Ph125a Class Notes

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Chapter 1

Week 1

1.1 Monday 28 Sept 2015

Office Hours TA hours: Sunday and Tuesday evening. Prof hours: Monday 11-1 (412 DWN). No recitations.

Review Consider 1 particle, 1D. Operators and eigenvalue equations:

$$X\hat{x} = x\hat{x} \tag{1.1}$$
$$P\hat{p} = p\hat{p} \tag{1.2}$$

Action of operators

$$X\Psi(x,t) = x\Psi(x,t) \tag{1.3}$$
$$P\Psi(x,t) = -i\hbar\frac{d}{dx}\Psi(x,t) \tag{1.4}$$

Commutators

$$XP - PX = i\hbar\boldsymbol{I} \tag{1.5}$$

Linear independence Given a set of vectors $\{|v_i\rangle\}, i = 1, \ldots, n$, if $\sum_i a_i|v_i\rangle = \mathbf{0} \implies a_i = 0, \forall i$ then the vectors are called linearly independent. There exists a maximum number of linear independent vectors, the dimension of that space.

Inner product

$$\langle w|v\rangle = \langle v|w\rangle^* \tag{1.6}$$

For QM:

$$\langle\Psi_2|\Psi_1\rangle = \int_{-\infty}^{\infty} dx\Psi_2^*(x)\Psi_1(x) \tag{1.7}$$

Linearity

$$\langle w|\alpha v_1 + \beta v_2\rangle = \alpha\langle w|v_1\rangle + \beta\langle w|v_2\rangle \tag{1.8}$$
$$\langle \alpha w_1 + \beta w_2|v\rangle = \alpha^*\langle w_1|v\rangle + \beta^*\langle w_2|v\rangle \tag{1.9}$$

Orthonormality

$$\langle e_i|e_j\rangle = \delta_{ij} \tag{1.10}$$

Summation convention

$$v_i|e_i\rangle \equiv \sum_i v_i|e_i\rangle \tag{1.11}$$

Linear Operators

$$\Omega|\alpha v + \beta w\rangle = \alpha\Omega|v\rangle + \beta\Omega|w\rangle \tag{1.12}$$

Hermitian Operators

$$\Omega = \Omega^\dagger \tag{1.13}$$

$$\text{s.t. } \langle v|\Omega w\rangle \equiv \langle \Omega^\dagger v|w\rangle \equiv \langle w|\Omega^\dagger v\rangle^* = \langle \Omega v|w\rangle \tag{1.14}$$

1.2 Wednesday, 30 Sept 2015

1.2.1 Analogue to matrices

Expansion Consider $|v\rangle = \sum_{i=1}^n v_i|e_i\rangle, v_j = \langle e_j|v\rangle$. Consider the linear operator Ω. Then:

$$\Omega|v\rangle = |w\rangle \implies \Omega\sum_{i=1}^n v_i|e_i\rangle = \sum_{j=1}^n w_j|e_j\rangle \implies w_j = \sum_{i=1}^n \langle e_j|\Omega|e_i\rangle v_i \tag{1.15}$$

Define the components of the operator:

$$\Omega_{ji} = \langle e_j|\Omega|e_i\rangle \tag{1.16}$$

Hermitian Adjoint of Matrix Recall:

$$\langle e_j|\Omega|e_i\rangle = \langle \Omega^\dagger e_j|e_i\rangle = \langle e_i|\Omega^\dagger|e_j\rangle^* \implies \Omega_{ji} = \left(\Omega^\dagger\right)^*_{ij} \implies \Omega^\dagger_{ij} = \Omega^*_{ji} \tag{1.17}$$

Identity expansion (completeness relation)

$$\boldsymbol{I} = \sum_{i=1}^n |e_i\rangle\langle e_i| \tag{1.18}$$

Subspaces Consider a subset of an orthonormal basis:

$$\{|e_i\rangle\}, \quad i = 1, 2, \ldots, s < n \tag{1.19}$$

Then the smaller set of orthonormal vectors spans a subspace. We can associate the projection of any vector in the original space onto the subspace:

$$\boldsymbol{P}_s = \sum_{i=1}^s |e_i\rangle\langle e_i| \tag{1.20}$$

The projection operator is also Hermitian. Note also that higher powers of the projection operator are equivalent:

$$\boldsymbol{P}_s^2 = \sum_{i=1}^s\sum_{j=1}^s |e_i\rangle\langle e_i|e_j\rangle\langle e_j| = \sum_{i=1}^s\sum_{j=1}^s |e_i\rangle\delta_{ij}\langle e_j| = \boldsymbol{P}_s \tag{1.21}$$

Hermitian operators Consider a Hermitian operator Ω with eigenvectors $|\omega_i\rangle$ with eigenvalues ω_i with $i = 1, 2$. By definition of the eigenvalue equation:

$$\Omega|\omega_i\rangle = \omega_i|\omega_i\rangle \tag{1.22}$$

Suppose further that Ω is self-adjoint: $\Omega = \Omega^\dagger$. Then:

$$\langle \omega_2 | \Omega \omega_1 \rangle = \omega_1 \langle \omega_2 | \omega_1 \rangle \tag{1.23}$$

We can also use the adjoint to write:

$$\langle \omega_2 | \Omega \omega_1 \rangle = \langle \Omega^\dagger \omega_2 | \omega_1 \rangle = \langle \omega_1 | \Omega^\dagger \omega_2 \rangle^* = \omega_2^* \langle \omega_2 | \omega_1 \rangle \tag{1.24}$$

Combining:

$$(\omega_1 - \omega_2^*) \langle \omega_2 | \omega_1 \rangle = 0 \tag{1.25}$$

Observe that if we have different eigenvalues then the eigenvectors must be orthogonal. If we have degenerate eigenvalues, then the eigenvectors do not have to be orthogonal, and they may span some subspace of the Hilbert space.

Position and Momentum Operators in QM Consider the momentum operator:

$$\boldsymbol{P} | \Psi_p \rangle = p | \Psi_p \rangle \tag{1.26}$$

where $|\Psi_p\rangle$ is an eigenvector of $\boldsymbol{P}$ in the Hilbert space. Recall:

$$-i\hbar \frac{d}{dx} \Psi_p(x) = p \Psi_p(x) \tag{1.27}$$

which is a first order differential equation with solution:

$$\Psi_p(x) = N e^{ip \cdot x / \hbar} \tag{1.28}$$

But ordinary normalization gives:

$$\int_{-\infty}^{\infty} dx \, |\Psi_p(x)|^2 = |N|^2 \cdot \infty \tag{1.29}$$

Note that we can ensure ordinary normalization works by imposing boundaries (draw a big enough box). Consider the circular boundary condition:

$$\Psi_p(0) = \Psi_p(L) \tag{1.30}$$

Check Hermiticity:

$$\langle \Psi_2 | \boldsymbol{P} \Psi_1 \rangle = \int_0^L dx \Psi_2^* \left(-i\hbar \frac{d}{dx} \Psi_1 \right) \tag{1.31}$$

Integrating by parts,

$$\langle \Psi_2 | \boldsymbol{P} \Psi_1 \rangle = -i\hbar \Psi_2^* \Psi_1 |_0^L + \int_0^L dx \left(-i\hbar \frac{d}{dx} \Psi_2 \right)^* \Psi_1 = \int_0^L dx \left(-i\hbar \frac{d}{dx} \Psi_2 \right)^* \Psi_1 = \langle \boldsymbol{P} \Psi_2 | \Psi_1 \rangle \tag{1.32}$$

In terms of wavenumbers, we can write $p = \hbar k$ so that the momentum eigenvectors go as $e^{ik \cdot x}$. At the boundary, we require that the wavefunction be periodic, so$e^{ikL} = e^{ik \cdot 0} = 1 \implies k = \frac{2\pi n}{L}, n = 0, \pm 1, \ldots$. Normalizing, we have the eigenvectors:

$$\Psi_n(x) = \frac{1}{\sqrt{L}} e^{i(2\pi n / L)x} \tag{1.33}$$

Momentum eigenvectors with infinite boundary conditions

$$\Psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \tag{1.34}$$

Recall that from Fourier transforms,

$$\tilde{f}(k) = \int_{-\infty}^{\infty} dx \frac{1}{\sqrt{2\pi}} e^{-ikx} F(x) \iff F(x) = \int_{-\infty}^{\infty} dk \frac{1}{\sqrt{2\pi}} e^{ikx} \tilde{f}(k) \tag{1.35}$$

Substituting the first equation into the second,

$$F(x) = \int_{-\infty}^{\infty} dk \frac{1}{\sqrt{2\pi}} e^{ikx} \int_{-\infty}^{\infty} dy \frac{1}{\sqrt{2\pi}} e^{-iky} F(y) \tag{1.36}$$

Exchanging the order of integration and abandoning mathematical rigor,

$$F(x) = \int_{-\infty}^{\infty} dy \left[\int_{-\infty}^{\infty} dk \frac{1}{2\pi} e^{-ik(y-x)} \right] F(y) \tag{1.37}$$

Consider a function with finite support. To satisfy the identity, we consider that the expression in the square brackets is a distribution, specifically, the Dirac Delta distribution. In fact, it should be $\delta(y-x)$. The defining property is:

$$f(0) = \int_{-\infty}^{\infty} dx \delta(z) f(z) \tag{1.38}$$

Derivative of delta function Integrate by parts:

$$\int_{-\infty}^{\infty} dz \partial_z \delta(z) f(z) = -\frac{df}{dz}\bigg|_{z=0} \tag{1.39}$$

since the delta function vanishes everywhere except at a point of measure zero.

