Review of Key Concepts from Quantum Physics 1

- Understanding wavefunctions

- Operators

- Eigenfunction expansions

- 1D cases
  - Infinite well, Finite well, Harmonic well, Delta function
  - Scattering from a step potential

- 3D cases
  - Infinite rectilinear well
  - Spherical symmetry and angular momentum
  - Coulomb potential and the H atom

- Spin

Probability density

- In quantum physics, we think about particles in terms of the probability that a particle will be found in a certain state, or in a range of positions, or in a range of momenta.

- The probability of finding a particle in a certain volume is given by $\int_V \Psi^* \Psi \, dV$. In one dimension, the probability of finding the particle between x1 and x2 is $\int_{x1}^{x2} \Psi^* \Psi \, dx$.

- The product of the wavefunction with itself $\Psi^* \Psi$ is called the probability density.

Connection between wave and particle parameters

- Momentum-Wavelength:
  - $\lambda = h/p; \; p = \hbar k$
- Energy – Wave frequency:
  - $E = \hbar \omega$
- Energy – Momentum
  - Classical kinetic energy: $T = p^2/2m$
  - $T = E - E_0 = \sqrt{p^2 c^2 + (mc^2)^2} - mc^2$

Working with wavefunctions

- Physical rules
  - Normalizable
  - Continuity
  - "Smoothity"
  - Single valued

- Consequences
  - Conservation rule: $\frac{\partial |\Psi|^2}{\partial t} + \nabla \cdot \vec{j} = 0$
  - $j_x = \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \quad \frac{\partial \Psi^*}{\partial x}$ (probability current)

Wavepackets and Transforms

- We can construct a free wavepacket with spatial envelope $\psi(x)$ from traveling wave eigenfunctions.

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int A(k) e^{ikx} dk$$

with $A(k) = \frac{1}{\sqrt{2\pi}} \int \psi(x) e^{-ikx} dx$

  – Note that this transform pair leads to the Heisenberg Uncertainty Principle

Averages and expectation values

- The average value of an observable $\langle q \rangle$ can be computed from the wavefunction:
$$\langle q \rangle = \int \Psi^* q_{op} \Psi \, dx$$

The operator for position is x_{op}

Momentum: $p_{op} = -i\hbar \frac{\partial}{\partial x}$

Kinetic energy: $T_{op} = \frac{p_{op}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

Orthogonality and Completeness

All physical solutions to the SE can be composed as a sum of eigenfunctions

$$\Psi(x,t) = c_1\Psi_1 + c_2\Psi_2 + \cdots$$

- The probability of observing Ψ in state Ψ_1 is $|c_1|^2$.
    - $c_1(0) = \int \Psi_1^* \Psi dx$
    - $1 = \Sigma_n |c_n|^2$

Linearity and Superposition

If there exist two distinct state functions of a system with Hamiltonian H, then for arbitrary constants c_1 and c_2 the linear combination $c_1\psi_1 + c_2\psi_2$ also satisfies the TDSE:

$$\left(\widehat{H} - \widehat{E}\right)\left(c_1\psi_1 + c_2\psi_2\right)$$
$$= \left(c_1\left(\widehat{H} - \widehat{E}\right)\psi_1 + c_2\left(\widehat{H} - \widehat{E}\right)\psi_2\right) = 0$$

An arbitrary linear combination represents a quantum state of the system.

This property of an operator is known as linearity.

Operators

- Operators must act on a function
- Operators act on every function to their right unless their action is constrained by brackets
- The product of operators implies successive operation (starting with the rightmost).
- The sequence of operations does not necessarily commute.
- addition or subtration of operators means to distribute the operations

Operators and Eigenvalues

In quantum physics, the form of the eigenvalue equation for an observable $\hat{A}$ with eigenstate ψ_a and eigenvalue a is:

$$\hat{A}\psi_a = a\psi.$$

The collection of all eigenvalues is called the spectrum of this operator.

The most familiar eigenstate is the stationary state.
$\Psi_E = \psi_E e^{-iEt/\hbar}$ which satisfies: $\hat{H}\Psi = E\Psi$

In an eigenstate of an observable, the uncertainty in that observable is zero.

Hermitian Operators/Hermiticity

$\hat{Q}$ is Hermitian if for any two physically admissible state functions:

$$\int \Psi_1^* \hat{Q} \Psi_2\, dx = \int (\widehat{Q}^* \Psi_1^*) \Psi_2\, dx$$

If an operator is Hermitian, the expectation value of that operator will be real.

All operators for physically measurable quantities are Hermitian.

Hermiticity: Real eigenvalues and orthonormal eigenfunctions

- The eigenvalues of a Hermitian operator are real.
- The eigenvalues of a Hermitian operator are the only values that we can observe in a measurement of that observable.

AND

The eigenfunctions of a Hermitian operator are orthogonal, constitute a complete set, and satisfy closure.

Dirac braket notation

It can be tiresome to write the same integrals repeatedly. Dirac notation saves some ink, and provides conceptual flexibility.

Dirac Notation − "bra"=⟨ | "ket"=| ⟩

$$\langle Q \rangle = \langle \Psi_1 | \hat{Q} \Psi_1 \rangle = \int_{allspace} \Psi_1{}^* \hat{Q} \Psi_1 \, dx = \text{expectation value}$$

$$\langle \Psi_1 | \hat{Q} \Psi_2 \rangle = \int_{allspace} \Psi_1{}^* \hat{Q} \Psi_2 \, dx = \text{matrix element}$$

$$\langle \Psi_1 | \Psi_1 \rangle = \int_{allspace} \Psi_1{}^* \Psi_2 \, dx = \text{overlap integral}$$

1) Take the complex conjugate of the function inside the ⟨ |
2) Act with the operator on the function to its right.
3) Integrate the integrand over all space.

Operator Example
The Parity Operator: $\hat{\Pi}$
What are its properties?

Definition

$$\hat{\Pi} f(\vec{r}) = f(-\vec{r})$$
$$\hat{\Pi} f(x, y, x) = f(-x, -y, -z)$$

__$\boldsymbol{\hat{\Pi}}$ is linear__

$$\hat{\Pi}[c_1 f_1(x) + c_2 f_2(x)]$$
$$= c_1 f_1(-x) + c_2 f_2(-x)$$
$$= [c_1 \hat{\Pi} f_1(x) + c_2 \hat{\Pi} f_2(x)]$$

$\widehat{\Pi}$ is Hermitian

$$\int \psi_1^*(x) \left[\widehat{\Pi}\psi_2(x)\right] dx = \int \left[\widehat{\Pi}\psi_1(x)\right]^* \left[\psi_2(x)\right] dx?$$

Working on the LHS:

$$\int \psi_1^*(x) \left[\widehat{\Pi}\psi_2(x)\right] dx = \int \psi_1^*(x) \left[\psi_2(-x)\right] dx$$

change the dummy variable of integration

$$\int_{-\infty}^{\infty} \psi_1^*(x)\, \psi_2(-x)\, dx = \int_{\infty}^{-\infty} \psi_1^*(-x)\, \psi_2(x)\, d(-x)$$

$$= -\int_{\infty}^{-\infty} \left[\widehat{\Pi}\psi_1(x)\right]^* \psi_2(x)\, dx = \int_{-\infty}^{\infty} \left[\widehat{\Pi}\psi_1(x)\right]^* \psi_2(x)\, dx$$

And since it is Hermitian it's eigenfunctions must form a complete, orthogonal set. – Let's check.

Physical meaning of expansions

- The collection of expansion coefficients in a state function is merely an alternate way to represent this physical state. They contain the same information as the state function itself.

- The expansion coefficients may be useful.
  - The wave function explicitly shows the dependence of the state function on space and time. If we are interested in another property, such as energy, it may be more informative to represent the state function in terms of energy eigenstates.
  - The coefficients c_q are properly called, the probability amplitudes for the observable Q.
  - Knowledge of the probability of a certain outcome may provide physical insight into the situation.

Commuting Operators

- The commutator is the combination of two operators in which the difference is taken between the operations performed in different order:

Commutator$\equiv \left[A_{op}, B_{op}\right] = \left(A_{op}B_{op} - B_{op}A_{op}\right)$

- Whether two operators commute or not can tell us a lot about the nature of the eigenfunctions of the operators without even solving the Schrodinger equation.

Information from the Commutator

- A complete set of simultaneous eigenfunctions of two Hermitian operators exists iff the operators commute.

- If two operators do not commute and their commutator can be expressed as $[A_{op}, B_{op}] = iC_{op}$ where C_{op} is a Hermitian operator, then an uncertainty relation of the form $\Delta A \Delta B \geq \left| \frac{\langle C \rangle}{2} \right|$ must hold.

Uncertainty

- The uncertainty of an arbitrary observable is given by: $\Delta A = \sqrt{\langle (A - \langle A \rangle)^2 \rangle} = \sqrt{\langle A \rangle - \langle A \rangle^2}$

- If many measurements are analyzed, then ΔA is the standard deviation of the measurements.

- The variance is defined as $(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2$

- If we define $U_{op} = A_{op} - \langle A \rangle$, then

$$\int \psi^* U_{op}^2 \psi dx = (\Delta A)^2$$

Spin Matrices 2

Let's find the matrix for S_{op}^2.

We know that a particle in a spin up state satisfies:

$$S_{op}^2 \chi_+ = \left(s(s+1) \right) \hbar^2 \chi_+ = \frac{3}{4} \hbar^2 \chi_+$$

$$S_{op}^2 \chi_- = \left(s(s+1) \right) \hbar^2 \chi_- = \frac{3}{4} \hbar^2 \chi_-$$

To find the eigenfunctions and values we write S^2 as a matrix with unknown elements:

$$S_{op}^2 = \begin{pmatrix} e & f \\ g & h \end{pmatrix}$$

So that $S_{op}^2 \chi_+ = \begin{pmatrix} e & f \\ g & h \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{3}{4} \hbar^2 \begin{pmatrix} e \\ g \end{pmatrix} = \frac{3}{4} \hbar^2 \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

And thus $\begin{pmatrix} e \\ g \end{pmatrix} = \begin{pmatrix} \frac{3}{4} \hbar^2 \\ 0 \end{pmatrix}$. Similarly, $f = 0 \ and \ g = \frac{3}{4} \hbar^2$

Spin 3

Putting the coefficients into the matrix representation:

$$S_{op}^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

We can also deduce the operators for S_x and S_y.

