$$n\lambda = 2d \sin \theta$$



n = order of reflection (number of lattice planes in depth)

λ = wavelength of the incident wave [m]

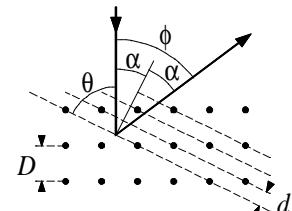
d = distance between **lattice planes** (interatomic spacing in this case) [m]

θ = angle of incidence; the angle between the incident wave and the surface of the material

ELECTRON SCATTERING

Electrons directed into a crystalline material are scattered (reflected) at various angles depending on the arrangement of **lattice planes**. There is more than one set of lattice planes in a crystal. The technique can be used to explore the characteristics of a material. Compare to BRAGG'S LAW above.

$$n\lambda = D \sin \phi$$



n = order of reflection (number of lattice planes in depth)

λ = wavelength of the incident wave [m]

D = interatomic spacing [m]

d = distance between lattice planes [m]

ϕ = angle between the incident and reflected waves

K CLASSICAL KINETIC ENERGY

Two expressions for kinetic energy:

$$\frac{p^2}{2m} = K = \frac{3}{2} kT$$

lead to a **momentum-temperature relation** for particles:

$$p^2 = 3mkT$$

p = momentum [kg-m/s]

m = particle mass [kg]

K = kinetic energy [J]

k = Boltzmann's constant $1.380658 \times 10^{-23} \text{ J/K}$

T = temperature in Kelvin ($273.15 \text{ K} = 0^\circ \text{C}$, $\Delta K = \Delta \text{C}$)

(see page 5 for RELATIVISTIC KINETIC ENERGY)

WAVES

Y WAVE FUNCTIONS

Classical Wave Equation

We did not use this equation:

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2}$$

This **wave function** fits the classical form, but is not a solution to the Schrödinger equation:

$$\Psi(x,t) = A \sin(kx - \omega t + \phi)$$

More **general wave functions** which are solutions to the Schrödinger equation are:

$$\Psi(x,t) = A e^{i(kx - \omega t)} = A [\cos(kx - \omega t) + i \sin(kx - \omega t)]$$

k WAVE NUMBER

A component of a wave function representing the **wave density** relative to distance, in units of radians per unit distance [rad/m].

$$k = \frac{2\pi}{\lambda}$$

w ANGULAR FREQUENCY

A component of a wave function representing the **wave density** relative to time (better known as frequency), in units of radians per second [rad/s].

$$\omega = \frac{2\pi}{T}$$

v_{ph} PHASE VELOCITY

The velocity of a point on a wave, e.g. the velocity of a wave peak
[m/s].

$$v_{\text{ph}} = \frac{\lambda}{T} = \frac{\omega}{k}$$

f PHASE CONSTANT

The angle by which the wave is offset from zero, i.e. the angle by which the wave's zero amplitude point is offset from $t=0$. [radians or degrees].

Y SUM OF TWO WAVES

(see also WaveSummingExample.pdf)

$$\Psi_1 + \Psi_2 = 2A \cos\left(\frac{\Delta k}{2}x - \frac{\Delta \omega}{2}t\right) \underbrace{\cos(k_{\text{av}}x - \omega_{\text{av}}t)}_{\text{internal wave}}$$

A = harmonic amplitude [various units?]

Δk = difference in wave numbers $k_1 - k_2$ [rad/m]

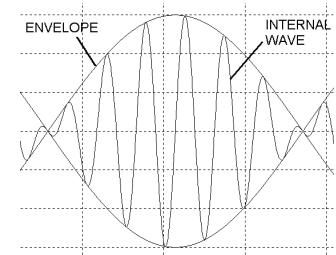
k_{av} = average wave number $(k_1 + k_2)/2$ [rad/m]

$\Delta \omega$ = difference in angular frequencies $\omega_1 - \omega_2$ [rad/s]

ω_{av} = average angular frequency $(\omega_1 + \omega_2)/2$ [rad/s]

x = distance [m]

t = time [s]



Phase Velocity:

$$v_{\text{ph}} = \omega_{\text{av}} / k_{\text{av}}$$

[m/s] velocity of a point on a wave

Group Velocity:

$$u_{\text{gr}} = \Delta \omega / \Delta k$$

[m/s] speed of the envelope

1 de BROGLIE WAVELENGTH

De Broglie extended the concept of waves to all matter.

$$\lambda = \frac{h}{p}$$

λ = wavelength [m]

h = Planck's constant $6.6260755 \times 10^{-34}$ J·s

p = momentum [kg·m/s], convertible to [eV/c] by multiplying by c/q .

WAVE UNCERTAINTIES

This has to do with the effects of combining different waves. In order to know precisely the position of the wave packet envelope (Δx small), we must have a large range of wave numbers (Δk large). In order to know precisely when the wave is at a given point (Δt small), we must have a large range of frequencies ($\Delta \omega$ large). Another result of this relationship, is that an electronic component must have a large bandwidth $\Delta \omega$ in order for its signal to respond in a short time Δt .

$$\Delta k \Delta x = 2\pi$$

$$\Delta \omega \Delta t = 2\pi$$

Δk = the range of wave numbers, see WAVE NUMBER

Δx = the width of the wave envelope

$\Delta \omega$ = the range of wave frequencies

Δt = a time interval

SCHRÖDINGER'S WAVE EQUATION

time-dependent form:

$$K + U = E$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x) \Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$$

time-independent form:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x)$$

$$\text{or } -\frac{\hbar^2}{2m\psi(x)} \frac{d^2 \psi(x)}{dx^2} = E - V(x)$$

\hbar = Planck's constant divided by 2π [J-s]

$\Psi(x,t)$ = wave function

V = voltage; can be a function of space and time (x,t)

m = mass [kg]

Two separate solutions to the time-independent equation have the form:

$$Ae^{ikx} + Be^{-ikx} \quad \text{where } k = \sqrt{2m(E-V)/\hbar}$$

$$\text{or } A\sin(kx) + B\cos(kx)$$

Note that the **wave number** k is consistent in both solutions, but that the constants A and B are **not** consistent from one solution to the other. The values of constants A and B will be determined from **boundary conditions** and will also depend on which solution is chosen.