More delta identities

$$\int_{-\epsilon}^{\epsilon} dx \delta(x) = 1 \tag{1.40}$$

$$\delta(ax) = \frac{1}{|a|} \delta(x) \tag{1.41}$$

To prove delta identities $\delta_1 = \delta_2$, show that:

$$\int_{-\infty}^{\infty} f(x) \delta_1 dx = \int_{-\infty}^{\infty} f(x) \delta_2 dx \tag{1.42}$$

for all $f(x)$.

1.3 Friday 2 Oct 2015

1.3.1 More on the Dirac Delta

Recall

$$\delta(z) = \int_{-\infty}^{\infty} dk \frac{e^{ikz}}{2\pi} \tag{1.43}$$

$$f(0) = \int dz \delta(z) f(z) \tag{1.44}$$

Momentum space eigenstates Consider the inner product (verify the normalization)

$$\langle p|p'\rangle = \int dx \Psi^*_{p'}(x)\Psi_p(x) \tag{1.45}$$
$$= \frac{1}{2\pi\hbar}\int dx e^{i(p-p')x/\hbar} \tag{1.46}$$
$$= \delta(p-p') \tag{1.47}$$

Position operator eigenstates

$$X|y\rangle = y|y\rangle \tag{1.48}$$

so that the wavefunctions behave as:

$$X\Psi_y(x) = x\Psi_y(x) = y\Psi_y(x) \implies \Psi_y(x) = \delta(x-y) \tag{1.49}$$

because $\Psi_y(x)$ must vanish everywhere except where $x = y$ since x is a variable and y is a constant (eigenvalue of position of the wavefunction).

Checking orthogonalization:

$$\langle y'|y\rangle = \int dx \Psi^*_{y'}(x)\Psi_y(x) = \int dx \delta(x-y')\delta(x-y) = \delta(y-y') \tag{1.50}$$

Moving into position space

$$\langle x|\Psi\rangle = \int dy \delta(y-x)\Psi(y) = \Psi(x) \tag{1.51}$$

Completeness (infinite dimensional)

$$I = \int dp|p\rangle\langle p| = \int dx|x\rangle\langle x| \tag{1.52}$$

We verify that it is the identity by plugging it directly:

$$\langle x|I|y\rangle = \int dp\langle x|p\rangle\langle p|y\rangle \tag{1.53}$$
$$= \int \frac{dp}{2\pi\hbar} e^{ip(x-y)/\hbar} \tag{1.54}$$
$$= \delta(x-y) \tag{1.55}$$
$$= \langle x|y\rangle \tag{1.56}$$

Functions of Operators Consider a linear diagonalizable operator Ω. Then:

$$\Omega|\omega_i\rangle = \omega_i|\omega_i\rangle \tag{1.57}$$

so that any vector can be written as a linear combination:

$$|v\rangle = \sum_{i=1}^{n} v_i|\omega_i\rangle \tag{1.58}$$

then the function of an operator is written as:

$$f(\Omega)|v\rangle = \sum_{i=1}^{n} v_i f(\Omega)|\omega_i\rangle = \sum_{i=1}^{n} v_i f(\omega_i)|\omega_i\rangle \tag{1.59}$$

Power series expansion of operators Recall that:

$$f(z) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0) z^n}{n!} \tag{1.60}$$

hence

$$f(\Omega) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0) \Omega^n}{n!} \tag{1.61}$$

1.3.2 Review of Classical Mechanics

There are the two canonical variables x, p, a Hamiltonian, Hamilton's equations:

$$\dot{p} = -\frac{\partial H}{\partial x} \tag{1.62}$$

$$\dot{x} = \frac{\partial H}{\partial p} \tag{1.63}$$

For a particle $H = \frac{p^2}{2m} + V(x)$ which can be shown to reduce to the definition of momentum $\dot{x} = \frac{p}{m}$ and N2L, $\dot{p} = -\frac{\partial V}{\partial x}$ by plugging into Hamilton's equations.

1.3.3 Moving into Quantum Mechanics

Examine the matrix representation of each of the operators in an orthonormal basis (position basis in this example):

$$\langle x|X|x'\rangle = x\delta(x - x') = x'\delta(x - x') \tag{1.64}$$

$$\langle x|P|x'\rangle = -i\hbar \frac{d}{dx}\delta(x - x') = i\hbar \frac{d}{dx'}\delta(x - x') \tag{1.65}$$

The difficulty of directly replacing variables with operators In QM, operators need to be Hermitian. Hence if a variable was originally xp, we cannot immediately replace it with the operators XP because X and P do not commute and hence the adjoint of XP is $P^\dagger X^\dagger = PX \neq XP$. To fix this, we take a bit of both:

$$\Omega = \frac{1}{2}(XP + PX) \tag{1.66}$$

Measurement A measurement with Ω will yield an eigenvalue of Ω. The probability of obtaining the eigenvalue is given by:

$$P(\omega_i) = |\langle \omega_i|\Psi\rangle|^2 \tag{1.67}$$

The system then changes to the corresponding eigenvector measured.

Example Consider $|\Psi\rangle = \sum_i |\omega_i\rangle\langle\omega_i|\Psi\rangle$. Then the probability is:

$$P(\omega) \propto |\langle\omega|\Psi\rangle|^2 = \langle\Psi|\omega\rangle\langle\omega|\Psi\rangle = \langle\Psi|P_\omega|\Psi\rangle \tag{1.68}$$

where we recognize the projection operator onto the eigenspace corresponding to the eigenvalue ω. We verify that the probability actually corresponds to this by checking the normalization:

$$P(\omega_i) = \frac{|\langle\omega_i|\Psi\rangle|^2}{\sum_i |\langle\omega_i|\Psi\rangle|^2} = \frac{|\langle\omega_i|\Psi\rangle|^2}{\sum_i \langle\Psi|\omega_i\rangle\langle\omega_i|\Psi\rangle} = \frac{|\langle\omega_i|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle} = \frac{\langle\Psi|P_\omega|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{1.69}$$

and if we assume that the state is normalized, the denominator just sums to unity. After the measurement, we are in the state $P_\omega|\Psi\rangle$, the projection of the original state onto the subspace.

Moving into continuous operators Recall that the continuous eigenfunctions are delta-function normalizable:

$$\langle \omega' | \omega \rangle = \delta(\omega - \omega') \tag{1.70}$$

Then the probability formula becomes a probability density formula:

$$\rho(\omega) = \frac{|\langle \omega | \Psi \rangle|^2}{\langle \Psi | \Psi \rangle} \tag{1.71}$$

Integrate over all ω to show normalization:

$$\int d\omega \rho(\omega) = \int d\omega \frac{|\langle \omega | \Psi \rangle|^2}{\langle \Psi | \Psi \rangle} = \int d\omega \frac{\langle \Psi | \omega \rangle \langle \omega | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 1 \tag{1.72}$$

Time evolution :

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H |\Psi(t)\rangle \tag{1.73}$$

To convert this to a differential equation, take the inner product with $\langle x|$ so that we enter the position basis:

$$i\hbar \frac{d}{dt} \langle x | \Psi(t) \rangle = \langle x | H | \Psi(t) \rangle \tag{1.74}$$

Inserting a complete set of states of position eigenvectors,

$$i\hbar \frac{d}{dt} \langle x | \Psi(t) \rangle = \int dy \langle x | H | y \rangle \langle y | \Psi(t) \rangle = \int dy \langle x | H | y \rangle \Psi(y, t) \tag{1.75}$$

Hence we need the position representation of the Hamiltonian. Consider the potential part of the Hamiltonian first (since it is a composition of position operators):

$$\int dy \langle x | V(x) | y \rangle \Psi(y, t) = \int dy V(x) \langle x | y \rangle \Psi(y, t) = V(x) \Psi(x, t) \tag{1.76}$$

Where we can expand $V(X)$ in a power series and re-write each term in terms of eigenvalues to achieve the RHS.