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \text{ and } S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

and using a standard notation: $S_x = \frac{\hbar}{2}\sigma_x$

Where $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\ldots$

The sigma's are called the Pauli spin matrices.

Special 1D Cases

The Schrodinger Equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + U\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

which reduces to

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E-U)\psi = 0$$

with $\Psi = \psi(x)e^{\frac{-iEt}{\hbar}}$ in 1D if U is independent of time.

Piecewise constant potentials 1

Solution to the TISE in a region where V is a constant and E>V:

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + (E - V)\psi(x) = 0$$

Guess: $\psi = e^{ikx}$

$$-\frac{\hbar^2 k^2}{2m} = (E - V) \Rightarrow k = \pm\sqrt{\frac{2m(E - V)}{\hbar^2}}$$

$$\psi = Ae^{ikx} + Be^{-ikx}$$

Piecewise constant potentials 2

Solution to the TISE in a region where V is a constant and E<V:

$$\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} - |E - V|\psi(x) = 0$$

Guess: $\psi = e^{ikx}$

$$\frac{\hbar^2 k^2}{2m} = -|E - V| \qquad \Rightarrow \qquad k = \pm i\sqrt{\frac{2m|E - V|}{\hbar^2}}$$

Let $K = ik = \pm\sqrt{\frac{2m|E - V|}{\hbar^2}}$ ($\therefore$ K is a real number)

$\psi = Ae^{Kx} + Be^{-Kx}$ (exponential growth or decay)

Some "intuitive" rules for sketching wavefunctions*

1. Solutions for the Schrodinger equation curve toward the x-axis in classically allowed ($E > V$) regions and away from the axis in classically forbidden regions.

2. For bound states, the wavefunction must go to zero for large distances outside the well. (must be normalizable)

3. Curvature increases for larger $|E - V(x)|$.

4. Solutions are continuous and smooth if the potential has no infinite steps.

5. Energy eigenfunctions have an integer number of antinodes on classically allowed regions.

6. The wavefunction amplitude is usually larger in regions with small E>V.

* From https:''www.asc.ohio-state.edu/physics/ntg/H133/handouts/wavefunctions.pdf

Bound state wavefunctions for symmetric potentials
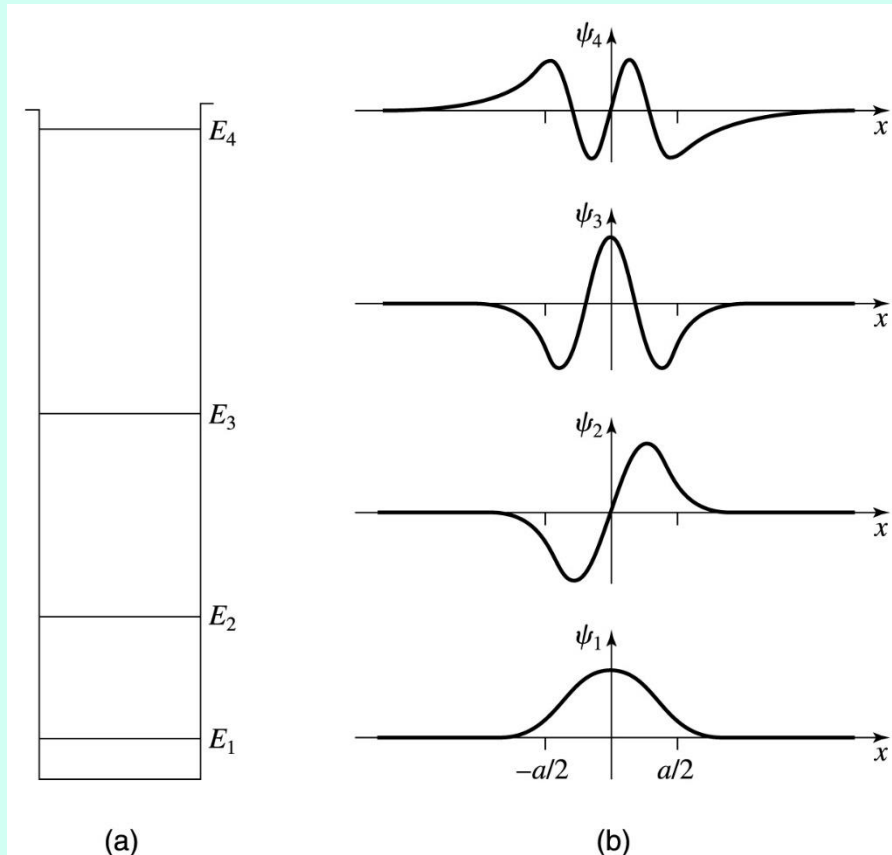
Figure 4.4 copyright 2009 University Science Books

Same rules: +
- Ground state has one antinode, centered
- Alternating odd and even functions.

The Finite Square Well

$$V(x) = \begin{cases} 0 \; ; & -\dfrac{a}{2} < x < \dfrac{a}{2} \\[2mm] 1; & |x| > \dfrac{a}{2} \end{cases}$$

$$\psi(x) = \begin{cases} Ce^{Kx} + De^{-Kx} \; for \; x < -\dfrac{a}{2} \\[2mm] A \sin k\,x + B \cos k\,x \; \text{for} \; -\dfrac{a}{2} < x < \dfrac{a}{2} \\[2mm] Fe^{Kx} + Ge^{-Kx} \; for \; x > \dfrac{a}{2} \end{cases}$$

where $k = \left| \dfrac{\sqrt{2mE}}{\hbar} \right|$ and $K = \left| \dfrac{\sqrt{2m(V_0 - E)}}{\hbar} \right|$

The physical requirement that the wavefunction must be normalizable means that it cannot blow up at $\pm\infty, so$

$$\psi(x) = \begin{cases} Ce^{Kx} \; for \; x < -\dfrac{a}{2} \\ A\sin k\,x + B\cos k\,x \; \text{for} \; -\dfrac{a}{2} < x < \dfrac{a}{2} \\ Ge^{-Kx} \; for \; x > \dfrac{a}{2} \end{cases}$$

Symmetry of the potential leads to the requirement that the probability density for an eigenfunction be an even function of x. This leads to the requirement that the eigenfunctions be either even or odd.

$$\psi_{even}(x) = \begin{cases} Ce^{Kx} \ for \ \ x < -\dfrac{a}{2} \\ B\cos k\,x \ \text{for} \ -\dfrac{a}{2} < x < \dfrac{a}{2} \\ Ce^{-Kx} \ for \ \ x > \dfrac{a}{2} \end{cases}$$ (Note that we set C=G.)

$$\psi_{odd}(x) = \begin{cases} Ce^{Kx} \ for \ \ x < -\dfrac{a}{2} \\ B\sin kx \ \text{for} \ -\dfrac{a}{2} < x < \dfrac{a}{2} \\ -Ce^{-Kx} \ for \ \ x > \dfrac{a}{2} \end{cases}$$ (Note that we set C=-G.)

Now we use the physical properties of the wavefunction at the boundaries to find the constants B and C, and the energies.

Considering the even solutions first:

1) The wavefunction must be continuous at the boundary at +a/2 and –a/2.

For x=-a/2 and +a/2: $B \cos \dfrac{ka}{2} = C e^{-\frac{Ka}{2}}$

2) The derivative of the wavefunction must be continuous at the boundaries.

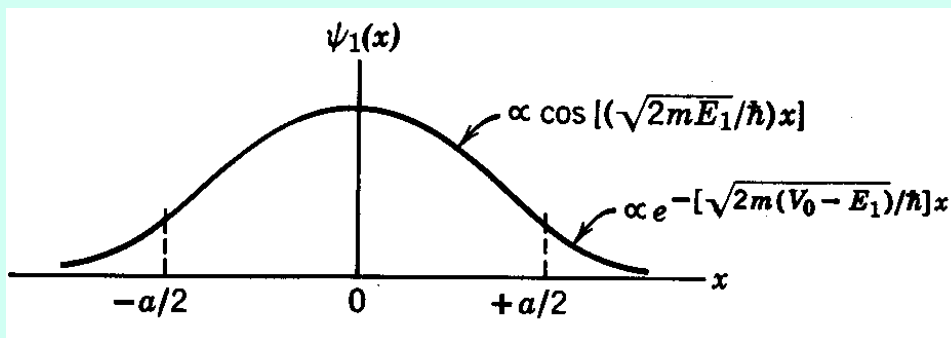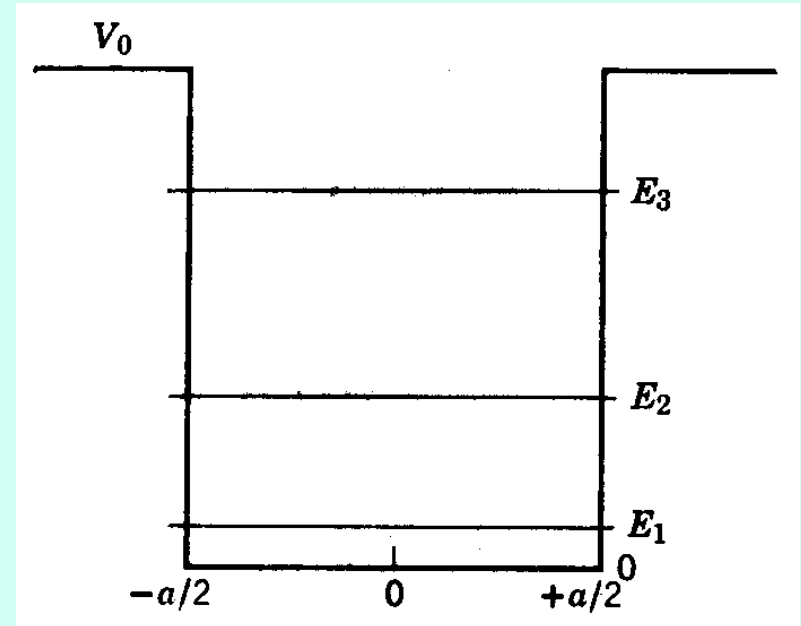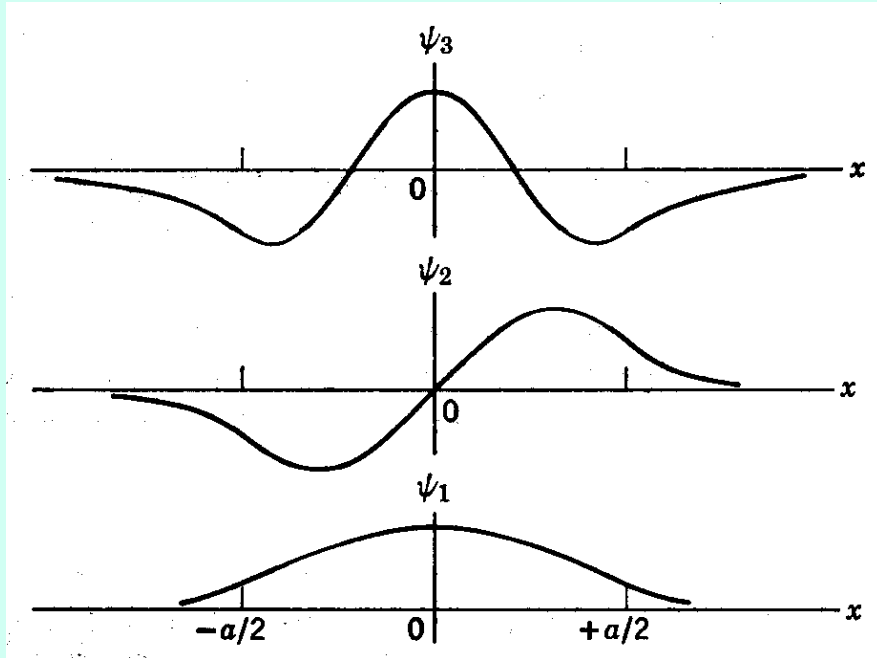For x=-a/2 and +a/2: $Bk \sin \dfrac{ka}{2} = CK e^{-\frac{Ka}{2}}$