PROBABILITY

A probability is a value from zero to one. The probability may be found by the following steps:

Multiply the function by its complex conjugate and take the integral from negative infinity to positive infinity with respect to the variable in question, multiply all this by the square of a constant c and set equal to one.

$$c^2 \int_{-\infty}^{\infty} F * F dx = 1$$

Solve for the probability constant c .

$$\text{The probability from } x_1 \text{ to } x_2 \text{ is: } P = c^2 \int_{x_1}^{x_2} F * F dx$$

PROBABILITY OF LOCATION

Given the wave function: $\psi(x,t)$

find the probability that a particle is located between x_1 and x_2 .

Normalize the wave function: $2 \int_0^{\infty} A^2 \psi^2 dx = 1$

with A known, find the probability: $P = \int_{x_1}^{x_2} A^2 \psi^2 dx$

EXPECTATION VALUES

average value:

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x) dx$$

average x^2 value:

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x) x^2 \psi(x) dx$$

\hat{p} MOMENTUM OPERATOR

An **operator** transforms one function into another function. The momentum operator is:

$$\hat{p} = -i\hbar \frac{d}{dx}$$

For example, to find the average momentum of a particle described by wave function ψ :

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \hat{p} \psi dx = \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{d}{dx} \psi \right) dx$$

SIMPLE HARMONIC MOTION

Examples of simple harmonic motion include a mass on a spring and a pendulum. The average potential energy equals the average kinetic energy equals half of the total energy. In simple harmonic motion, k is the spring constant, not the wave number.

$$\text{spring constant } k: \quad \omega = \sqrt{\frac{k}{m}} \quad \text{force: } F = kx$$

$$\text{potential energy } V: \quad V = \frac{1}{2}kx^2$$

Schrödinger Wave Equation for simple harmonic motion: $\frac{d^2\psi}{dx^2} = (\alpha^2 x^2 - \beta)\psi$

$$\text{where } \alpha^2 = \frac{mk}{\hbar^2} \quad \text{and } \beta = \frac{2mE}{\hbar^2}$$

The wave equation solutions are:

$$\psi_n = H_n(x) e^{-\alpha x^2/2}$$

where $H_n(x)$ are polynomials of order n , where $n = 0, 1, 2, \dots$ and x is the variable taken to the power of n . The functions $H_n(x)$ are related by a constant to the *Hermite polynomial functions*.

$$\psi_0 = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2} \quad \psi_1 = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2\alpha} xe^{-\alpha x^2/2}$$

$$\psi_2 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} (2\alpha x^2 - 1) e^{-\alpha x^2/2}$$

$$\psi_3 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}} (x\sqrt{\alpha})(2\alpha x^2 - 3) e^{-\alpha x^2/2}$$

...and they call this simple!

quantized energy levels:

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega$$

The **zero-point energy**, or Heisenberg

limit is the minimum energy allowed by the uncertainty principle; the energy at $n=0$:

$$E_0 = \frac{1}{2} \hbar\omega$$

HEISENBERG UNCERTAINTY PRINCIPLE

These relations apply to **Gaussian wave packets**. They describe the limits in determining the factors below.

$$\Delta p_x \Delta x \geq \hbar/2 \quad \Delta E \Delta t \geq \hbar/2$$

Δp_x = the uncertainty in the momentum along the x -axis

Δx = the uncertainty of location along the x -axis

ΔE = the uncertainty of the energy

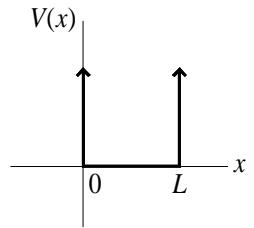
Δt = the uncertainty of time. This also happens to be the particle lifetime. Particles you can measure the mass of ($E=mc^2$) have a long lifetime.

INFINITE SQUARE-WELL POTENTIAL

or "Particle in a Box"

This is a concept that applies to many physical situations.

Consider a two-dimensional box in which a particle may be trapped by an infinite voltage potential on either side. The problem is an application of the **Schrödinger Wave Equation**.



The particle may have various energies represented by waves that must have an amplitude of zero at each boundary 0 and L. Thus, the energies are quantized. The probability of the particle's location is also expressed by a wave function with zero values at the boundaries.

$$\text{Wave function: } \psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right)$$

$$\text{Energy levels: } E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2}$$

Probability of a particle being found between x_1 and x_2 :

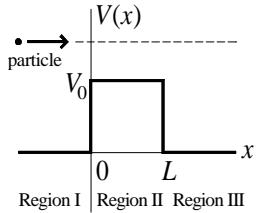
$$P = \int_{x=x_1}^{x_2} \Psi^* \Psi dx$$

$$A = \sqrt{\frac{2}{L}} \text{ normalization constant}$$

$$\text{a useful identity: } \sin^2 \theta = \frac{1}{2}(1 - \cos 2\theta)$$

POTENTIAL BARRIER

When a particle of energy E encounters a barrier of potential V_0 , there is a possibility of either a reflected wave or a transmitted wave.