Chapter 2

Week 2

2.1 Monday 5 Oct 2015

2.1.1 Dynamics: Time Evolution

Recall Schrodinger's Equation

$$H = \frac{P^2}{2m} + V(X) \tag{2.1}$$

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V(x)\Psi(x,t) \tag{2.2}$$

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle \tag{2.3}$$

Examining the kinetic energy term Consider the system in the position basis:

$$i\hbar\frac{d}{dt}\langle x|\Psi(t)\rangle = \langle x|H|\Psi(t)\rangle \tag{2.4}$$

$$= \int_{-\infty}^{\infty} dy\langle x|H|y\rangle\langle y|\Psi(t)\rangle \quad \text{inserting identity in position basis} \tag{2.5}$$

$$= \int_{-\infty}^{\infty} dy\langle x|H|y\rangle\Psi(y,t) \tag{2.6}$$

Note that the potential part fulfils:

$$\langle x|V|y\rangle = V(x)\delta(x-y) \tag{2.7}$$

The kinetic part is:

$$\begin{aligned}\langle x|\frac{P^2}{2m}|y\rangle &= \frac{1}{2m}\int dz\langle x|P|z\rangle\langle z|P|y\rangle \quad \text{inserting identity} \\ &= \frac{\hbar^2}{2m}\frac{d}{dx}\frac{d}{dy}\int dz\delta(x-z)\delta(y-z) \\ &= \frac{\hbar^2}{2m}\frac{d}{dx}\frac{d}{dy}\delta(x-y) \\ &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\delta(x-y)\end{aligned}$$

Solution of Schrodinger's Equation (Time Independent Hamiltonian)

$$i\hbar\frac{d}{dt}|\Psi\rangle = H|\Psi\rangle \iff |\Psi(t)\rangle = \exp\left(-\frac{iH(t-t_0)}{\hbar}\right)|\Psi(t_0)\rangle \tag{2.8}$$

Time Evolution Operator Define:

$$U(t, t_0) = \exp\left(-\frac{iH(t-t_0)}{\hbar}\right) \tag{2.9}$$

which is a unitary operator $U^\dagger U = UU^\dagger = I$. Unitary operators preserve inner products: $\langle \Psi_1 | \Psi_2 \rangle = \langle U\Psi_1 | U\Psi_2 \rangle$.

Measurement and Interpretation Consider a system in state $|\omega\rangle$ which is an eigenstate of operator Ω. Suppose we want to perform the operator measurement Λ. Then we need to decompose $|\omega\rangle$ into a linear superposition of eigenstates of Λ.

We can calculate the expectation value:

$$\begin{aligned}
\langle \Omega \rangle &= \sum_i \omega_i P(\omega_i) && (2.10)\\
&= \sum_i \omega_i |\langle \omega_i | \Psi \rangle\rangle|^2 && (2.11)\\
&= \sum_i \omega_i \langle \Psi | \omega_i \rangle \langle \omega_i | \Psi \rangle && (2.12)\\
&= \sum_i \langle \Psi | \Omega | \omega_i \rangle \langle \omega_i | \Psi \rangle && (2.13)\\
&= \langle \Psi | \Omega | \Psi \rangle && (2.14)
\end{aligned}$$

and the variance:

$$\begin{aligned}
\langle (\Delta\Omega)^2 \rangle &= \sum_i P(\omega_i)(\omega_i - \langle \Omega \rangle)^2 && (2.15)\\
&= \langle \Psi | (\Omega - \langle \Omega \rangle)^2 | \Psi \rangle && (2.16)
\end{aligned}$$

Compatible operators are ones that commute. They are simultaneously diagonalizable and the eigenvectors are mutually orthogonal.

$$\langle \omega_l, \lambda_m | \omega_i, \lambda_j \rangle = \delta_{li}\delta_{mj} \tag{2.17}$$

Consider a state $|\Psi\rangle = \alpha|\omega_3, \lambda_3\rangle + \beta|\omega_1, \lambda_2\rangle + \gamma|\omega_2, \lambda_2\rangle$. Assume that the coefficients are such that the state is normalized $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$. Suppose a measurement of Ω yields ω_3. Now we measure Λ. We know that we can only get λ_3. On the other hand, if we measured Λ and got λ_3, then we know we will get ω_3. Hence:

$$\begin{aligned}
P(\omega_3, \lambda_3) &= |\alpha|^2 && (2.18)\\
P(\lambda_3, \omega_3) &= |\alpha|^2 && (2.19)
\end{aligned}$$

However, if we obtain λ_2 first, then the state will be:

$$\mathbb{P}_{\lambda_2}|\Psi\rangle = \frac{\beta|\omega_1, \lambda_2\rangle + \gamma|\omega_2, \lambda_2\rangle}{\sqrt{|\beta|^2 + |\gamma|^2}} \tag{2.20}$$

hence

$$P(\lambda_1, \omega_1) = (|\beta|^2 + |\gamma|^2)\frac{|\beta|^2}{|\beta|^2 + |\gamma|^2} = |\beta|^2 = P(\omega_1, \lambda_2) \tag{2.21}$$

hence if the operators commute, the order of taking them does not matter.

Binary state system Consider a Hilbert space with two eigenstates: $|1\rangle, |2\rangle$. Then any state can be written as a two-dimensional vector:

$$|\Psi(t)\rangle = \Psi_1(t)|1\rangle + \Psi_2(t)|2\rangle \tag{2.22}$$

Let the Hamiltonian be time-independent and written as a linear combination of Pauli matrices (2x2 matrices which are Hermitian and unitary). 4 Pauli matrices (including the identity) span the space of Hermitian 2x2 matrices:

$$H = g_0 I + \vec{g} \cdot \vec{\sigma} \tag{2.23}$$

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2.24}$$

$$\sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{2.25}$$

$$\sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.26}$$

where we collect the coefficients of σ^i into a vector $\vec{g}$. For electron spin in a magnetic field,

$$\vec{g} \cdot \vec{\sigma} = -\frac{\mu}{2} \vec{B} \cdot \vec{\sigma} \tag{2.27}$$

Property of Pauli matrices:

$$[\sigma_i, \sigma_j] = \epsilon^{ijk} \sigma_k \tag{2.28}$$

so that:

$$H = \begin{pmatrix} g_0 + g_3 & g_1 - ig_2 \\ g_1 + ig_2 & g_0 - g_3 \end{pmatrix} \tag{2.29}$$

Note that we chose this combination because H has to be Hermitian (hence the complex numbers in σ^2). Note that we can throw out the identity part because all it does is shift the energy levels by a fixed amount. See this energy displacement by direct substitution into the Schrodinger equation. Then:

$$H = \begin{pmatrix} g_3 & g_1 - ig_2 \\ g_1 + ig_2 & -g_3 \end{pmatrix} \tag{2.30}$$

Define $\vec{g} = g\hat{g}$.

Hence the propagator is:

$$U = \exp\left(\frac{-iHt}{\hbar}\right) = \exp\left(\frac{-i(g\hat{g} \cdot \vec{\sigma})t}{\hbar}\right) \tag{2.31}$$

$$= \sum_{n=0}^{\infty} \left(\frac{-igt}{\hbar}\right)^n \frac{1}{n!} (\hat{g} \cdot \vec{\sigma})^n \tag{2.32}$$

For $n = 0, (\hat{g} \cdot \vec{\sigma})^0 = 1, n = 1, (\hat{g} \cdot \vec{\sigma})^1 = \hat{g} \cdot \vec{\sigma}$.

Observe that for $n = 2$,

$$(\hat{g}\cdot\vec{\sigma})^2 = \sum_i \sum_j \hat{g}_i \hat{g}_j \sigma^i \sigma^j \tag{2.33}$$

$$= \sum_{i,j} \hat{g}_i \hat{g}_j \left(\frac{\sigma^i \sigma^j + \sigma^j \sigma^i}{2} \right) \quad \text{symmetric about } i \leftrightarrow j \tag{2.34}$$

$$= \sum_{i,j} \hat{g}_i \hat{g}_j \delta_{ij} I \tag{2.35}$$

$$= \sum_i \hat{g}_i \hat{g}_i I \tag{2.36}$$

$$= (\hat{g}\cdot\hat{g}) I \tag{2.37}$$

$$= I \tag{2.38}$$

Hence for even n, $(\hat{g}\cdot\vec{\sigma})^n = I$ and for odd n, $(\hat{g}\cdot\vec{\sigma})^n = \hat{g}\cdot\vec{\sigma}$.

