
QUANTUM MECHANICS (PHYS4010) LECTURE NOTES

LECTURE NOTES BASED ON A COURSE GIVEN BY ROMAN KONIUK.
THE COURSE BEGINS WITH A FORMAL INTRODUCTION INTO QUANTUM MECHANICS AND THEN
MOVES TO SOLVING DIFFERENT QUANTUM SYSTEMS AND ENTANGLEMENT

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I. UNDERLYING PRINCIPLES OF QUANTUM MECHANICS

Lecture 1 - Sept. 7th 2011

The course website is <http://www.yorku.ca/koniuk/PHYS4010/index.htm> .

A. Postulates of Quantum Mechanics

1. To every observable there corresponds an operator. For example to the observable A (e.g. energy, momentum, position, etc.) there corresponds an operator \hat{A} . Every measurement of A gives a value, a , s.t. a is an eigenvalue of the operator \hat{A} . i.e. for an eigenfunction of A , ϕ , $\hat{A}\phi = a\phi$.
2. Measurement of observable A yields the value a , and then leaves the state in the state ϕ_a . i.e.

$$A\phi_a = a\phi_a$$

3. All possible information is contained in the wavefunction, $\Psi(\mathbf{r}, t)$.
4. Ψ develops in time according to the Schrodinger wave equation (SWE)

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \hat{H}\Psi(\mathbf{r}, t) \quad (\text{I.1})$$

B. Important Properties

The average value (expectation value) of an observable C at time t is given by

$$\langle C \rangle(t) = \int \Psi^*(\mathbf{r}, t) \hat{C} \Psi(\mathbf{r}, t) d\mathbf{r} \quad (\text{I.2})$$

Experimentally this would be done by preparing an ensemble of identical initial states $\Psi(\mathbf{r}, 0)$ and measure C at time t . This will generate a set of values, $c_1, c_2, c_3, \dots, c_N$ (where N is the number of measurements)

$$\langle C \rangle = \frac{1}{N} \sum_{i=1}^N c_i \quad (\text{I.3})$$

We can also interpret this as

$$\langle C \rangle = \sum_i c_i P(c_i) \quad (\text{I.4})$$

The uncertainty (or standard deviation) in c is given by Δc :

$$\Delta c = \sqrt{\langle c^2 \rangle - \langle c \rangle^2} \quad (\text{I.5})$$

The modulus of Ψ is given by

$$\Psi^*(\mathbf{r}, t) \Psi(\mathbf{r}, t) = |\Psi(\mathbf{r}, t)|^2 \quad (\text{I.6})$$

$$|\Psi|^2 dx = \overbrace{P(x) dx}^{\text{probability to find particle at point } x} \quad (\text{I.7})$$

The normalization condition is:

$$\int_{-\infty}^{\infty} P(x) dx = 1 \quad (\text{I.8})$$

C. The Time Evolution Operator

Suppose \hat{H} doesn't depend on time. (i.e. $\hat{H} = \hat{H}(\mathbf{r})$). Assume $\Psi(\mathbf{r}, t) = \phi(\mathbf{r})T(t)$ Plugging this result into the SWE:

$$i\hbar \frac{\partial(\phi T)}{\partial t} = \hat{H} \phi T \quad (\text{I.9})$$

$$i\hbar \phi \frac{\partial T}{\partial t} = T \hat{H} \phi \quad (\text{I.10})$$

Divide both sides by ψ :

$$\overbrace{i\hbar \frac{1}{T} \frac{\partial T}{\partial t}}^f = \overbrace{\frac{1}{\phi} \hat{H} \phi}^g \quad (\text{I.11})$$

Thus $f(t) = g(\mathbf{r})$ (regardless of t and \mathbf{r}) The only way this can be true is if $f(t) = g(\mathbf{r}) = E$ where E is some constant. This generates two equations

$$i\hbar \frac{\partial T}{\partial t} = ET \quad (\text{I.12})$$

and

$$\hat{H} \phi = E \phi \quad (\text{I.13})$$

Notice that equation I.13 contains all the physics of the problem while the time equation contains no physics (does not contain the Hamiltonian). Equation I.12 can be solved by:

$$T(t) = e^{-iEt/\hbar} \quad (\text{I.14})$$

Thus if the problem is separable then the time dependence is always given by the above equation. All this term does is change the phase of the wavefunction (shifts the magnitude of the wavefunction from the real and complex part of the wavefunction). This time dependence is often referred to as trivial time dependence.

Equation I.13 is an eigenvalue problem. E is the eigenvalue and ϕ is the eigenfunction of the operator \hat{H} . There are typically infinitely many solutions:

$$\hat{H} \phi_n = E_n \phi_n \quad (\text{I.15})$$

With

$$\Psi_n(\mathbf{r}, t) = \phi_n(\mathbf{r})T(t) \quad (\text{I.16})$$

$$\Psi_n(\mathbf{r}, t) = \phi_n(\mathbf{r})e^{-iE_n t/\hbar} \quad (\text{I.17})$$

The probability density can depend on time if we don't have an eigenfunction.

The initial value problem: If we know the $\Psi(\mathbf{r}, 0)$ then we can determine Ψ for all time (i.e. $\Psi(\mathbf{r}, t)$)

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi \quad (\text{I.18})$$

$$\Rightarrow \frac{\partial \Psi}{\partial t} = \frac{-i}{\hbar} \hat{H} \Psi \quad (\text{I.19})$$

$$\Rightarrow \frac{\partial \Psi}{\partial t} + i \frac{\hat{H}}{\hbar} \Psi = 0 \quad (\text{I.20})$$

$$\Rightarrow \frac{\partial}{\partial t} \left(\exp(it\hat{H}/\hbar) \Psi(\mathbf{r}, t) \right) = 0 \quad (\text{I.21})$$

Note: For this to be true we have to assume that $\hat{H} = \hat{H}(\mathbf{r})$

Comments:

1. Notice that in the factor $\exp\left(\frac{it\hat{H}}{\hbar}\right)$, \hat{H} is an operator (could be a matrix). This can be understood by the real definition of the exponential function (a power series expansion):

$$\exp(it\hat{H}/\hbar) = 1 + \frac{it\hat{H}}{\hbar} + \frac{(it\hat{H})^2}{\hbar^2 2!} + \dots \quad (\text{I.22})$$

This operator is defined as:

$$\boxed{\hat{U}^{-1} \equiv \exp\left(\frac{it\hat{H}}{\hbar}\right)} \quad (\text{I.23})$$

Lets carry on with our solution:

$$\int_0^{t'} \frac{\partial}{\partial t} \left(\exp(it\hat{H}f/\hbar)\Psi(\mathbf{r}, t) \right) dt = \int_0^{t'} 0 dt \quad (\text{I.24})$$

By the fundamental theorem of calculus:

$$\exp(it'\hat{H}f/\hbar)\Psi(\mathbf{r}, t') - \exp(0)\Psi(\mathbf{r}, 0) = 0 \quad (\text{I.25})$$

You are free to change the dummy variable t' to t and multiplying by \hat{U} :

$$\boxed{\Psi(\mathbf{r}, t') = \exp(-it'\hat{H}f/\hbar)\Psi(\mathbf{r}, 0)} \quad (\text{I.26})$$

The operator \hat{U} is called the time evolution operator.

Note that this is true for *any* state. Now suppose the initial state is an eigenstate (also called stationary states) of \hat{H} . Hence:

$$\Psi(\mathbf{r}, 0) = \phi_n(\mathbf{r}) \quad (\text{I.27})$$

$$\Rightarrow \Psi(\mathbf{r}, t) = \hat{U}\phi_n(\mathbf{r}) \quad (\text{I.28})$$

$$= \exp(-i\hat{H}t/\hbar)\phi_n(\mathbf{r}) \quad (\text{I.29})$$

$$= \exp(-iE_n t/\hbar)\phi_n(\mathbf{r}) \quad (\text{I.30})$$

Hence in this special case the time ordering operator is just the trivial phase found earlier.

Lecture 3

II. PARTICLE IN A BOX

Step 1:

Write down the potential

$$V(x) = \begin{cases} V = 0 & 0 < x < a \\ V(x) = \infty & x \leq 0, x \geq a \end{cases} \quad (\text{II.1})$$

Step 2:

Write down the S.E.

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

The time portion is given by (assuming a separable solution)

$$T(t) = \exp(-iEt/\hbar) \quad (\text{II.3})$$

Thus the time independent problem is now given by

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \phi(x) + V(x)\phi(x) = E\phi(x) \quad (\text{II.4})$$

Step 3:

Outside the box the solution is trivial. It is zero.

Inside the box the equation is given by

$$\frac{\partial^2}{\partial x^2} \phi(x) = -k^2 \phi(x) \quad (\text{II.5})$$

Where k is given by

$$k^2 = \frac{2mE}{\hbar^2} \quad (\text{II.6})$$

The solution is given by

$$\phi(x) = A \sin(kx) + B \cos(kx) \quad (\text{II.7})$$

Step 4:

Check the boundary conditions

$$\phi(0) = 0 = B \quad (\text{II.8})$$

$$\phi(a) = 0 = A \sin(ka) \quad (\text{II.9})$$

$$(\text{II.10})$$

Hence we have the trivial solution (no particle) unless

$$ka = n\pi \quad (\text{ n is an integer}) \quad (\text{II.11})$$

$$\sqrt{\frac{2mE}{\hbar^2}} a = n\pi \quad (\text{II.12})$$

$$\Rightarrow E_n = \left(\frac{n\pi}{a}\right)^2 \frac{\hbar^2}{2m} \quad (\text{II.13})$$

Hence E developed an index and energy quantization came out. Note that k also has an index:

$$k_n = \frac{n\pi}{a} \quad \text{The wave-number is also quantized} \quad (\text{II.14})$$

$$\phi_n(x) = A \sin\left(\frac{n\pi x}{a}\right) \quad (\text{II.15})$$

Note the energy levels rise rapidly they go as n^2 . Note we were dealing with a homogeneous differential equation and hence isn't fixed yet. This can be done using the normalization condition:

$$\int_{-\infty}^{\infty} |\phi_n|^2 dx = \int_0^a A^2 \sin^2\left(\frac{n\pi x}{a}\right) dx \quad (\text{II.16})$$

$$A^2 \frac{a}{2} = 1 \quad (\text{II.18})$$

Hence

$$A = \sqrt{\frac{2}{a}} \quad (\text{II.19})$$

Notice that the normalization constant is independent of the particular quantum number n. Therefore

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad E_n = \frac{n^2 \hbar^2 \pi^2}{2ma^2} \quad (\text{II.20})$$

Since the energy increases with decreasing a it means that quantum mechanics opposes this motion. This can be thought of as a quantum mechanical pressure on the outside of the box. Note that n can equal any integer

$$n = 1, 2, \dots \quad (\text{Infinity many bound states}) \quad (\text{II.21})$$

Note the dimensions of ϕ are $1/\sqrt{L}$ and the dimensions of the P (the probability density) is $1/L$. The energy levels

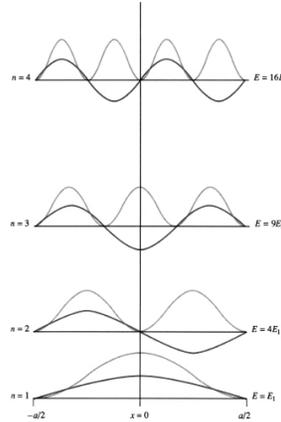


FIG. 1. The Wavefunctions of the Square Well and Their Corresponding Probability Densities

as well as the corresponding wavefunctions are shown in figure 1. Typically there are as many quantum numbers as dimensions of the problem.

Def 1. In any problem as $\hbar \rightarrow 0$ we recover classical physics. Equivalently we can recover classical physics as $E \rightarrow \infty$.

In our problem as E becomes large we should recover the classical distribution. The classical distribution is given by

$$P(x) = \begin{cases} 1/a & 0 < x < a \\ 0 & x \leq 0, x \geq a \end{cases} \quad (\text{II.22})$$

In the limit of large E , we have a highly oscillating function from 0 to $2/a$. For any experiment that tries to measure how likely it is we will get to any finite region it will be $1/a$.

Assignment: Demonstrate by direct substitution that the first 5 eigenfunctions of the 1d well are indeed eigenfunctions of the potential. Plot the first 5 eigenfunctions as well as the first 5 probability distributions. Due date: Wednesday.

Lecture 4 (September 14th, 2011)

Note: *Assignment 2 is up.*

III. DIRAC NOTATION

The Dirac notation is a more abstract notation than was used up till now though it is more powerful. There is a corresponding notation in geometry referred to as coordinate free notation. The idea is a vector has a meaning before a coordinate system is assigned to it. Similarly in quantum mechanics we have states which are independent of a particular representation.

A state labeled by a quantum number α is denoted by a “ket”. The symbol for the ket of α

$$|\alpha\rangle \quad (\text{III.1})$$

In the spatial representation the state $|\alpha\rangle$ is given by $\Psi_\alpha(x)$. For example

$$\langle\alpha|\beta\rangle = \int_{-\infty}^{\infty} \psi_\beta^*(x)\psi_\alpha(x)dx \quad (\text{III.2})$$

Note that this is analogous to

$$\mathbf{A} \cdot \mathbf{B} \quad (\text{III.3})$$

The analogy is even more evident by writing the integral as

$$\lim_{\substack{\Delta x_i \rightarrow 0 \\ N \rightarrow \infty}} \sum_{i=1}^N \psi_{\beta}^*(x_i) \psi_{\alpha}(x_i) \Delta x \quad (\text{III.4})$$

Thus the wavefunctions are infinite dimension vectors. In coordinate free notation equation III.2 is given by

$$\langle \beta | \alpha \rangle \quad (\text{III.5})$$

The “thing you dot kets with” is called a bra:

$$\langle \beta | \quad (\text{III.6})$$

Bras and kets obey the following rules (a is some constant)

$$\langle \beta | a \alpha \rangle = a \langle \beta | \alpha \rangle \quad (\text{III.7})$$

$$\langle a \beta | \alpha \rangle = a^* \langle \beta | \alpha \rangle \quad (\text{III.8})$$

$$\langle \beta | \alpha \rangle^* = \langle \alpha | \beta \rangle \quad (\text{III.9})$$

$$\langle \alpha | + \langle \beta | = \langle \alpha + \beta | \quad (\text{III.10})$$

The state $|x'\rangle$ is an eigenstate of the position operator \hat{x} .

$$\hat{x} |x'\rangle = \overbrace{x'}^{\text{eigenvalue}} |x'\rangle \quad (\text{III.11})$$

$$\langle x' | x \rangle = \delta(x' - x) \quad \text{The Dirac Delta Function} \quad (\text{III.12})$$

This makes sense since this expression reads what is the amplitude that a state $|x'\rangle$ coincides with the state $|x\rangle$. These two states are distinctly different unless $x = x'$. The overlap of a position with the state α is

$$\langle x' | \alpha \rangle = \psi_{\alpha}(x') \quad (\text{III.13})$$

This expression can be read as what is the amplitude that a state α is at x . Suppose you have a complete set of states labeled by integers (an orthonormal set):

$$\sum_n |n\rangle \langle n| = \hat{I} \quad (\text{III.14})$$

To see that this is truly the identity:

$$\hat{I} |m\rangle = \sum_n |n\rangle \langle n|m\rangle \quad (\text{III.15})$$

$$= \sum_n |n\rangle \delta_{nm} \quad (\text{III.16})$$

$$= |m\rangle \quad (\text{III.17})$$

Lecture 5: September 16, 2011
Notes for the assignment:

$$\langle x \rangle = \int P(x, t) x dx \quad (\text{III.18})$$

$$P(x, t) = \Psi^*(x, t) \Psi(x, t) \quad (\text{III.19})$$

$$\Psi(x, t) = \frac{1}{\sqrt{2}} (\phi_1(x)e^{-i\omega_1 t} + \phi_2(x)e^{-i\omega_2 t}) \quad (\text{III.20})$$

$$E_1 = \hbar\omega_1 = \frac{\hbar^2\pi^2}{2ma^2} \quad (\text{III.21})$$

Continuing with the lecture

$$\langle x|\alpha\rangle = \psi_\alpha(x) \quad (\text{III.22})$$

$$\langle \beta|x\rangle = \psi_\beta(x)^* \quad (\text{III.23})$$

$$|\alpha\rangle = \text{ket, "vector"} \quad (\text{III.24})$$

$$\langle \beta| = \text{bra, "dual vector"} \quad (\text{III.25})$$

Dual vectors are the objects that come from the scalar product with kets.

$$\langle \alpha|\beta\rangle = \int \psi_\alpha^*(x)\psi_\beta(x)dx \quad (\text{III.26})$$

Aside (Cultural): The place where these are completely different objects are in differential geometry (general relativity). The objects dual to vectors are called one-forms. Maxwell's equals can be written in differential geometry language as:

$$dF = 0 \quad (\text{III.27})$$

$$d * F = J \quad (\text{III.28})$$

IV. HILBERT SPACE

Recall Cartesian 3-space. We have vectors:

$$\mathbf{v} = (v_x, v_y, v_z) \quad (\text{IV.1})$$

$$\mathbf{v} = \hat{e}_x v_x + \hat{e}_y v_y + \hat{e}_z v_z \quad (\text{IV.2})$$

We say that $(\hat{e}_x, \hat{e}_y, \hat{e}_z)$ form a *basis* that *spans* the vector space. In other words we can build any vector in the vector space by a linear combination of the basis vectors.

Inner Product:

$$\mathbf{v} \cdot \mathbf{u} = v_x u_x + v_y u_y + v_z u_z \quad (\text{IV.3})$$

Length:

$$\sqrt{\mathbf{v} \cdot \mathbf{u}} = |\mathbf{v}| \quad (\text{IV.4})$$

1. The Hilbert space (\mathcal{H}) is analogous to this space.

The space is linear

For a constant "a" $a\phi$ is also in the Hilbert space

If ψ and ϕ are in \mathcal{H} then so is $\psi + \phi$.

2. There is an inner product

$$\langle \alpha|\beta\rangle = \int \psi_\alpha^*(x)\psi_\beta(x)dx \quad (\text{IV.5})$$

3. Any element of \mathcal{H} has a "length"

$$\langle \alpha|\alpha\rangle = \|\alpha\|^2 \quad (\text{IV.6})$$

4. \mathcal{H} is complete: Every *Cauchy sequence* of functions (or states) in \mathcal{H} converges to an element in \mathcal{H} .
i.e. \mathcal{H} contains the limit points)

To understand this definition we need to define the Cauchy sequence:

Def 2. Cauchy Sequence: A sequence that as we go on in the sequence the difference gets smaller and smaller between neighboring number.

Mathematically, given the sequence $\{x_i\}$ any ϵ for some i :

$$|x_{i+1} - x_i| \leq \epsilon \quad (\text{IV.7})$$

A Cauchy sequence can converge to a number that is not rational (the limit point can be outside the set). We say the irrationals *complete* the rationals.