for $E > V_0$:

$$\text{kinetic energy: } K = E - V_0$$

$$\text{wave number: } k_I = k_{III} = \sqrt{2mE}/\hbar$$

$$k_{II} = \sqrt{2m(E - V_0)}/\hbar$$

$$\text{incident wave: } \phi_I = Ae^{ik_I x}$$

$$\text{reflected wave: } \phi_I = Be^{-ik_I x}$$

$$\text{transmitted wave: } \phi_{III} = Fe^{k_I x}$$

$$\text{trans. probability: } T = \left(1 + \frac{V_0^2 \sin^2(k_{II}L)}{4E(E - V_0)} \right)^{-1}$$

$$\text{reflection probability: } R = 1 - T$$

for $E < V_0$: Classically, it is not possible for a particle of energy E to cross a greater potential V_0 , but there is a quantum mechanical possibility for this to happen called **tunneling**.

$$\text{kinetic energy: } K = V_0 - E$$

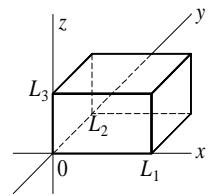
$$\text{wave #, region II: } \kappa = \sqrt{2m(V_0 - E)}/\hbar$$

$$\text{trans. probability: } T = \left(1 + \frac{V_0^2 \sinh^2(\kappa L)}{4E(V_0 - E)} \right)^{-1}$$

$$\text{when } \kappa L \gg 1: T = 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0} \right) e^{-2\kappa L}$$

3D INFINITE POTENTIAL BOX

Consider a three-dimensional box with zero voltage potential inside the box and infinite voltage outside. A particle trapped in the box is described by a wave function and has quantized energy levels.



Time-independent Schrödinger Wave Equation in three dimensions:

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + V\Psi = E\Psi$$

Wave equation for the 3D infinite potential box:

$$\Psi_{n_1 n_2 n_3} = A \sin\left(\frac{n_1 \pi x}{L_1}\right) \sin\left(\frac{n_2 \pi y}{L_2}\right) \sin\left(\frac{n_3 \pi z}{L_3}\right)$$

$$\text{Energy levels: } E_{n_1 n_2 n_3} = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2} \right)$$

Degenerate energy levels may exist—that is, different combinations of n -values may produce equal energy values.

SCHRÖDINGER'S EQUATION – 3D SPHERICAL

spherical coordinate form:

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \Psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \Psi}{\partial \phi^2} + \frac{2m}{\hbar^2} (E - V) \Psi = 0$$

separation of variables using: $\Psi(r, \theta, \phi) = R(r) f(\theta) g(\phi)$

We can obtain a form with terms of g on one side and terms of R and f on the other. These are set equal to the constant m_l^2 . m_l turns out to be an integer.

Another separation is performed for R and f and the constant is $l(l+1)$, where l is an integer. The three equations are:

Azimuthal equation:

$$\frac{1}{g} \frac{d^2 g}{d\phi^2} + m_l^2 = 0 \Rightarrow g = A e^{im_l \phi}$$

Radial equation:

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2m}{\hbar^2} (E - V) R - \frac{l(l+1)}{r^2} R = 0$$

Angular Equation:

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{df}{d\theta} \right) + \left[l(l+1) - \frac{m_l^2}{\sin^2 \theta} \right] f = 0$$

m_l = magnetic quantum number; integers ranging from $-l$ to $+l$

l = orbital angular momentum quantum number

\hbar = Planck's constant divided by 2π [J-s]

E = energy

V = voltage; can be a function of space and time (x, t)

m = mass [kg]

NORMALIZING WAVE FUNCTIONS

To normalize a function, multiply the function by its complex conjugate and by the square of the **normalization constant A** . Integrate the result from $-\infty$ to ∞ and set equal to 1 to find the value of A . The normalized function is the original function multiplied by A .

To normalize the **wave function $\Psi(x)$** :

$$\int_{-\infty}^{\infty} |A\Psi|^2 dx \rightarrow A^2 \int_{-\infty}^{\infty} \Psi^2 dx$$

Where Ψ is an even function, we can simplify to:

$$2A^2 \int_0^{\infty} \Psi^2 dx \text{ and find } A: 2A^2 \int_0^{\infty} \Psi^2 dx = 1$$

Some relations for definite integrals will be useful in solving this equation; see CalculusSummary.pdf page 3.

To normalize the **wave function $\Psi(r)$** , where r is the radius in spherical coordinates:

$$\int_0^{\infty} r^2 |A\Psi|^2 dr \rightarrow A^2 \int_0^{\infty} r^2 \Psi^2 dr = 1$$

Note that we integrate from 0 to ∞ since r has no negative values.

To normalize the **wave function $\Psi(r, \theta, \phi)$** :

$$A^2 \int_0^{\infty} dr r^2 |A\Psi|^2 \int_0^{\pi} d\theta \sin \theta \int_0^{2\pi} d\phi = 1$$

Note that dr , $d\theta$, and $d\phi$ are moved to the front of their respective integrals for clarity.