Note that we used this identity for Pauli matrices:

$$\sigma^i \sigma^j + \sigma^j \sigma^i = 2\delta_{ij} I \tag{2.39}$$

We hence write the Hamiltonian as the sum over even and odd parts:

$$U = \sum_{n=0}^{\infty} \left(-\frac{igt}{\hbar} \right)^{2n} \frac{1}{(2n)!} I + \sum_{n=0}^{\infty} \left(-\frac{igt}{\hbar} \right)^{2n+1} \frac{1}{(2n+1)!} (\hat{g}\cdot\vec{\sigma}) \tag{2.40}$$

$$= \cos\left(\frac{gt}{\hbar}\right) I - i \sin\left(\frac{gt}{\hbar}\right) (\hat{g}\cdot\vec{\sigma}) \tag{2.41}$$

Example calculation Consider the probability that the state will change from state 1 to 2 over time t:

$$P(1\to 2) = \left| \langle 2| \exp\left(-\frac{iHt}{\hbar}\right) |1\rangle \right|^2 \tag{2.42}$$

$$= \left| -i \sin\left(\frac{gt}{\hbar}\right) (0,1) \exp\left(-\frac{iHt}{\hbar}\right) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right|^2 \tag{2.43}$$

$$= \left| -i \sin\left(\frac{gt}{\hbar}\right) (0,1) \begin{pmatrix} g_3 & g_1 - ig_2 \\ g_1 + ig_2 & -g_3 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right|^2 \tag{2.44}$$

$$= \sin^2\left(\frac{gt}{\hbar}\right) \left| \frac{g_1 + ig_2}{g} \right|^2 \tag{2.45}$$

$$= \sin^2\left(\frac{\sqrt{g_1^2 + g_2^2 + g_3^3}\, t}{\hbar} \right) \left(\frac{g_1^2 + g_2^2}{g_1^2 + g_2^2 + g_3^2} \right) \tag{2.46}$$

2.2 Wednesday, 7 Oct 2015

2.2.1 Example: Neutrino Mixing

Mechanism of neutron decay Neutron goes in black box, out comes proton, electron and anti electron neutrino.

More decay schemes:

$$\pi^- \to \mu^- + \bar{\nu}_\mu \tag{2.47}$$

$$\pi^+ \to \bar{\mu} + \nu_\mu \tag{2.48}$$

The muon can then decay to form the muon neutrino/antineutrino. The anticipated ratio of muon neutrino to electron neutrino is 2. But the experimental ratio is significantly different:

2.2.2 More on Neutrino mixing

Pion decay chain

$$\pi^- \to \mu^- \bar{\nu}_\mu \to e^- \nu_\mu \bar{\nu}_e \bar{\nu}_\mu \tag{2.49}$$
$$\pi^+ \to \mu^+ \nu_\mu \to e^+ \bar{\nu}_\mu \nu_e \nu_\mu \tag{2.50}$$

Incident electron neutrinos interact with neutrons to form an electron and a proton. Similarly a muon neutrino can interact with a neutron to form a muon and a proton. The electron antineutrinos interact with a proton to form an antielectron and a neutron.

Approximation using two-state QM Consider the muon-tau neutrino mixing. Define the mass (Hamiltonian) eigenstates $|v_1\rangle, |v_2\rangle$. Write the weak force eigenstates $|\nu_\mu\rangle, |\nu_\tau\rangle$ as linear combinations of the mass eigenstates related with a unitary matrix $\boldsymbol{U}$:

$$\begin{pmatrix} |\nu_\mu\rangle \\ |\nu_\tau\rangle \end{pmatrix} = \boldsymbol{U} \begin{pmatrix} |v_1\rangle \\ |v_2\rangle \end{pmatrix} \tag{2.51}$$
$$\boldsymbol{U}^\dagger \boldsymbol{U} = 1 \tag{2.52}$$

We parametrize this matrix using angles:

$$\begin{pmatrix} |\nu_\mu\rangle \\ |\nu_\tau\rangle \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} |v_1\rangle \\ |v_2\rangle \end{pmatrix} \tag{2.53}$$

Consider the propagator in time:

$$e^{-iHt/\hbar}|\nu_\mu\rangle = \cos\theta e^{-iE_1 t/\hbar}|v_1\rangle + \sin\theta e^{-iE_2 t/\hbar}|v_2\rangle \tag{2.54}$$

We obtain the energy using the Einstein mass-momentum relation and expand it to first order:

$$E_= \sqrt{p^2c^2 + m_{v_1}^2 c^4} \approx pc + \frac{1}{2}\frac{m_{v_1}^2 c^4}{pc} + \dots \tag{2.55}$$

so that:

$$e^{-iHt/\hbar}|\nu_\mu\rangle = e^{-ipct/\hbar}\left[\cos\theta e^{-i(m_{v_1}^2 c^3 t/2p\hbar)}|v_1\rangle + \sin\theta e^{-i(m_{v_2}^2 c^3 t/2p\hbar)}|v_2\rangle\right] \tag{2.56}$$

Define the distance travelled in propagation $L = ct$ and let the momentum be $p \approx \frac{E}{c}$.

$$e^{-iHt/\hbar}|\nu_\mu\rangle = e^{-ipct/\hbar}\left[\cos\theta e^{-i(m_{v_1}^2 c^3 L/2E\hbar)}|v_1\rangle + \sin\theta e^{-i(m_{v_2}^2 c^3 L/2E\hbar)}|v_2\rangle\right] \tag{2.57}$$

To consider the probability that a purely muon neutrino state will become a tau neutrino state (i.e. the muon disappears) is given by the overlap:

$$\langle\nu_\tau|e^{-iHt/\hbar}|\nu_\mu\rangle = e^{ipct/\hbar}\left[-\sin\theta\cos\theta e^{-i(m_{v_1}^2 c^3 L/2E\hbar)} + \sin\theta\cos\theta e^{-i(m_{v_2}^2 c^3 L/2E\hbar)}\right] \tag{2.58}$$

Note that the probability (magnitude squared) depends on the difference in the square of the masses $\Delta m_\nu^2 = m_{v_2}^2 - m_{v_1}^2$. After some algebra, the probability of a muon neutrino turning into a tau neutrino is:

$$P_{\nu_\mu - \nu_\tau}(L) = 4\sin^2\theta\cos^2\theta\sin^2\left(\frac{\Delta m_\nu^2 c^3 L}{4E\hbar}\right) \tag{2.59}$$

2.2.3 Derivation of the Heisenburg uncertainty principle

Recall that:

$$\langle \Omega \rangle = \langle \psi | \Omega | \psi \rangle \tag{2.60}$$

$$\Delta\Omega = |\langle \psi | (\Omega - \langle \Omega \rangle)^2 | \psi \rangle|^{1/2} \tag{2.61}$$

Consider two non-commutating Hermitian observables:

$$[\Omega, \Lambda]^\dagger = (\Omega\Lambda - \Lambda\Omega)^\dagger = -[\Omega, \Lambda] \tag{2.62}$$

Observe that the commutator is anti-Hermitian. Note that we can turn any Hermitian operator into an anti-Hermitian operator by multiplying it by i. Hence we write the commutator as:

$$[\Omega, \Lambda] = i\Gamma \tag{2.63}$$

Define the fluctuation operators:

$$\hat{\Omega} = \Omega - \langle \Omega \rangle I \tag{2.64}$$

$$\hat{\Lambda} = \Lambda - \langle \Lambda \rangle I \tag{2.65}$$

Consider the product:

$$(\Delta\Omega)^2 (\Delta\Lambda)^2 = \langle \psi | \hat{\Omega}^2 | \psi \rangle \langle \psi | \hat{\Lambda}^2 | \psi \rangle \tag{2.66}$$

$$= \langle \hat{\Omega}\psi | \hat{\Omega}\psi \rangle \langle \hat{\Lambda}\psi | \hat{\Lambda}\psi \rangle \tag{2.67}$$

$$\geq |\langle \hat{\Omega}\psi | \hat{\Lambda}\psi \rangle|^2 \quad \text{Cauchy-Schwarz} \tag{2.68}$$

$$\geq |\langle \psi | \hat{\Omega}\hat{\Lambda} | \psi \rangle|^2 \tag{2.69}$$

Note that the expectation value of an anti-Hermitian operator is an imaginary number and that of a Hermitian operator is real. The commutator of two Hermitian operators is anti-Hermitian and the anti-commutator is Hermitian. We decompose the operator product into these two parts accordingly so that we can take the absolute value by taking the sum of the real part squared and the imaginary part squared:

$$|\langle \psi | \hat{\Omega}\hat{\Lambda} | \psi \rangle|^2 = |\langle \psi | \frac{\{\hat{\Omega}, \hat{\Lambda}\}}{2} + \frac{[\hat{\Omega}, \hat{\Lambda}]}{2} | \psi \rangle|^2 \tag{2.70}$$