Lecture 6: September 19, 2011

A quick summary of the different notations is given below

3-D	Representation	Bro-ket
$\mathbf{v} \cdot \mathbf{v} = 0$	$\int \psi_\alpha^*(x) \psi_\beta(x) dx = 0$	$\langle \alpha \beta \rangle = 0$
$(\hat{e}_1, \hat{e}_2, \hat{e}_3)$	(ψ_1, ψ_2, \dots)	$(1\rangle, 2\rangle, 3\rangle, \dots)$
$\mathbf{v} = \sum_i a_i \hat{e}_i$	$\phi(x) = \sum_n a_n \phi_n(x)$	$ \alpha\rangle = \sum_n a_n n\rangle$
$\hat{e}_i \cdot \hat{e}_j = \delta_{i,j}$	$\int \phi_n^*(x) \phi_m(x) dx = \delta_{n,m}$	$\langle n m \rangle = \delta_{n,m}$
$\hat{e}_n \cdot \mathbf{v} = a_n$	$\int \phi_n^*(x) \psi_\alpha(x) dx = a_n$	$\langle n \alpha \rangle = a_n$

$$|\alpha\rangle = \sum_m a_m |m\rangle \quad (\text{IV.8})$$

$$\langle n | \alpha \rangle = \sum_m \langle n | a_m | m \rangle \quad (\text{IV.9})$$

$$= \sum_m a_m \langle n | m \rangle \quad (\text{IV.10})$$

$$= \sum_m a_m \delta_{n,m} \quad (\text{IV.11})$$

$$= a_n \quad (\text{IV.12})$$

Word of warning: Sometimes we choose basis sets in \mathcal{H} that are labeled by a continuous valued label. An example of this is the wave number: $|k\rangle$. This can be used as:

$$\langle x | k \rangle = e^{ikx} \quad (\text{IV.13})$$

$$\left\langle k \left| \int_x |x\rangle \langle x| k \right\rangle dx = \int_{-\infty}^{\infty} (1) dx = \infty \quad (\text{IV.14})$$

The reason the overlap is infinity is because the plane waves are **non-normalizable**.

V. HERMITIAN OPERATORS

Consider the operator \hat{A} such that $\hat{A}|\alpha\rangle$ is also in \mathcal{H} and $\langle \beta | \hat{A} | \alpha \rangle$. If there is another operator designated by \hat{A}^\dagger such that

$$\langle \hat{A}^\dagger \beta | \alpha \rangle = \langle \beta | \hat{A} \alpha \rangle \quad (\text{V.1})$$

Then we say that \hat{A}^\dagger is the Hermitian adjoint of \hat{A} (It does not mean that \hat{A} is hermitian). Simplest possible operator $\hat{A} = a$ (where a is some number)

$$\langle a^\dagger \beta | \alpha \rangle = \langle \beta | a \alpha \rangle = a \langle \beta | \alpha \rangle = \langle a^* \beta | \alpha \rangle \quad (\text{V.2})$$

Hence $a^\dagger = a^*$. i.e. the hermitian adjoint of a complex number is its complex conjugate. Consider the operator $\hat{D} = \frac{\partial}{\partial x}$.

$$\langle \beta | \hat{D} \alpha \rangle = \int_{-\infty}^{\infty} dx \psi_\beta^*(x) \frac{\partial}{\partial x} \psi_\alpha(x) \quad (\text{V.3})$$

By integration by parts:

$$= \cancel{\psi_\beta^*(x)\psi_\beta(x)} \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} dx \left(\frac{\partial}{\partial x} \psi_\beta^*(x) \right) \psi_\alpha(x) \quad (\text{V.4})$$

The surface terms cancel due to normalization condition. Hence

$$\hat{D}^\dagger = -\hat{D} \quad (\text{V.5})$$

In the special case where

$$\hat{A}^\dagger = \hat{A} \quad (\text{V.6})$$

we say the operators are Hermitian.

Lecture 7 - Sept 21, 2011 Recall $\frac{\partial}{\partial x}$ is not Hermitian, but $\left(\frac{\partial}{\partial x}\right)^\dagger = -\frac{\partial}{\partial x}$. Consider

$$\hat{A}|n\rangle = a_n|n\rangle \quad (\text{V.7})$$

Then

$$\langle n|\hat{A}|n\rangle = \langle n|a_n|n\rangle \quad (\text{V.8})$$

$$= a_n \langle n|n\rangle \quad (\text{V.9})$$

$$(\text{V.10})$$

But if \hat{A} is Hermitian then

$$\langle \hat{A}n|n\rangle = \langle a_n n|n\rangle \quad (\text{V.11})$$

$$= a_n^* \langle n|n\rangle \quad (\text{V.12})$$

Hence $a_n = a_n^*$ (a_n is real). Consider now

$$\langle m|\hat{A}|n\rangle = \langle m|a_n|n\rangle \quad (\text{V.13})$$

$$= a_n \langle m|n\rangle \quad (\text{V.14})$$

But

$$\langle m|\hat{A}|n\rangle = \langle \hat{A}^\dagger m|n\rangle \quad (\text{V.15})$$

$$= \langle \hat{A}m|n\rangle \quad (\text{V.16})$$

$$= \langle a_m m|n\rangle \quad (\text{V.17})$$

$$= a_m^* \langle m|n\rangle = a_m \langle m|n\rangle \quad (\text{V.18})$$

Therefore

$$(a_n - a_m) \langle m|n\rangle = 0 \quad (\text{V.19})$$

If $a_n \neq a_m$ then

$$\langle m|n\rangle = 0 \quad (\text{V.20})$$

Therefore eigenstate of Hermitian operators are orthogonal.

VI. FOURIER SERIES

Suppose $f(x)$ is periodic with period 2. i.e. For some a and all n :

$$f(x + na) = f(x) \quad (\text{VI.1})$$

Then we can write

$$f(x) = \begin{cases} \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(nx) & \text{for odd } f \\ \sum_{n=1}^{\infty} b_n \sin(n\pi x) & \text{for odd } f \end{cases} \quad (\text{VI.2})$$

Where for all n :

$$a_n = \int_0^2 f(t) \cos(n\pi t) dt \quad b_n = \int_0^2 f(t) \sin(n\pi t) dt \quad (\text{VI.3})$$

Exercise: Prove that any function can be written as a Fourier expansion

For any interval $-L$ to L for a general periodic function:

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left(a_n \cos\left(\frac{n\pi x}{L}\right) + b_n \sin\left(\frac{n\pi x}{L}\right) \right) \quad (\text{VI.4})$$

Where

$$a_n = \frac{1}{L} \int_{-L}^L f(t) \cos\left(\frac{n\pi t}{L}\right) dt \quad (\text{VI.5})$$

$$b_n = \frac{1}{L} \int_{-L}^L f(t) \sin\left(\frac{n\pi t}{L}\right) dt \quad (\text{VI.6})$$

For an example consider the square wave:

$$f(x) = \begin{cases} 0 & -\pi < x < 0 \\ 1 & 0 < x < \pi \end{cases} \quad (\text{VI.7})$$

$$a_0 = 1 \quad (\text{VI.8})$$

$$a_n = \frac{1}{\pi} \int_0^{\pi} \cos(nt) dt = 0 \quad \text{It is an odd function shifted upwards} \quad (\text{VI.9})$$

$$b_n = \frac{1}{\pi} \int_0^{\pi} \sin(nt) dt \quad (\text{VI.10})$$

$$= \frac{1}{\pi} \left(\frac{1}{n} - \frac{\cos n\pi}{n} \right) \quad (\text{VI.11})$$

$$= \frac{1}{n\pi} (1 - (-1)^n) \quad (\text{VI.12})$$

Therefore

$$b_n = \begin{cases} \frac{2}{n\pi} & \text{odd } n \\ 0 & \text{even } n \end{cases} \quad (\text{VI.13})$$

$$f(x) = \frac{1}{2} + \frac{2}{\pi} \left(\sin x + \frac{\sin 3x}{3} + \dots \right) \quad (\text{VI.14})$$

The orthogonality statement

$$\int_0^{2\pi} \sin(mx) \sin(nx) = \pi \delta_{nm} \quad \text{Unless } m = n = 0 \quad (\text{VI.15})$$

$$\int_0^{2\pi} \cos(mx) \cos(nx) = \pi \delta_{nm} \quad (\text{VI.16})$$

$$\int_0^{2\pi} \sin(mx) \cos(nx) = \pi \delta_{nm} = 0 \quad \text{Unless } m = n = 2\pi \quad (\text{VI.17})$$

VII. FOURIER TRANSFORM

Lecture 8 - September 23rd, 2011

The Fourier series of a function f is given by

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi x}{L}\right) + b_n \sin\left(\frac{n\pi x}{L}\right) \quad (\text{VII.1})$$

Where

$$a_n = \frac{1}{L} \int_{-L}^L f(t) \cos\left(\frac{n\pi t}{L}\right) dt \quad (\text{VII.2})$$

$$b_n = \frac{1}{L} \int_{-L}^L f(t) \sin\left(\frac{n\pi t}{L}\right) dt \quad (\text{VII.3})$$

Explicitly:

$$f(x) = \frac{1}{2L} \int_{-L}^L f(t) dt + \frac{1}{L} \cos\left(\frac{\pi n x}{L}\right) \int_{-L}^L f(t) \cos\left(\frac{n\pi t}{L}\right) dt + \frac{1}{L} \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right) \int_{-L}^L f(t) \sin\left(\frac{n\pi t}{L}\right) dt \quad (\text{VII.4})$$

$$= \frac{1}{2L} \int_{-L}^L f(t) dt + \frac{1}{L} \sum_{n=1}^{\infty} \int_{-L}^L f(t) \cos\left(\frac{n\pi}{L}(t-x)\right) dt \quad (\text{VII.5})$$

Now let $L \rightarrow \infty$ (non-periodic function). Set

$$\frac{n\pi}{L} = \omega \quad (\text{VII.6})$$

This is equivalent to making the spacing between neighboring ω 's ($\Delta\omega = \frac{\pi}{L}$) goes to 0. i.e. ω is continuous. In this limit:

$$f(x) = \frac{1}{\pi} \sum_{n=1}^{\infty} \Delta\omega \int_{-\infty}^{\infty} f(t) \cos(\omega(t-x)) dt \quad (\text{VII.7})$$

Notice the first integral went to zero due to the $\frac{1}{L}$ dependence and no infinite summation over n . $\frac{1}{\pi} \sum_{n=1}^{\infty} \Delta\omega$ is just the definition of an integral. Thus

$$f(x) = \frac{1}{\pi} \int_0^{\infty} d\omega \int_{-\infty}^{\infty} f(t) \cos(\omega(t-x)) dt \quad (\text{VII.8})$$

Notice that in the integrand we have an even function of ω . Therefore we can divide by 2 and change the ω integral to:

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} f(t) \cos(\omega(t-x)) dt \quad (\text{VII.9})$$

Now notice that the limits are symmetric so we can add an odd function of ω in the integrand (it will just go to zero anyways)

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} f(t) \cos(\omega(t-x)) + i f(t) \sin(\omega(t-x)) dt \quad (\text{VII.10})$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} f(t) e^{-i\omega(t-x)} dt \quad (\text{VII.11})$$

$$= \frac{1}{2\pi} \overbrace{\int_{-\infty}^{\infty} e^{i\omega x} d\omega}^{\mathcal{F}^{-1}(x)} \overbrace{\int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt}^{\mathcal{F}(\omega)} \quad (\text{VII.12})$$

Each of these \mathcal{F} are transformations on the function $f(t)$. Whatever the first one does, the second one undoes. \mathcal{F} is called the Fourier transform of $f(t)$. $\mathcal{F}^{-1}(x)$ is the inverse Fourier transform of $g(\omega)$.

$$f(t) \xrightarrow{\mathcal{F}} g(\omega) \quad f(t) \xleftarrow{\mathcal{F}^{-1}} g(\omega) \quad (\text{VII.13})$$

$g(\omega)$ is analogous to a_n .

Lecture 9 - Sept 30th, 2011
 Make up lecture Tuesday 2:30 pm.
 Recall:

$$f(x) = \int_{-\infty}^{\infty} f(t) \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(t-x)\omega} d\omega \right) dt \quad (\text{VII.14})$$

Definitions:

$$g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt \quad (\text{VII.15})$$

We say that $g(\omega)$ is the Fourier transform of the function $f(t)$. The function

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(\omega) e^{i\omega t} d\omega \quad (\text{VII.16})$$

is called the inverse Fourier transform.

A. Example: Finite Wave Train

$$f(t) = \begin{cases} \sin \omega_0 t & |t| < \frac{N\pi}{\omega_0} \\ 0 & |t| \geq \frac{N\pi}{\omega_0} \end{cases} \quad (\text{VII.17})$$

The reason it is $\frac{N\pi}{\omega_0}$ is because $\sin \omega_0 t \rightarrow \sin \left(\frac{\omega N\pi}{\omega_0} \right) = 0$. Note that this is an odd function. Remember that

$$e^{i\omega t} = \cos \omega t + i \sin \omega t \quad (\text{VII.18})$$

Since $f(t)$ has a particular parity (i.e. is either odd or even) then only one cos or sin survive. The Fourier transform can be split into two integrals:

$$g_s(\omega) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} f(t) \sin \omega t dt \quad \text{Fourier-Sin Transform} \quad (\text{VII.19})$$

$$g_c(\omega) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} f(t) \cos \omega t dt \quad \text{Fourier-Cos Transform} \quad (\text{VII.20})$$

Since we have an odd function we only have to do the sin integral:

$$g_s(\omega) = \sqrt{\frac{2}{\pi}} \int_0^{N\pi/\omega_0} \sin \omega_0 t \sin \omega t dt \quad (\text{VII.21})$$

$$= \sqrt{\frac{2}{\pi}} \int_0^{N\pi/\omega_0} \frac{1}{2} (\cos(\omega_0 - \omega)t - \cos(\omega_0 + \omega)t) dt \quad (\text{VII.22})$$

$$= \frac{1}{\sqrt{2\pi}} \left(\frac{\sin((\omega_0 - \omega)N\pi/\omega_0)}{\omega_0 - \omega} - \frac{\sin((\omega_0 + \omega)N\pi/\omega_0)}{\omega_0 + \omega} \right) \quad (\text{VII.23})$$

Consider the case in which $\omega \gg 1$. Further lets focus on the region where $\omega \sim \omega_0$. This allows us to concentrate on the first term.

$$g_s \omega \sim \frac{1}{\sqrt{2\pi}} \frac{\sin(\omega_0 - \omega)N\pi/\omega_0}{\omega_0 - \omega} \quad (\text{VII.24})$$

Taking the limit as $\omega_0 \rightarrow \omega$

$$\lim_{x \rightarrow 0} g_s(\omega) = \frac{1}{\sqrt{2\pi}} \frac{N\pi}{\omega_0} \quad (\text{VII.25})$$

At what values does $g_s(\omega)$ vanish?

$$\sin\left((\omega_0 - \omega) \frac{N\pi}{\omega_0}\right) = 0 \quad (\text{VII.26})$$

$$\Rightarrow (\omega_0 - \omega) \frac{N\pi}{\omega_0} = n\pi \quad (\text{VII.27})$$

$$\Rightarrow \omega_0 - \omega = \frac{n\omega_0}{N} = \Delta\omega \quad (\text{VII.28})$$

Thus the distance between nodes (node spacing) is ω_0/N . The width of the main peak is given by $2\omega_0/N$. The

Lecture 10 - Oct 3rd, 2011

Test 1: Nov 2nd

Test 2: Nov. 21st

B. Generalize Fourier Transforms to Three Dimensions

Recall the 1d definition

$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \quad (\text{VII.29})$$

The three dimensional analog is

$$g(\mathbf{k}) = \left(\frac{1}{\sqrt{2\pi}}\right)^3 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y, z) e^{-i\mathbf{k}\cdot\mathbf{x}} dx dy dz \quad (\text{VII.30})$$

VIII. MOMENTUM REPRESENTATION

$$\langle x|\alpha\rangle = \psi_\alpha(x) \quad (\text{VIII.1})$$

This is equal to probability amplitude to find a particle at position x for the state $|\alpha\rangle$. Analogously,

$$\langle p|\alpha\rangle = \phi_\alpha(p) \quad (\text{VIII.2})$$

is the probability amplitude to find a particle with momentum p for the state $|\alpha\rangle$. The functions $\psi_\alpha(x)$ and $\phi_\alpha(p)$ are Fourier transforms of one another

$$\psi_\alpha(x) \xrightarrow{FT} \phi_\alpha(p) \quad (\text{VIII.3})$$

The probability density in momentum (p) space is given by

$$P_\alpha(p) = \phi_\alpha^* \phi_\alpha(p) \quad (\text{VIII.4})$$

The dimensionless quantity that represents the probability of finding the particle with momentum between p and $p + dp$ is:

$$P_\alpha(p) dp \quad (\text{VIII.5})$$

In three dimensions:

$$\phi_\alpha(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int \int \int \psi_\alpha(\mathbf{r}) e^{i(\mathbf{r}\cdot\mathbf{p})/\hbar} d\mathbf{r} \quad (\text{VIII.6})$$

A. Example 1: Hydrogen in the 1s state

$$\psi_{1s}(\mathbf{r}) = \left(\frac{1}{\pi a_0^3} \right)^{1/2} e^{-r/a_0} \quad (\text{VIII.7})$$

Where $a_0 = \frac{\hbar^2}{m e^2}$ is the Bohr radius. Notice that the wave function is spherically symmetrical. Note if we want to find the probability of finding the electron between radius r and $r + dr$ is

$$\psi_{1s}^*(\mathbf{r})\psi_{1s}(\mathbf{r})r^2 dr \quad (\text{VIII.8})$$

The probability density is the greatest at the origin. However the radius of a spherical shell around the origin is so small that the probability to find an electron at that *radius* is zero. The most likely radius to find the electron is a_0 . However the most likely *place* to find the electron is the origin since that is where there are the highest density. The Fourier transform of this functions turns out to be (not proven)

$$\phi_{1s}(\mathbf{p}) = \frac{2^{3/2}}{\pi} \frac{a_0^{3/2} \hbar^{5/2}}{(a_0^2 p^2 + \hbar^2)^2} \quad (\text{VIII.9})$$

Notice the Fourier transforms are really different functions. The expectation value of position is given by

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x)x\psi(x)dx \quad (\text{VIII.10})$$

There are two ways to find the expectation value of momentum:

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x) dx \quad (\text{VIII.11})$$

$$= \int_{-\infty}^{\infty} \phi^*(p)p\phi(p)dp \quad (\text{VIII.12})$$

B. Example 2: Harmonic Oscillator

The representations of the harmonic oscillator (ground?) state in position and momentum space are given by

$$\psi(x) \propto e^{-(\sqrt{m}k/(2\hbar))x^2} \quad (\text{VIII.13})$$

$$\phi(p) \propto e^{\frac{-1}{2\hbar\sqrt{m}k}p^2} \quad (\text{VIII.14})$$

Notice the functional forms are the same but one gets narrower as the other gets wider with α .

Lecture 11 - October 5th, 2011

Makelectures delayed to October 25, and November 1st

IX. COMMUTATORS

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad (\text{IX.1})$$

If $[\hat{A}, \hat{B}] = 0$ we say the operators commute.

$$[\hat{x}, \hat{p}] = \left[x, \frac{\hbar}{i} \frac{\partial}{\partial x} \right] \quad (\text{IX.2})$$

$$= \frac{\hbar}{i} \left(x \frac{\partial}{\partial x} - \left(\frac{\partial}{\partial x} + \frac{\hbar}{i} x \frac{\partial}{\partial x} \right) \right) = i\hbar \quad (\text{IX.3})$$

If $[\hat{A}, \hat{B}] = 0$ then one can find simultaneous eigenfunctions of \hat{A} and \hat{B} . I.e.

$$\hat{A}\psi = \lambda\psi \quad (\text{IX.4})$$

$$\hat{B}\psi = \lambda'\psi \quad (\text{IX.5})$$

If $[\hat{A}, \hat{B}] \neq 0$ then one **cannot** find simultaneous eigenfunctions.