Even solutions: Plot both the left hand and

right hand side of $\tan \xi \ = \dfrac{\sqrt{\xi_0^2 - \xi^2}}{\xi}$ as a function of ξ.
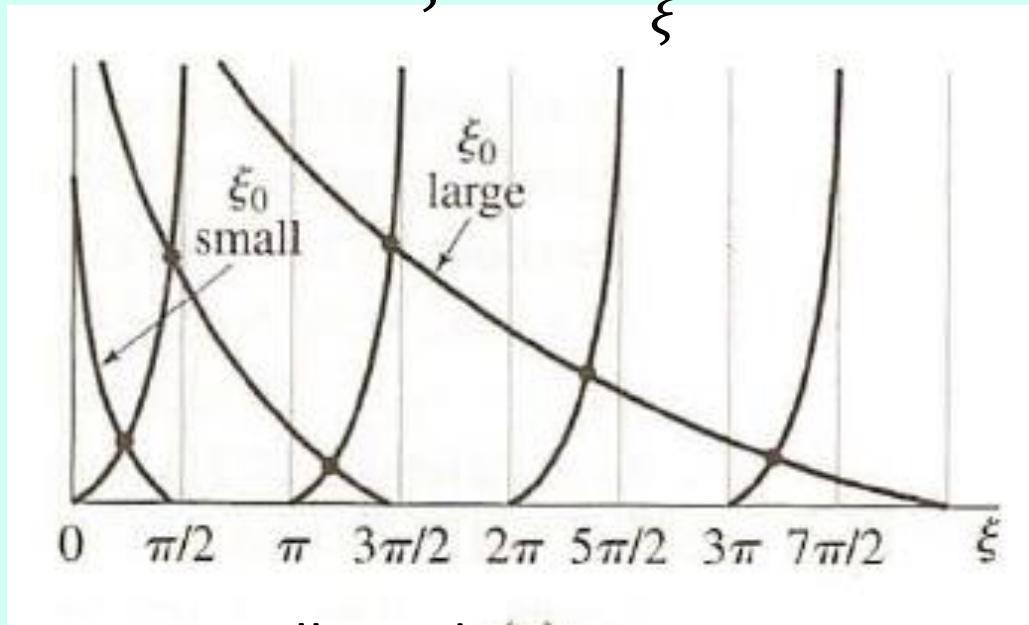
- Intersections are allowed energies
- $\tan \xi$ goes to ∞ each time ξ goes through odd $\dfrac{\pi}{2}$.
- If well depth is small, then only one solution can be found.
- If well depth is large, solutions approach infinite well.

- Summary of eigenfunctions and eigenvalues

$$\psi_1(x)$$

$$\propto \cos\left[(\sqrt{2mE_1}/\hbar)x\right]$$

$$\propto e^{-\left[\sqrt{2m(V_0 - E_1)}/\hbar\right]x}$$

The Harmonic Oscillator

To be consistent with Appendix B1 in Townsend, we change variables to avoid writing constants repeatedly. $(Let\ y = \sqrt{\frac{m\omega}{\hbar}}\ x, and\ \epsilon = \frac{2E}{\hbar\omega})$

$$\frac{\partial^2 \psi}{\partial y^2} = (y^2 - \epsilon)\psi$$

Find the approximate solution for large *y*.

$$\frac{\partial^2 \psi}{\partial y^2} \approx y^2 \psi$$

Solution:

$$\psi(very\ large\ y) = A y^n e^{-\frac{y^2}{2}}$$

- Any polynomial in y, times the exponential decay term $e^{-\frac{y^2}{2}}$ will satisfy the large y equation.

- Now we can see what polynomials ($H(y)$) can satisfy the full equation, and what conditions they impose on the energy.

$$\frac{d^2 H(y)e^{-\frac{y^2}{2}}}{dy^2} = (y^2 - \epsilon)H(y)e^{-\frac{y^2}{2}}$$

$$\frac{d\psi}{dy} = -yH(y)e^{-\frac{y^2}{2}} + e^{-\frac{y^2}{2}}\frac{dH}{dy}$$

$$\frac{d^2\psi}{dy^2} = -He^{-\frac{y^2}{2}} - y\frac{dH}{dy}e^{-\frac{y^2}{2}} + e^{-\frac{y^2}{2}}\frac{d^2 H}{dy^2}$$

Hermite Polynomials

$$H_0(\xi) = 1$$

$$H_1(\xi) = 2\xi$$

$$H2(\xi) = 4\xi^2 - 2$$

$$H3(\xi) = 8\xi^3 - 12\xi$$

-

-

Figure 5-9

Energy levels and eigenfunctions for the first four stationary states of the harmonic oscillator. Shaded areas represent the penetration of the wave function into regions where classical motion is forbidden.

ψ_3 $E_3 = \frac{7\hbar\omega_0}{2}$

ψ_2 $E_2 = \frac{5\hbar\omega_0}{2}$

ψ_1 $E_1 = \frac{3\hbar\omega_0}{2}$

ψ_0 $E_0 = \frac{\hbar\omega_0}{2}$

$V = 0$
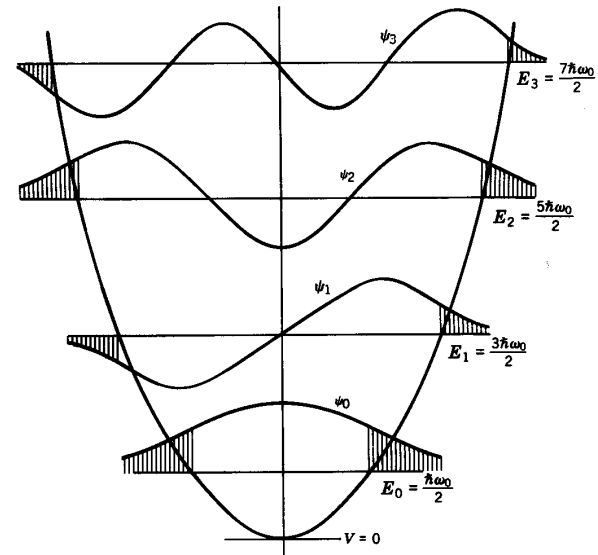
The delta function potential

$$\hat{H}\psi = \hat{E}\psi$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + \lambda\delta(x)\psi = E\psi$$

with λ negative, for an attractive potential.

http://galileo.phys.virginia.edu/classes/751.mf1i.fall02/OneDimSchr.htm

We expect to have at least one bound state for a symmetric attractive potential.

Away from the origin, we expect solutions of the form:

$$\psi = Ae^{Kx} + Be^{-Kx}$$

So for negative x, we have $\psi^- = Ae^{Kx}$

and for positive x, we have $\psi^+ = Be^{-Kx}$

Continuity of the wavefunction gives $\psi^- = \psi^+ \Rightarrow A = B$.

The slope on the two sides is discontinuous due to the infinite δ function.

$$\left.\frac{d\psi}{dx}\right|_{-\beta} = KA; \quad \left.\frac{d\psi}{dx}\right|_{\beta} = -KA; \text{ for small } \beta, \text{ so } \left.\frac{d\psi}{dx}\right|_{-\beta} \quad \left.\frac{d\psi}{dx}\right|_{\beta} - \left.\frac{d\psi}{dx}\right|_{-\beta} = -2KA;$$

Returning to the Schrodinger equation,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + \lambda\delta(x)\psi = E\psi$$

We integrate both sides once in x, from $-\beta$ to $+\beta$.

$$-\int_{-\beta}^{\beta}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi\,dx + \int_{-\beta}^{\beta}\lambda\delta(x)\psi\,dx = \int_{-\beta}^{\beta}E\psi\,dx$$

The rhs goes to zero as $\beta \Rightarrow 0$ because the integrand is finite.

so, $\displaystyle\int_{-\beta}^{\beta} \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi dx = \int_{-\beta}^{\beta} \lambda\delta(x)\psi dx$