$$= \frac{1}{4} |\langle \psi | \{\hat{\Omega}, \hat{\Lambda}\} | \psi \rangle|^2 + \frac{1}{4} |\langle \psi | [\hat{\Omega}, \hat{\Lambda}] | \psi \rangle|^2 \tag{2.71}$$

where $\{A, B\}$ is the anticommutator $AB + BA$. Combining this with the inequality earlier:

$$\Omega = x \tag{2.72}$$

$$\Lambda = p \tag{2.73}$$

$$[x, p] = i\hbar I \tag{2.74}$$

$$\Delta x \Delta p \geq \frac{\hbar}{2} \tag{2.75}$$

Chapter 3

Week 3

3.1 Monday, 12 Oct 2015

3.1.1 Uncertainty Principle and the Classical Limit

Gaussian wavefunction Define the state in the position representation:

$$\langle x|x_0, p_0, \Delta\rangle = \frac{1}{(\pi\Delta^2)^{1/4}} e^{ip_o x/\hbar} e^{-(x-x_0)^2/2\Delta^2} \tag{3.1}$$

$$\langle P\rangle = p_0 \tag{3.2}$$

$$\langle x\rangle = x_0 \tag{3.3}$$

$$\Delta x = \Delta \tag{3.4}$$

$$\Delta p = \frac{\hbar}{2\Delta} \tag{3.5}$$

Time variation of expectation value

$$\frac{d}{dt}\langle\Omega\rangle = -\frac{i}{\hbar}\langle\psi|[\Omega, H]|\psi\rangle \tag{3.6}$$

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle\psi|P|\psi\rangle \tag{3.7}$$

through using commutator identities to split the $\frac{p^2}{2m}$ in the Hamiltonian. For the momentum:

$$\frac{d}{dt}\langle p\rangle = -\frac{i}{\hbar}\langle[P, V]\rangle \tag{3.8}$$

$$= -\left\langle\frac{\partial V}{\partial X}\right\rangle \tag{3.9}$$

Note that this is not the same as a potential operator operating on an expectation value of x, which will be closest to the classical calculation which only uses a single coordinate value. Recall that we can write $X = \langle x\rangle I + \hat{x}$ in terms of the fluctuation operator. Perform an expansion about the expectation value:

$$V(X) = V(\langle x\rangle I + \hat{x}) = V(\langle x\rangle) + \hat{x}V'(\langle x\rangle) + \dots \tag{3.10}$$

$$\implies \frac{\partial V}{\partial X} = \frac{\partial V}{\partial \hat{x}} = V'(\langle x\rangle) + \hat{x}V''(\langle x\rangle) + \dots \tag{3.11}$$

Note that the first term $V'(\langle x\rangle)$ is the classical expression for the potential, the odd terms have zero expectation value (by definition of the fluctuation operator, which has mean zero), and only the even terms contribute to the correction to the classical approximation:

$$\frac{d}{dt}\langle p\rangle = -V'(\langle x\rangle) - \frac{1}{2}\langle\hat{x}^2\rangle V'''(\langle x\rangle) + \dots \tag{3.12}$$

Example: Number of spatial dimensions Recall the time evolution operator:

$$U(t,t_0) = e^{-iH(t-t_0)/\hbar} \tag{3.13}$$

$$|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle \tag{3.14}$$

$$\psi(x,t) = \langle x|\psi(t)\rangle = \int_{-\infty}^{\infty} dz \langle x|U(t,t_0)|z\rangle\langle z|\psi(t_0)\rangle = \int_{-\infty}^{\infty} dz \langle x|U(t,t_0)|z\rangle\psi(z,t_0) \tag{3.15}$$

Hence we want to calculate the matrix elements of the propagator. Consider a free particle. The state can be decomposed (in principle) into energy eigenstates:

$$|\psi(t_0)\rangle = \sum_n c_n(t_0)|E_n\rangle \tag{3.16}$$

$$\implies |\psi(t)\rangle = \sum_n c_n(t_0)e^{-iE_n(t-t_0)/\hbar}|E_n\rangle \tag{3.17}$$

the coefficients are:

$$c_n(t_0) = \langle E_n|\psi(t_0)\rangle \tag{3.18}$$

hence we can write:

$$|\psi(t)\rangle = \sum_n e^{-iE_n(t-t_0)/\hbar}|E_n\rangle\langle E_n\rangle|\psi(t_0)\rangle \tag{3.19}$$

hence the time evolution operator has formal expression:

$$U(t,t_0) = \sum_n e^{-iE_n(t-t_0)/\hbar}|E_n\rangle\langle E_n| \tag{3.20}$$

Doing this explicitly for the free particle, we have:

$$H = \frac{P^2}{2m} \tag{3.21}$$

$$U(t,0) = U(t) = \int_{-\infty}^{\infty} dp|p\rangle\langle p|e^{-ip^2t/2m\hbar} \tag{3.22}$$

substituting the eigenstates of the momentum operator:

$$U(t) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp e^{ip\cdot(x-x')}e^{-ip^2t/2m\hbar} \tag{3.23}$$

Completing the square in the exponent, we will get the components of the propagator. The complete expression will imply that $|\psi(x,t)|^2$ is a Gaussian with a width that increases in time almost linearly like $\Delta(t) \approx \frac{\hbar t}{m\Delta}$.

3.2 Wednesday 14 Oct 2015

Nature of space-time Consider an additional spatial dimension that is periodic like a circle. Let its momentum be quantized $p_4 = \frac{2\pi n\hbar}{L}$. The energy is now written in terms of the Einstein relation:

$$E^2 = c^2p^2 + c^2p_4^2 + m^2c^4 \tag{3.24}$$

The wavefunctions can then be written as:

$$\psi_{\vec{p},n}(\vec{x},x) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\vec{p}\cdot\vec{x}/\hbar} \frac{1}{\sqrt{L}} e^{i2\pi x/L} \tag{3.25}$$

Note that since the energy is quantized, if we do not have sufficient energy to excite the first excited state $n = 1$, then we won't be able to see the extra dimension (remain in $n = 0$). When excited, the particle will appear to have a larger mass corresponding to a non-zero value of p_4.

We can set a limit on L based on the energy range we have access to and noting that we have not observed such extra dimensions. The LHC has energy on order of $1000 m_p c^2$. We hence want:

$$\frac{2\pi\hbar c}{L} \geq 1000 m_p c^2 \tag{3.26}$$

$$\implies L \leq 10^{-16} cm \tag{3.27}$$

3.2.1 Path Integral Formulation

Review of Classical Physics Consider n particles in 3 dimensions. The classical path corresponds to the stationary action. Note that the extremum in action does not need to be a minimum. Consider the Harmonic oscillator example where the Lagrangian is:

$$L = \frac{1}{2}\dot{x}^2 - \frac{1}{2}x^2 \tag{3.28}$$

$$t_i = 0, \quad t_f = 2\pi \tag{3.29}$$

Note that the classical path correspond to the periodic motion $x(t) = x_0 \cos t$. We parametrize the neighbouring paths:

$$x(\alpha, t) = (1-\alpha)x_0 \cos t + \alpha x_0 \tag{3.30}$$

We may hence calculate the action for each of the parametrized paths:

$$S[\alpha] = -\pi\alpha^2 x_0^2 \tag{3.31}$$

which is maximized at $\alpha = 0$ for the classical path.

Feynman Path Integral Formulation Suppose we want to calculate:

$$\langle x_f | U(t_f, t_i) | x_i \rangle \tag{3.32}$$

This is the QM amplitude to go from $|x_i\rangle$ at t_i to $|x_f\rangle$ at t_f. The path integral formulation says that you can sum over all paths $x(t)$ where $x(t_i) = x_i$ and $x(t_f) = x_f$,

$$\langle x_f | U(t_f, t_i) | x_i \rangle = \sum_{x(t)} e^{iS[x(t)]/\hbar} \tag{3.33}$$

3.3 Friday 16 Oct 2015

3.3.1 More on the path integral formulation

What is a sum over paths Recall that an integral can be represented by a discrete sum with a finite measure:

$$\int dx f(x) = \sum_i \Delta f(x_i) \tag{3.34}$$

The sum over paths is usually dominated by the classical path, especially when the action is large compared to $\hbar$. We may hence approximate the sum over paths by the single term corresponding to the classical path:

$$\langle x_f|U(t_f,t_i)|x_i\rangle = e^{iS[x_{class}(t)]/\hbar} \tag{3.35}$$

This is called the **Method of stationary phase**. We perform a Taylor expansion of the exponent around the stationary point (noting that the first order term vanishes):

$$S(x) = S(x_0) + \frac{1}{2}S''(x_0)(x-x_0)^2 + \dots \tag{3.36}$$

Substituting this into the integral and changing variables $y = x - x_0$,

$$I = \exp\left(\frac{iS(x_0)}{\hbar}\right)\int_{a-x_0}^{b-x_0} dy \exp\left(\frac{iy^2S''(x_0)}{2\hbar} + \dots\right) \tag{3.37}$$