The expectation value of the distance from the average value is given by

$$\Delta_A^2 \equiv \left\langle \left(\hat{A} - \langle \hat{A} \rangle \right)^2 \right\rangle \quad (\text{IX.6})$$

This value is referring the uncertainty. To avoid confusion lets expand this definition:

$$\left\langle \left(\hat{A} - \langle \hat{A} \rangle \right)^2 \right\rangle = \left\langle \hat{A}^2 - 2\hat{A}\langle \hat{A} \rangle + \hat{A}^2 \right\rangle \quad (\text{IX.7})$$

$$= \left\langle \hat{A}^2 \right\rangle - 2\langle \hat{A} \rangle^2 + \left\langle \hat{A}^2 \right\rangle \quad (\text{IX.8})$$

$$= \left\langle \hat{A}^2 \right\rangle - \langle \hat{A} \rangle^2 \quad (\text{IX.9})$$

Remember its implied that there is some state α at either end. i.e.

$$\Delta_A^2 = \left\langle \alpha \left| \left(\hat{A} - \langle \hat{A} \rangle \right) \left(\hat{A} - \langle \hat{A} \rangle \right) \right| \alpha \right\rangle \quad (\text{IX.10})$$

$$= \left\langle \left(\hat{A} - \langle \hat{A} \rangle \right) \alpha \left| \left(\hat{A} - \langle \hat{A} \rangle \right) \right| \alpha \right\rangle \quad (\text{IX.11})$$

Call this term $\langle f|f \rangle$ where

$$|f\rangle \equiv \left(\hat{A} - \langle \hat{A} \rangle \right) |\alpha\rangle \quad (\text{IX.12})$$

likewise

$$\Delta_B^2 = \langle g|g \rangle \quad (\text{IX.13})$$

Where $|g\rangle = \left(\hat{B} - \langle \hat{B} \rangle \right) |\alpha\rangle$. But recall from mathematics the Schwarz inequality says:

$$\langle f|f \rangle \langle g|g \rangle \geq |\langle f|g \rangle|^2 \quad (\text{IX.14})$$

Therefore

$$\Delta_A^2 \Delta_B^2 = \langle f|f \rangle \langle g|g \rangle \geq |\langle f|g \rangle|^2 \quad (\text{IX.15})$$

remember that in general $\langle f|g \rangle$ is in general a complex number. Lets call this number z . Then

$$|z|^2 = (\Re z)^2 + (\Im z)^2 \geq (\Im z)^2 = \left(\frac{z - z^*}{2i} \right)^2 \quad (\text{IX.16})$$

Thus

$$\Delta_A^2 \Delta_B^2 \geq \left(\frac{1}{2i} [\langle f|g \rangle - \langle g|f \rangle] \right)^2 \quad (\text{IX.17})$$

Consider

$$\langle f|g \rangle = \left\langle \left(\hat{A} - \langle \hat{A} \rangle \right) \left(\hat{B} - \langle \hat{B} \rangle \right) \right\rangle \quad (\text{IX.18})$$

$$= \left\langle \hat{A}\hat{B} - \langle \hat{A} \rangle \hat{B} - \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \langle \hat{B} \rangle \right\rangle \quad (\text{IX.19})$$

$$= \left\langle \hat{A}\hat{B} \right\rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle \quad (\text{IX.20})$$

$$\langle g|f \rangle = \langle \hat{B}\hat{A} \rangle - \langle \hat{B} \rangle \langle \hat{A} \rangle \quad (\text{IX.21})$$

$$\langle f|g \rangle - \langle g|f \rangle = \langle \hat{A}\hat{B} \rangle - \langle \hat{B}\hat{A} \rangle \quad (\text{IX.22})$$

$$= \langle \hat{A}\hat{B} - \hat{B}\hat{A} \rangle \quad (\text{IX.23})$$

$$= \langle [\hat{A}, \hat{B}] \rangle \quad (\text{IX.24})$$

Hence

$$\Delta_A^2 \Delta_B^2 \geq \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2 \quad (\text{IX.25})$$

Example:

$$[\hat{x}, \hat{p}] = i\hbar \quad (\text{IX.26})$$

For momentum and position then:

$$\Delta_x^2 \Delta_p^2 \geq \left(\frac{i\hbar}{2i} \right)^2 \quad (\text{IX.27})$$

Equivalently:

$$\Delta_x^2 \Delta_p^2 \geq \frac{\hbar^2}{4} \quad (\text{IX.28})$$

$$\Delta_x \Delta_p \geq \frac{\hbar}{2} \quad (\text{IX.29})$$

When none commuting operators correspond to observables, we can them incompatible observables.

Lecture 12 - Oct. 7th, 2011

X. HARMONIC OSCILLATOR (OPERATOR METHOD)

Recall the classical harmonic oscillator

$$F = -kx \quad (\text{X.1})$$

$$m \frac{d^2x}{dt^2} = -kx \quad (\text{X.2})$$

$$\Rightarrow x = A \sin \omega t + B \cos \omega t \quad (\text{X.3})$$

$$V = \frac{kx^2}{2} \quad (\text{X.4})$$

The use of the harmonic oscillator model is that almost any potential can be approximated as a harmonic oscillator. Now lets work with the quantum analogue. The Hamiltonian is given by

$$\mathcal{H} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \psi \quad (\text{X.5})$$

The S.E. is given by

$$\frac{1}{2m} (p^2 + (m\omega x)^2) \psi = E\psi \quad (\text{X.6})$$

The key idea is to factor the operator $p^2 + (m\omega x)^2$. Consider if we were factoring two numbers u and v :

$$u^2 + v^2 = (iu + v)(-iu + v) \quad (\text{X.7})$$

Lets define

$$a_- \equiv \frac{1}{\sqrt{2\hbar m\omega}}(ip + m\omega x); \quad a_+ \equiv \frac{1}{\sqrt{2\hbar m\omega}}(-ip + m\omega x) \quad (\text{X.8})$$

Now if everything commuted then we would have $\mathcal{H} = a_- a_+$. However this is not the case as shown below:

$$a_- a_+ = \frac{1}{2\hbar m\omega}(ip + m\omega x)(-ip + m\omega x) \quad (\text{X.9})$$

$$= \frac{1}{2\hbar m\omega}(p^2 + m^2\omega^2 x^2 + im\omega(px - xp)) \quad (\text{X.10})$$

$$= \frac{1}{2\hbar m\omega}(p^2 + m^2\omega^2 x^2 - im\omega i\hbar) \quad (\text{X.11})$$

$$= \frac{1}{\hbar\omega}\mathcal{H} + \frac{1}{2} \quad (\text{X.12})$$

In the future we require $a_+ a_-$ so we may as well calculate it here:

$$a_+ a_- = \frac{1}{2\hbar m\omega}(-ip + m\omega x)(ip + m\omega x) \quad (\text{X.13})$$

$$= \frac{1}{2\hbar m\omega}(p^2 + m^2\omega^2 x^2 - im\omega(px - xp)) \quad (\text{X.14})$$

$$= \frac{1}{\hbar\omega}\left(\mathcal{H} - \frac{1}{2}i\omega(i\hbar)\right) \quad (\text{X.15})$$

$$= \left(\frac{1}{\hbar\omega}\mathcal{H} - \frac{1}{2}\right) \quad (\text{X.16})$$

Rearranging gives

$$\mathcal{H} = \hbar\omega\left(a_+ a_- + \frac{1}{2}\right) \quad (\text{X.17})$$

The commutator of a_+, a_- is

$$[a_+, a_-] = \left(\frac{1}{\hbar\omega}\mathcal{H} - \frac{1}{2}\right) - \left(\frac{1}{\hbar\omega}\mathcal{H} + \frac{1}{2}\right) \quad (\text{X.18})$$

$$= -1 \quad (\text{X.19})$$

Hence

$$\mathcal{H}\psi = E\psi \quad (\text{X.20})$$

$$\hbar\omega\left(a_+ a_- + \frac{1}{2}\right)\psi = E\psi \quad (\text{X.21})$$

Now suppose that we take

$$\mathcal{H}(a_+ \psi_n) = \left(a_+ a_- + \frac{1}{2}\right)a_+ \psi_n \quad (\text{X.22})$$

$$= \hbar\omega a_+ \left(\frac{1}{\hbar\omega}\mathcal{H} + 1\right)\psi_n \quad (\text{X.23})$$

$$= \hbar\omega a_+ \left(\frac{E_n}{\hbar\omega} + 1\right)\psi_n \quad (\text{X.24})$$

$$= (E + \hbar\omega)a_+ \psi_n \quad (\text{X.25})$$

Hence the energy of the state acted on or “raised” by a_+ is increased by a factor of $\hbar\omega$.

Now if we apply a_- continuously to some state ψ then at one point you will get the state with no particle there at all (zero)

$$a_- \psi_0 = 0 \quad (\text{X.26})$$

Hence

$$\frac{1}{\sqrt{2\hbar m\omega}} (ip + m\omega x) \psi_0 = 0 \quad (\text{X.27})$$

$$\hbar \frac{\partial \psi}{\partial x} + m\omega x \psi = 0 \quad (\text{X.28})$$

$$\frac{\partial \psi}{\partial x} = -m \frac{\omega}{\hbar} x \psi \quad (\text{X.29})$$

$$\psi = e^{-\frac{m\omega}{2\hbar} x^2} \quad (\text{X.30})$$

XI. CLASSICAL HARMONIC OSCILLATOR

$$F = ma \quad (\text{XI.1})$$

$$-kx = ma \quad (\text{XI.2})$$

$$m \frac{d^2 x}{dt^2} + kx = 0 \quad (\text{XI.3})$$

$$\frac{d^2 x}{dt^2} + \omega_o^2 x = 0 \quad (\text{XI.4})$$

$$x(t) = A \cos \omega_o t \quad (\text{XI.5})$$

$$E(t) = \frac{1}{2} m \dot{x}^2(t) + \frac{1}{2} k x^2(t) \quad (\text{XI.6})$$

Plugging the solution into the energy gives

$$E(t) = \frac{1}{2} m A^2 \omega_o^2 \sin^2 \omega_o t + \frac{1}{2} k A^2 \cos^2 \omega_o t \quad (\text{XI.7})$$

$$= \frac{1}{2} k A^2 \quad (\text{XI.8})$$

Alternatively we can write

$$\frac{1}{2} m \dot{x}^2 + \frac{1}{2} k x^2 = \frac{1}{2} k A^2 \quad (\text{XI.9})$$

$$\dot{x} = \omega_o \sqrt{A^2 - x^2} \quad (\text{XI.10})$$

The probability to be between x and dx is

$$P(x) dx = \frac{dt}{T/2} \quad (\text{XI.11})$$

Where T is the period of oscillation. The period is given by $T = \frac{2\pi}{\omega_o}$. Thus:

$$P(x)dx = \frac{dt}{T/2} \quad (\text{XI.12})$$

$$= \frac{2\omega_o dt}{2\pi} \quad (\text{XI.13})$$

$$= \frac{2\omega_o dx}{2\pi \dot{x}} \quad (\text{XI.14})$$

$$= \frac{2\omega_o}{2\pi} \frac{dx}{\omega_o \sqrt{A^2 - x^2}} \quad (\text{XI.15})$$

$$= \frac{dx}{\pi \sqrt{A^2 - x^2}} \quad (\text{XI.16})$$

The probability of finding the particle everywhere should be 1. Hence:

$$= \int_{-A}^A P(x)dx \quad (\text{XI.17})$$

$$= \int_{-A}^A \frac{1}{\pi} \frac{dx}{\sqrt{A^2 - x^2}} = 1 \quad (\text{XI.18})$$

Let $x = Ay$, $dx = A dy$.

$$= \int_{-A}^A \frac{A}{\pi} \frac{dy}{\sqrt{A^2 - A^2 y^2}} \quad (\text{XI.19})$$

$$= \int_{-A}^A \frac{1}{\pi} \frac{dy}{\sqrt{1^2 - y^2}} \quad (\text{XI.20})$$

$$= 1 \quad (\text{XI.21})$$

Note that the probability density is infinite at $x = A$, however its not a problem since the probability is finite (as it must be since our probability density is normalized)

XII. TIME DEVELOPMENT OF EXPECTATION VALUES

Consider

$$\langle \hat{A} \rangle \quad (\text{XII.1})$$

In the x-representation for example we integrate this over all positions x. Hence the expectation value isn't a function of x. In other words:

$$\frac{d\langle \hat{A} \rangle}{dt} = \frac{\partial \langle \hat{A} \rangle}{\partial t} \quad (\text{XII.2})$$

$$\frac{\partial \langle \hat{A} \rangle}{\partial t} = \frac{\partial}{\partial t} \int_{-\infty}^{\infty} \psi_{\alpha}^*(x) \hat{A} \psi_{\alpha}(x) dx \quad (\text{XII.3})$$

$$= \int_{-\infty}^{\infty} \frac{\partial}{\partial t} (\psi_{\alpha}^*(x) \hat{A} \psi_{\alpha}(x)) dx \quad (\text{XII.4})$$

$$= \int_{-\infty}^{\infty} \frac{\partial \psi_{\alpha}^*(x)}{\partial t} \hat{A} \psi_{\alpha}(x) + \psi_{\alpha}^*(x) \frac{\partial \hat{A}}{\partial t} \psi_{\alpha}(x) + \psi_{\alpha}^*(x) \hat{A} \frac{\partial \psi_{\alpha}(x)}{\partial t} dx \quad (\text{XII.5})$$

Now the Schrodinger equation says that:

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi; \quad -\hbar \frac{\partial \psi^*}{\partial t} = H \psi^* \quad (\text{XII.6})$$

Thus

$$\int_{-\infty}^{\infty} \frac{\partial \psi^* \hat{A} \psi}{\partial t} dx = \int_{-\infty}^{\infty} \frac{i}{\hbar} \left(\hat{H} \psi^* \hat{A} \psi - \psi^* \hat{A} \hat{H} \psi + \frac{\hbar}{i} \psi^* \frac{\partial \hat{A}}{\partial t} \psi \right) dx \quad (\text{XII.7})$$

Using representation free notation:

$$\frac{d \langle \hat{A} \rangle}{dt} = \frac{i}{\hbar} \left(\langle \hat{H} \alpha | \hat{A} \alpha \rangle - \langle \alpha | \hat{A} \hat{H} | \alpha \rangle + \frac{\hbar}{i} \left\langle \alpha \left| \frac{\partial \hat{A}}{\partial t} \right| \alpha \right\rangle \right) \quad (\text{XII.8})$$

But the Hamiltonian is Hermitian. Hence

$$\frac{d \langle A \rangle}{dt} = \frac{i}{\hbar} \langle [\hat{H}, \hat{A}] \rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle \quad (\text{XII.9})$$

In most cases $\frac{\partial \hat{A}}{\partial t} = 0$. In other words we're mostly interested in operators that don't have explicit time dependence. In this case

$$\boxed{\frac{d \langle \hat{A} \rangle}{dt} = \frac{i}{\hbar} \langle [\hat{H}, \hat{A}] \rangle} \quad (\text{XII.10})$$

If $[\hat{H}, \hat{A}] = 0$, then $\frac{d \hat{A}}{dt} = 0$. Therefore if \hat{A} commutes with the Hamiltonian then $\langle \hat{A} \rangle$ is a constant of motion. As an example consider the free case of $V = 0$. Then:

$$[\hat{p}, \hat{H}] = 0; \quad \hat{H} = \frac{\hat{p}^2}{2m} \quad (\text{XII.11})$$

Hence momentum is conserved. Now consider the non free case:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V \quad (\text{XII.12})$$

$$\frac{d \langle x \rangle}{dt} = \frac{i}{\hbar} \langle [H, x] \rangle = \frac{i}{\hbar} \left\langle \left[\frac{\hat{p}^2}{2m} + V, x \right] \right\rangle \quad (\text{XII.13})$$

But V will certainly commute with x since V contains no derivatives but is just a function of x. Hence:

$$\frac{d \langle x \rangle}{dt} = \frac{i}{\hbar} \left\langle \left[\frac{\hat{p}^2}{2m}, x \right] \right\rangle \quad (\text{XII.14})$$

$$= \frac{i}{2m\hbar} \langle [\hat{p}^2, x] \rangle \quad (\text{XII.15})$$

$$= \frac{i}{2m\hbar} \left\langle \hat{p} \hat{p} x - x \hat{p} \hat{p} - \overbrace{\hat{p} x \hat{p}}^0 + \hat{p} x \hat{p} \right\rangle \quad (\text{XII.16})$$

$$= \frac{i}{2m\hbar} \langle \hat{p} [\hat{p}, x] + [\hat{p}, x] \hat{p} \rangle \quad (\text{XII.17})$$

$$= \frac{i}{2m\hbar} \langle -i\hbar \hat{p} - i\hbar \hat{p} \rangle \quad (\text{XII.18})$$

$$= \frac{i}{2m\hbar} \langle -i\hbar \hat{p} - i\hbar \hat{p} \rangle \quad (\text{XII.19})$$

$$= \frac{\langle p \rangle}{m} \quad (\text{XII.20})$$

This is an example of Ehrenfest's principle which says that classical physics emerges as an average of quantum probabilities. Next consider

$$[\hat{H}, \hat{p}] = [V, p] \quad (\text{XII.21})$$

$$= i\hbar \frac{\partial V}{\partial x} \quad (\text{XII.22})$$

but

$$\frac{d\langle\hat{p}\rangle}{dt} = \frac{i}{\hbar} \langle [\hat{H}, \hat{p}] \rangle \quad (\text{XII.23})$$

$$\frac{d\langle\hat{p}\rangle}{dt} = - \left\langle \frac{\partial V}{\partial x} \right\rangle \quad (\text{XII.24})$$

This is Newton's second law!

XIII. CONSERVATION LAWS

- In classical physics one can show that the invariance of physics under time translations leads to energy conservation.
- In a previous lecture we have derived the time evolution operator:

$$U = \exp\left(\frac{-i\hat{H}t}{\hbar}\right); \quad U^\dagger = U^{-1} \quad (\text{XIII.1})$$

Consider the expectation value of a time evolved state α :

$$\langle U\alpha | H | U\alpha \rangle = \langle \alpha | U^\dagger H U | \alpha \rangle \quad (\text{XIII.2})$$

Note that

$$U = \exp(-iHt/\hbar) = 1 - i\frac{Ht}{\hbar} + \left(\frac{-iHt}{\hbar}\right)^2 \frac{1}{2} + \dots \quad (\text{XIII.3})$$

Hence U commutes with H. Thus

$$\langle U\alpha | H | U\alpha \rangle = \langle \alpha | H | \alpha \rangle \quad (\text{XIII.4})$$

So the expectation values of \hat{H} is constant. In other words

$$\frac{d\langle E \rangle}{dt} = 0 \quad (\text{XIII.5})$$

This conservation of the energy. This can also be shown by the formula derived in the previous section for the expectation value of an operator.