$R_{nl}(r)$ RADIAL WAVE FUNCTIONS for the hydrogen atom

n	l	$R_{nl}(r)$
1	0	$\frac{2}{a_0^{3/2}} e^{-r/a_0}$
2	0	$\left(w - \frac{r}{a_0} \right) \frac{e^{-r/2a_0}}{(2a_0)^{3/2}}$
2	1	$\frac{r}{a_0} \frac{e^{-r/2a_0}}{\sqrt{3}(2a_0)^{3/2}}$
3	0	$\frac{1}{(a_0)^{3/2}} \frac{2}{81\sqrt{3}} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2} \right) e^{-r/3a_0}$
3	1	$\frac{1}{(a_0)^{3/2}} \frac{4}{81\sqrt{6}} \left(6 - \frac{r}{a_0} \right) \frac{r}{a_0} e^{-r/3a_0}$
3	2	$\frac{1}{(a_0)^{3/2}} \frac{4}{81\sqrt{30}} \frac{r^2}{a_0^2} e^{-r/3a_0}$

a_0 = Bohr radius 5.29177×10^{-11} m

$P(r)dr$ RADIAL PROBABILITY

The radial probability is a value from 0 to 1 indicating the probability of a particle occupying a certain area radially distant from the center of orbit. The value is found by integrating the right-hand side of the expression over the interval in question:

$$P(r) dr = r^2 |R(r)|^2 dr$$

r = orbit radius

$R(r)$ = radial wave function, normalized to unity

$P(r)$ RADIAL PROBABILITY DENSITY

The radial probability density depends only on n and l .

$$P(r) = r^2 |R(r)|^2$$

r = orbit radius

$R(r)$ = radial wave function, normalized to unity

\bar{r} RADIAL EXPECTATION VALUE

average radius (radial wave function):

$$\langle r \rangle = \int_{r=0}^{\infty} r P(r) dr = \int_{r=0}^{\infty} r^3 R(r) dr$$

$P(r)$ = probability distribution function $P(r) = r^2 |R(r)|^2 dr$

$R(r)$ = radial wave function, normalized to unity

ATOMS

QUANTUM NUMBERS

n = **principal quantum number**, shell number, may have values of 1, 2, 3, ...

l = **orbital angular momentum quantum number**, subshell number, may have values of 0 to $n-1$. These values are sometimes expressed as letters: $s=0, p=1, d=2, f=3, g=4, h=5, \dots$

m_l = **magnetic quantum number**, may have integer values from $-l$ to $+l$ for each l . (p251)

m_s = **magnetic spin quantum number**, may have values of $+\frac{1}{2}$ or $-\frac{1}{2}$

Then we introduce these new ones:

s = **intrinsic quantum number**, $s=1/2$ (p238)

j = **total angular momentum quantum number**, $j = l \pm s$, but j is not less than 0. (p257)

m_j = **magnetic angular momentum quantum number**, may have values from $-j$ to $+j$ (p257)

Example, for $n = 3$:

$l =$	0	1			2			
$j =$	1/2	1/2		3/2	3/2		5/2	
$m_j =$	-1/2 +1/2	-1/2 +1/2	-3/2 -1/2 +1/2 +3/2	-3/2 -1/2 +1/2 +3/2			-5/2 -3/2 -1/2 +1/2 +3/2 +5/2	
$m_l =$	0	-1	0	+1	-2	-1	0	+1
$m_s =$	-1/2 +1/2	-1/2 +1/2	-1/2 +1/2	-1/2 +1/2	-1/2 +1/2	-1/2 +1/2	-1/2 +1/2	-1/2 +1/2

L ORBITAL ANGULAR MOMENTUM

Classically, orbital angular momentum is rr or mvr .

The orbital angular momentum L is a vector quantity. Its components are as follows:

Magnitude: $L = \hbar \sqrt{l(l+1)}$

Z-axis value: $L_z = m_l \hbar$

The values of L_x and L_y cannot be determined exactly but obey the following relation:

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

\hbar = Planck's constant divided by 2π [J-s]

l = orbital angular momentum quantum number

m_l = magnetic quantum number; integers ranging from $-l$ to $+l$

The orbital angular momentum quantum number was originally given letter values resulting from early visual observations: sharp, principal, diffuse, fundamental

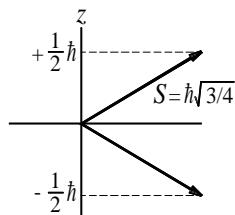
$l = 0 \ 1 \ 2 \ 3 \ 4 \ 5$
s p d f g h

S SPIN ANGULAR MOMENTUM

The spin angular momentum is (insert some illuminating explanation here).

Magnitude:

$$|\mathbf{S}| = \hbar\sqrt{s(s+1)} = \hbar\sqrt{3/4}$$



z component:

$$S_z = m_s \hbar = \pm \hbar / 2$$

J TOTAL ANGULAR MOMENTUM

The vector sum of the orbital angular momentum and the spin angular momentum. This applies to 1-electron and many-electron atoms.

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

J (the magnitude?) is an integer value from $|L-S|$ to $L+S$.

ALLOWED TRANSITIONS

The allowed energy level transitions for 1-electron atoms are

$$\Delta n: \text{any} \quad \Delta l: \pm 1 \quad \Delta m_l: 0, \pm 1 \quad \Delta j: 0, \pm 1$$

ZEEMAN SPLITTING ("ZAY· mahn")

When a single-electron atom is under the influence of an external magnetic field (taken to be in the z -axis direction), each energy level ($n=1, 2, 3, \dots$) is split into multiple levels, one for each quantum number m_l .

The difference in energy is:

$$\Delta E = \mu_B B m_l$$

ΔE = difference in energy between two energy levels [J]

μ_B = Bohr magneton 9.274078×10^{-24} J/T

B = magnetic field [T]

m_l = magnetic quantum number; integers ranging from $-l$ to $+l$

m MAGNETIC MOMENT

Both the magnetic moment \mathbf{m} and the orbital angular momentum \mathbf{L} are vectors:

$$\mathbf{m} = -\frac{e}{2m} \mathbf{L}$$

m = mass of the orbiting particle [kg]

MANY-ELECTRON ATOMS

SPECTROSCOPIC SYMBOLS

The energy state of an atom having 1 or 2 electrons in its outer shell can be represented in the form

$$n^{2s+1} L_j$$

n = shell number

S = intrinsic spin angular momentum quantum number; $1/2$ for a single-electron shell, 0 or 1 ($S_1 + S_2$) for the 2-electron shell

L = angular momentum quantum number; l for single-electron shell, $L_1 + L_2$ for a 2-electron shell, expressed as a capital letter: $S=0, P=1, D=2, F=3, G=4, H=5, I=6$.

j = total angular momentum quantum number $j = l \pm s$. I'm not sure how to tell whether it's plus or minus, but I think it has to be the lower value of j to be in the ground state. j is positive only.