Doing both integrals separately, $\displaystyle \frac{\hbar^2}{2m}\frac{\partial\psi}{\partial x}\Big|_{-\beta}^{\beta} = \lambda\psi(0)$

and substituting $\displaystyle \frac{\partial\psi}{\partial x}\Big|_{-\beta}^{\beta} = -2AK$ (from the previous slide),

we have $\displaystyle -\frac{\hbar^2 K}{m} = \lambda$

$$K = -\frac{\lambda m}{\hbar^2} \quad \Rightarrow \quad E = \frac{\hbar^2 K^2}{2m} = -\frac{m\lambda^2}{2\hbar^2}$$
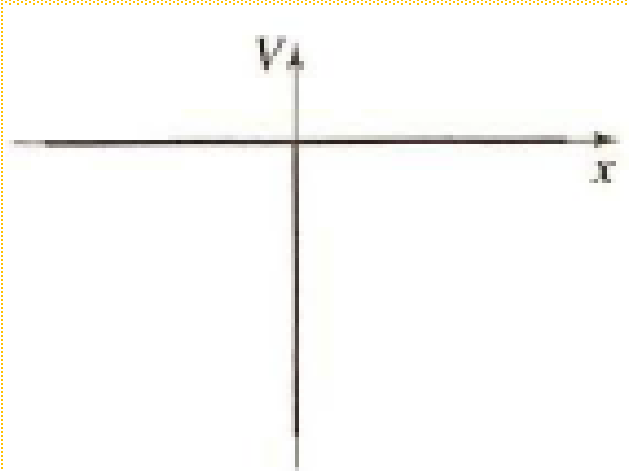
Figure 4.14 The Dirac delta function potential energy (4.77).
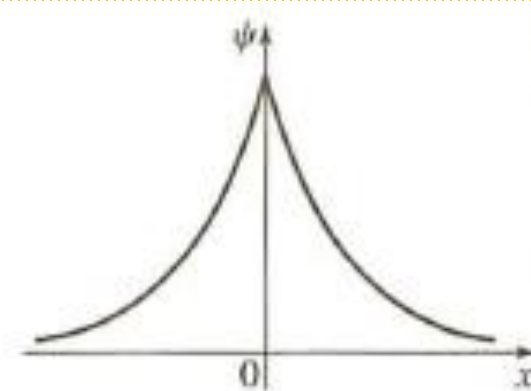
Figure 4.15 The wave function (4.85) for a particle bound in a Dirac delta function potential energy well.

$$\psi(x) = A \exp\left(-\frac{\lambda m}{\hbar^2}|x|\right)$$

is the only bound state.

A Model Molecule

We will use the Dirac Delta function as a simplified representation of an electron bound to an atom.

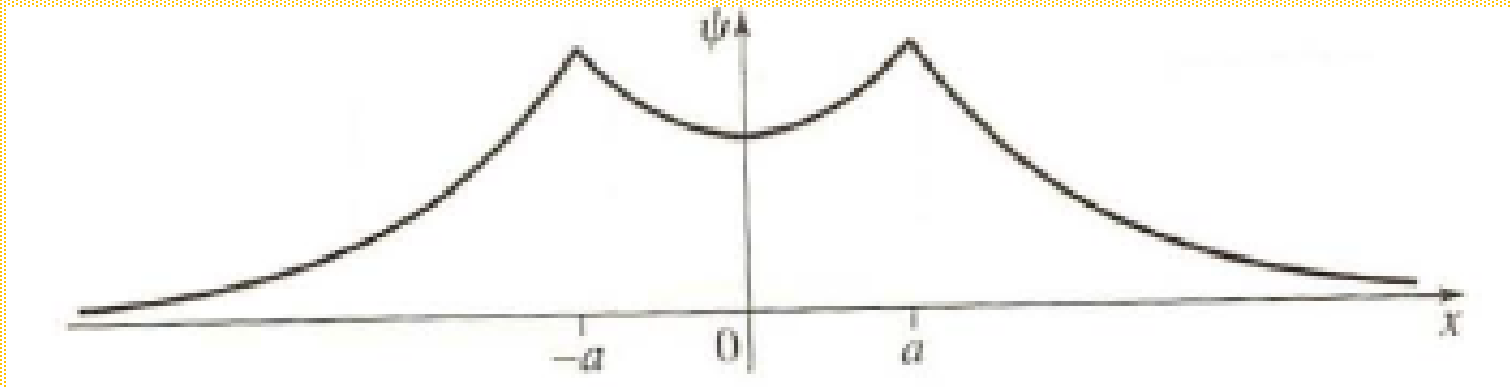We will address the case of an electron bound to a proton in a Coulomb potential later in this course.

Consider two delta function potentials near one another.

$$\frac{2m}{\hbar^2} V(x) = -\frac{\lambda}{a}\left[\delta(x-a) + \delta(x+a)\right]$$

Model Molecule Wavefunction Shape

- We expect that the solution will look something like this:.

Model Molecule Wavefunction

- Since $E < V$ everywhere except for the two points a and –a, and the wavefunction must be normalizable, the solutions must be of the form:

$$\psi(x) = \begin{cases} Ce^{Kx} \ for \ x < -a \\ A\exp(Kx) + B\exp(-Kx) \ for -a < x < a \\ D\exp(-Kx) \ for \ a < x \end{cases}$$

- Where $K = \sqrt{\dfrac{2m|E|}{\hbar^2}}$

- The lowest energy solution must be an even function, so C=D and A=B.

Model Wavefunction (2)

Applying the symmetry conditions:

$$\psi(x) = \begin{cases} Ce^{Kx} \ for \ x < -a \\ A\cosh Kx \ for \ -a < x < a \\ C\,e^{-Kx} \ for \ a < x \end{cases}$$

Continuity at x=a yields:

$$A\cosh Ka = Ce^{-Ka}$$

And the condition on the discontinuity in the derivative at x=a yields:

$$-KCe^{-Ka} - AK\sinh Ka = -\frac{\lambda}{a}A\cosh Ka$$
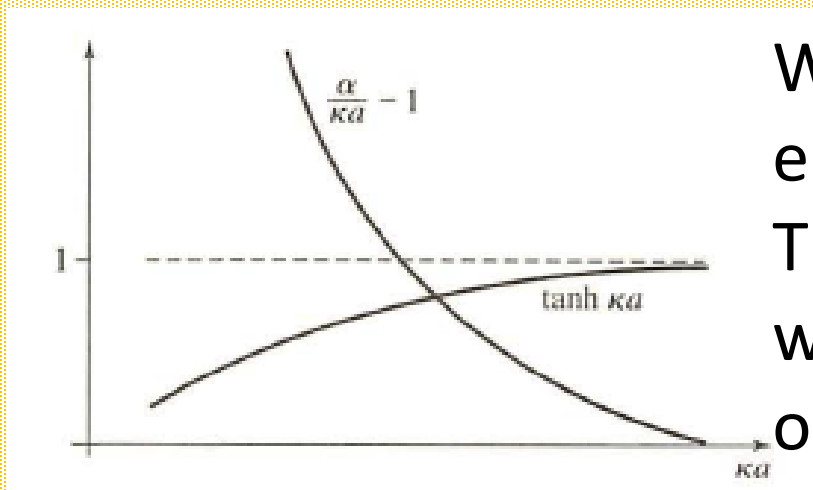
Putting the two conditions together:

$$-KA \cosh Ka - A \sinh Ka = -\frac{\lambda}{a} A \cosh Ka$$

And dividing by $A \cosh Ka$

$$\tanh Ka = \frac{\lambda}{a} - 1$$

Which can be solved numerically.
Here is a graphical representation to illustrate

Where the dashed line is the energy for a single well.
The particle has lower energy when bound to two wells near one another – binding.

The Step Potential

U

E - - - - - - →

0

x=0

x
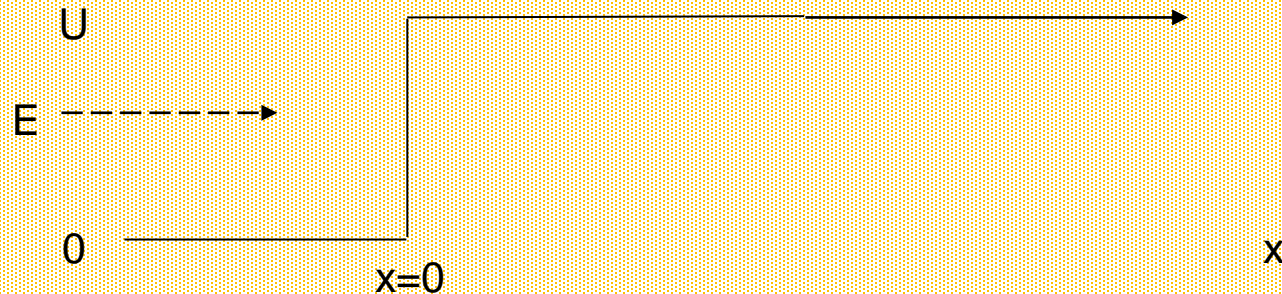
- State general solutions in each region.
- Carefully eliminate non-physical possibilities.
- Match wavefunctions the boundary.
  - Two possibilities E>V and E<V.

http://www.abdn.ac.uk/physics/vpl/qstep/index.html

An example

- Let's consider the situation where a wave is incident from the left onto a barrier at x=0.