Consider any old function:

$$f(x + \xi) = f(x) + f'(x)(\xi) + \frac{1}{2!} f''(x)(\xi^2) + \dots \quad (\text{XIII.6})$$

$$= \exp\left(\xi \frac{\partial}{\partial x}\right) f(x) \quad (\text{XIII.7})$$

Consider the operator we just derived:

$$T \equiv \exp\left(\xi \frac{\partial}{\partial x}\right) = \exp\left(\frac{i}{\hbar} \xi \frac{\hbar}{i} \frac{\partial}{\partial x}\right) \quad (\text{XIII.8})$$

$$= \exp\left(\frac{i}{\hbar} \xi \hat{p}\right) \quad (\text{XIII.9})$$

Comparing with the time evolution operator we infer that this is the spatial translation operator. Alternatively by looking at the definition you can see that when you let the operator act on some function $f(x)$ and it brings you to the function $f(x + \xi)$.

For the free Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m}$,

$$[T, \hat{H}] = 0 \quad (\text{XIII.10})$$

Therefore

$$\left\langle \frac{d\hat{p}}{dt} \right\rangle = 0 \quad (\text{XIII.11})$$

Thus invariance under spatial transformation gives us momentum conservation. Now consider rotations:

$$f(\phi) = f(\phi + \Delta\phi) \quad (\text{XIII.12})$$

$$= \exp\left(\frac{i}{\hbar}\Delta\phi\frac{\hbar}{i}\frac{\partial}{\partial\phi}\right)f(\phi) \quad (\text{XIII.13})$$

$$= \exp\left(\frac{i}{\hbar}\Delta\phi\hat{L}_z\right) \quad (\text{XIII.14})$$

Define this operator as

$$R(\Delta\phi) = \exp\left(\frac{i}{\hbar}\Delta\phi\hat{L}_z\right) \quad (\text{XIII.15})$$

This operator rotates the function by an amount $\Delta\phi$. If the rotation operator commutes with the Hamiltonian then angular momentum will be conserved. i.e.

$$[L_z, H] = 0 \Rightarrow \frac{d\langle L_z \rangle}{dt} = 0 \quad (\text{XIII.16})$$

Next consider the parity operator (\mathcal{P}).

$$\mathcal{P}f(x) = f(-x) \quad (\text{XIII.17})$$

If $f(x) = f(-x)$ then we say $f(x)$ even. If $f(x) = -f(-x)$ then we say that $f(x)$ is odd. For even f the eigenvalue of \mathcal{P} is 1 if f is odd then the eigenvalue of \mathcal{P} is -1 . If

$$[\mathcal{P}, H] = 0 \Rightarrow \frac{d\langle \mathcal{P} \rangle}{dt} = 0 \quad (\text{XIII.18})$$

Weak interactions violate parity conservation.

Lecture 15: October 21st, 2011

XIV. TUNNELING

Test 1: November 1

Make up lecture is in room HNE on Nov. 1st, Nov 8th

Consider the potential

$$V = \begin{cases} x < -a & V = 0 \\ -a < x < a & V = V_0 \\ x > a & V = 0 \end{cases} \quad (\text{XIV.1})$$

Consider particles coming from the left

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi \quad (\text{XIV.2})$$

For $x < a$:

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad (\text{XIV.3})$$

$$\psi = \overbrace{Ae^{ik_1x}}^{\text{Particles from left}} + \overbrace{Be^{-ik_1x}}^{\text{Particles from right}} ; \quad E = \frac{\hbar^2 k_1^2}{2m} \quad (\text{XIV.4})$$

We keep both terms because particles may reflect back off the barrier.
In the region $-a < x < a$:

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V_o\psi = E\psi \quad (\text{XIV.5})$$

Bring the potential to the other side we have the same equation we have before with a new k:

$$\psi = \overbrace{Ce^{ik_2x}}^{\text{Particles from left}} + \overbrace{De^{-ik_2x}}^{\text{Particles from right}} \quad (\text{XIV.6})$$

Where $k_2 = \frac{2m}{\hbar^2} (E - V_o)$.
In $x > a$:

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} \psi = E\psi \quad (\text{XIV.7})$$

$$\psi = \overbrace{Ge^{ik_1x}}^{\text{Particles from left}} + \overbrace{Ge^{-ik_1x}}^{\text{Particles from right}} ; \quad E = \frac{\hbar^2 k_1^2}{2m} \quad (\text{XIV.8})$$

But here we can't have any left movers, thus

$$\psi = \overbrace{Fe^{ik_1x}}^{\text{Particles from left}} ; \quad E = \frac{\hbar^2 k_1^2}{2m} \quad (\text{XIV.9})$$

In this situation we can choose the energy E and $|A|^2$. E corresponds to the energy of the particles and $|A|^2$ corresponds to how many particles per second are incoming. B,C,D, and F are output that we get from the boundary conditions. We require continuity of the wavefunction as well as first derivative in order to have continuity of the second derivative (for S.E.).

The boundary conditions are (where the points where the S.E. was solved now correspond to the labels, I,II, and III):

$$\psi_I(-a) = \psi_{II}(-a) \quad (\text{XIV.10})$$

$$\psi'_I(-a) = \psi'_{II}(-a) \quad (\text{XIV.11})$$

$$\psi_{II}(a) = \psi_{III}(a) \quad (\text{XIV.12})$$

$$\psi'_{II}(a) = \psi'_{III}(a) \quad (\text{XIV.13})$$

All we really care to know is the transmission and reflection coefficients so we may as well set $A = 1$. If $A = 1$ then we know that

$$1 = |B|^2 + |F|^2 \quad (\text{XIV.14})$$

The boundary conditions tell us that

$$e^{-ik_1a} + Be^{ika} = Ce^{-k_2a} + De^{ik_2a} \quad (\text{XIV.15})$$

$$ik_1(e^{-k_1a} - Be^{ik_1a}) = ik_2(Ce^{-k_2a} - De^{ik_2a}) \quad (\text{XIV.16})$$

$$Ce^{ik_2a} + De^{-ik_2a} = Fe^{ik_1a} \quad (\text{XIV.17})$$

$$ik_2(Ce^{ik_2a} + De^{-ik_2a}) = ik_1Fe^{ik_1a} \quad (\text{XIV.18})$$

These equations can be solved using Mathematica. Switching to dimensionless variables: Define $y = E/V_o$ and $\eta = \frac{8ma^2V_o}{\hbar^2}$ the transmission coefficient comes out to

$$T = \frac{1}{\frac{\sinh^2(\sqrt{1-y})}{4(1-y)y} + 1} \quad (\text{XIV.19})$$

The points where the transmission is one are called transmission resonances. The transmission function in different regimes is shown in figure 2.

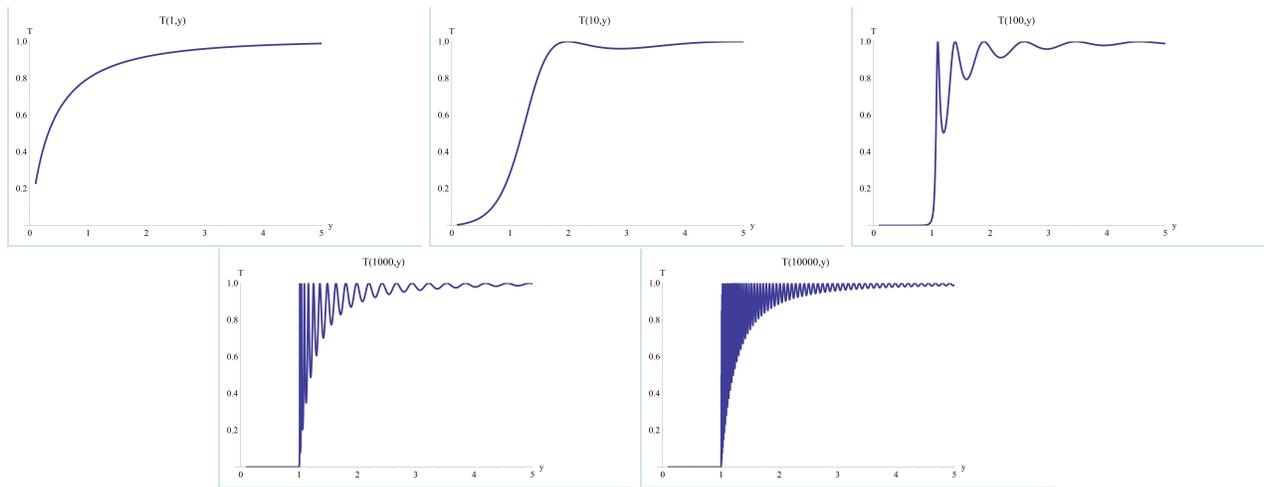
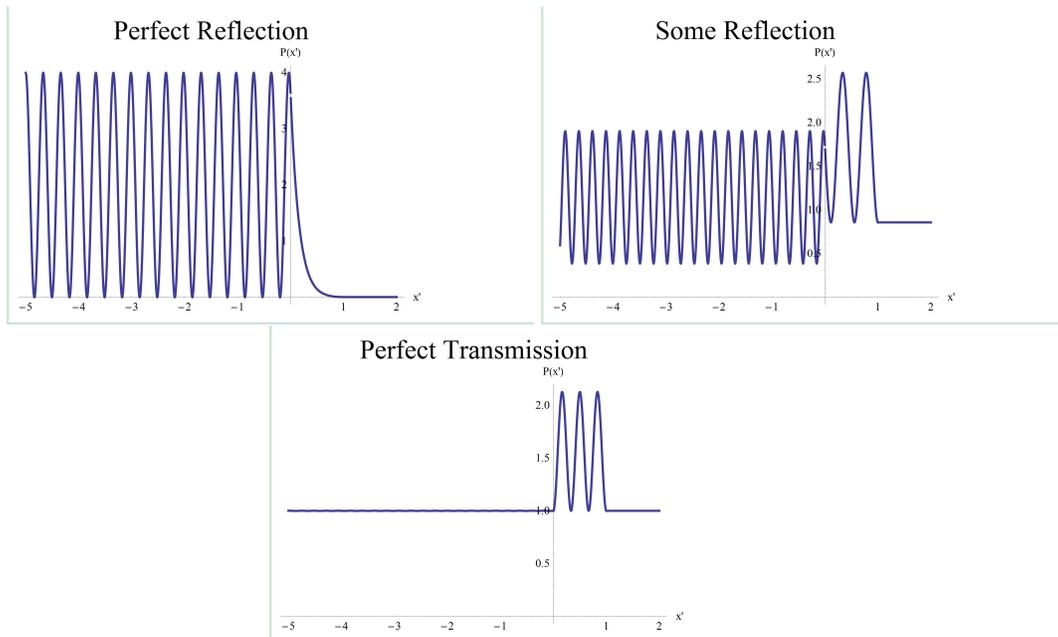


FIG. 2. The transmission function in different regimes $T(\eta, y)$. The greater the value of η the more classical the transmission function



Lecture 16 - Oct. 24, 2011

The probability density for different types of transmission are shown in figure 3 Note that on a test we may be required to sketch these probability densities for different amounts of reflection or transmission.

XV. ANGULAR MOMENTUM

Classically:

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \tag{XV.1}$$

$$= \det \begin{pmatrix} \hat{x} & \hat{y} & \hat{z} \\ x & y & z \\ p_x & p_y & p_z \end{pmatrix} \tag{XV.2}$$

$$= \hat{x}(yp_z - yp_y) + \hat{y}(zp_x - xp_z) + \hat{z}(xp_y - yp_x) \tag{XV.3}$$

$$\tag{XV.4}$$

Quantumly:

$$L_x = y \frac{\hbar}{i} \frac{\partial}{\partial z} - z \frac{\hbar}{i} \frac{\partial}{\partial y} \tag{XV.5}$$

The 3d operator angular momentum operator can be written

$$\mathbf{L} = \frac{\hbar}{i} \mathbf{r} \times \nabla \tag{XV.6}$$

In order to find the following commutator makes use the the commutator:

$$[p_x, f(x)] = (p_x f(x)) + f p_x - f p_x \tag{XV.7}$$

$$= p_x f(x) \tag{XV.8}$$

$$[L_x, L_y] = L_x L_y - L_y L_x \tag{XV.9}$$

$$= (yp_z - zp_y)(zp_x - xp_z) - (zp_x - xp_z)(yp_z - zp_y) \tag{XV.10}$$

$$= \frac{\hbar}{i} yp_x - \frac{\hbar}{i} xp_y \tag{XV.11}$$

$$= \frac{\hbar}{i} (-L_z) \tag{XV.12}$$

$$= i\hbar L_z \tag{XV.13}$$

Exercise: Do this . The commutators can be summarized by the following

$$\boxed{[L_i, L_j] = i\hbar \epsilon^{ijk} L_k} \tag{XV.14}$$

Where the symbol ϵ^{ijk} is called the Levi-Cevita and is defined as

$$\epsilon^{ijk} \equiv \begin{cases} 1 & ijk \text{ cyclic} \\ -1 & ijk \text{ anti-cyclic} \\ 0 & \text{otherwise} \end{cases} \tag{XV.15}$$

Lecture 17 - October 26th, 2011

$$L^2 = L_x^2 + L_y^2 + L_z^2 \tag{XV.16}$$

Using this it is straightforward to show that

$$[L_x, L^2] = 0 \tag{XV.17}$$

$$[L_y, L^2] = 0 \tag{XV.18}$$

$$[L_z, L^2] = 0 \tag{XV.19}$$

We can pick a component (typically we pick L_z) and find simultaneous eigenfunctions of L_z, L^2 .

Note on notation: L is used for orbital angular momentum while S is used for spin angular momentum (intrinsic). J is used for total angular momentum e.g. $L + S, L_1 + L_2$. No matter what the type of angular momentum we are dealing with is, L, J, or S the commutation relations are identical. e.g.

$$[J_x, J_y] = \hbar J_z \quad (\text{XV.20})$$

Define the ladder operators as:

$$\boxed{J_+ = J_x + iJ_y} \quad (\text{XV.21})$$

$$\boxed{J_- = J_x - iJ_y} = J_+^\dagger \quad (\text{XV.22})$$

List of commutation relations:

$$[J_z, J_+] = \hbar J_+ \quad (\text{XV.23})$$

$$[J_z, J_-] = -\hbar J_- \quad (\text{XV.24})$$

$$[J^2, J_+] = 0 \quad (\text{XV.25})$$

$$[J^2, J_-] = 0 \quad (\text{XV.26})$$

Further we can show that

$$J^2 = J_\mp J_\pm + J_z^2 \pm \hbar J_z \quad (\text{XV.27})$$

$$[J_+, J_-] = 2\hbar J_z \quad (\text{XV.28})$$

Let

$$J_z |m\rangle = m\hbar |m\rangle \quad (\text{XV.29})$$

Consider

$$J_z (J_+ \phi_m) = (\hbar J_+ + J_+ J_z) \phi_m \quad (\text{XV.30})$$

$$= \hbar J_+ + J_+ m\hbar \phi_m \quad (\text{XV.31})$$

$$= J_+ (m + 1) \hbar \phi_m \quad (\text{XV.32})$$

Thus the state $J_+ \phi_m$ is an eigenfunction of J_z with the eigenvalue $\hbar(m + 1)$. Thus J_+ is called a raising or ladder operator.

$$J_+ \phi_m \propto \phi_{m+1} \quad (\text{XV.33})$$

$$J_- \phi_m \propto \phi_{m-1} \quad (\text{XV.34})$$

Now

$$[J^2, J_z] = 0 \quad (\text{XV.35})$$

Therefore

$$J^2 \phi_m = \hbar^2 K^2 \phi_m \quad (\text{XV.36})$$

Where K is some value (not yet known). Consider

$$J_+ J^2 \phi_m = J_+ \hbar^2 K^2 \phi_m \quad (\text{XV.37})$$

$$= \hbar^2 K^2 J_+ \phi_m \quad (\text{XV.38})$$

$$\propto \hbar^2 K^2 \phi_{m+1} \quad (\text{XV.39})$$

$J_+ \phi_m$ has the same eigenvalue as J^2 .

$$\langle J^2 \rangle = \hbar K^2 = \langle J_x^2 \rangle + \langle J_y^2 \rangle + \langle J_z^2 \rangle \quad (\text{XV.40})$$

$$= \langle J_x^2 \rangle + \langle J_y^2 \rangle + \hbar^2 m^2 \quad (\text{XV.41})$$

$$(\text{XV.42})$$

Now $\langle J_x^2 \rangle$ and $\langle J_y^2 \rangle$ are positive definite quantities. The proof of this is shown below. Here $|\alpha\rangle$ is some state in the J_z basis and $|\alpha\rangle$ is some state in the i basis, J'_i is the operator in the diagonalized basis and U is the matrix that diagonalizes J_x .

$$\langle J_i^2 \rangle = \langle \alpha | J_i^2 | \alpha \rangle \quad (\text{XV.43})$$

$$= \langle \alpha | U^\dagger U J_i U^\dagger U J_i U^\dagger U | \alpha \rangle \quad (\text{XV.44})$$

$$= \langle \alpha' | J_i'^2 | \alpha' \rangle \quad (\text{XV.45})$$

$$= j_i^2 \quad (\text{XV.46})$$

Where here j_i is the eigenvalue of J_i . Thus $\langle J_x^2 \rangle$ and $\langle J_y^2 \rangle$ are positive definite which means that

$$\hbar^2 K^2 \geq \hbar^2 m^2 \quad (\text{XV.47})$$

and hence

$$|K| \geq |m| \quad (\text{XV.48})$$

This means that a given sequence of m 's must lie between $|K|$ and $-|K|$. Therefore

$$J_+ |m_{max}\rangle = 0 \quad (\text{XV.49})$$

$$J_- |m_{min}\rangle = 0 \quad (\text{XV.50})$$

$$J^2 |m_{max}\rangle = (J_x^2 + J_y^2 + J_z^2) |m_{max}\rangle \quad (\text{XV.51})$$

$$= \left(\left(\frac{J_+ + J_-}{2} \right)^2 + \left(\frac{J_+ - J_-}{2i} \right)^2 + J_z^2 \right) |m_{max}\rangle \quad (\text{XV.52})$$

$$= \frac{1}{4} (J_+ J_- + J_- J_+ + J_+ J_- + J_- J_+) |m_{max}\rangle \quad (\text{XV.53})$$

$$= \frac{1}{2} ((J_+ J_- + J_- J_+ + 2J_z^2) |m_{max}\rangle) \quad (\text{XV.54})$$

$$\hbar^2 K^2 |m_{max}\rangle = (\hbar J_z + J_z^2) |m_{max}\rangle \quad (\text{XV.55})$$

Similarly

$$\hbar^2 K^2 = \hbar^2 m_{min} (m_{min} - 1) \quad (\text{XV.56})$$

Solving these equations says that

$$m_{max} = -m_{min} \quad (\text{XV.57})$$

or

$$m_{min} = m_{max} + 1 \quad (\text{XV.58})$$

We can throw out the second solution on physical grounds (we can't have a maximum m be smaller than the minimum m).