Define the new parameter $z = y\sqrt{\frac{S''(x_0)}{2\hbar}}$. This produces a Gaussian integral:

$$I = \exp\left(\frac{iS(x_0)}{\hbar}\right)\sqrt{\frac{2\hbar}{S''(x_0)}}\int_{\sqrt{\frac{S''(x_0)}{2\hbar}}(a-x_0)}^{\sqrt{\frac{S''(x_0)}{2\hbar}}(b-x_0)} dz e^{iz^2+\dots} \tag{3.38}$$

for small $\hbar$, we can extend the limits of integration to the whole z line:

$$I \approx \exp\left(\frac{iS(x_0)}{\hbar}\right)\sqrt{\frac{2\hbar}{S''(x_0)}}\int_{-\infty}^{\infty} dz e^{iz^2+\dots} \tag{3.39}$$

$$= \exp\left(\frac{iS(x_0)}{\hbar}\right)\sqrt{\frac{2\hbar}{S''(x_0)}}(1+i)\sqrt{\frac{\pi}{2}} \tag{3.40}$$

$$= \exp\left(\frac{iS(x_0)}{\hbar}\right)\sqrt{\frac{2\pi i\hbar}{S''(x_0)}} \tag{3.41}$$

Note that even though the $\hbar$ is in the numerator, it does not have a large effect because the exponential term increases even more rapidly.

Free particle wavefunction The Lagrangian is just $\frac{1}{2}mv^2$ so that the action along the classical path (constant velocity) is simply:

$$S[x_{cl}(t)] = \frac{1}{2}mv^2(t_f - t_i) = \frac{m}{2}\frac{(x_f-x_i)^2}{t_f-t_i} \tag{3.42}$$

so that we may approximate the path integral as:

$$\langle x_f|U(t_f,t_i)|x_i\rangle \approx e^{im(x_f-x_i)^2/2\hbar(t_f-t_i)} \tag{3.43}$$

1D Harmonic Oscillator Define the Hamiltonian:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \tag{3.44}$$

The expectation value of the Hamiltonian is:

$$\langle H\rangle = \frac{1}{2m}\langle P^2\rangle + \frac{m\omega^2}{2}\langle X^2\rangle = \frac{1}{2m}\langle P\psi|P\psi\rangle + \frac{m\omega^2}{2}\langle X\psi|X\psi\rangle \tag{3.45}$$

Clearly, the eigenvalues of the Hamiltonian have to be positive because the inner products are positive definite.

Harmonic Oscillator - Position space Write Schrodinger's equation:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right)\psi(x)=E\psi(x) \tag{3.46}$$

Non-dimensionalize the equations by the substitution:

$$x=\left(\frac{\hbar}{m\omega}\right)^{1/2}y \tag{3.47}$$

$$E=\hbar\omega\epsilon \tag{3.48}$$

so that the Schrodinger's equation is:

$$\frac{d^2\psi}{dx^2}+(2\epsilon-y^2)\psi=0 \tag{3.49}$$

Examine the asymptotic behavior. For large y, neglect ϵ, and hence we have the differential equation:

$$\frac{d^2\psi}{dx^2}-y^2\psi=0 \implies \psi\sim e^{-y^2/2} \tag{3.50}$$

where we throw the positive root away because it is non-physical. Hence we write the wavefunction as a product:

$$\psi(y)=u(y)e^{-y^2/2} \tag{3.51}$$

Chapter 4

Week 4

4.1 Monday, 19 Oct 2015

Midterm Measurement, Observables, Time evolution, Path Integral (Stationary phase, quantum amplitude)

4.1.1 More on the Harmonic Oscillator

Recall change of variables equation

$$\frac{d^2\psi}{dy^2} + (2\epsilon - y^2)\psi = 0 \tag{4.1}$$

For large y, the function went like $e^{-y^2/2}$. Writing the wavefunction in terms of this ansatz, $\psi(y) = u(y)e^{-y^2/2}$, there is a differential equation for the coefficient $u(y)$:

$$u''(y) - 2yu'(y) + (2\epsilon - 1)u(y) = 0 \tag{4.2}$$

Proceed by power series. Make the ansatz:

$$u(y) = \sum_{n=0}^{\infty} c_n y^n \tag{4.3}$$

to get the recursion relation:

$$c_n n(n-1)y^{n-2} - 2nc_n y^n + (2\epsilon - 1)c_n y^n = 0, \quad \forall n \tag{4.4}$$

$$\implies c_{n+2} = -\frac{2\epsilon - 1 - 2n}{(n+1)(n+2)}c_n \tag{4.5}$$

For a normalizable solution, the series cannot be infinite and must terminate. That is, $2\epsilon - 1 - 2n = 0$ for some n. This gives $\epsilon = n + \frac{1}{2}$. Then the energies are quantized:

$$E = \hbar\omega\left(n + \frac{1}{2}\right) \tag{4.6}$$

The solutions are Hermite polynomials. The recursion relation for these polynomials is:

$$H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1}(y) \tag{4.7}$$

$$H_n'(y) = 2nH_{n-1}(y) \tag{4.8}$$

Features of the Harmonic oscillator solution :

1. Energy eigenvalues are evenly spaced.
2. Ground state energy is nonzero: $E_0 = \frac{\hbar\omega}{2}$.
3. There are even and odd solutions.
4. Wavefunction extends past classical turning points.

Raising and Lowering Operators Consider the Hamiltonian operator again:

$$\left(\frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2\right)|E\rangle = E|E\rangle \tag{4.9}$$

$$[X, P] = i\hbar \tag{4.10}$$

Define the operators:

$$a = \sqrt{\frac{m\omega}{2\hbar}}X + i\sqrt{\frac{1}{2m\omega\hbar}}P \tag{4.11}$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}X - i\sqrt{\frac{1}{2m\omega\hbar}}P \tag{4.12}$$

The commutator of the two is:

$$[a, a^\dagger] = 1 \tag{4.13}$$

and the Hamiltonian can be written as:

$$H = \hbar\omega\left[a^\dagger a + \frac{1}{2}\right] \tag{4.14}$$

Define the number operator:

$$\hat{N} = a^\dagger a \tag{4.15}$$

so that we have the eigenvalue equation:

$$\hat{N}|n\rangle = n|n\rangle \tag{4.16}$$

with bound state normalization:

$$\langle n|n'\rangle = \delta_{nn'} \tag{4.17}$$

The commutator with a is:

$$[a, N] = a \tag{4.18}$$

$$[a^\dagger, N] = -a^\dagger \tag{4.19}$$

We examine the operation of N with the a operators:

$$Na^\dagger|n\rangle = (a^\dagger N - [a^\dagger, N])|n\rangle = (a^\dagger N + a^\dagger)|n\rangle = (n+1)a^\dagger|n\rangle \tag{4.20}$$

Observe that $a^\dagger|n\rangle$ is an eigenvector of N with eigenvalue $(n+1)$. Then $|n+1\rangle \propto a^\dagger|n\rangle$. Proceed similarly for $Na|n\rangle$. Define the constants of proportionality:

$$a^\dagger|n\rangle = d_{n+1}|n+1\rangle \tag{4.21}$$
$$a|n\rangle = c_n|n-1\rangle \tag{4.22}$$

Observe that there must be a lowest state because the energy was bounded. Define $c_0 = 0$ so that the eigenstate $|0\rangle$ satisfies:

$$a|0\rangle = \mathbf{0} \tag{4.23}$$

The inner product is:

$$\langle an|an\rangle = |c_n|^2 \tag{4.24}$$
$$\implies \langle n|a^\dagger a|n\rangle = \langle n|N|n\rangle = |c_n|^2 \tag{4.25}$$

Define the phase relation $c_n = \sqrt{n}$ without any additional imaginary phase. A similar calculation for $\langle a^\dagger n|a^\dagger n\rangle$ yields:

$$d_{n+1} = \sqrt{n+1} \tag{4.26}$$

Then the operation of the raising and lowering operators is as follows:

$$a|n\rangle = \sqrt{n}|n-1\rangle \tag{4.27}$$
$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \tag{4.28}$$

Observe that we may also write the position and momentum operators in terms of the raising and lowering operators:

$$X = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a) \tag{4.29}$$
$$P = i\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a) \tag{4.30}$$

This gives us the matrix elements of the operators:

$$\langle n'|X|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}\right) \tag{4.31}$$
$$\langle n'|P|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}\left(\sqrt{n}\delta_{n',n-1} - \sqrt{n+1}\delta_{n',n+1}\right) \tag{4.32}$$

Summary of Harmonic Oscillator

$$a = \sqrt{\frac{m\omega}{2\hbar}}X + i\sqrt{\frac{1}{2m\omega\hbar}}P \tag{4.33}$$
$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}X - i\sqrt{\frac{1}{2m\omega\hbar}}P \tag{4.34}$$
$$\hat{N} = a^\dagger a \tag{4.35}$$

4.2 Wednesday, 21 Oct 2015

Transition matrix elements Consider $\langle 3|x^3|2\rangle$. Note that we only need to consider operator terms with one more $a^\dagger$ than a since the eigenstates are orthogonal. Then:

$$\langle 3|x^3|2\rangle = \left(\frac{\hbar}{2m\omega}\right)^{3/2} \langle 3|a(a^\dagger)^2 + a^\dagger a a^\dagger + (a^\dagger)^2 a|2\rangle \tag{4.36}$$

Then use equations (4.28) and (4.27).