- The wavefunction for pure momentum wave moving left is:

$$\Psi(x,t) = Ae^{ikx - i\omega t}$$

- What can the wave do?
  - It can bounce back, going the other way.

    $$\Psi(x,t) = Be^{-ikx - i\omega t}$$

  - It can pass through the boundary.

    $$\Psi(x,t) = Ce^{ikx - i\omega t}$$

Solutions in two regions

$$\psi_1(x,t) = (Ae^{ik_1x} + Be^{-ik_1x})$$

$$\psi_2(x,t) = Ce^{ik_2x}$$

1) $A + B = C$ (continuity)

2) $ik_1A - ik_1B = ik_2C$ ("smoothity")

$$B = C - A \quad \Rightarrow \quad i2k_1A = i(k_2 + k_1)C \quad \Rightarrow \quad C = \frac{2k_1}{k_2 + k_1}A$$

$$B = \frac{k_1 - k_2}{k_2 + k_1}A$$

In terms of energy: $\dfrac{C}{A} = \dfrac{2\sqrt{2mE/\hbar^2}}{\sqrt{2mE/\hbar^2} + \sqrt{2m(E-V)/\hbar^2}} = \dfrac{2\sqrt{E}}{\sqrt{E} + \sqrt{(E-V)}}$

For E>>V, C/A $\Rightarrow$ 1.   For E=V, C/A $\Rightarrow 2/\sqrt{V}$

Probability current in two regions

$$j(x,t) = \frac{-i\hbar}{2m}\left(\Psi^* \frac{\partial}{\partial x}\Psi - \Psi\frac{\partial}{\partial x}\Psi^*\right)$$

which for a pure momentum state is:

$$j = k\Psi^*\Psi$$

$$j_{incident} = +\frac{\hbar k_1}{m}A^2$$

$$j_{reflected} = -\frac{\hbar k_1}{m}B^2$$

$$j_{transmitted} = +\frac{\hbar k_2}{m}C^2$$

$$T \equiv \frac{j_{transmitted}}{j_{incident}} = \frac{k_2 C^2}{k_1 A^2} = \frac{k_2}{k_1}\left(\frac{2k_1}{k_2+k_1}\right)^2 = \frac{2k_1 k_2}{(k_2+k_1)^2}$$

The Step Barrier

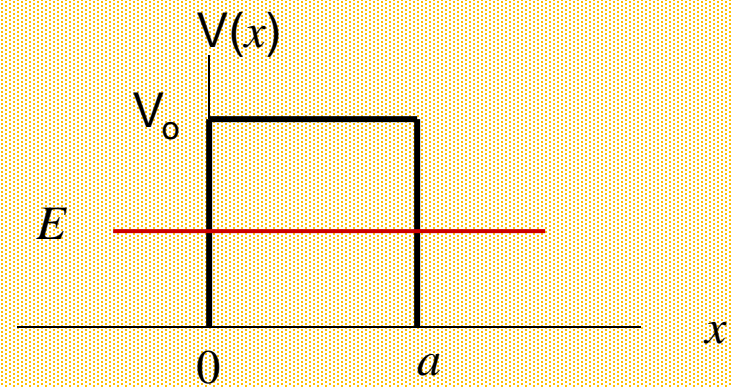# Barrier Potential

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & 0 < x < a \\ 0, & x > a \end{cases}$$

Figure 5-21

Reflection and transmission of a classical particle by a rectangular potential energy barrier.

Reflection if $E < V_0$

Transmission if $E > V_0$
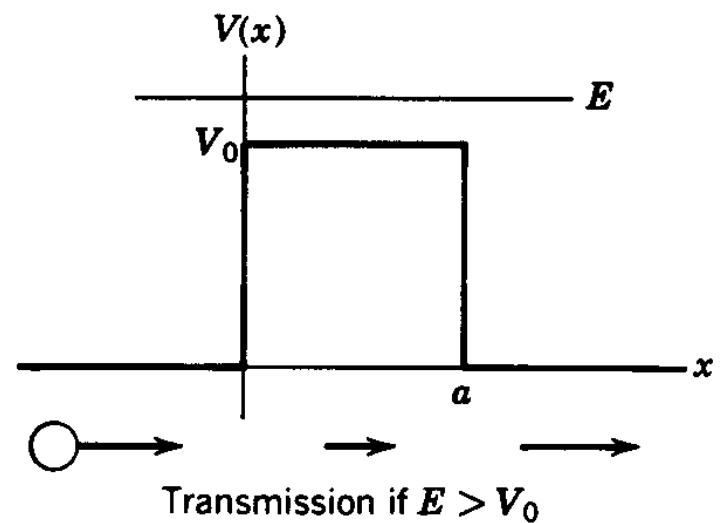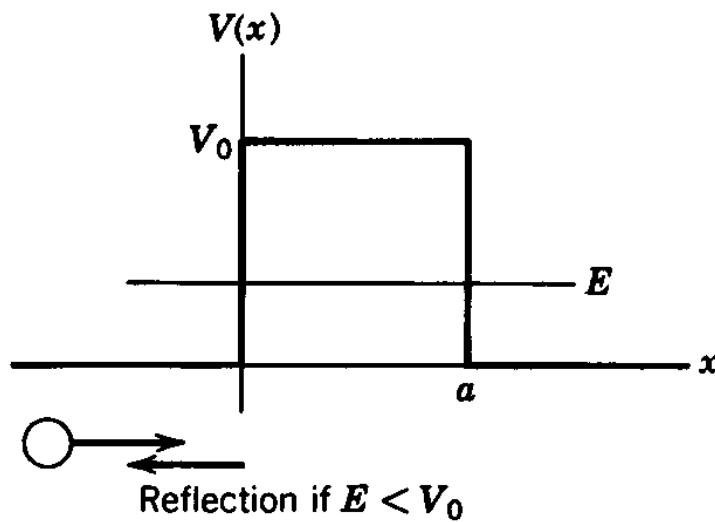
Case 1 $E < V_0$

$$\psi(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1} & x<0 \\ Ce^{-k_2 x} + De^{k_2 x} & 0<x<a \\ \hat{A}e^{ik_1 x} + \hat{B}e^{-ik_1 x} & x>a \end{cases} \quad (5\text{-}73)$$
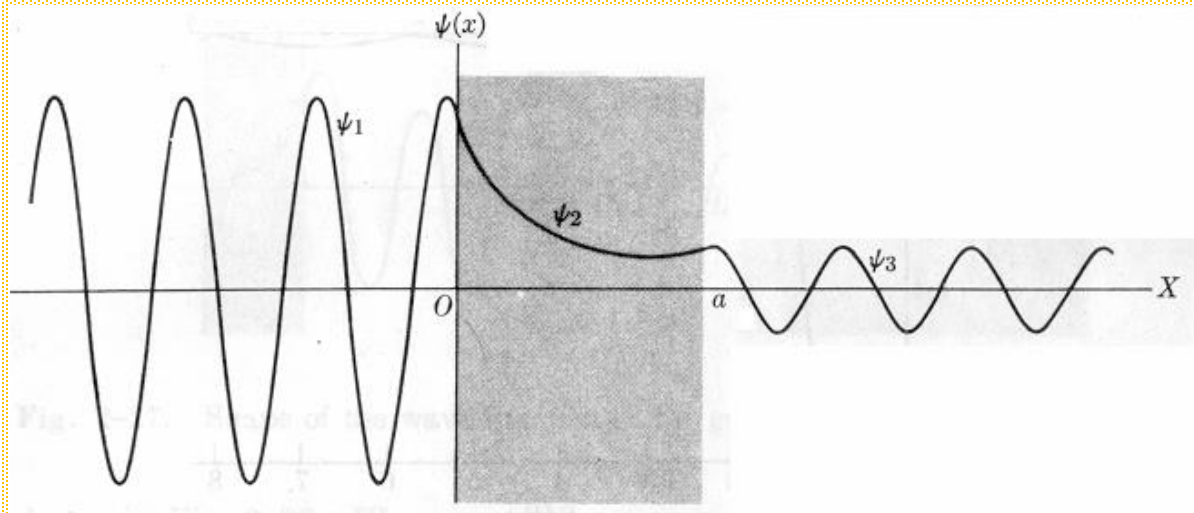
where $\begin{cases} k_1 = \dfrac{\sqrt{2mE}}{\hbar} \\ k_2 = \dfrac{\sqrt{2m(V_0 - E)}}{\hbar} \end{cases}$

use $\qquad \hat{B}=0 \qquad$ for $\qquad x > a$

$$\left.\begin{array}{l} \psi(o)\ \text{continuous} \\ \psi'(o) \qquad " \end{array}\right\} \text{at } x=0$$

$$\left.\begin{array}{l} \psi(a)\ \text{continuous} \\ \psi'(a) \qquad " \end{array}\right\} \text{at } x=a$$

Express $B, C, D, \hat{A}$ in terms of A.

$$x=0$$

$\psi(x):$ $Ae^{ik_1x} + Be^{-ik_1x}$ $= Ce^{-k_2x} + De^{k_2x}$

$\psi(0):$ $A \quad + \quad B$ $= C \quad + \quad D$ (1)

$\psi'(x):$ $ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x}$ $= -k_2Ce^{-k_2x} + k_2De^{k_2x}$

$\psi'(0):$ $ik_1(A-B)$ $= -k_2(C-D)$ (2)

$$x=a \qquad \text{Note} \quad \hat{B}=0 \quad \text{for} \quad x > a$$

$\psi(x):$ $Ce^{-k_2x} + De^{k_2x}$ $= \hat{A}e^{ik_1x}$ (3)

$\psi(a):$ $Ce^{-k_2a} + De^{k_2a}$ $= \hat{A}e^{ik_1a}$

$\psi'(x):$ $-k_2\left(Ce^{-k_2x} - De^{k_2x}\right)$ $= ik_1\hat{A}e^{ik_1x}$ (4)

$\psi'(a):$ $-k_2\left(Ce^{-k_2a} - De^{k_2a}\right)$ $= ik_1\hat{A}e^{ik_1a}$

Approximate transmission coefficient when

$$a \rangle\rangle \frac{1}{k_2}$$

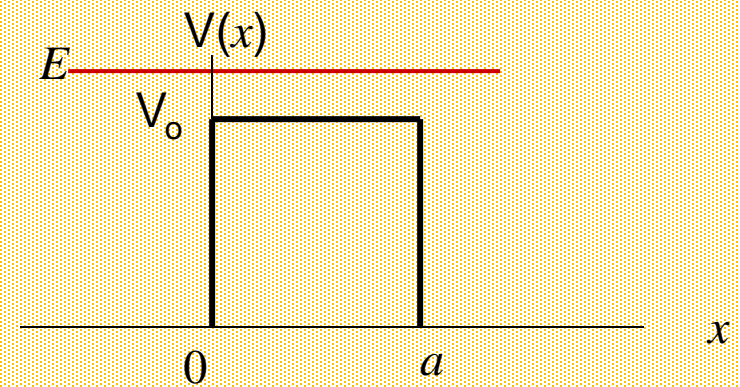$$T = 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0} \right) e^{-2k_2 a}$$

$$\sinh u = \frac{1}{2} \left(e^u - e^{-u} \right) \quad and \quad u = k_2 a$$

This form is frequently used as an approximation in tunnelling calculations.
Examples: STM, Quantum wells and barriers in semiconductors, nuclear decay

Case 2 $E > V_0$

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & x<0 \\ \\ Ce^{ik_3x} + De^{-ik_3x} & 0 < x < a \quad \text{note } k_3 \\ \hat{A}e^{ik_1x} + \hat{B}e^{-ik_1x} & x>a \end{cases}$$

$$\text{where} \begin{cases} k_1 = \dfrac{\sqrt{2mE}}{\hbar} \\ \\ k_3 = \dfrac{\sqrt{2m(E-V_0)}}{\hbar} \end{cases}$$