Therefore if $m_{max} = j$ (define j this way) then $m_{min} = -j$ and therefore

$$m = (-j, -j + 1, \dots, j - 1, j) \quad (\text{XV.59})$$

$$J^2 |m\rangle = \hbar^2 j(j + 1) |m\rangle \quad (\text{XV.60})$$

XVI. ORBITAL ANGULAR MOMENTUM

Now lets specialize to eigenfunctions of orbital angular momentum.

$$L^2 \phi_{lm} = \hbar^2 l(l + 1) \phi_{lm} \quad (\text{XVI.1})$$

$$L_z \phi_{lm} = m \hbar \phi_{lm} \quad (\text{XVI.2})$$

We want explicit constructions of ϕ_{lm} . Recall:

$$L_z = \frac{\hbar}{i} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \quad (\text{XVI.3})$$

We could proceed in this way but its more natural to move to spherical coordinates. The coordinate system is shown in figure 3 Exercise: Transform L_z into spherical coordinates. This can be found by finding the transformation from

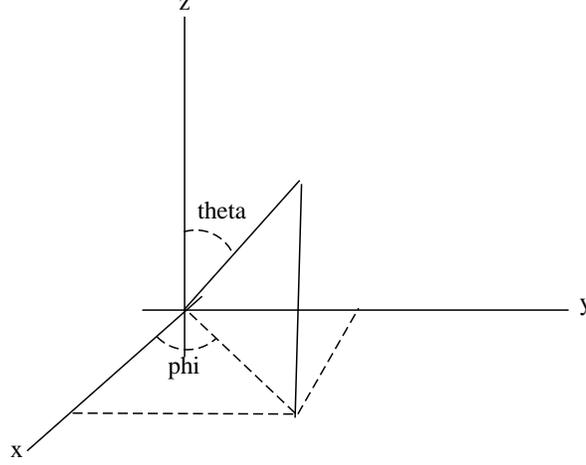


FIG. 3. The spherical coordinate system

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} r \\ \theta \\ \phi \end{pmatrix} \quad (\text{XVI.4})$$

and then taking the inverse of the transformation. This gives the following

$$\frac{\partial}{\partial y} = (\sin \theta \sin \phi) \frac{\partial}{\partial r} + \left(\frac{\sin \theta \sin \phi}{r} \right) \frac{\partial}{\partial \theta} + \left(\frac{\cos \theta}{r \sin \theta} \right) \frac{\partial}{\partial \phi} \quad (\text{XVI.5})$$

$$\frac{\partial}{\partial x} = (\sin \theta \cos \phi) \frac{\partial}{\partial r} + \left(\frac{\cos \theta \cos \phi}{r} \right) \frac{\partial}{\partial \theta} - \left(\frac{\sin \phi}{r \sin \theta} \right) \frac{\partial}{\partial \phi} \quad (\text{XVI.6})$$

By substitution (ideally blended with astute observations)

$$L_z = \frac{\hbar}{i} \left(0 \frac{\partial}{\partial r} + 0 \frac{\partial}{\partial \theta} + \frac{r \sin \theta \cos \phi \omega \phi}{r \sin \theta} + \frac{r \sin \theta \sin \phi \sin \phi}{r \sin \theta} \frac{\partial}{\partial \theta} \right) \quad (\text{XVI.7})$$

$$= \frac{\hbar}{i} \frac{\partial}{\partial \theta} \quad (\text{XVI.8})$$

The other operators are not as compact

$$L_y = i\hbar \left(-\cos \phi \frac{\partial}{\partial \theta} + \cot \phi \sin \phi \frac{\partial}{\partial \phi} \right) \quad (\text{XVI.9})$$

$$L_x = i\hbar \left(\sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right) \quad (\text{XVI.10})$$

$$L^2 = L_x^2 + J_y^2 + J_z^2 \quad (\text{XVI.11})$$

$$= -\hbar^2 \left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) \quad (\text{XVI.12})$$

$$L^2\phi_{lm} = \hbar^2 l(l+1)\phi_{lm} \quad (\text{XVI.13})$$

$$L_z\phi_{lm} = m\hbar\phi_{lm} \quad (\text{XVI.14})$$

The solutions to the differential equation is

$$\phi_{lm}(\theta, \phi) = Y_{lm}(\theta, \phi) \quad (\text{XVI.15})$$

The spherical harmonics are properly normalized:

$$\int |Y_{lm}(\theta, \phi)|^2 d\Omega = 1 \quad (\text{XVI.16})$$

$$L_z Y_{lm}(\theta, \phi) = m\hbar Y_{lm}(\theta, \phi) \quad (\text{XVI.17})$$

$$\Rightarrow Y_{lm}(\theta, \phi) \propto e^{im\phi} \quad (\text{XVI.18})$$

Singlevaluedness of these solutions forces

$$e^{im\phi} = e^{im\phi + im2\pi} \quad (\text{XVI.19})$$

Hence

$$e^{2im\pi} = 1 \quad (\text{XVI.20})$$

In other words $m \in \mathbb{Z}$. In order to keep the ϕ component normalized we require that the ϕ component is

$$\frac{1}{\sqrt{2\pi}} e^{im\phi} \quad (\text{XVI.21})$$

Now subbing into the spherical harmonics says that

$$Y_{lm}(\theta, \phi) = \frac{e^{im\phi}\Theta(\theta)}{\sqrt{2\pi}} \quad (\text{XVI.22})$$

Plugging this into

$$L^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm} \quad (\text{XVI.23})$$

$$\Rightarrow \frac{1}{\sin\theta} \left(\frac{d}{d\theta} \left(\sin\theta \frac{d\Theta(\theta)}{d\theta} \right) \right) + \left(l(l+1) - \frac{m^2}{\sin^2\theta} \right) \Theta(\theta) = 0 \quad (\text{XVI.24})$$

This is an ugly differential equation. Define

$$\mu = \cos\theta \quad (\text{XVI.25})$$

$$\Theta(\theta)_{lm} = P_l^m(\mu) \quad (\text{XVI.26})$$

Where these are the associated Legendre Polynomials.

$$P_l^m(\mu) = (-1)^m (1-\mu^2)^{m/2} \frac{d^m}{d\mu^m} P_l(\mu) \quad (\text{XVI.27})$$

Where $P_l(\mu)$ are the Legendre Polynomials defined as

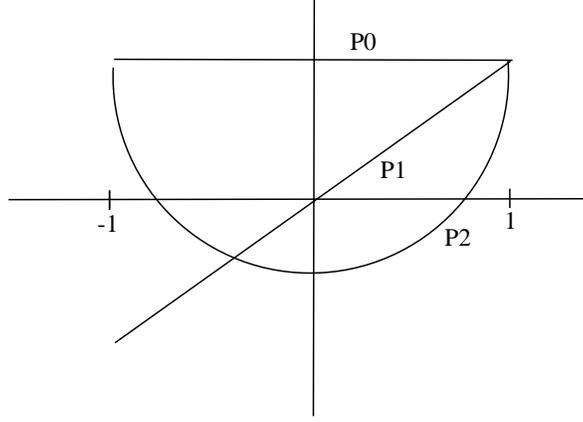
$$P_l(\mu) = \frac{1}{2^l l!} \frac{d^l}{d\mu^l} (\mu^2 - 1)^l \quad (\text{XVI.28})$$

The first few Legendre Polynomials are

$$P_0(\mu) = 1 \quad (\text{XVI.29})$$

$$P_1(\mu) = \mu \quad (\text{XVI.30})$$

$$P_2(\mu) = \frac{1}{8} \frac{d^2}{d\mu^2} (\mu^4 - 2\mu^2 + 1) = \frac{3\mu^2 - 1}{2} \quad (\text{XVI.31})$$



The first few Associated Legendre Polynomials are

$$P_{00}(\mu) = 1 = 1 \tag{XVI.32}$$

$$P_{10}(\mu) = \mu = \cos \theta \tag{XVI.33}$$

$$P_{11}(\mu) = -\sqrt{1 - \mu^2} = -\sin \theta \tag{XVI.34}$$

Putting this all together we can write the spherical harmonics.

$$Y_{lm}(\theta, \phi) \tag{XVI.35}$$

with

$$L^2 Y_{lm} = \hbar^2 l(l + 1) Y_{lm}; \quad L_z Y_{lm} = m\hbar \tag{XVI.36}$$

$$Y_{lm}(\theta, \phi) = \left(\frac{2l + 1}{4\pi} \frac{(l - m)!}{(l + m)!} \right)^{1/2} P_{lm}(\cos \theta) e^{im\phi} \tag{XVI.37}$$

The spherical harmonics are orthonormal:

$$\int Y_{lm}^*(\theta, \phi) Y_{l'm'}(\theta, \phi) d\Omega = \delta_{m,m'} \delta_{l,l'} \tag{XVI.38}$$

Due to the phase we have

$$Y_{l,-m} = (-1)^m Y_{lm}^* \tag{XVI.39}$$

The first few are tabulated below

$$\begin{aligned} Y_{0,0} &= \frac{1}{\sqrt{4\pi}} \\ Y_{1,1} &= -\frac{1}{2} \left(\frac{3}{2\pi} \right)^{1/2} \sin \theta e^{i\phi} \\ Y_{1,0} &= \frac{1}{2} \left(\frac{3}{\pi} \right)^{1/2} \cos \theta \\ Y_{1,-1} &= \frac{1}{2} \left(\frac{3}{\pi} \right)^{1/2} \sin \theta e^{-i\phi} \end{aligned}$$

In order to plot these we can plot $|Y_{lm}|$ and set $|Y_{lm}| = r$. In other words the distance from the origin being large implies that the function is large (note this is only for plotting purposes). Its important to note there is no ϕ dependence. So the plot is independent of the angle in the x,y plane.

XVII. HYDROGEN

$$H = -\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{4\pi\epsilon_0} \frac{q^2 Z}{r} \tag{XVII.1}$$

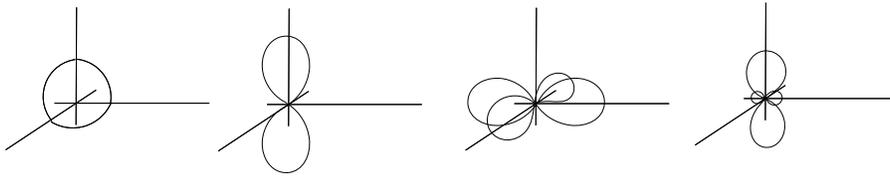


FIG. 4. Spherical Harmonics

In this class we will use cgs units:

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\epsilon_0}\frac{q^2Z}{r} \quad (\text{XVII.2})$$

Note that $V = V(r)$ so its natural to go into spherical coordinates. Thus

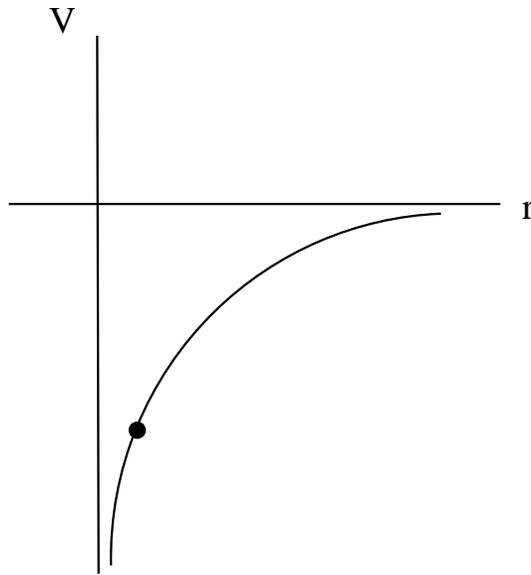


FIG. 5. The Hydrogen potential energy

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\overbrace{\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\theta^2}\right)}^{L^2} \quad (\text{XVII.3})$$

$$-\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{L^2}{2mr^2} \quad (\text{XVII.4})$$

$$= \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} \quad (\text{XVII.5})$$

Theorem: The ground state of a system has the full symmetry of the problem.
This lovely coincidence that L^2 showed up was of course not actually a coincidence.

$$L^2 = (\mathbf{r} \times \mathbf{p})^2 \quad (\text{XVII.6})$$

$$= r^2 p^2 - (\mathbf{r} \cdot \mathbf{p})^2 \quad (\text{XVII.7})$$

$$r^2 p^2 = (\mathbf{r} \cdot \mathbf{p})^2 + L^2 \quad (\text{XVII.8})$$

$$\frac{p^2}{2m} = \frac{(\mathbf{r} \cdot \mathbf{p})^2}{r^2} + \mathbf{L}^2 r^2 \quad (\text{XVII.9})$$

$$= (\hat{r} \cdot \mathbf{p})^2 + \frac{L}{2mr^2} \quad (\text{XVII.10})$$

$$= \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} \quad (\text{XVII.11})$$

Thus

$$\left(\frac{p_r^2}{2m} + \frac{L^2}{2mr^2} - \frac{Ze^2}{r} \right) \psi(r, \theta, \phi) = E\psi(r, \theta, \phi) \quad (\text{XVII.12})$$

Using the relation $[L^2, H] = 0$ (easy to see by looking at the Hamiltonian term by term), we know that they share eigenfunctions. Hence

$$\psi(r, \theta, \phi) = R(r)Y_{lm}(\theta, \phi) \quad (\text{XVII.13})$$

Note it is always the case that if $V = V(r)$ then $\psi = R(r)Y_{lm}(\theta, \phi)$.

Lecture 18 - November 1st, 2011

Recall (switched to MKS)

$$\left(-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{L^2}{2mr^2} - \frac{Ze^2}{4\pi\epsilon_0 r} \right) \psi(r, \theta, \phi) = E\psi(r, \theta, \phi) \quad (\text{XVII.14})$$

Since we have a central potential (i.e. $V = V(r)$) we can write $\psi(r) = R(r)Y_{lm}(\theta, \phi)$

$$[H, L^2] = 0 \Rightarrow \begin{cases} H\psi = E\psi \\ L^2\psi = \hbar^2 l(l+1)\psi \end{cases} \quad (\text{XVII.15})$$

Plugging in $\psi(\mathbf{r}) = R(r)Y_{lm}(\theta, \phi)$ into our equation.

$$\left(-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{l(l+1)}{2mr^2} - \frac{Ze^2}{4\pi\epsilon_0 r} \right) R(r) = ER(r) \quad (\text{XVII.16})$$

Note we have reduced a 3D problem to 1D. Introduce a new function $U(r) \equiv rR(r)$ to simplify the differential equation. This gives

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r} \right) U(r) = EU(r) \quad (\text{XVII.17})$$

The nice thing about this equation is that this looks just like 1D quantum mechanics in the variable r , but the potential term is an effective potential given by

$$V_{eff}(r) = \frac{\hbar^2 l(l+1)}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r} \quad (\text{XVII.18})$$

Note that when $l = 0$ The potential is just the Coloumb potential. The effective potential is shown in figure 6 What is the natural scale for this problem? We can build the scale from the constants in the problem:

$$[m]^\alpha [\hbar]^\beta \left[\frac{e^2}{4\pi\epsilon_0} \right]^\gamma = L \quad (\text{XVII.19})$$

$$[M]^\alpha \left[\frac{ML^2}{T} \right]^\beta \left[\frac{ML^3}{T^2} \right]^\gamma = L \quad (\text{XVII.20})$$

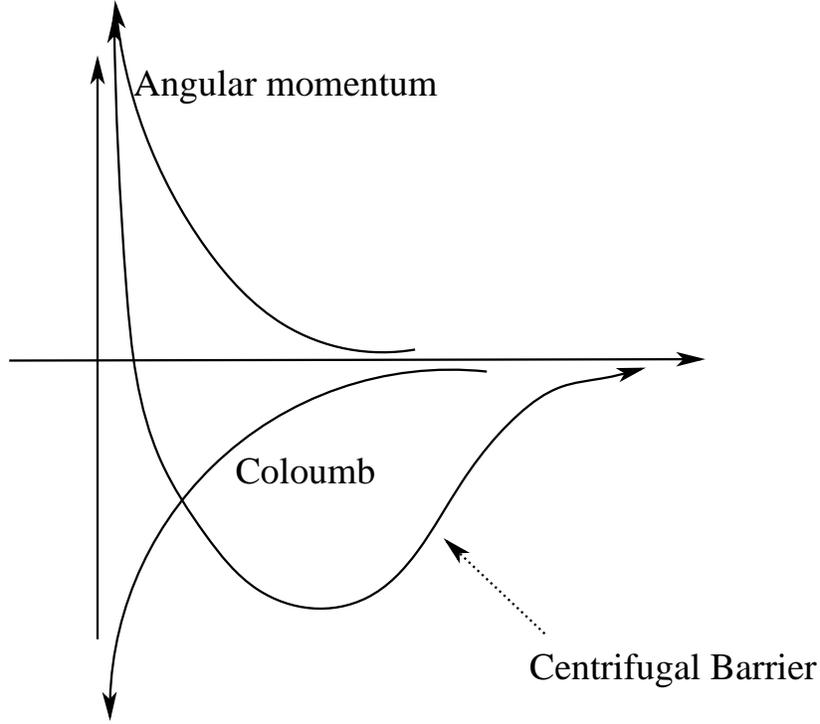


FIG. 6. The Effective potential of Hydrogen

So we know that

$$\alpha + \beta + \gamma = 0 \quad (\text{XVII.21})$$

$$-\beta - 2\gamma = 0 \quad (\text{XVII.22})$$

$$2\beta + 2\gamma = 1 \quad (\text{XVII.23})$$

The solution of this set of equations is

$$\alpha = -1 \quad (\text{XVII.24})$$

$$\beta = 2 \quad (\text{XVII.25})$$

$$\gamma = -1 \quad (\text{XVII.26})$$

Thus

$$[L] = \frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.53 \times 10^{-10}m \equiv a_o \quad (\text{XVII.27})$$

Note that with little work we already know the natural scale for atomic systems (\AA).

Its also convenient to introduce

$$\kappa \equiv \sqrt{\frac{-2mE}{\hbar}}; \quad \rho \equiv \kappa r; \quad \rho_o = \frac{2}{a_o\kappa} \quad (\text{XVII.28})$$

With these changes we get

$$\frac{d^2v}{d\rho^2} = \left(1 - \frac{\rho_o}{\rho} + \frac{l(l+1)}{\rho^2}\right)v \quad (\text{XVII.29})$$

Consider $\rho \rightarrow \infty$.

$$\frac{d^2v}{d\rho^2} = v \quad (\text{XVII.30})$$

$$\Rightarrow u(\rho) = Ae^{-\rho} + Be^{\rho} \quad (\text{XVII.31})$$

B must be zero due to normalization requirements. Now consider $\rho \rightarrow 0$:

$$\frac{d^2 v}{d\rho^2} = \frac{l(l+1)}{\rho^2} v \quad (\text{XVII.32})$$

$$u(\rho) = C\rho^{l+1} + D\rho^{-l} \quad (\text{XVII.33})$$

Where for normalization we require $D = 0$. Substitute $u(\rho) = \rho^{l+1}e^{-l}v(\rho)$ into the radial equation

$$\rho \frac{d^2 v}{d\rho^2} + 2(l+1-\rho) \frac{dv}{d\rho} + (l_0 - 2(l+1))v = 0 \quad (\text{XVII.34})$$

Frobenius method gives that the result is the associated Laguerre polynomials.

$$L_{q-p}^p(x) \equiv (-1)^p \left(\frac{d}{dx}\right)^p L_q(x)$$

$$L_q \equiv e^x \left(\frac{d}{dx}\right)^q (e^{-x}x^q)$$

$$L_0 = 1$$

$$L_1 = 1 - x$$

$$L_2 = x^2 - 4x + 2$$

$$L_0^0 = 1$$

$$L_1^0 = -x + 1$$

$$L_2^0 = x^2 - 4x + 2$$

Reassemble our radial wavefunctions:

$$R_{nl} = \frac{1}{r} \rho^{l+1} e^{-\rho} L_{n-l-1}^{2l+1}(2\rho) \quad (\text{XVII.35})$$

Where $\kappa = \frac{1}{a_0 n}$, $\rho = \frac{r}{a_0 n}$. The energies are

$$E_n = \frac{E_1}{n^2} \quad (\text{XVII.36})$$

Where

$$E_1 = -\frac{1}{2} m c^2 \alpha^2; \quad \alpha \equiv \frac{e^2}{4\pi\epsilon_0 \hbar c} \approx \frac{1}{137} \quad (\text{XVII.37})$$

α is called the fine structure constant. It is a measure of the electromagnetic interaction.