ORDER OF ELECTRON FILLING

Here's a way to remember the order in which the outer shells of atoms are filled by electrons:

Form groups of l -numbers like this. The first group is just the lowest value for l : s . The next value of l is p ; form a new group of p with s . The third value of l is d ; form the third group with d , p , and s . You get a list of groups like this:

s	p	d	f	g
p	d p	d p s	f d p s	g f d p s
d	p s	f d p s	h g f d p s	
f				
g				
h				

Now, in a column, write each group twice beginning with the single s that is the first group.

Next number each s beginning with 1, placing the number in front of the s . This is as far as I have gone with the list at right.

The next step is to number each p beginning with the number 2.

Then number each d beginning with the number 3.

Number each f beginning with 4, and so on.

The result will be the order of filling (there are a few exceptions) and will look like this:

1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 4f 5d
and so on.

1s	2s	p	3s	p	4s	d	5s	f	6s	f	7s
2s		d p	p	4s	p	5s	d	6s	p	7s	
p		f d p s	f	5s	d	6s	p	7s			
d		g f d p s	g	5s	p	6s	f	7s			
f			h g f d p s	h	6s	f					
g				7s							
h											

and so on.

g LANDÉ g FACTOR

A dimensionless number that helps make physics complicated. Used in ANOMALOUS ZEEMAN SPLITTING

$$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

ALLOWED PHOTON TRANSITIONS

The allowed photon energy level transitions for many-electron atoms are

ΔL : ± 1 ΔJ : $0, \pm 1$, but J can't transition from 0 to 0.

ΔS : 0 Δm_s : $0, \pm 1$, but can't transition from 0 to 0 when $\Delta J=0$.

Other transitions are possible—just not likely.

q MINIMUM ANGLE BETWEEN J AND THE Z-AXIS

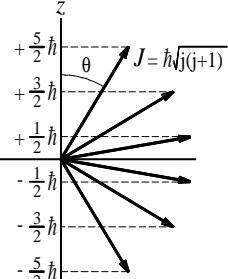
There were exercises where we had to calculate this. I don't know what the significance is. This is done similarly for L and S as well.

Example: $j = \frac{5}{2}$

$$\cos \theta = \frac{j \times \hbar}{\hbar \sqrt{j(j+1)}} \rightarrow$$

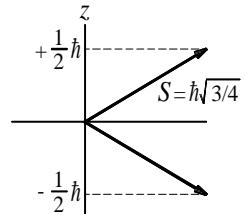
$$\cos^2 \theta = \frac{j^2}{j(j+1)} \rightarrow \cos^2 \theta = \frac{j}{(j+1)}$$

$$\cos \theta = \sqrt{\frac{j}{j+1}}$$



SPLITTING DUE TO SPIN

For each state described by quantum numbers n, l, m_l , there are two states defined by the magnetic spin numbers $m_s = \pm 1/2$. These two levels have the same energy except when the atom is influenced by an external magnetic field.



The lower of the two energy levels is aligned with the magnetic field.

$$|\Delta E| = \frac{hc}{\lambda^2} |\Delta \lambda|$$

ΔE = difference in energy between two (split) energy levels

$$m_s = \pm 1/2 \text{ [J]}$$

$\Delta \lambda$ = difference in wavelengths for the transitions to the ground state for each energy level [m]

λ = wavelength for the transitions to the ground state for the lower of the two energy levels (the greater of the two wavelengths) [m]

$$h = \text{Planck's constant } 6.6260755 \times 10^{-34} \text{ J-s}$$

$$c = \text{speed of light } 2.998 \times 10^8 \text{ m/s}$$

SPIN-ORBIT ENERGY SPLITTING

Spin-orbit energy splitting is the splitting of energy levels caused by an internal magnetic field due to spin. This produces a greater ΔE than the spin splitting described above. p265

$$\text{P.E. due to spin } V = -\mathbf{i}_s \cdot \mathbf{B}$$

$$\text{z-component } \mu_z = -g_s \left(\frac{e\hbar}{2m_e} \right) \frac{J_z}{\hbar}$$

$$\text{energy level difference } \boxed{\Delta E = g_s \frac{e\hbar}{m_e} B}$$

$$e = q = \text{electron charge } 1.6022 \times 10^{-19} \text{ C}$$

$$\hbar = \text{Planck's constant divided by } 2\pi \text{ [J-s]}$$

$$j_z = \text{z-component of the total angular momentum}$$

$$\Delta E = \text{difference in energy between two (split) energy levels}$$

$$m_s = \pm 1/2 \text{ [J]}$$

$$g_s = 2, \text{ the gyromagnetic ratio}$$

$$m_e = \text{mass of an electron } 9.1093897 \times 10^{-31} \text{ kg}$$

$$B = \text{internal magnetic field [T]}$$

ANOMALOUS ZEEMAN SPLITTING

("ZAY· mahn")

In addition to the Zeeman splitting of the m_l energy levels described previously, and the spin-orbit energy splitting described above, there is a splitting of the m_j levels when an external magnetic field is present.