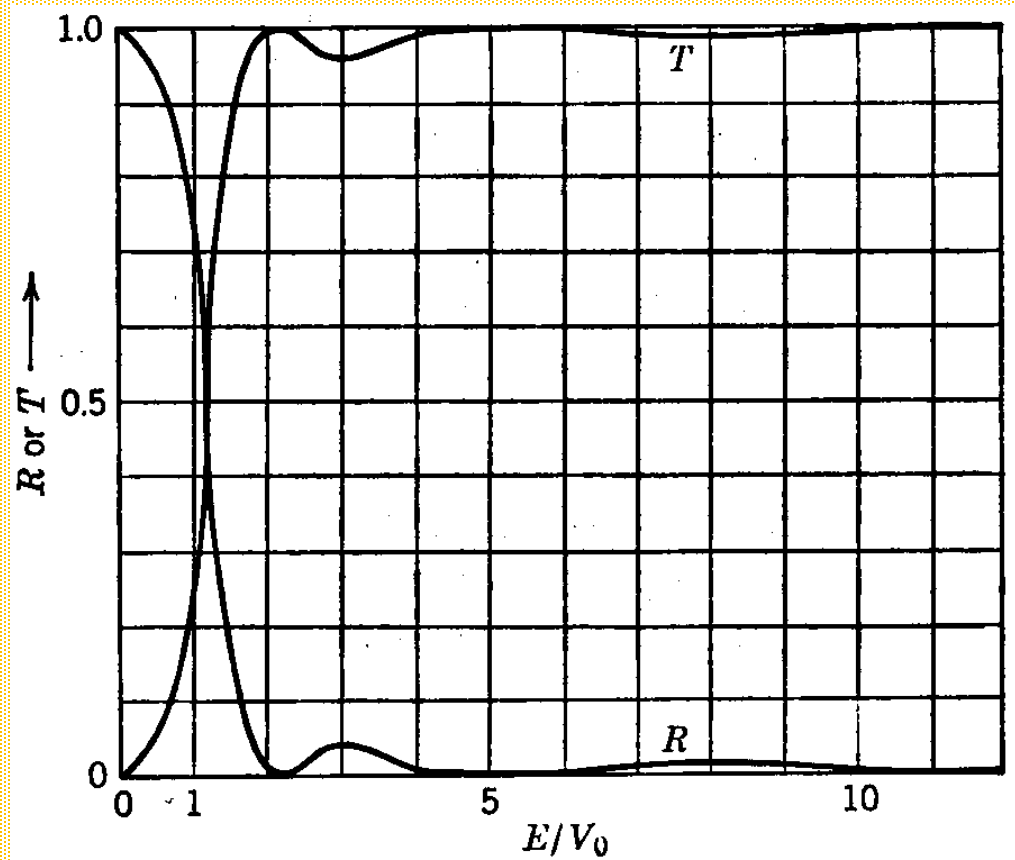Follow the method used in case $1 \left(E < V_0 \right)$

$\vdots$

$$T = \cfrac{1}{1 + \cfrac{\sin^2 k_3 a}{4 \dfrac{E}{V_0}\left(\dfrac{E}{V_0} - 1\right)}}$$

Ramsauer effect:

Note if $k_3 a = \pi, 2\pi, 3\pi ...,$
then

$T = 1$ and $R = 0$.

3D Box

The 3-D Rectangular Box (TISE)

$$V(x,y,z) = \begin{cases} 0 & 0 < x < L_x \\ 0 & 0 < y < L_y \\ 0 & 0 < z < L_z \end{cases} \quad \text{and infinite otherwise}$$

The standard approach: Assume that a product solution exists inside the box—

$$\psi(x,y,z) = X(x)Y(y)Z(z)$$

$$-\frac{\hbar^2}{2m}\left(ZY\frac{\partial^2 X}{\partial x^2} + XZ\frac{\partial^2 Y}{\partial y^2} + XY\frac{\partial^2 Z}{\partial z^2}\right)\psi = EXYZ$$

$$\left(\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right) + \frac{2m}{\hbar^2}E = 0$$

Pulling all terms in z to one side:

$$\left(\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}\right) + \frac{2m}{\hbar^2}E = -\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}$$

which can only be true if each side is separately equal to the same constant which we set to: $\frac{2mE_z}{\hbar^2}$

$$\left(\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}\right) + \frac{2m}{\hbar^2}E = \frac{2m}{\hbar^2}E_z$$

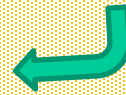$$-\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = \frac{2m}{\hbar^2}E_z$$

Solving the z equation

$$\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} + k_z^2 = 0 \quad \text{where } k_z \equiv \sqrt{\frac{2m}{\hbar^2}(E_z)}$$

$$Z = A \sin k_z z + B \cos k_z z$$

The z=0 boundary condition
leads to: B=0
The z=L$_z$ boundary condition
gives $Z(z = L_z) = A \sin k_z L_z = 0$
which has non−trival solutions if

$$k_z = \frac{n_z \pi}{L_z} \text{ with } E_z = \frac{\hbar^2 k_z^{\,2}}{2m}$$

$$so \ E_z = \frac{\hbar^2 n_z^{\,2} \pi^2}{2m L_z^2}$$

$$-\left(\frac{1}{X}\frac{\partial^2 X}{\partial x^2}\right) - \frac{2m}{\hbar^2}E + \frac{2m}{\hbar^2}E_z + \frac{2m}{\hbar^2}E_y = 0$$

$$= \left(\frac{1}{X}\frac{\partial^2 X}{\partial x^2}\right) - \frac{2m}{\hbar^2}E_x = 0 \quad (defining\ E_x \equiv E - E_y - E_z)$$

$$\frac{\partial^2 X}{\partial x^2} + \frac{2m}{\hbar^2}E_x X = 0$$

which has solutions: $X = A\sin k_x x + B\cos k_x x$

The x=0 condition gives: B=0

The x=L_x condition gives: $X(L_x) = A\sin k_x L_x = 0$
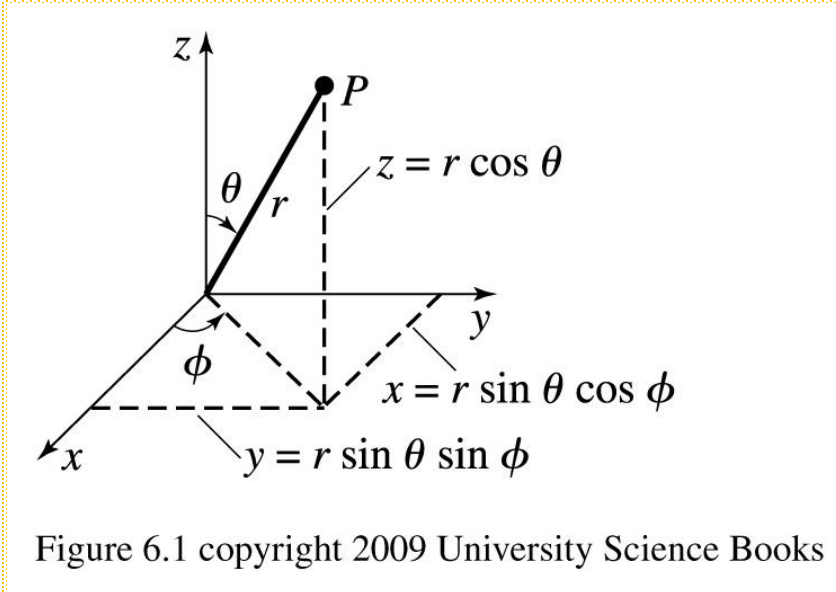
which has non−trival solutions if

$$k_x = \frac{n_x \pi}{L_x} \text{ with } E_x = \frac{\hbar^2 k_x{}^2}{2m}$$

$$E = E_x + E_y + E_z = \frac{\hbar^2}{2m}\left(k_x{}^2 + k_y{}^2 + k_z{}^2\right) = \frac{\hbar^2 \pi^2}{2m}\left(\frac{n_x{}^2}{L_x^2} + \frac{n_y{}^2}{L_y^2} + \frac{n_z{}^2}{L_z^2}\right)$$

Three dimension – Three quantum numbers

Spherical Potential

Spherical Coordinates

Figure 6.1 copyright 2009 University Science Books

$$x = r \sin(\theta) \cos(\phi)$$
$$y = r \sin(\theta) \sin(\phi)$$
$$z = r \cos(\theta)$$

$$r = \sqrt{x^2 + y^2 + z^2}$$
$$\theta = \arccos\left(\frac{z}{r}\right)$$
$$\phi = \arctan\left(\frac{y}{x}\right)$$

$$\nabla^2 = \left(\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \Psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \Psi}{\partial \phi^2} \right)$$

Solutions for Central Potentials

Let's address the case where the potential only depends on distance from the center.

The 3D time−independent Schrodinger Eq: $\hat{H}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi$

In spherical coordinates:

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

Assuming that the solution can be expressed as a product: $\Psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$

$$-\frac{\hbar^2}{2m}\left(\frac{\Theta\Phi}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{R\Phi}{r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{R\Theta}{r^2\sin^2\theta}\frac{d^2\Phi}{\partial d}\right) + (V-E)R\Theta\Phi = 0$$

Assuming: $V=V(r)$, dividing through by $R\Theta\Phi$, and multiplying through by $\sin^2\theta\, r^2 2m/\hbar^2$, we can separate the azimuthal term:

$$\sin^2\theta\left(\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left(\frac{2m}{\hbar^2}\right)(E-V)r^2\right) + \frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = -\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = m_l^2$$

Which has solutions: $\Phi(\phi) = e^{\pm im_l\phi}$.
In order for Φ to be single-valued for any ϕ , m_l must be an integer.