November 7th, 2011

The radial equation is

$$\left(-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r}\right) + \hbar^2 \frac{l(l+1)}{2mr^2} - \frac{e^2}{4\pi\epsilon_0} \frac{1}{r}\right) R(r) = ER(r) \quad (\text{XVII.38})$$

Notice that the only place where we have l dependence is in the middle term. Also notice that there is no m dependence in the Schrodinger equation. This reflects the fact that our problem is rotationally invariant. m measures the projection of l into the z axis and our choice of z is arbitrary. We can break this rotational symmetry (by for example adding a magnetic field) in this case the energy would depend on m . Note there has been a change in notation (at least with his online notes):

$$\rho \equiv 2\kappa r; \quad a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2} = 0.53 \text{ \AA}; \quad \kappa = \frac{\sqrt{-2mE}}{\hbar} \quad (\text{XVII.39})$$

The new differential equation is

$$\frac{d^2 u}{d\rho^2} = \left(\frac{1}{4} - \frac{n}{\rho} + \frac{l(l+1)}{\rho^2}\right) u \quad (\text{XVII.40})$$

Where $n = \frac{1}{a_o \kappa}$. The result is

$$u(\rho) = \rho^{l+1} e^{-\rho/2} u(\rho) \quad (\text{XVII.41})$$

Using the Frobenius method we find that we don't have well behaved solutions unless the series Frobenius series terminates. The ones that are finite are the Laguerre polynomials. They occur when n is an integer. Now we can find the radial term:

$$R_{nl}(\rho) = \rho^l e^{-\rho/2} L_{n+l}^{2l+1}(\rho) \quad (\text{XVII.42})$$

Notice that the $R_{nl}(\rho)$ depends on n and l and we call n the principle quantum number.

$$E_n = -\frac{1}{2} \frac{mc^2 \alpha^2}{n^2}; \quad \alpha \equiv \frac{e^2}{4\pi\epsilon_o \hbar c} \approx \frac{1}{137} \quad (\text{XVII.43})$$

Notice the eigenvalues don't have any angular dependence! Thus two very different eigenfunctions

$$R_{20} = \left(\frac{1}{2a_o}\right)^{3/2} \left(2 - \frac{r}{a_o}\right) e^{-r/2a_o} \quad (\text{XVII.44})$$

$$R_{21} = \left(\frac{1}{2a_o}\right)^{3/2} \frac{1}{\sqrt{3}} \left(\frac{r}{a_o}\right) e^{-r/2a_o} \quad (\text{XVII.45})$$

have the same eigenvalues! This mysterious degeneracy in the eigenvalues is due to a hidden symmetry in the problem.

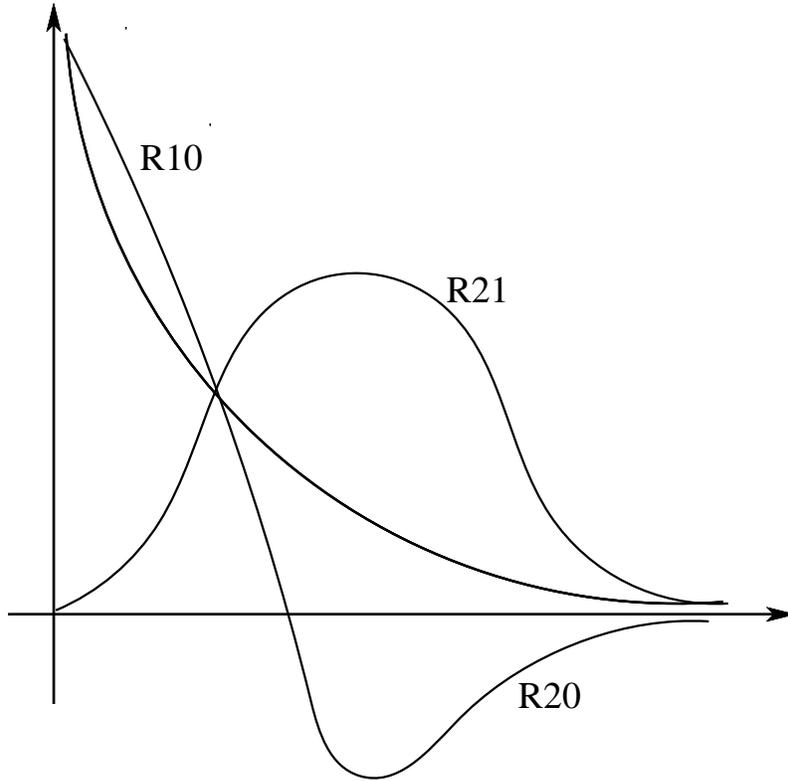


FIG. 7. The Radial terms of the Hydrogen wavefunction

$$\psi_{nlm}(\mathbf{r}) = R_{nl}(r) Y_{lm}(\phi, \theta) \quad (\text{XVII.46})$$

$$\int \psi_{n'l'm'}^* \psi_{nlm} r^2 \sin \theta dr d\theta d\phi = \delta_{n'n} \delta_{l'l} \delta_{m'm} \quad (\text{XVII.47})$$

The radial probability distribution is

$$P(r) = r^2 R_{nl}^2(r) \quad (\text{XVII.48})$$

For the state 1s state:

$$P_{1,0}(r) = r^2 R_{10}^2(r) \quad (\text{XVII.49})$$

To find the maximum we take the derivative and set it to zero:

$$\frac{dP_{10}}{dr} = 0 \quad (\text{XVII.50})$$

$$2re^{\frac{2r}{a_o}} - \frac{2}{a_o} e^{-2r/a_o} = 0 \quad (\text{XVII.51})$$

$$\left(r - \frac{r^2}{a_o}\right) e^{-2r/a_o} = 0 \quad (\text{XVII.52})$$

This is zero at $r = 0, r = \infty, r = a_o$. It is a minima at ∞ and 0. It is a maximum at a_o .

$$\langle r \rangle = \int R_{10}(r) r R_{10}(r) r^2 dr \quad (\text{XVII.53})$$

$$= \int_0^\infty P_{10} r dr \quad (\text{XVII.54})$$

Where $P_{10}(r)$ is the radial probability distribution.

$$\langle r \rangle = \int_0^\infty \frac{4}{a_o^3} r^2 e^{-2r/a_o} r dr \quad (\text{XVII.55})$$

Define $x = 2r/a_o \rightarrow dx = 2dr/a_o$

$$\langle r \rangle = \int_0^\infty \frac{a_o}{4} x^3 e^{-x} dx \quad (\text{XVII.56})$$

$$= \frac{a_o}{4} 3! \quad (\text{XVII.57})$$

$$= \frac{3a_o}{2} \quad (\text{XVII.58})$$

Another interesting quantity is

$$\langle \mathbf{r} \rangle = \langle x \rangle \hat{x} + \langle y \rangle \hat{y} + \langle z \rangle \hat{y} \quad (\text{XVII.59})$$

$$= 0 \quad (\text{XVII.60})$$

This must be zero since we have reflection symmetry. This is true for all Hydrogen eigenstates (but not for the linear combinations)

Lecture 19 - November 19th, 2011

XVIII. MATRIX MECHANICS

Consider some basis set

$$B_1 = (\phi_1, \phi_2, \dots, \phi_n) \quad (\text{XVIII.1})$$

We have already encountered some basis sets

$$\left(\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi y}{a}\right) \right) \quad (\text{XVIII.2})$$

$$\left(A_n H_n(\xi) e^{-\xi^2/2} \right) \quad (\text{XVIII.3})$$

$$\left(R_{nl}(r) Y_{lm}(\phi, \theta) \right) \quad (\text{XVIII.4})$$

Recall in Dirac notation

$$|\alpha\rangle = \sum_n |n\rangle \langle n|\alpha\rangle \quad (\text{XVIII.5})$$

$$\langle n|\alpha\rangle = a_n \quad (\text{XVIII.6})$$

$$|\alpha\rangle = \sum_n a_n |n\rangle \quad (\text{XVIII.7})$$

Knowing what basis \mathcal{B} and all the a_n is equivalent to knowing $|\alpha\rangle$.

Consider an operator F (arbitrary). Let

$$F|\alpha'\rangle = |\alpha\rangle \quad (\text{XVIII.8})$$

Now lets construct $\langle q|\alpha\rangle$. Where $|q\rangle$ is some basis state.

$$\langle q|\alpha\rangle = \langle q|F|\alpha'\rangle \quad (\text{XVIII.9})$$

$$= \sum_n \langle q|F|n\rangle \langle n|\alpha'\rangle \quad (\text{XVIII.10})$$

$$a_q = \sum_n F_{qn} a'_n \quad (\text{XVIII.11})$$

Where we have defined

$$F_{qn} \equiv \langle q|F|n\rangle \quad (\text{XVIII.12})$$

$$= \int \phi_q^* F \phi_n d\mathbf{r} \quad (\text{XVIII.13})$$

We call F_{qn} a matrix element.

$$a_q = \sum_n F_{qn} a'_n \quad (\text{XVIII.14})$$

$$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} F_{11} & F_{12} & \dots \\ F_{21} & F_{22} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a'_1 \\ a'_2 \\ \vdots \end{pmatrix} \quad (\text{XVIII.15})$$

We also call F_{qn} the matrix representation of the operator F .

Consider

$$G|n\rangle = g_n |n\rangle \quad (\text{XVIII.16})$$

This is an eigenvalue equation.

$$G = \begin{pmatrix} g_1 & 0 & 0 \\ 0 & g_2 & 0 \\ 0 & 0 & \ddots \end{pmatrix} \quad (\text{XVIII.17})$$

The eigenfunctions are just

$$|n\rangle = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad (\text{XVIII.18})$$

Recall some matrix properties

1. Matrix multiplication:

$$(AB)_{nq} = \sum_p A_{np} B_{pq} \quad (\text{XVIII.19})$$

2. Inverse:

$$A^{-1}A = I \quad (\text{XVIII.20})$$

$$A^{-1} = \frac{1}{\det A} A_{adj}; \quad A_{adj} = A_{cofactor}^T; \quad A_{cof} = (-1)^{i+j} M_{ij} \quad (\text{XVIII.21})$$

3. Determinant:

$$\det(A) = \sum_{\sigma \in S_n} \text{sgn}(\sigma) \prod_{i=1}^n A_{i,\sigma(i)} \quad (\text{XVIII.22})$$

Where σ is the particular permutation. S_n is the set of permutations. $\text{sgn}(\sigma) = +1, -1$ depending on if we have an even or odd permutation.

4. Symmetry: If

$$A^T = A \quad (\text{XVIII.23})$$

Then A is symmetric. If

$$A_T = -A \quad (\text{XVIII.24})$$

Then A is antisymmetric.

5. Trace:

$$\text{Tr}(A) = \sum_n A_{nn} \quad (\text{XVIII.25})$$

6. Hermitian Adjoint:

$$A^\dagger = A^{*T} \quad (\text{XVIII.26})$$

$$A_{qn}^\dagger = A_{nq}^* \quad (\text{XVIII.27})$$

For Hermitian operators:

$$A^\dagger = A \quad (\text{XVIII.28})$$

The proof of Hermitian operators corresponding to real numbers in terms of matrices is straightforward. It also shows that Hermitian operators correspond to Hermitian matrices. Exercise try this!

7. Unitary:

$$U^\dagger = U^{-1} \quad (\text{XVIII.29})$$

We have seen one unitary operator already. The time evolution

$$e^{-iHt/\hbar} \quad (\text{XVIII.30})$$

The importance of unitary operators is that they maintain inner products.

$$\langle \beta' | \alpha' \rangle = \langle U\beta | U\alpha \rangle \quad (\text{XVIII.31})$$

$$= \langle \beta | U^\dagger U | \alpha \rangle \quad (\text{XVIII.32})$$

$$= \langle \beta | \alpha \rangle \quad (\text{XVIII.33})$$

How operators transform?

$$F|\alpha\rangle = |\beta\rangle \quad (\text{XVIII.34})$$

$$FU^{-1}|\alpha'\rangle = U^{-1}|\beta'\rangle \quad (\text{XVIII.35})$$

$$UFU^{-1}|\alpha'\rangle = UU^{-1}|\beta'\rangle \quad (\text{XVIII.36})$$

$$F'|\alpha'\rangle = |\beta'\rangle \quad (\text{XVIII.37})$$

Hence

$$F' = UFU^{-1} \quad (\text{XVIII.38})$$

Lecture 22 - November 11, 2011

Recall the harmonic oscillator

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega_o c^2 \quad (\text{XVIII.39})$$

$$\mathcal{B} = e^{-\xi^2/2} (A_0 H_0(\xi), A_1 H_1(\xi), \dots) \quad (\text{XVIII.40})$$

Where $\xi^2 = \beta^2 x^2$, $\beta^2 = \frac{m\omega_o}{\hbar}$. Another way to denote the basis is

$$\mathcal{B} = (|0\rangle, |1\rangle, |2\rangle, \dots) \quad (\text{XVIII.41})$$

The action of the Hamiltonian

$$H|n\rangle = \left(n + \frac{1}{2}\right) \hbar\omega_o |n\rangle \quad (\text{XVIII.42})$$

In this basis the Hamiltonian:

$$H = \begin{pmatrix} \frac{1}{2}\hbar\omega_o & 0 & \dots \\ 0 & \frac{3}{2}\hbar\omega_o & 0 \\ \vdots & 0 & \ddots \end{pmatrix} \quad (\text{XVIII.43})$$

Since we are in the eigenbasis We see that H is diagonal. Now consider

$$x_{mn} = \langle m|x|n\rangle \quad (\text{XVIII.44})$$

We can evaluate these matrix elements:

$$x_{mn} = \int A_m H_m(\xi) x A_n H_n(\xi) dx \quad (\text{XVIII.45})$$

However alternatively we can be clever and use ladder operators.

$$a_+ = \frac{1}{\sqrt{2\hbar m\omega}} (-ip + m\omega x) \quad (\text{XVIII.46})$$

$$a_- = \frac{1}{\sqrt{2\hbar m\omega}} (ip + m\omega x) \quad (\text{XVIII.47})$$

$$a_+ |n\rangle = (n+1)^{1/2} |n+1\rangle \quad (\text{XVIII.48})$$

$$a_- |n\rangle = (n)^{1/2} |n-1\rangle \quad (\text{XVIII.49})$$

We can write the x operator as

$$x = \frac{1}{\sqrt{2}} \frac{1}{\beta} (a_- + a_+) \quad (\text{XVIII.50})$$

What is the a_+ matrix?

$$(a_+)_{mn} = \langle m | a_+ | n \rangle \quad (\text{XVIII.51})$$

$$= \langle m | (n+1)^{1/2} | n \rangle \quad (\text{XVIII.52})$$

$$= (n+1)^{1/2} \langle m | n+1 \rangle \quad (\text{XVIII.53})$$

$$= (n+1)^{1/2} \delta_{m,n+1} \quad (\text{XVIII.54})$$

$$(a_-)_{mn} = n^{1/2} \delta_{m,n-1} \quad (\text{XVIII.55})$$

Now we can construct the x

$$x = \frac{1}{\sqrt{2}} \frac{1}{\beta} \begin{pmatrix} 0 & 1 & 0 & 0 & \dots \\ 1 & 0 & \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 \\ 0 & 0 & \sqrt{3} & \ddots & \ddots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix} \quad (\text{XVIII.56})$$

This is a tridiagonal matrix.

For bonus marks: Find the eigenvectors of this matrix numerically using Mathematica.

What is $a_+ a_-$

$$a_+ a_- = \begin{pmatrix} 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & \dots \\ 0 & 0 & 2 & \ddots \\ \vdots & \vdots & \ddots & \ddots \end{pmatrix} \quad (\text{XVIII.57})$$

This is simply the number operator. Thus we can write

$$H = \hbar \omega_o \left(N + \frac{1}{2} \right) \quad (\text{XVIII.58})$$

Angular momentum:

$$[L^2, L_z] = 0 \quad (\text{XVIII.59})$$

$$L^2 |lm\rangle = \hbar^2 l(l+1) |lm\rangle \quad (\text{XVIII.60})$$

$$L_z |lm\rangle = m\hbar |lm\rangle \quad (\text{XVIII.61})$$

$$L^2 = \hbar^2 \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots \end{pmatrix} \quad (\text{XVIII.62})$$

$$L_z = \hbar^2 \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots \end{pmatrix} \quad (\text{XVIII.63})$$

$$L_+ = L_x + iL_y \quad (\text{XVIII.64})$$

$$L_- = L_x - iL_y \quad (\text{XVIII.65})$$

$$L_{\pm} |l, m\rangle = ((l \mp m)(l \pm m + 1))^{1/2} |l, m \pm 1\rangle \quad (\text{XVIII.66})$$

$$\langle l, m | L_{\pm} |l' m'\rangle = (l' \mp m') (l' \pm m' + 1)^{1/2} \hbar \delta_{ll'} \delta_{m, m' \pm 1} \quad (\text{XVIII.67})$$

Let's look at the $l = 1$ subspace:

$$L^2 = \hbar^2 \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad (\text{XVIII.68})$$

$$L_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad (\text{XVIII.69})$$

$$L_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad (\text{XVIII.70})$$

$$L_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (\text{XVIII.71})$$

The eigenvectors of L_z are

$$|l = 1, m = 1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}; \quad |l = 1, m = 0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}; \quad |l = 1, m = -1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (\text{XVIII.72})$$

Lecture 23 - November 14th, 2011

On the test:

- Tunneling
- Angular momentum
- Hydrogen

The eigenvalues of L^2 are $2\hbar^2$ (the same for all m). To diagonalize L_x is to

$$L_x v = \lambda v \quad (\text{XVIII.73})$$

$$(L_x - \lambda) v = 0 \quad (\text{XVIII.74})$$

One solution is the trivial solution $v = 0$, but this isn't interesting. To get interesting solutions:

$$\det(L_x - \lambda) \quad (\text{XVIII.75})$$

$$\det \begin{pmatrix} -\lambda & \frac{\hbar}{\sqrt{2}} & 0 \\ \frac{\hbar}{\sqrt{2}} & -\lambda & \frac{\hbar}{\sqrt{2}} \\ 0 & \frac{\hbar}{\sqrt{2}} & -\lambda \end{pmatrix} = 0 - \lambda(\lambda^2 - \hbar^2/2) + \lambda\hbar^2/2 = 0 \quad (\text{XVIII.76})$$

This gives eigenvalues are $0, \pm\hbar$. To get eigenvectors plug λ 's back in. Plugging in $\lambda = \hbar$:

$$\begin{pmatrix} -\hbar & \frac{\hbar}{\sqrt{2}} & 0 \\ \frac{\hbar}{\sqrt{2}} & -\hbar & \frac{\hbar}{\sqrt{2}} \\ 0 & \frac{\hbar}{\sqrt{2}} & -\hbar \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = 0 \quad (\text{XVIII.77})$$

$$\hbar \begin{pmatrix} -1 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -1 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = 0 \quad (\text{XVIII.78})$$

Solving the systems gives the following eigenvalues:

$$\lambda = \hbar \frac{1}{2} \rightarrow \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} \quad (\text{XVIII.79})$$

$$\lambda = 0 \rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \quad (\text{XVIII.80})$$

$$\lambda = -\hbar \rightarrow \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} \quad (\text{XVIII.81})$$

The transformation is a Unitary Matrix (as expected):

$$U = \frac{1}{2} \begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix} \quad (\text{XVIII.82})$$

In order to diagonalize L_x :

$$UL_x U^{-1} = \frac{1}{2} \begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix} \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix} \quad (\text{XVIII.83})$$

$$= \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (\text{XVIII.84})$$

In terms of spherical harmonics what are the eigenvectors? Thus the eigenvector for $\lambda = \hbar$:

$$\frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} \rightarrow \frac{1}{2} = \left(Y_{1,1}(\phi, \theta) + \sqrt{2}Y_{1,0}(\phi, \theta) + Y_{1,-1}(\phi, \theta) \right) \quad (\text{XVIII.85})$$

$$= \frac{1}{4} \sqrt{\frac{3}{2\pi}} (\sin \theta e^{-i\phi} + 2 \cos \theta + \sin \theta e^{i\phi}) \quad (\text{XVIII.86})$$

$$= \frac{1}{2} \sqrt{\frac{3}{2\pi}} (\cos \theta + -i \sin \theta \sin \phi) \quad (\text{XVIII.87})$$

$$P(\phi, \theta) = \frac{1}{4} \frac{3}{2\pi} (\cos^2 \theta + \sin^2 \theta \sin^2 \phi) \sin \theta \quad (\text{XVIII.88})$$

$$\int P(\phi, \theta) d\theta d\phi = 1 \quad (\text{XVIII.89})$$

Notice that since these aren't eigenfunctions of z we know longer have rotational symmetry of ϕ ! Now we can check whether this truly is an eigenfunction of $L_x = i\hbar \left(\sin \phi \frac{\partial}{\partial \theta} + \cos \theta \cos \phi \frac{\partial}{\partial \phi} \right)$. Notice that finding the eigenfunction of this operator is very difficult without the matrix formulation.

$$L_x |1, 1\rangle_x = \hbar |1, 1\rangle_x \quad (\text{XVIII.90})$$

Note that these are $m = 1$ eigenfunctions in the \mathbf{x} basis.