The difference in energy between levels is:

$$V = \mu_B B_{\text{ext}} g m_j$$

V = difference in energy between two energy levels [J]

μ_B = Bohr magneton 9.274078×10^{-24} J/T

B_{ext} = external magnetic field [T]

g = Landé factor [no units]

m_j = magnetic angular momentum quantum number; half-integers ranging from $-j$ to $+j$

STATISTICAL PHYSICS

$v^*, \bar{v}, v_{\text{rms}}$ MOLECULAR SPEEDS [m/s]

Maxwell speed distribution:

$$F(v) dv = 4\pi C e^{-\frac{1}{2}\beta mv^2} v^2 dv$$

v^* most probable speed:

$$v^* = \sqrt{\frac{2}{\beta m}} = \sqrt{\frac{2kT}{m}}$$

\bar{v} mean speed:

$$\bar{v} = \frac{4}{\sqrt{2\pi}} \sqrt{\frac{kT}{m}}$$

v_{rms} root mean square speed:

$$v_{\text{rms}} = \left[\bar{v}^2 \right]^{1/2} = \sqrt{\frac{3kT}{m}}$$

v = velocity [m/s]

C = normalization constant

k = Boltzmann's constant 1.380658×10^{-23} J/K

T = temperature [K]

m = mass of the molecule [kg]

β = the parameter $1/kT$ [J⁻¹]

ENERGY DISTRIBUTION

Derived from Maxwell's speed distribution:

$$F(E) = \frac{8\pi C}{\sqrt{2m^{3/2}}} e^{-\beta E} E^{1/2}$$

F_{MB} MAXWELL-BOLTZMANN FACTOR

The Maxwell-Boltzmann factor is a value between 0 and 1 representing the probability that an energy level E is occupied by an electron (at temperature T). This is for **classical systems, such as ideal gases**. One way to determine if Maxwell-Boltzmann statistics are valid is to compare the de Broglie wavelength $\lambda = h/p$ of a typical particle with the average interparticle spacing d . If $\lambda \ll d$ then Maxwell-Boltzmann statistics are generally acceptable.

$$F_{MB} = A e^{-\beta E}$$

$$d = \left(\frac{V}{N} \right)^{1/3}$$

A = normalization constant

β = the parameter $1/kT$ [J⁻¹]

d = space between atoms [m]

N = number of particles in volume V . Note that

Avogadro's number, 6.022×10^{23} , is the number of gas molecules in 22.4 liters, or 22.4×10^{-3} m³, at 0°C and 1 atmosphere. Also, gas volume is proportional to temperature: $V_1/T_1 = V_2/T_2$.

F_{FD} FERMI-DIRAC DISTRIBUTION

A value between 0 and 1 indicating the probability than an energy state is occupied by an electron. The Fermi-Dirac distribution is valid for **fermions**, particles with **half-integer spins** that obey the Pauli principle. Atoms and molecules consisting of an even number of fermions must be considered bosons when taken as a whole because their total spin will be zero or an integer.

$$F_{FD} = \frac{1}{B_1 e^{\beta E} + 1}$$

B_1 = normalization constant

β = the parameter $1/kT$ [J^{-1}]

F_{BE} BOSE-EINSTEIN DISTRIBUTION

The Bose-Einstein distribution is valid for **bosons**, particles with **zero or integer spins** that do no obey the Pauli principle. Photons, pions, and liquid 4He are bosons.

$$F_{BE} = \frac{1}{B_2 e^{\beta E} - 1}$$

B_2 = normalization constant

β = the parameter $1/kT$ [J^{-1}]

E_F FERMI ENERGY [eV]

The Fermi energy depends on the density of electrons in the material. The Fermi-Dirac distribution is modified to include the Fermi energy:

$$F_{FD} = \frac{1}{e^{[\beta(E - E_F)]} + 1}$$

The relationship between the Fermi energy and the number density of particles is:

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

F_{FD} = Fermi-Dirac distribution, a value from 0 to 1 indicating the probability that an energy state is occupied

β = the parameter $1/kT$ [J^{-1}]

h = Planck's constant $6.6260755 \times 10^{-34}$ J-s

m = mass of the particle [kg]

N/L^3 = number density of the particles [m^{-3}]

T_F FERMI TEMPERATURE

The Fermi temperature may be quite high, 80,000 K for copper.

$$T_F = \frac{E_F}{k}$$

E_F = Fermi Energy [eV]

k = Boltzmann's constant 1.380658×10^{-23} J/K

u_F FERMI SPEED

$$\text{The Fermi speed, } u_F = \sqrt{\frac{2E_F}{m}}$$

comes from the definition: $E_F = \frac{1}{2}mu_F^2$

E_F = Fermi Energy [eV]

m = mass (probably of the electron) [kg]

ENERGY STATES IN "PHASE SPACE"

The points in the 1/8 sphere represent the energy states of a particle in a cube, see 3D INFINITE POTENTIAL BOX p13.

Energy level at radius r

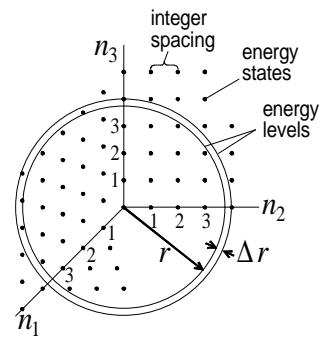
$$E = r^2 E_1$$

where $E_1 = h^2 / 8mL^2$

(a constant equal to 1/3 of the ground state energy)

and $r = \sqrt{n_1^2 + n_2^2 + n_3^2}$

and E is whatever energy the problem is concerned with.