θ solution for central potential

We are now left with the other two variables, r and θ.
Separating the angular terms from the radial terms:

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - r^2\frac{2m(E-V(r))}{\hbar^2} = +\frac{m_l^2}{\sin^2\theta} - \frac{1}{\Theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial\Theta}{\partial\theta}\right] = l(l+1)$$

The angular part of Laplace's equation is called the Legendre Equation.

$$+\frac{m_l^2}{\sin^2\theta} - \frac{1}{\Theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial\Theta}{\partial\theta}\right] = l(l+1)$$

Making the substitution x=cosθ

$$\frac{d}{d\theta} = \frac{dx}{d\theta}\frac{d}{dx} = -\sin\theta\frac{d}{dx} = -\sqrt{1-x^2}\frac{d}{dx}, \text{ so}$$

In standard form, this is known as the Legendre Equation:

$$\frac{d}{dx}\left[(1-x^2)\frac{d\Theta_{lm}}{dx}\right] + (l(l+1) - \frac{m_l^2}{1-x^2})\Theta_{lm} = 0$$

And the solutions are the Associated Legendre Polynomials

$\Theta(\theta)$ solutions for a central potential

We will not solve the Associated Legendre Equation here. You can find a good step by step solution to the Legendre equation in Appendix B.2 in Townsend.

Legendre Polynomials P_l are the solutions to the $m_l = 0$ Legendre Equation:

$$\frac{d}{dx}\left[(1-x^2)\frac{dP_l}{dx}\right] + (l(l+1))P_l = 0$$

and they appear as solutions to many physical problems, so we will discuss some of their properties here.

Associated Legendre Polynomials are the solutions to the wave equation for non-zero m_l

We will not solve the m $\neq$ 0 case now, but we will state the relation between the Legendre functions (m=0) and the full solutions (the associated Legendre functions).

$$\Theta_{lm}(x) = (1 - x^2)^{|m|/2}\frac{d^{|m|}P_l}{dx^{|m|}}$$

from which we can find

$$\Theta_{00} = 1,$$

$$\Theta_{10} = x, \quad \Theta_{1,\pm 1} = (1 - x^2)^{1/2},$$

$$\Theta_{20} = 1 - 3x^2, \quad \Theta_{2,\pm 1} = (1 - x^2)^{1/2}x$$

Angular solutions put together – Spherical Harmonics

The θ and φ solutions can now be combined
$F_{lm}(\theta, \varphi) = \Theta_{lm}(\theta)\Phi_m(\varphi)$ and when normalized, yields the Spherical Harmonics:
$$Y_l^m = \left(\frac{2l+1}{4\pi}\right)\frac{(l-m)!}{(l+m)!}\Theta_l^m(\cos\theta)e^{im\varphi}$$

The orthonormality relation is: $\iint Y_l^m Y_{l'}^{m'} \sin\theta d\theta d\varphi = \delta_{ll'}\delta_{mm'}$

l	m	$Y_{lm}(\varphi, \theta)$
0	0	$(4\pi)^{-1/2}$
1	0	$(3/4\pi)^{1/2}\cos\theta$
1	1	$-(3/8\pi)^{1/2}\sin\theta\, e^{i\varphi}$
2	0	$(5/16\pi)^{1/2}(3\cos^2\theta - 1)$

The radial equation for the Coulomb potential

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

Setting $u(r) = rR(r)$

$$-\frac{\partial^2(u(r))}{\partial r^2} + \frac{l(l+1)}{r^2}u(r) + \frac{2m}{\hbar^2}\left(-\frac{e^2}{4\pi\varepsilon_0 r}\right)u(r) = Eu(r)$$

Let $\rho = \dfrac{r}{a_0}$ where $a_0 = 4\pi\varepsilon_0\dfrac{\hbar^2}{me^2}$

Let $\varepsilon = \dfrac{E}{E_R}$ where $E_R = \dfrac{me^4}{(4\pi\varepsilon_0)^2 2\hbar^2}$

and so: $-\dfrac{\partial^2(u(\rho))}{\partial\rho^2} + \dfrac{l(l+1)}{\rho^2}u(\rho) + \dfrac{2}{\rho}u(\rho) = \varepsilon u(\rho)$

l=0 + Coulomb potential

Let's look at forms of the radial equation for $l = 0$ in the large r limit:

$$\text{when } \rho \to \infty, \quad \frac{d^2 u}{d\rho^2} + \varepsilon u = 0 \quad \Rightarrow u \propto e^{i\sqrt{\varepsilon}\rho} = e^{-\sqrt{|\varepsilon|}\rho}$$

(Remember that ε is negative because these are bound states and the potential is negative.)

We now search for solutions to the full equation using the polynomial expansion approach.

The lowest order polynomial with the right behavior *as $\rho \to 0$ is $u(\rho) = \rho e^{-\sqrt{|\varepsilon|}\rho}$.

$$*\int r^2 R^2 dr \text{ must be finite.}$$

Higher order l=0 Coulomb solutions

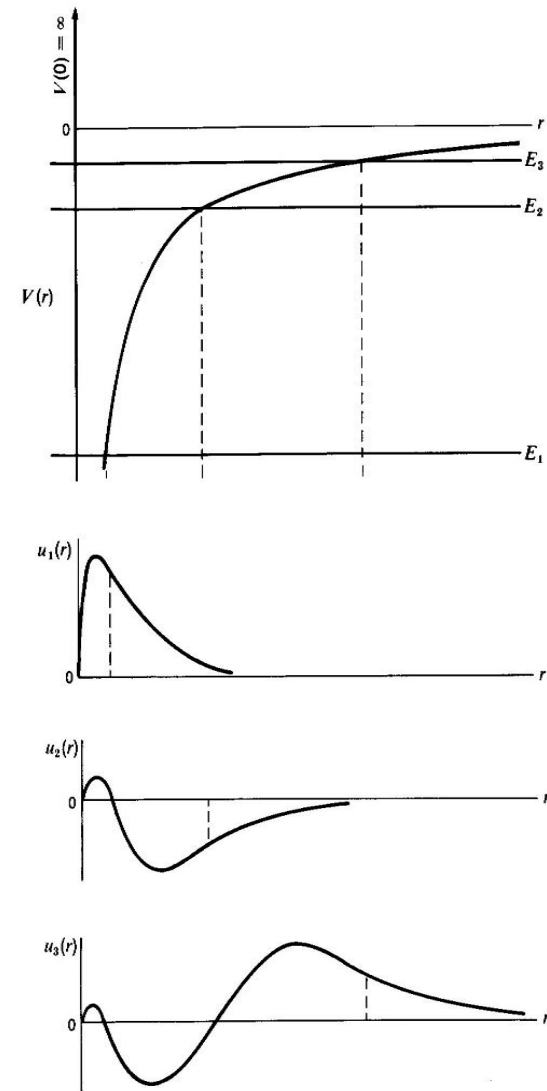We look for solutions of increasing polynomial order in similar manner and can find:
$$u_2 \propto [2\rho - \rho^2]e^{-\rho/2}$$
$$u_3 \propto [27\rho - 18\rho^2 + 2\rho^3]e^{-\rho/3}$$
and we find that the energies are:

$$E_n = \frac{E_1}{n^2}$$

A general solution for all *l* is outline
Appendix B3 in Townsend.

Probability density

- The <u>probability density</u> yields the probability of d=finding the electron in a volume dv and is given by $\Psi^*\Psi$, which for the ground state of the H atom is

$$P = \frac{1}{a_0^3 \pi} e^{-\frac{2r}{a_0}}$$

- The <u>radial probability density</u> is the probability of finding the electron in the volume between r and $r + dr$.

Radial Probability density $P(r)dr = dvP = \frac{4r^2}{a_0^3} e^{-\frac{2r}{a_0}} dr$
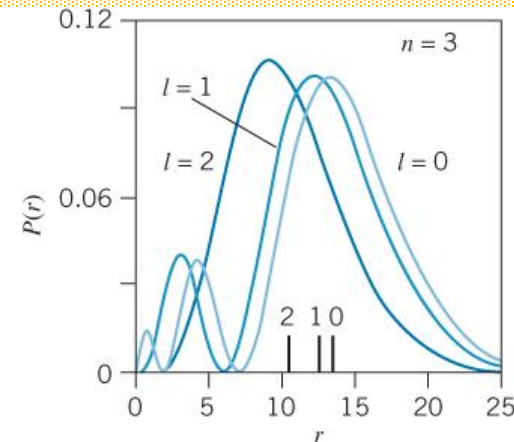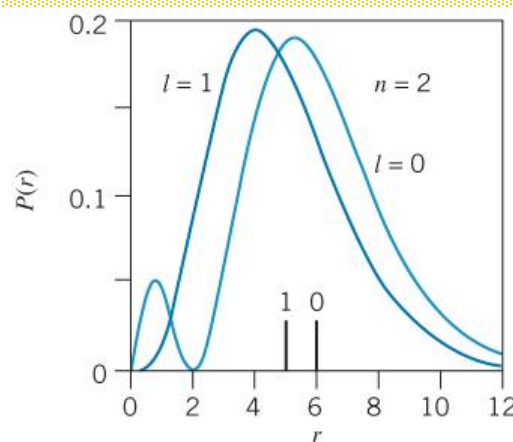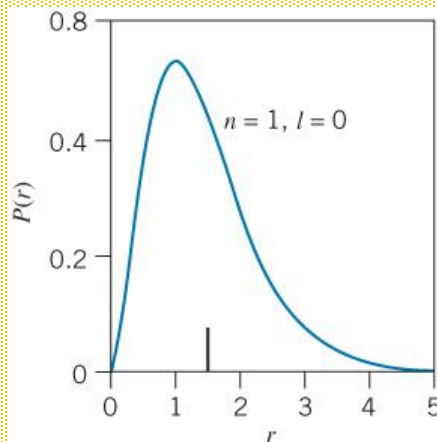
Orbital Magnetic Moment and Angular Momentum

A classical analogy leads to the proposal that a charge in a state with angular momentum has a magnetic moment:

$$\vec{\mu} = \frac{q}{2m}\vec{L}$$

If this state is placed in a magnetic field, the energy of the state shifts by:

$$\Delta E_B = \frac{qB}{2m}m_l\hbar = \mu_B B m_l$$

where $\mu_B = \frac{e\hbar}{2m} \approx 5.79 \times 10^{-5}$ eV/T is called the Bohr magneton.

The theory of orbital angular momentum and magnetic moment is predicts small but measurable shifts in optical transition energies known as the Zeeman Effect.