XIX. SPIN

Spin is the intrinsic angular momentum of a particle. There is no coordinate representation for spin since it doesn't exist in real space. We will construct the matrix representation. We still expect the angular momentum commutation relations to hold. For example

$$[S_x, S_y] = i\hbar S_z; \quad (\text{XIX.1})$$

or more generally we expect

$$[S_i, S_j] = i\hbar \epsilon^{ijk} S_k \quad (\text{XIX.2})$$

We can define

$$S_+ = S_x + iS_y; \quad S_- = S_x - iS_y \quad (\text{XIX.3})$$

We expect $S^2 = S_x^2 + S_y^2 + S_z^2$ to obey

$$S^2 |s, m_s\rangle = s(s+1) \hbar^2 |s, m_s\rangle \quad (\text{XIX.4})$$

$$S_z |s, m_s\rangle = m_s |s, m_s\rangle \quad (\text{XIX.5})$$

$$(\text{XIX.6})$$

Where $m_s = (-s, -s+1, \dots, s-1, s)$. Pions, mesons, etc all carry $s = 0$. Electrons, protons, neutrons, neutrinos, etc. all carry $s = \frac{1}{2}$. The force carriers such as photons, W and Z bosons, gluons, carry $s = 1$. The graviton (if it exists) carries $s = 2$. We will focus on spin half objects since all stable matter is mostly made up of spin half particles.

$$S^2 \left| \frac{1}{2}, \frac{1}{2} \right\rangle = \frac{1}{2} \frac{3}{2} \hbar^2 \left| \frac{1}{2}, \frac{1}{2} \right\rangle \quad (\text{XIX.7})$$

$$S_z \left| \frac{1}{2}, \frac{1}{2} \right\rangle = \frac{1}{2} \hbar \left| \frac{1}{2}, \frac{1}{2} \right\rangle \quad (\text{XIX.8})$$

Recall

$$L_{\pm} |l, m\rangle = \hbar (l(l+1) - m(m \pm 1))^{1/2} |l, m \pm 1\rangle \quad (\text{XIX.9})$$

$$S_- \left| \frac{1}{2}, \frac{1}{2} \right\rangle = \left(\frac{1}{2} \left(\frac{1}{2} + 1 \right) - \frac{1}{2} \left(\frac{1}{2} - 1 \right) \right)^{1/2} \quad (\text{XIX.10})$$

$$= \hbar \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \quad (\text{XIX.11})$$

$$S_+ \left| \frac{1}{2}, \frac{1}{2} \right\rangle = 0 \quad (\text{XIX.12})$$

$$S^2 \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \frac{3}{4} \hbar^2 \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \quad (\text{XIX.13})$$

$$S_z \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = -\frac{1}{2} \hbar \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \quad (\text{XIX.14})$$

$$S_+ \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \hbar \left| \frac{1}{2}, \frac{1}{2} \right\rangle \quad (\text{XIX.15})$$

$$S_- \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = 0 \quad (\text{XIX.16})$$

Lets denote $|\uparrow\rangle \rightarrow |\alpha\rangle$, $|\downarrow\rangle \rightarrow |\beta\rangle$.

$$S_+ |\alpha\rangle = 0 \quad (\text{XIX.17})$$

$$S_- |\alpha\rangle = \hbar |\beta\rangle \quad (\text{XIX.18})$$

$$S_+ |\beta\rangle = \hbar |\alpha\rangle \quad (\text{XIX.19})$$

$$S_- |\beta\rangle = 0 \quad (\text{XIX.20})$$

$$S_{\pm} = S_x \pm iS_y \quad (\text{XIX.21})$$

$$S_x |\alpha\rangle = \frac{\hbar}{2} |\beta\rangle \quad (\text{XIX.22})$$

$$S_y |\alpha\rangle = i \frac{\hbar}{2} |\beta\rangle \quad (\text{XIX.23})$$

$$S_z |\alpha\rangle = \frac{\hbar}{2} |\alpha\rangle \quad (\text{XIX.24})$$

$$S_x |\beta\rangle = \frac{\hbar}{2} |\alpha\rangle \quad (\text{XIX.25})$$

$$S_y |\beta\rangle = -i \frac{\hbar}{2} |\alpha\rangle \quad (\text{XIX.26})$$

$$S_z |\beta\rangle = -\frac{\hbar}{2} |\beta\rangle \quad (\text{XIX.27})$$

To construct the S_x matrix:

$$S_x = \begin{pmatrix} \langle \alpha | S_x | \alpha \rangle & \langle \alpha | S_x | \beta \rangle \\ \langle \beta | S_x | \alpha \rangle & \langle \beta | S_x | \beta \rangle \end{pmatrix} \quad (\text{XIX.28})$$

$$\frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (\text{XIX.29})$$

$$S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (\text{XIX.30})$$

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{XIX.31})$$

$$|\alpha\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad |\beta\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (\text{XIX.32})$$

We can write $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$. Where

$$\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \quad (\text{XIX.33})$$

$$S^2 = S_x^2 + S_y^2 + S_z^2 \quad (\text{XIX.34})$$

$$= \hbar^2 \left(\frac{1}{2} + 1\right) \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (\text{XIX.35})$$

$$= \hbar^2 \frac{3}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (\text{XIX.36})$$

Hence any two component vector is an eigenstate of S^2 . Note that these spinors are **not** a vector in the sense of R^3 or R^2 . Of course its a vector in Hilbert space. The geometrical meaning is **not** a 2D or 3D geometrical vector but its a new geometric object called a spinor. Geometrically there are scalars, vectors, and tensors. Spinors fit in between scalars and vectors. Under rotations spinors do not behave transform like vectors but like spinors.

$$S_x S_y + S_y S_x = \frac{\hbar^2}{4} \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) \quad (\text{XIX.37})$$

$$= 0 \quad (\text{XIX.38})$$

Doing this for all directions:

$$\{S_x, S_y\} = 0 \quad (\text{XIX.39})$$

Where $\{ , \}$ is the anticommutator. This relation implies the Pauli-Exclusion principle.

Spin has many important consequences. The electron is charge. Can think of electron as a spinning ball of charge (though this is a very incorrect picture). Thus we have a current loop and hence a magnet. The electron has a magnetic moment. The potential associated with this magnetic moment is

$$V = -\boldsymbol{\mu} \cdot \mathbf{B} \quad (\text{XIX.40})$$

Where

$$\boldsymbol{\mu} = \frac{e}{mc} \mathbf{S} \quad (\text{XIX.41})$$

Lecture 25- November 16, 2011

There was a small change in the notes:

$$U = \frac{1}{2} \begin{pmatrix} 1 & \sqrt{2} & 1 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix} \quad (\text{XIX.42})$$

If you compare this with L_y you can see that

$$U = I + iL_y - L_y^2 \quad (\text{XIX.43})$$

But

$$e^{i\theta L_y} = I + i \sin \theta L_y + \cos \theta L_y^2 - L_y^2 \quad (\text{XIX.44})$$

is the rotation operator for rotations. If $\theta = \frac{\pi}{2}$ then this is just the U !. This makes sense since the matrix that diagonalizes L_x can be interpreted as a rotation about the y axis.

XX. ADDITION OF ANGULAR MOMENTUM

Examples

An electron with both orbital and spin angular momentum:

$$\mathbf{J} = \mathbf{L} + \mathbf{S} \quad (\text{XX.1})$$

Two electron system (e.g. Helium):

$$\mathbf{J} = \mathbf{S}_1 + \mathbf{S}_2 \quad (\text{XX.2})$$

We will now consider two electrons:

$$J^2 = (S_1 + S_2)^2 \quad (\text{XX.3})$$

Where the subscript denotes which electron we are talking about.

$$[S_1, S_2] = 0 \quad (\text{XX.4})$$

Since the operators act on completely different spaces.

$$J^2 = S_1^2 + S_2^2 + 2S_1 \cdot S_2 \quad (\text{XX.5})$$

but

$$(S_1 + S_2)^2 = S_1^2 + S_2^2 + 2S_1 \cdot S_2 \quad (\text{XX.6})$$

Which implies that

$$2\mathbf{S}_1 \cdot \mathbf{S}_2 = S_{+,1}S_{-,2} + S_{-,1}S_{+,2} + 2S_{z,1}S_{z,2} \quad (\text{XX.7})$$

Hence

$$J^2 = S_1^2 + S_2^2 + S_{+,1}S_{-,2} + S_{-,1}S_{+,2} + 2S_{z,1}S_{z,2} \quad (\text{XX.8})$$

$$S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \quad S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad (\text{XX.9})$$

Hence

$$S_+ |\uparrow\rangle = 0; \quad S_- |\uparrow\rangle = \hbar |\downarrow\rangle \quad (\text{XX.10})$$

$$S_+ |\downarrow\rangle = \hbar |\uparrow\rangle; \quad S_- |\downarrow\rangle = 0 \quad (\text{XX.11})$$

$$J^2 |\uparrow\uparrow\rangle = S_1^2 + S_2^2 + S_{+,1}S_{-,2} + S_{-,1}S_{+,2} + 2S_{z,1}S_{z,2} |\uparrow\uparrow\rangle \quad (\text{XX.12})$$

$$= \frac{3}{4}\hbar^2 |\uparrow\uparrow\rangle + \frac{3}{4}\hbar^2 |\uparrow\uparrow\rangle + \frac{\hbar^2}{2} |\uparrow\uparrow\rangle \quad (\text{XX.13})$$

$$= 2\hbar^2 |\uparrow\uparrow\rangle \quad (\text{XX.14})$$

$$= J(J+J); \quad \text{Where } J = 1 \quad (\text{XX.15})$$

$$J^2 |\uparrow\downarrow\rangle = S_1^2 + S_2^2 + S_{+,1}S_{-,2} + S_{-,1}S_{+,2} + 2S_{z,1}S_{z,2} |\uparrow\downarrow\rangle \quad (\text{XX.16})$$

$$= \left(\frac{3}{4}\hbar^2 + \frac{3}{4}\hbar^2\right) |\uparrow\downarrow\rangle + 0 + \hbar^2 |\uparrow\downarrow\rangle - \frac{\hbar^2}{2} |\uparrow\downarrow\rangle \quad (\text{XX.17})$$

$$= \hbar^2 (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \quad (\text{XX.18})$$

This is **not** an eigenfunction of J^2 . By symmetry of electrons 1 and 2 we know that

$$J^2 |\uparrow\downarrow\rangle = \hbar^2 (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \quad (\text{XX.19})$$

but adding the two results above:

$$J^2 (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) = 2\hbar^2 (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \quad (\text{XX.20})$$

We can also subtract them

$$J^2 (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = 0 \quad (\text{XX.21})$$

$$J^2 |\downarrow\downarrow\rangle = 2\hbar^2 |\downarrow\downarrow\rangle \quad (\text{XX.22})$$

This gives us the spin singlet and the spin triplet states. Thus electrons in Helium can be in both spin singlet and spin triplet.

Exercise: take $L = 1$ and $S = \frac{1}{2}$ and find the eigenfunctions of $J = L + S$. Also try $S_1 + S_2 + S_3$.

In general if we do

$$\mathbf{J} = \mathbf{L}_1 + \mathbf{L}_2 \quad (\text{XX.23})$$

$$|l_1 l_2, j m\rangle = \sum_{m_1=-l_1}^{l_1} \sum_{m_2=-l_2}^{l_2} |l_1 m_1\rangle |l_2 m_2\rangle \langle l_1 m_1, l_2 m_2 | j m\rangle \quad (\text{XX.24})$$

$$J_z |\uparrow\uparrow\rangle = (S_z^1 + S_z^2) |\uparrow\uparrow\rangle \quad (\text{XX.25})$$

$$= \left(\frac{\hbar}{2} + \frac{\hbar}{2} \right) |\uparrow\uparrow\rangle \quad (\text{XX.26})$$

$$(\text{XX.27})$$

$$J^2 |\uparrow\uparrow\rangle = 1(2)\hbar^2 |\uparrow\uparrow\rangle \quad (\text{XX.28})$$

The spin triplet is formed by $J = 1$:

$$|\uparrow\uparrow\rangle \quad (\text{XX.29})$$

$$\frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \quad (\text{XX.30})$$

$$|\downarrow\downarrow\rangle \quad (\text{XX.31})$$

The spin singlet is formed by $J = 0$:

$$\frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad (\text{XX.32})$$

$$J_z \left(\frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \right) = (S_z^1 + S_z^2) \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \quad (\text{XX.33})$$

$$= \frac{1}{\sqrt{2}} \left(\frac{\hbar}{2} |\uparrow\downarrow\rangle - \frac{\hbar}{2} |\downarrow\uparrow\rangle - \frac{\hbar}{2} |\uparrow\downarrow\rangle + \frac{\hbar}{2} |\downarrow\uparrow\rangle \right) \quad (\text{XX.34})$$

$$= 0 \quad (\text{XX.35})$$

The spin states are orthonormal:

$$\langle \uparrow | \uparrow \rangle = 1 \quad (\text{XX.36})$$

$$\langle \downarrow | \downarrow \rangle = 1 \quad (\text{XX.37})$$

$$\langle \uparrow | \downarrow \rangle = 0 \quad (\text{XX.38})$$

$$\langle \downarrow | \uparrow \rangle = 0 \quad (\text{XX.39})$$

Lets find the matrix U that diagonalizes the $S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ matrix.

$$\det \begin{pmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{pmatrix} = 0 \Rightarrow \lambda = \pm \frac{\hbar}{2} \quad (\text{XX.40})$$

$$\frac{\hbar}{2} \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 0 \quad (\text{XX.41})$$

Hence the eigenvector is (after normalization)

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (\text{XX.42})$$

The other eigenvector (easy to check) is

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (\text{XX.43})$$

Thus the transformation matrix is

$$U^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = U^{-1} \quad (\text{XX.44})$$

Here we are changing the quantization axis from z to x. So the rotation matrix is (rotation about the y axis)

$$e^{i\theta S_y/\hbar} = 1 + \frac{i\theta\sigma_y}{2} + \frac{(i\theta)^2\sigma_y^2}{4} + \frac{(i\theta)^3\sigma_y^3}{2^3} + \frac{(i\theta)^3\sigma_y^3}{6} \dots \quad (\text{XX.45})$$

But the squares the Pauli spin matrices are 1!. Thus

$$e^{i\theta S_y/\hbar} = 1 + \frac{i\theta\sigma_y}{2} - \frac{\theta^2}{4} \frac{1}{2} - \frac{\theta^3\sigma_y}{2^3} \frac{1}{6} + \dots \quad (\text{XX.46})$$

$$= \cos(\theta/2) + i \sin(\theta/2) \sigma_y \quad (\text{XX.47})$$

$$= \begin{pmatrix} \cos(\theta/2) & \sin(\theta/2) \\ -\sin(\theta/2) & \cos(\theta/2) \end{pmatrix} \quad (\text{XX.48})$$

For $\theta = \pi/2$:

$$e^{i\pi S_y/2\hbar} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \quad (\text{XX.49})$$

Notice that for $\theta = 2\pi$

$$U(\theta = 2\pi) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{XX.50})$$

Thus when we rotate by 2π we don't get the identity!

We can split the eigenstates of S_x into eigenstates of S_z :

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle) \quad (\text{XX.51})$$

One notation for this vector is

$$|\rightarrow\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle) \quad (\text{XX.52})$$

XXI. ENTANGLEMENT

The idea of entanglement first came out in the paper called the “EPR paper” by Einstein, Podolsky, and Rosen (1935). This paper discussed the philosophy of entanglement but never thought that the different interpretations of quantum mechanics could really be proved right or wrong. However a paper by Bell showed that they could and Bell produced Bell’s inequalities. Einstein’s problem with quantum mechanics was that he thought that “Quantum mechanics is not complete, it doesn’t describe objective reality”.

The EPR experiment is as follows. Consider a π^0 particle which has spin $J = 0$. It decays through

$$\pi^0 \rightarrow e^+ + e^- \quad (\text{XXI.1})$$

Angular momentum is conserved and therefore the e^+, e^- pair has total $J = 0$. Hence the spin configuration is

$$|0, 0\rangle = \frac{1}{\sqrt{2}} (\uparrow\downarrow - \downarrow\uparrow) \quad (\text{XXI.2})$$

Entanglement is displayed in figure 8

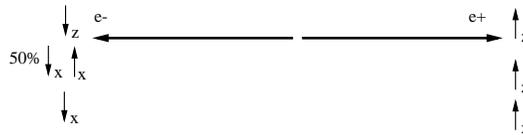


FIG. 8. Entanglement of a positron and electron pair

Lecture 27 -November 25th, 2011

Interesting paper: “Is the moon there when nobody looks? Reality and quantum theory”, Physics Today, April 1985, by David Mermin.

Consider two operators O_1 and O_2 . Define the correlator as

$$\frac{\langle O_1 O_2 \rangle}{\sqrt{\langle O_1^2 \rangle \langle O_2^2 \rangle}} \quad (\text{XXI.3})$$

If $O_1 = O_2$, then the correlator is equal to 1. The most common use of correlators is

$$\langle O(x_1, t_1) O(x_2, t_2) \rangle \quad (\text{XXI.4})$$

Def 3. Entanglement: We say a state is entangled if it cannot be written as a simple product of one particle states.