N_r Number of energy states in a sphere of radius r , i.e. the number of energy states there are with energy less than E :

$$N_r = 2 \left(\frac{1}{8} \right) \left(\frac{4}{3} \pi r^3 \right) \quad \text{or} \quad N_r = \frac{\pi}{3} \left(\frac{E}{E_1} \right)^{3/2}$$

where the factor of 2 is due to spin degeneracy, and the factor of 1/8 is because the energy states only occupy 1/8 of the sphere where n_1, n_2, n_3 are all positive.

$g(E)$ DENSITY OF ENERGY STATES

Number of states per unit energy

$$g(E) = \frac{\pi}{2} E_1^{-3/2} E^{1/2} \quad g(E) = \frac{\Delta N_r}{\Delta E} = \frac{dN_r}{dE}$$

N_r = number of energy states in a sphere of radius r

E_1 = a constant equal to 1/3 of the ground state energy

$n(E)$ DENSITY OF OCCUPIED STATES

Number of occupied states per unit energy

$$n(E) = F_{FD} \cdot g(E)$$

$$\text{at } T=0, n(E) = \begin{cases} g(E), & \text{for } E < E_F \\ 0, & \text{for } E > E_F \end{cases}$$

F_{FD} = Fermi-Dirac distribution, a value from 0 to 1 indicating the probability that an energy state is occupied

APPENDIX

CONSTANTS

Avogadro's number

$$[\text{molecules/mole}] \quad N_A = 6.0221367 \times 10^{23}$$

$$\text{Bohr magneton} \quad \mu_B = \frac{q\hbar}{2m_e} = 9.27407836 \times 10^{-24} \text{ J/T}$$

$$\text{Boltzmann's constant} \quad k = 1.380658 \times 10^{-23} \text{ J/K}$$

or

$$K = 8.62 \times 10^{-5} \text{ eV/K}$$

Earth to Moon distance

$$\approx 384 \times 10^6 \text{ m}$$

Elementary charge

$$q = 1.60 \times 10^{-19} \text{ C}$$

Electron mass

$$m_e = 9.1093897 \times 10^{-31} \text{ kg}$$

$$m_e = 0.51100 \text{ MeV/c}^2$$

Neutron mass

$$m_{neutron} = 1.6749 \times 10^{-27} \text{ kg}$$

$$m_{neutron} = 939.57 \text{ MeV/c}^2$$

Proton mass

$$m_p = 1.6726231 \times 10^{-27} \text{ kg}$$

$$m_p = 938.27 \text{ MeV/c}^2$$

Permittivity of free space

$$\epsilon_0 = 8.8541878 \times 10^{-12} \text{ F/m}$$

Planck's constant

$$h = 6.6260755 \times 10^{-34} \text{ J-s}$$

$$= 4.14 \times 10^{-15} \text{ eV-s}$$

Rydberg constant

$$R = 1.097373 \times 10^7 \text{ m}^{-1}$$

kT @ room temperature

$$kT = 0.0259 \text{ eV}$$

Speed of light

$$c = 2.998 \times 10^8 \text{ m/s}$$

Speed of sound (air 0°C)

$$v_s = 331.29 \text{ m/s}$$

1 Å (angstrom)

$$10^{-8} \text{ cm} = 10^{-10} \text{ M}$$

1 µm (micron)

$$10^{-4} \text{ cm}$$

1 nm = 10Å = 10⁻⁷ cm

$$273.15 \text{ K} = 0^\circ \text{C}$$

1 eV = 1.6 × 10⁻¹⁹ J

$$1 \text{ W} = 1 \text{ J/S} = 1 \text{ VA}$$

1 V = 1 J/C

$$1 \text{ N/C} = 1 \text{ V/m}$$

$$1 \text{ J} = 1 \text{ N} \cdot \text{m} = 1 \text{ C} \cdot \text{V}$$

BINOMIAL EXPANSION

For $|x| < 1$:

$$(1 \pm x)^n = 1 \pm nx + \frac{n(n-1)}{2!} x^2 \pm \frac{n(n-1)(n-2)}{3!} x^3 + \dots$$

When x is much less than 1: $(1 \pm x)^n = 1 \pm nx$

WAVELENGTH SPECTRUM

BAND	METERS	ANGSTROMS
Longwave radio	1 - 100 km	$10^{13} - 10^{15}$
Standard Broadcast	100 - 1000 m	$10^{12} - 10^{13}$
Shortwave radio	10 - 100 m	$10^{11} - 10^{12}$
TV, FM	0.1 - 10 m	$10^9 - 10^{11}$
Microwave	1 - 100 mm	$10^7 - 10^9$
Infrared light	0.8 - 1000 μm	$8000 - 10^7$
Visible light	360 - 690 nm	3600 - 6900
violet	360 nm	3600
blue	430 nm	4300
green	490 nm	4900
yellow	560 nm	5600
orange	600 nm	6000
Red	690 nm	6900
Ultraviolet light	10 - 390 nm	100 - 3900
X-rays	5 - 10,000 pm	0.05 - 100
Gamma rays	100 - 5000 fm	0.001 - 0.05
Cosmic rays	< 100 fm	< 0.001

UNITS

Energy: Joules $\times \left[\frac{1}{q} \right] = \text{eV}$

Mass: Kg $\times \left[\frac{c^2}{q} \right] = \text{eV/c}^2$

Momentum: $\frac{\text{kg} \cdot \text{m}}{\text{s}} \times \left[\frac{c}{q} \right] = \frac{\text{eV}}{\text{c}}$