Degeneracy Let ψ_1 and ψ_2 satisfy the TISE and let them not be proportional to each other. Consider the difference between the ODEs:

$$\psi_2\psi_1'' - \psi_1\psi_2'' = 0 \tag{4.37}$$

But we can write this as:

$$\frac{d}{dx}\left(\psi_2\psi_1' - \psi_1\psi_2'\right) = 0 \tag{4.38}$$

which means that the term inside the brackets is some constant, which has to be zero considering boundary conditions at infinity (bound state). Then, rearranging,

$$\frac{d}{dx}\ln\psi_1 = \frac{d}{dx}\ln\psi_2 \implies \ln\psi_1 = \ln\psi_2 + C \implies \psi_1 \propto \psi_2 \tag{4.39}$$

Hence they are actually the same state! There are hence no degeneracies in the 1D bound state problem.

Eigenfunctions can be chosen to be real Observe that ψ, ψ^* both satisfy the TISE. But we know that they correspond to the same state. Hence we can always pick real ψ.

Multiple particles - Direct product Consider two vector spaces $\mathbb{V}^n, \mathbb{V}^m$ with dimensions n and m respectively. We construct the direct product $\mathbb{V}^n \otimes \mathbb{V}^m$, which has dimension $m \times n$. Observe that any element in the direct product space can be written in terms of the basis elements of each of the vector spaces:

$$|V\rangle \in \mathbb{V}^n \tag{4.40}$$

$$|W\rangle \in \mathbb{V}^m \tag{4.41}$$

$$|V\rangle \otimes |W\rangle = \left(\sum_i v_i|e_i\rangle\right) \otimes \left(\sum_i w_i|f_i\rangle\right) = \sum_{i,j} v_i w_j |e_i\rangle \otimes |f_j\rangle = \sum_{i,j} a_{ij}|e_i\rangle \otimes |f_j\rangle \tag{4.42}$$

Notation-wise:

$$|V\rangle \otimes |W\rangle \equiv |VW\rangle \equiv |V\rangle|W\rangle \tag{4.43}$$

Define the sum in the direct product space as:

$$\alpha|A\rangle + \beta|B\rangle = \sum_{i,j} \left(\alpha a_{ij} + \beta b_{ij}\right)|e_i\rangle \otimes |f_j\rangle \tag{4.44}$$

and the inner product inherited from the lower dimensional vector spaces:

$$\langle e_i f_j | e_k f_l\rangle = \langle e_i|e_k\rangle\langle f_j|f_l\rangle \tag{4.45}$$

Linear operators can also be used on the outer product space (another name for the direct product space):

$$\Omega|e_i\rangle|f_j\rangle = |\Omega e_i\rangle|f_j\rangle \tag{4.46}$$

so that if it is defined on one of the constituent product spaces, it acts as the identity for the other vectors.

Define the coordinate basis for the Hilbert space with N particles:

$$|x_1\rangle \cdots |x_N\rangle \tag{4.47}$$

such that the position operators for each of the particles satisfies:

$$X_i|x_1\rangle \cdots |x_N\rangle = x_i|x_1\rangle \cdots |x_N\rangle \tag{4.48}$$

and the inner product is delta-function normalized:

$$\langle x'_1, \ldots, x'_N|x_1, \ldots, x_N\rangle = \delta(x'_1 - x_1) \cdots \delta(x'_N - x_N) \tag{4.49}$$

Define the momentum operators with usual commutation relations:

$$[X_i, X_j] = 0 \tag{4.50}$$
$$[P_i, P_j] = 0 \tag{4.51}$$
$$[X_i, P_j] = i\hbar\delta_{ij} \tag{4.52}$$

with position basis representation:

$$\langle x_1, \ldots, x_N|P_j|\psi\rangle = -i\hbar\frac{\partial}{\partial x_j}\psi(x_1, \ldots, x_N) \tag{4.53}$$

Distinguishable particles - 3D harmonic oscillator Consider the Hamiltonian:

$$H = \frac{1}{2m}(P_1^2 + P_2^2 + P_3^2) + \frac{1}{2}m\omega^2(X_1^2 + X_2^2 + X_3^2) \tag{4.54}$$

Consider the separable ansatz:

$$\psi_E(x_1, x_2, x_3) = \psi_{E_1}(x_1)\psi_{E_2}(x_2)\psi_{E_3}(x_3) \tag{4.55}$$

and substitute into the ODE to get the energies:

$$E = \hbar\omega\left(n_1 + n_2 + n_3 + \frac{3}{2}\right) \tag{4.56}$$

Observe that we can write the Hamiltonian as the sum of commuting Hamiltonians:

$$H = H_1 + H_2 + H_3 \tag{4.57}$$

and it turns out that they form a complete set of commuting observables to uniquely defined each state in terms of n_1, n_2, n_3.

4.3 Friday 23 Oct 2015

3D Harmonic Oscillator Recall the 3D quantum harmonic oscillator Hamiltonian:

$$H = \frac{1}{2m}\left(P_x^2 + P_y^2 + P_z^2\right) + \frac{1}{2}m\omega^2(X^2 + Y^2 + Z^2) \tag{4.58}$$

The solutions are separable. The solutions are also invariant under rotations.

Important potentials :

- Harmonic oscillator $V(r) = \frac{1}{2}m\omega^2 r^2$
- Coulomb $V(r) = \frac{-e^2}{r}$
- Screened Coulomb $V(r) = \frac{-e^2}{r}e^{-r/\lambda}$

Converting to spherical coordinates Recall that positions can be parametrized by r, θ, ϕ in Cartesian coordinates by:

$$\vec{r} = (r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta) \tag{4.59}$$

Conservation laws Key equations: Continuity

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{J} = 0 \implies \frac{d}{dt}\int_V \rho(\vec{r},t)d^3x = -\oint_S \vec{J}\cdot d\vec{A} \tag{4.60}$$

Current density: $\vec{J} = \rho\vec{v}$.

Note that the probability density is conserved whenever the Hamiltonian is Hermitian. Hence the analogue to conservation of charge in QM is the conservation of probability. Consider the Schrodinger equation for the wavefunction and its complex conjugate

$$i\hbar\frac{d}{dt}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \tag{4.61}$$

$$-i\hbar\frac{d}{dt}\psi^* = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^* \tag{4.62}$$

where we note that V must be real to be Hermitian. We multiply the top equation by ψ^* and the bottom by ψ, then subtract them:

$$i\hbar\frac{d}{dt}(\psi^*\psi) = -\frac{\hbar^2}{2m}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*) \tag{4.63}$$

Note that the RHS can be combined:

$$\frac{d}{dt}(\psi^*\psi) = -\frac{\hbar}{2mi}\nabla\cdot(\psi^*\nabla\psi - \psi\nabla\psi^*) \tag{4.64}$$

Define the probability current:

$$\vec{J} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*) \tag{4.65}$$

so that we have the conservation law:

$$\frac{d}{dt}P = \frac{d}{dt}(\psi^*\psi) = -\nabla\cdot\vec{J} \tag{4.66}$$

Classical Electrodynamics Recall the Lorentz force law:

$$\vec{F} = q\left(\vec{E} + \frac{1}{c}\vec{v} \times \vec{B}\right) \tag{4.67}$$

We also introduce the scalar and vector potentials:

$$\vec{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t} \tag{4.68}$$

$$\vec{B} = \nabla \times \vec{A} \tag{4.69}$$

Relativistic Free Particle First consider the Lagrangian:

$$L = -mc^2\sqrt{1 - \frac{\dot{x}^2}{c^2}} \tag{4.70}$$

The action is given by:

$$S = \int dtL = -mc^2 \int dt\sqrt{1 - \frac{v^2}{c^2}} \tag{4.71}$$

We parametrize the path using the proper length, which is a Lorentz invariant:

$$d\tau^2 = c^2dt^2 - d\vec{x}^2 \implies d\tau = c\sqrt{1 - \frac{1}{c^2}\left(\frac{d\vec{x}}{dt}\right)^2}\,dt \tag{4.72}$$

So the action is given by:

$$S = -mc\int d\tau \tag{4.73}$$

and it is clearly Lorentz invariant.