For example: If we could write the Helium atom as

$$\psi_1(x)\psi_2(x) \quad (\text{XXI.5})$$

then we don’t have an entangled state. However

$$\frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad (\text{XXI.6})$$

is entangled.

Consider a box with a button on it There a few key points

1. Brick stops light from flashing
2. Everytime both random number generators has pointers pointing in the same direction we get perfect anticorrelation. In other words we have GR or RG if we have 11,22, or 33.

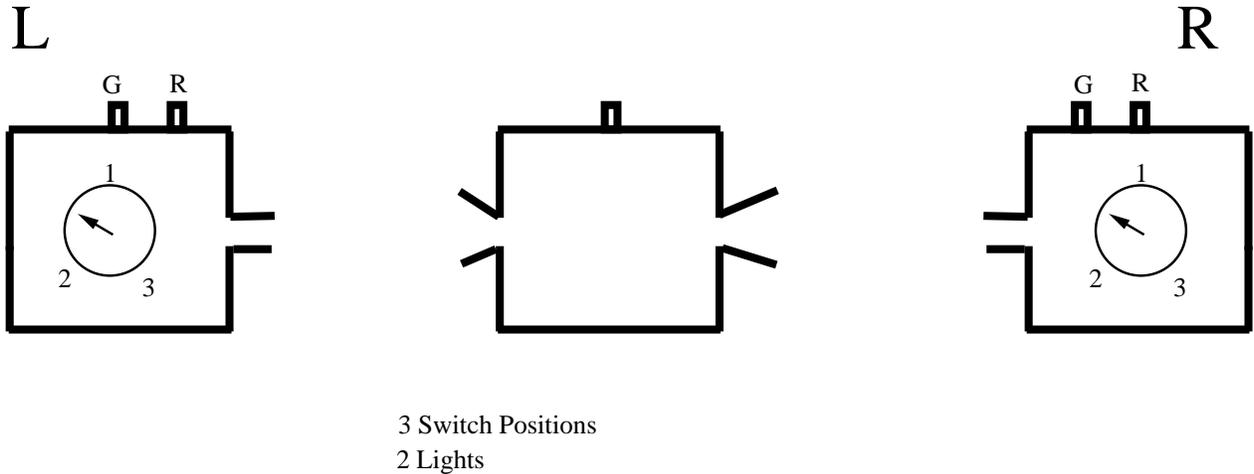


FIG. 9. Entanglement figure

3. There are four possible outcomes

4. If one pays attention to the point directions then half the time we have GG or RR and half the time we have GR and RG

Classical point of view says that particles have genes. In order for the particles to have perfect anticorrelation we require the particles 1 and 2 have the following gene table.

Particle one genes	Particle two genes
123	123
<i>GGG</i>	<i>RRR</i>
<i>GGR</i>	<i>RRG</i>
<i>GRG</i>	<i>RGR</i>
<i>RGG</i>	<i>GRR</i>
<i>RRG</i>	<i>GGR</i>
<i>RGR</i>	<i>GRG</i>
<i>GRR</i>	<i>RGG</i>
<i>RRR</i>	<i>GGG</i>

Consider the GGR -RRG row. There are 9 possible pointer settings:

$$11, 12, 21, 22, 33 \\ 13, 23, 31, 32$$

The top row gives anti-correlation while the bottom row gives the same colours. For this gene the probability is 5/9 for anti-correlation. The row that we analyzed is the same form as all the rows but the first and last ones. On row 1 and row 8 we get perfect anti-correlation. Therefore identical results for 6 of the 8 rows (genes) and perfect anti-correlation for the other two rows.

The classical conclusion is that if we pay no attention to pointer positions we will get anti-correlation with a probability greater than 5/9. This is the simplest way to state Bell's inequality. The experiment violates Bell's inequality. This refutes the EPR claim of the existence of an element of physical reality.

The EPR reality criteria is: "If without in any way disturbing the system we can predict with certainty the value of a physical quantity then there exists an element of physical reality corresponding to this physical quantity." Recall

$$\pi^0 \rightarrow \chi = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad (\text{XXI.7})$$

Recall that

$$J^2 \chi = 0 \chi \quad (\text{XXI.8})$$

We want to know that correlator:

$$\langle \chi | S_1^z S_2^z | \chi \rangle \quad (\text{XXI.9})$$

First lets do the simpler correlator

$$S_1^z S_2^z |\uparrow\downarrow\rangle = -\hbar^2 \frac{1}{2} \frac{1}{2} |\uparrow\downarrow\rangle \quad (\text{XXI.10})$$

$$S_1^z S_2^z |\downarrow\uparrow\rangle = -\frac{\hbar^2}{4} |\downarrow\uparrow\rangle \quad (\text{XXI.11})$$

Now

$$S_1^z S_2^z \chi = -\frac{\hbar^2}{4} \chi \quad (\text{XXI.12})$$

We can finally compute the normalized correlator:

$$\frac{\langle \chi | S_1^z S_2^z | \chi \rangle}{\sqrt{\langle \chi | (S_1^z)^2 | \chi \rangle \langle \chi | (S_2^z)^2 | \chi \rangle}} = -1 \quad (\text{XXI.13})$$

This tells you that the spins in this state are perfectly anti-correlated. Now consider the operators in the x direction

$$\frac{\langle \chi | S_1^x S_2^x | \chi \rangle}{\sqrt{\langle \chi | (S_1^x)^2 | \chi \rangle \langle \chi | (S_2^x)^2 | \chi \rangle}} \quad (\text{XXI.14})$$

To get this correlator we need

$$S_1^x S_2^x |\uparrow\downarrow\rangle = \frac{\hbar^2}{4} |\downarrow\uparrow\rangle \quad (\text{XXI.15})$$

$$S_1^x S_2^x |\downarrow\uparrow\rangle = \frac{\hbar^2}{4} |\uparrow\downarrow\rangle \quad (\text{XXI.16})$$

$$S_1^x S_2^x |\downarrow\uparrow\rangle = \frac{\hbar^2}{4} |\uparrow\downarrow\rangle \quad (\text{XXI.17})$$

$$S_1^x S_2^x \chi = -\frac{\hbar^2}{4} \chi \quad (\text{XXI.18})$$

Thus

$$\frac{\langle \chi | S_1^x S_2^x | \chi \rangle}{\sqrt{\langle \chi | (S_1^x)^2 | \chi \rangle \langle \chi | (S_2^x)^2 | \chi \rangle}} = -1 \quad (\text{XXI.19})$$

The same is true for the $S_1^y S_2^y$ we have perfect anti-correlation.

$$C(S_1^x S_2^z) |\uparrow\downarrow\rangle = (S_1^x \uparrow) (S_2^z) \quad (\text{XXI.20})$$

$$= \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (\text{XXI.21})$$

$$= -\frac{\hbar^2}{4} |\downarrow\downarrow\rangle \quad (\text{XXI.22})$$

Similarly

$$S_1^x S_2^z |\downarrow\uparrow\rangle = \frac{\hbar^2}{4} |\uparrow\uparrow\rangle \quad (\text{XXI.23})$$

$$S_1^x S_2^z \chi = -\frac{\hbar^2}{4} \frac{1}{\sqrt{2}} (\downarrow\downarrow + \uparrow\uparrow) \quad (\text{XXI.24})$$

$$|\chi\rangle S_1^x S_2^z |\chi\rangle = 0 \quad (\text{XXI.25})$$

Hence there is no correlation.

Lecture 28 - November 30th, 2011

Recall the EPR experiment:

$$\pi^0 \rightarrow e^+ + e^- \quad (\text{XXI.26})$$

The results were

1. If the spin measurements are on the same axis then perfect anti-correlation
2. If you don't pay attention to which axis then no-correlation

Classical thinking:

If you construct gene tables to satisfy the first condition then the second condition will produce correlation.

Quantum thinking :

$$\pi^0 \rightarrow \frac{1}{\sqrt{2}} (\uparrow\downarrow - \downarrow\uparrow) \equiv \chi; J = 0, J_z = 0 \quad (\text{XXI.27})$$

The three pointers in the experiment are actually the directions in which we are actually measuring the spin: The vectors are $(\hat{n}_1 = \hat{e}_z, \hat{n}_2 = \frac{\sqrt{3}}{2}\hat{e}_x - \frac{1}{2}\hat{e}_z, \hat{n}_3 = -\frac{\sqrt{3}}{2}\hat{e}_x - \frac{1}{2}\hat{e}_z)$. Recall the definition of \mathbf{S}

$$\mathbf{S} = \frac{\hbar}{2} \boldsymbol{\sigma} \quad (\text{XXI.28})$$

Where $\boldsymbol{\sigma}_1$ is the spin matrix corresponding to particle 1. To find the correlator we first find the relations:

$$S_1^z S_2^z \uparrow\downarrow = \frac{-\hbar^2}{4} \uparrow\downarrow \quad (\text{XXI.29})$$

The correlator of $\mathbf{S}_1 \cdot \hat{n}_1 \mathbf{S}_2 \cdot \hat{n}_2$ (without normalization) is

$$\langle \chi | \mathbf{S}_1 \cdot \hat{n}_1 \mathbf{S}_2 \cdot \hat{n}_2 | \chi \rangle = \langle \chi | S_1^z S_2^z | \chi \rangle \quad (\text{XXI.30})$$

$$= -1 \quad (\text{XXI.31})$$

Now lets calculate

$$\langle \chi | (\mathbf{S}_1 \cdot \hat{n}_2) (\mathbf{S}_2 \cdot \hat{n}_1) | \chi \rangle = \langle \chi | \left(\frac{\sqrt{3}}{2} S_1^x - \frac{1}{2} S_1^z \right) \left(\frac{\sqrt{3}}{2} S_2^x - \frac{1}{2} S_2^z \right) | \chi \rangle \quad (\text{XXI.32})$$

$$= \langle \chi | \frac{3}{4} S_1^x S_2^x + \frac{1}{4} S_1^z S_2^z - \frac{\sqrt{3}}{4} S_1^z S_2^x - \frac{\sqrt{3}}{4} S_1^x S_2^z | \chi \rangle \quad (\text{XXI.33})$$

Define this operator in the bracket as \mathcal{O} .

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (\text{XXI.34})$$

$$S_x \uparrow = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (\text{XXI.35})$$

$$\frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (\text{XXI.36})$$

$$S_x \downarrow = -\uparrow \quad (\text{XXI.37})$$

$$\mathcal{O} \uparrow\downarrow = \frac{\hbar^2}{4} \left(\frac{3}{4} \downarrow\uparrow - \frac{1}{4} \uparrow\downarrow - \frac{\sqrt{3}}{4} \uparrow\uparrow + \frac{\sqrt{3}}{4} \downarrow\downarrow \right) \quad (\text{XXI.38})$$

$$\mathcal{O} \downarrow\uparrow = \frac{\hbar^2}{4} \left(\frac{3}{4} \uparrow\downarrow - \frac{1}{4} \downarrow\uparrow + \frac{\sqrt{3}}{4} \downarrow\downarrow - \frac{\sqrt{3}}{4} \uparrow\uparrow \right) \quad (\text{XXI.39})$$

Finally

$$\mathcal{O}\chi = \mathcal{O} \frac{1}{\sqrt{2}} (\uparrow\downarrow - \downarrow\uparrow) \quad (\text{XXI.40})$$

$$= -\frac{\hbar^2}{4} \chi \quad (\text{XXI.41})$$

Thus these are perfectly anti-correlated.

If we don't pay any attention to the spin then we should get zero for the following: ($i \neq j$)

$$\sum_{i,j} \langle \chi | \mathbf{S}_1 \cdot \hat{n}_i \mathbf{S}_2 \cdot \hat{n}_j | \chi \rangle = \langle \chi | \sum_i \mathbf{S}_1 \cdot \hat{n}_i \sum_j \mathbf{S}_2 \cdot \hat{n}_j | \chi \rangle \quad (\text{XXI.42})$$

$$= \langle \chi | \mathbf{S}_1 \cdot \left(\sum_i \hat{n}_i \right) \mathbf{S}_2 \cdot \left(\sum_j \hat{n}_j \right) | \chi \rangle \quad (\text{XXI.43})$$

$$= 0 \quad (\text{XXI.44})$$

Since the vector sum over all the three vectors is trivially zero. To summarize: Bell's inequality follows from classical thinking. Bell's inequality is violated by experiment and quantum mechanics. Bell's inequality is a statistical statement. In other words you have to do many measurements and sum the results. This is the way things stood until GHZ came along (Greenburger, Horne, and Zolnger) and they proposed an experiment and carried it out which is not a statistical experiment (one-shot experiment). In this experiment 100% of the time quantum mechanics predicts one thing and classical mechanics predicts another. You are responsible for this experiment for the exam.

We have solved most of the exactly solvable problems in quantum mechanics but we have approximation schemes for the others.

- Time-dependant perturbation theory
- Time-independant perturbation thoery
- Degenerate perturbation theory
- WKB approximation
- Variational method

Lecture 29 - December 1st, 2011

XXII. VARIATIONAL METHOD

This is an approximation technique. If $|\alpha\rangle$ is some trial state to the equation:

$$H\psi = E\psi \quad (\text{XXII.1})$$

Then we consider

$$\langle \alpha | H | \alpha \rangle \quad (\text{XXII.2})$$

As an approximation to the energy. To get the trial state we make an educated guess. There is no way we'll get the exact solution. If we minimize

$$\langle \alpha | H | \alpha \rangle \quad (\text{XXII.3})$$

this quantity with respect to a parameter then we assured of getting as closed as possible the exact solution. Mathematically:

$$\frac{d \langle \alpha | H | \alpha \rangle}{da} = 0 \quad (\text{XXII.4})$$

For some parameter a is the best possible solution. We call a a variational parameter and we use it to parametrize our wavefunction. e.g. $\psi(x, a)$. Why does it work? This works because

$$|\alpha\rangle = \sum_n a_n |n\rangle \quad (\text{XXII.5})$$

$$\langle \alpha | H | \alpha \rangle = \sum_{n, n'} a_n a_{n'}^* \langle n' | H | n \rangle \quad (\text{XXII.6})$$

but since this is an exact solution $H |n\rangle = E_n |n\rangle$

$$\langle \alpha | H | \alpha \rangle = \sum_{n, n'} a_n^* a_{n'} E_n \delta_{n, n'} = \sum_n |a_n|^2 E_n \quad (\text{XXII.7})$$

$$\geq E_o \sum_n |a_n|^2 \quad (\text{XXII.8})$$

$$\geq E_o \quad (\text{XXII.9})$$

Minimizing the energy is maximizing a_o . As an example consider Hydrogen

$$\left\{ -\frac{\hbar^2}{2m} \left(\frac{1}{r} \frac{d^2 r}{dr^2} \right) + \frac{1}{2m} \frac{L^2}{r^2} - \frac{Ze^2}{r} \right\} \psi(r, \phi, \theta) = E \psi(r, \phi, \theta) \quad (\text{XXII.10})$$

Because the problem has rotational symmetry we know that $\psi(r, \phi, \theta) = R(r) Y_{lm}(\phi, \theta)$. Substituting in we will get

$$H = -\frac{\hbar^2}{2m} \left(\frac{1}{r} \frac{d^2 r}{dr^2} \right) + \frac{\hbar^2}{2mr^2} l(l+1) - \frac{Ze^2}{r} \quad (\text{XXII.11})$$

We will discuss $l = 0$. Thus

$$H = -\frac{\hbar^2}{2m} \left(\frac{1}{r} \frac{d^2 r}{dr^2} \right) - \frac{Ze^2}{r} \quad (\text{XXII.12})$$

Our trial solution is $R(r) = 2 \left(\frac{1}{a} \right)^{3/2} e^{-r/a}$, where a is the variational parameter (not a_o). This is silly since we know that $R(r)$ above contains within it the exact solution. Note once we decide we want to try an exponential solution we are essentially forced to this form by dimensions and normalization (even the 2!). First lets find this (define γ in this way).

$$H R(r) = \left(-\frac{\hbar^2}{2m} \left(\frac{1}{4} \frac{d^2 r}{dr^2} \right) - \frac{Ze^2}{r} \right) \gamma e^{-r/a} \quad (\text{XXII.13})$$

$$= \gamma \left(-\frac{\hbar^2}{2m} \left(-\frac{2}{ar} + \frac{1}{a^2} \right) - \frac{Ze^2}{r} \right) e^{-r/a} \quad (\text{XXII.14})$$

$$\langle a | H | a \rangle = \int_0^\infty \gamma^2 r^2 dr \left(-\frac{\hbar^2}{2m} \left(-\frac{2}{ar} + \frac{1}{a^2} \right) - \frac{Ze^2}{r} \right) e^{-r/a} \quad (\text{XXII.15})$$

$$= \frac{4}{a^3} \int_0^\infty \left(\left(\frac{\hbar^2}{ma} - \frac{Ze^2}{r} \right) r e^{-r/a} - \frac{\hbar^2}{2ma^2} r^2 e^{-r/a} \right) dr \quad (\text{XXII.16})$$

but

$$\int_0^{\infty} r^2 e^{-r/a} dr = \frac{a^3}{4} \quad (\text{XXII.17})$$

and

$$\int_0^{\infty} r e^{-r/a} dr = \frac{a^2}{4} \quad (\text{XXII.18})$$

$$\langle a | H | a \rangle = \frac{4}{a^3} \left(\left(\frac{\hbar^2}{ma} - Ze^2 \right) \frac{a^2}{4} - \frac{\hbar^2}{2ma^2} \frac{a^3}{4} \right) \quad (\text{XXII.19})$$

$$= \frac{4}{a^3} \left(\frac{\hbar^2 a}{8m} - Z \frac{e^2 a^2}{4} \right) \quad (\text{XXII.20})$$

$$= \left(\frac{\hbar^2}{2ma^2} - Z \frac{e^2}{a} \right) \quad (\text{XXII.21})$$

$$(\text{XXII.22})$$

We have calculated the energy as a function of our variational parameter a .

$$E(a) = \frac{\hbar^2}{2ma^2} - Z \frac{e^2}{a} \quad (\text{XXII.23})$$

The Coloumb term is pushing the electron inwards while the Quantum mechanics forms the repulsive term pushing

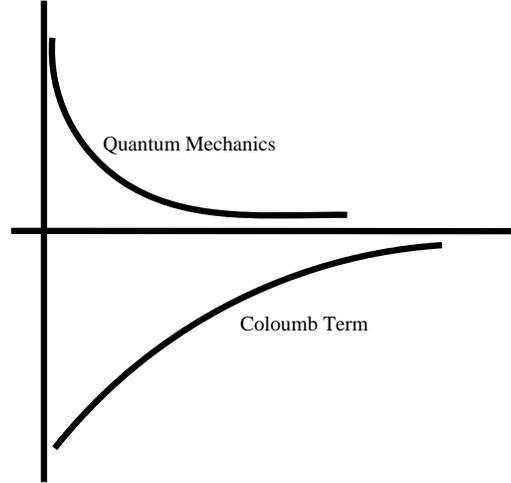


FIG. 10. The energy contributions from the varitional method

the electron outwards.

$$E'(a) = -\frac{\hbar^2}{ma^3} + \frac{Ze^2}{a^2} = 0a \quad = \frac{\hbar^2}{2e^2m} \quad (\text{XXII.24})$$

To no suprise $E'(a)$ is minimized at the Bohr radius. Plugging this back in you get the exact energy, $E(a) = -\frac{1}{2}mc^2\alpha^2$.