The energy of a magnetic dipole assumes discrete energies associated with the magnetic moment.

$$\Delta E_B = -\vec{\mu} \cdot \vec{B} = -\mu_{L,z}B = -m_l\mu_B B$$
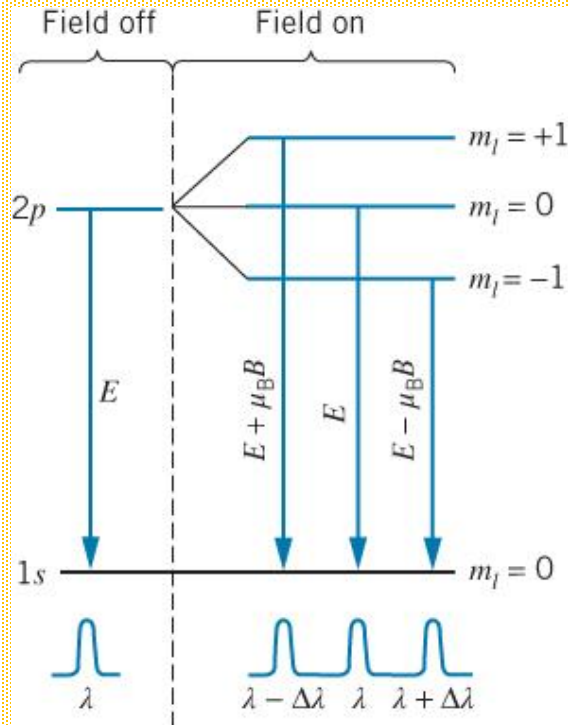
For B=1 T (strong!)
$$\Delta E \sim 10^{-4} \, eV$$
And $\frac{\Delta\lambda}{\lambda} = \frac{\lambda^2}{hc}$ and $\Delta\lambda \sim 0.03 \, nm$
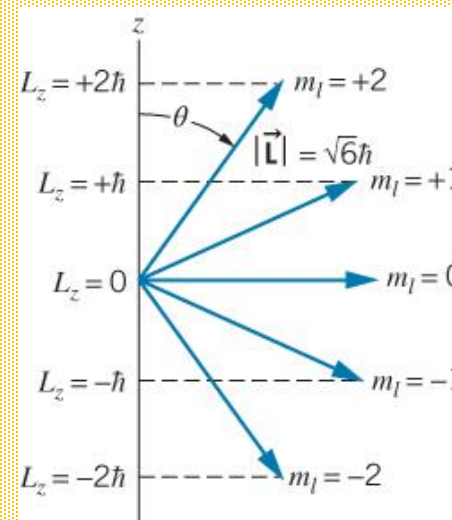(out of about 600 nm for a typical optical transition.)

Quantum Angular Momentum

It can be shown that $[L^2_{op}, L_{z,op}] = 0$, therefore it is possible to

simultaneously find eigenfunctions of the total angular momentum and the z-component of the angular momentum.

$$L^2_{op}\Psi = l(l+1)\hbar^2\Psi$$

$$L_{z,op}\Psi = m_l\hbar\Psi$$

$$where\ m_l = 0, \pm 1, \pm l$$

Electron Spin

The observed splittings imply that the electron has a magnetic moment.
A new spin quantum number m_S was proposed to explain the experiments. The intrinsic **spin** angular momentum is $\vec{S}$ where $|\vec{S}| = \sqrt{s(s+1)}\hbar$
and $S_z = m_s\hbar$ and $m_s = -s, ..., s$ in integer steps
(2*s* + 1 allowed values)

m_S must be two-valued (Stern-Gerlach Exp.) and does not appear to have a term with $\mu=0$, so it was proposed that

s = 1/2 and
m_S = -1/2 or + 1/2

Two independent indices m_l and m_S are used to specify states according to the *z* component of **L** and **S**

Electron Spin Magnetic Moment

The electron magnetic moment can be found from the splittings, but also can be derived from first principles (too hard for this course).

$$\vec{\mu}_s = -\frac{q_e}{m}\vec{S}$$

(Note that this relation differs by a factor of two from the angular momentum – moment relation.)

$$\Delta E = -\vec{\mu_s} \cdot \vec{B} = -\mu_{s_z}B$$

Total angular momentum

- We now have two sources of magnetic moment and consequent energy shift.

- We are tempted to think that they are just two effects that are independent of one another, but no, it is more complicated.

- The two magnetic moments are coupled. (Orbital angular momentum creates a magnetic field that defines a z-direction for the spin moment (and vice versa).)

- Because $\vec{L}$ and $\vec{S}$ are coupled, they interact with an external magnetic field in such a way that the total angular momentum: $\vec{J} = \vec{L} + \vec{S}$ is a conserved quantity

Total angular momentum

The total angular momentum (J) is the vector sum of the orbital and electron angular momenta (spin).

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

The total angular momentum is conserved in all interactions (and not necessarily L or S individually). The total angular momentum has the value:

$$|J| = \sqrt{j(j+1)}\hbar \text{ with possible values}$$
$$j = |l-s|, |l-s|+1, |l-s|+2, \ldots |l+s|$$
$$\text{and with } j_z = m_z\hbar$$

Spectroscopic notation

In spectroscopic notation we label the value of the total angular momentum quantum number j with a subscript following the letter code for orbital angular momentum.

As an example: The notation $3p_{3/2}$ denotes a single electron in the n=3, l=1, j=3/2 state.

Spectroscopic notation can also be used to describe the state of an atom with more than one electron. The angular momentum and spin are the sum for all the electrons in the system.

As an example: The notation $3P_{1/2}$ can denote a sodium atom with its electron in the n=3, l=1, j=1/2 state. The electrons in the filled shells are paired off in such a way that the total angular momentum and spin are zero.

Summary

- Orbital angular momentum gives rise to an orbital magnetic moment
  - The energy shift of states due to magnetic moment interaction with external field is observed as the Zeeman effect
- Electron spin also gives rise to a magnetic moment
  - Evidence for electron spin of ½ unit is found from the Anomalous Zeeman and Stern-Gerlach experiments (even splittings)
  - Fine structure spectroscopic energy shifts indicate that the spin and orbital magnetic moments interact with one another.
- The total spin and orbital angular momentum couple to one another so that the total angular momentum $\vec{J} = \vec{L} + \vec{S}$, with $|J| = \sqrt{j(j+1)}\hbar$ with possible values $j = |l - s|, |l - s| + 1, |l - s| + 2, \ldots |l + s|$ and with $j_z = m_z\hbar$.
- Spectroscopic Notation

Identical Particles

- Wavefunctions of multiple particles must account for the fact that identical particles are indistinguishable.

- Pauli Exclusion Principle: No two electrons in the same system can be in the same state.

- These effects lead to profound changes in the physical world.

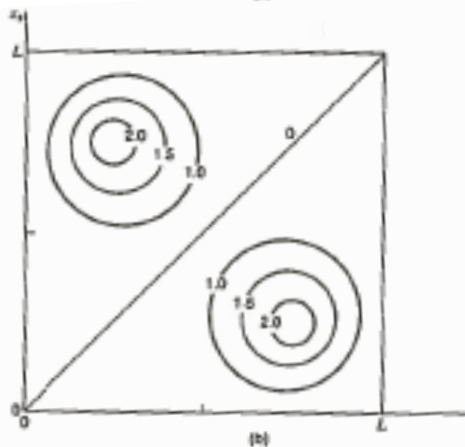- How does particle symmetry requirement affect properties of atoms?

Constructing a probability density that does not change under particle exchange
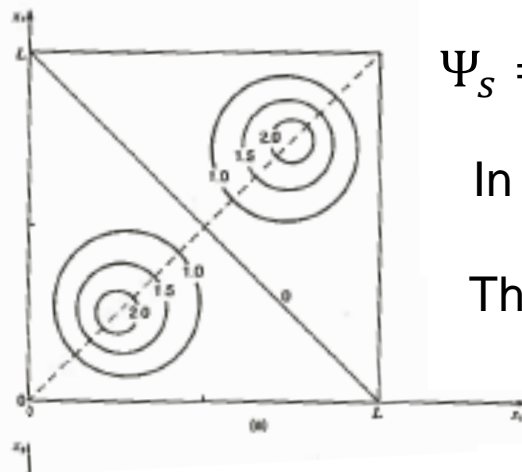
$$\Psi_S = \frac{1}{\sqrt{2}}(\psi_A(x_1)\psi_B(x_2) + \psi_A(x_2)\psi_B(x_1))$$

In the symmetric state, $P(x_1,x_2)$ is a maximum when the particles are close together.
They act as though they are attracted to one another even though there is no force between them.

$$\Psi_a = \frac{1}{\sqrt{2}}(\psi_A(x_1)\psi_B(x_2) - \psi_A(x_2)\psi_B(x_1))$$

In the antisymmetric state, P is a maximum when the particles are far apart and is zero along the $x_1=x_2$ line.
They act as though they are repelling one another, even though there is no force between them.

Identical Particles

3 Identical Particles: Antisymmetric Case
The Slater Determinant

$$\Psi_A(1,2,3)$$

$$= \frac{1}{\sqrt{6}} \begin{vmatrix} \psi_\alpha(1) & \psi_\alpha(2) & \psi_\alpha(3) \\ \psi_\beta(1) & \psi_\beta(2) & \psi_\beta(3) \\ \psi_\alpha(1) & \psi_\alpha(2) & \psi_\alpha(3) \end{vmatrix}$$

To make the symmetric case, just switch all (-) signs to (+).

Which choice, Symmetric or Antisymmetric, does nature take?

- The answer is: Sometimes one, sometimes the other, depending on the type of particle involved, but ...

- to address this question properly we need to consider the complete wavefunction, which includes properties like intrinsic spin, isospin, strangeness, charm, beauty ...

- We'll just worry about spin for now.

Total Wavefunction symmetry

- The total wavefunction for two identical particles is the product of one of the possible spatial wavefunction combinations and one of the possible spin wavefunctions.

$$\Psi = \psi(x_1, x_2)\chi(s_1, s_2)$$

- It is the <u>overall symmetry</u> of the total wavefunction that is important for exchange symmetry and the Pauli Exclusion Principle.

Consequences of Exchange Symmetry

- Pauli exclusion principle leads to building up of electrons in multi-electron atoms.

- Corrections to the energies of multi-particle states.

- The Simplest Testable Example:
  The Helium Atom