GREEK ALPHABET

A	α	alpha	I	ι	iota	P	ρ	rho
B	β	beta	K	κ	kappa	Σ	σ	sigma
X	χ	chi	Λ	λ	lambda	T	τ	tau
Δ	δ	delta	M	μ	mu	Y	υ	upsilon
E	ε	epsilon	N	ν	nu	Ω	ω	omega
Φ	φ	phi	O	ο	omicron	Ξ	ξ	xi
Γ	γ	gamma	Π	π	pi	Ψ	ψ	psi
H	η	eta	Θ	θ	theta	Z	ζ	zeta

TRIG IDENTITIES

$$i2 \sin x = e^{ix} - e^{-ix}$$

$$2 \cos x = e^{ix} + e^{-ix}$$

$$2 \sinh x = e^x - e^{-x}$$

$$2 \cosh x = e^x + e^{-x}$$

$$e^{ix} = \cos x + i \sin x$$

$$\sin(A \pm B) = \sin A \cos B \pm \cos A \sin B$$

$$\cos(A \pm B) = \cos A \cos B \mp \sin A \sin B$$

$$\sin A + \sin B = 2 \sin\left(\frac{A+B}{2}\right) \cos\left(\frac{A-B}{2}\right)$$

$$\cos A + \cos B = 2 \cos\left(\frac{A+B}{2}\right) \cos\left(\frac{A-B}{2}\right)$$

GEOMETRY

SPHERE

$$\text{Area } A = 4\pi r^2$$

$$\text{Volume } V = \frac{4}{3}\pi r^3$$

ELLIPSE

$$\text{Area } A = \pi AB$$

Circumference

$$L \approx 2\pi \sqrt{\frac{a^2 + b^2}{2}}$$

COORDINATE SYSTEMS

Cartesian or Rectangular Coordinates:

$$\mathbf{r}(x, y, z) = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}$$

$$|\mathbf{r}| = \sqrt{x^2 + y^2 + z^2}$$

Spherical Coordinates:

$\mathbf{P}(r, \theta, \phi)$ r is distance from center

θ is angle from vertical

ϕ is the CCW angle from the x -axis

$\hat{\mathbf{r}}$, $\hat{\mathbf{e}}$, and $\hat{\mathbf{f}}$ are functions of position—their orientation depends on where they are located.

Cylindrical Coordinates:

$\mathbf{C}(r, \phi, z)$ r is distance from the vertical (z) axis

ϕ is the CCW angle from the x -axis

z is the vertical distance from origin

COORDINATE TRANSFORMATIONS

Rectangular to Cylindrical:

$$\text{To obtain: } \mathbf{A}(r, \phi, z) = \hat{\mathbf{r}}A_r + \hat{\mathbf{f}}A_\phi + \hat{\mathbf{z}}A_z$$

$$A_r = \sqrt{x^2 + y^2} \quad \hat{\mathbf{r}} = \hat{\mathbf{x}} \cos \phi + \hat{\mathbf{y}} \sin \phi$$

$$\phi = \tan^{-1} \frac{y}{x} \quad \hat{\mathbf{f}} = -\hat{\mathbf{x}} \sin \phi + \hat{\mathbf{y}} \cos \phi$$

$$z = z \quad \hat{\mathbf{z}} = \hat{\mathbf{z}}$$

Cylindrical to Rectangular:

$$\text{To obtain: } \mathbf{r}(x, y, z) = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}$$

$$x = r \cos \phi \quad \hat{\mathbf{x}} = \hat{\mathbf{r}} \cos \phi - \hat{\mathbf{f}} \cos \phi$$

$$y = r \sin \phi \quad \hat{\mathbf{f}} = \hat{\mathbf{r}} \sin \phi + \hat{\mathbf{y}} \cos \phi$$

$$z = z \quad \hat{\mathbf{z}} = \hat{\mathbf{z}}$$

Rectangular to Spherical:

$$\text{To obtain: } \mathbf{A}(r, \theta, \phi) = \hat{\mathbf{r}}A_r + \hat{\mathbf{e}}A_\theta + \hat{\mathbf{f}}A_\phi$$

$$A_r = \sqrt{x^2 + y^2 + z^2}$$

$$\hat{\mathbf{r}} = \hat{\mathbf{x}} \sin \theta \cos \phi + \hat{\mathbf{y}} \sin \theta \sin \phi + \hat{\mathbf{z}} \cos \theta$$

$$\theta = \frac{z \cos^{-1}}{\sqrt{x^2 + y^2 + z^2}}$$

$$\hat{\mathbf{e}} = \hat{\mathbf{x}} \cos \theta \cos \phi + \hat{\mathbf{y}} \cos \theta \sin \phi - \hat{\mathbf{z}} \sin \theta$$

$$\phi = \tan^{-1} \frac{y}{x} \quad \hat{\mathbf{f}} = -\hat{\mathbf{x}} \sin \phi + \hat{\mathbf{y}} \cos \phi$$

Spherical to Rectangular:

$$\text{To obtain: } \mathbf{r}(x, y, z) = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}$$

$$x = r \sin \theta \cos \phi$$

$$\hat{\mathbf{x}} = \hat{\mathbf{r}} \sin \theta \cos \phi - \hat{\mathbf{e}} \cos \theta \cos \phi - \hat{\mathbf{f}} \sin \phi$$

$$y = r \sin \theta \sin \phi$$

$$\hat{\mathbf{y}} = \hat{\mathbf{r}} \sin \theta \sin \phi + \hat{\mathbf{e}} \cos \theta \sin \phi + \hat{\mathbf{f}} \cos \phi$$

$$z = r \cos \theta \quad \hat{\mathbf{z}} = \hat{\mathbf{r}} \cos \theta - \hat{\mathbf{e}} \sin \theta$$