Relativistic Hamiltonian We obtain the Hamiltonian from the Lagrangian:

$$H = \vec{p}\cdot\vec{v} - L \tag{4.74}$$

$$\vec{p} = \frac{\partial L}{\partial \dot{x}} = \frac{mc^2}{c^2}\frac{\vec{v}}{\sqrt{1 - v^2/c^2}} \tag{4.75}$$

and inverting,

$$\vec{v}/c = \frac{c\vec{p}}{\sqrt{m^2c^2 + p^2}} \tag{4.76}$$

which simplifies to the correct mass-energy relation:

$$H = \sqrt{m^2c^4 + p^2c^2} \tag{4.77}$$

Relativistic EM Lagrangian

$$L = -mc^2\sqrt{1-\frac{v^2}{c^2}} + \frac{q}{c}\vec{v}\cdot\vec{A} - q\phi \tag{4.78}$$

The canonical momentum is:

$$\vec{p} = \frac{m\vec{v}}{\sqrt{1-\frac{v^2}{c^2}}} + \frac{q\vec{A}}{c} \tag{4.79}$$

so the Hamiltonian is:

$$H = \vec{p}\cdot\vec{v} - L = \sqrt{m^2c^4 + \left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 c^2} + q\phi \tag{4.80}$$

The non-relativistic EM Lagrangian is:

$$L = \frac{1}{2}mv^2 - q\phi + \frac{q}{c}\vec{v}\cdot\vec{A} \tag{4.81}$$

and the canonical momentum is:

$$\vec{p} = m\dot{\vec{x}} + \frac{q}{c}\vec{A} \tag{4.82}$$

with Hamiltonian:

$$H = \frac{\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2}{2m} + q\phi \tag{4.83}$$

Moving into quantum mechanics, we promote the x and p into operators and symmetrize them

$$H = \frac{\vec{P}^2}{2m} - \frac{q}{2mc}\left(\vec{P}\cdot\vec{A} + \vec{A}\cdot\vec{P}\right) + \frac{q^2}{2mc^2}\vec{A}^2 + q\phi \tag{4.84}$$

Note that we can usually neglect the $\frac{q^2}{c^2}\vec{A}^2$ term because of the c^2 in the denominator.

Chapter 5

Week 5

5.1 Monday, 26 Oct 2015

Coulomb problem Just considering the proton as the source of the electric field in the hydrogen atom, we have the potential:

$$\phi(\vec{x}) = \frac{e}{|\vec{x}|} \tag{5.1}$$

Two body problem Consider the Lagrangian:

$$L = \frac{\vec{P}_1^2}{2m_1} + \frac{\vec{P}_2^2}{2m_2} - V(|\vec{x}_1 - \vec{x}_2|) \tag{5.2}$$

We move into the CM frame:

$$\vec{x}_{CM} = \frac{m_1\vec{x}_1 + m_2\vec{x}_2}{m_1 + m_2} \tag{5.3}$$
$$\vec{x} = \vec{x}_{rel} = \vec{x}_1 - \vec{x}_2 \tag{5.4}$$
$$m_+ = m_1 + m_2 \tag{5.5}$$
$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \tag{5.6}$$

so that the Lagrangian becomes:

$$L = \frac{1}{2}m_+\dot{\vec{x}}_{CM}^2 + \frac{1}{2}\mu\dot{\vec{x}}^2 - V(|\vec{x}|) \tag{5.7}$$

The canonical momenta are:

$$\vec{p}_{CM} = m_+\dot{\vec{x}}_{CM} \tag{5.8}$$
$$\vec{p} = \mu\dot{\vec{x}} \tag{5.9}$$

and the Hamiltonian is:

$$H = \frac{\vec{p}_{CM}^2}{2m_+} + \frac{\vec{p}^2}{2\mu} + V(|\vec{x}|) \tag{5.10}$$

and moving into QM, we use the commutation relations:

$$[P^i, X^j] = -i\hbar\delta^{ij} \tag{5.11}$$

$$[P^i_{CM}, X^j_{CM}] = -i\hbar\delta^{ij} \tag{5.12}$$

This gives a separable system. The CM coordinate behaves as a free particle:

$$\psi_E(\vec{x}_{CM}, \vec{x}) = \frac{e^{i\vec{p}_{CM}\cdot\vec{x}_{CM}/\hbar}}{\sqrt{2\pi\hbar}}\psi_{E_{rel}}(\vec{x}) \tag{5.13}$$

$$E = \frac{p^2_{CM}}{2m_+} + E_{rel} \tag{5.14}$$

and the relative part satisfies the TISE:

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2_{\vec{x}} + V\right)\psi_{E_{rel}}(\vec{x}) = E_{rel}\psi_{E_{rel}} \tag{5.15}$$

Identical particles First consider two particles. The Hilbert space of the two particle system is spanned by the position eigenstates:

$$\{|x_1, x_2\rangle\} \tag{5.16}$$

Note that for different (distinguishable) particles, the states $|a, b\rangle$ and $|b, a\rangle$ with $a \neq b$ are orthogonal. But for distinguishable particles, we require that the system remains in the same state (up to overall phase) when we exchange the particles. Hence when we write the state of a system, we have to take linear combinations of $|a, b\rangle$ and $|b, a\rangle$:

$$|\psi\rangle = \frac{\beta|a, b\rangle + \gamma|b, a\rangle}{\sqrt{\beta^2 + \gamma^2}} \tag{5.17}$$

Making the switch $a \leftrightarrow b$:

$$|\psi'\rangle = \frac{\beta|b, a\rangle + \gamma|a, b\rangle}{\sqrt{\beta^2 + \gamma^2}} \tag{5.18}$$

and we want the exchanged system to be equal to the original system up to some overall phase:

$$|\psi'\rangle = e^{i\alpha}|\psi\rangle \tag{5.19}$$

Hence upon comparison of the coefficients, we want:

$$\beta = e^{i\alpha}\gamma \tag{5.20}$$

$$\gamma = e^{i\alpha}\beta = e^{i\alpha}e^{i\alpha}\gamma \tag{5.21}$$

Observe that this can be satisfied if we pick $\alpha = 0, \pi$. Hence we have two possibilities:

$$|\psi_S\rangle = \frac{|a, b\rangle + |b, a\rangle}{\sqrt{2}} \tag{5.22}$$

$$|\psi_A\rangle = \frac{|a, b\rangle - |b, a\rangle}{\sqrt{2}} \tag{5.23}$$

Observe that if $a = b$, then the antisymmetric state does not exist.

The Hilbert space of two particles $\mathbb{V}_2 = \mathbb{V} \otimes \mathbb{V}$ can be decomposed into two subspaces corresponding to the symmetric and antisymmetric states. Write this symbolically as $\mathbb{V}_A \oplus \mathbb{V}_S = \mathbb{V}_2$.

Bosonic state Consider the probability that a bosonic system $|\psi_S\rangle$ has a particle in the state with eigenvalue ω_1 and another in the state with eigenvalue ω_2. This is written as:

$$P(\omega_1, \omega_2) = |\langle \omega_1, \omega_2, S|\psi_S\rangle|^2 \tag{5.24}$$

The normalization condition is:

$$1 = \langle \psi_S|\psi_S\rangle = \sum_{\text{distinct}} |\langle \omega_1, \omega_2, S|\psi_S\rangle|^2 \tag{5.25}$$

$$= \sum_{\omega_2=\omega_{min}}^{\omega_{max}} \sum_{\omega_1=\omega_{min}}^{\omega_2} |\langle \omega_1, \omega_2, S|\psi_S\rangle|^2 \tag{5.26}$$

Chapter 6

Week 6

6.1 Monday 2 Nov 2015

6.1.1 More on identical particles

Hilbert space Note that if two particles are distinct, the Hilbert space is just $\mathbb{V} \otimes \mathbb{V}$. But of the particles are identical, the Hilbert space is written as the direct sum of two vector spaces $\mathbb{V}_s \oplus \mathbb{V}_A$, the symmetric and antisymmetric spaces. Particles either belong to the symmetric or antisymmetric spaces alone.

Quantum entanglement Consider the Hermitian operator:

$$O = \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{6.1}$$

and define the up state to be $(1,0)^T$ and the down state to be $(0,1)^T$. Then we can specify the state of two particles in terms of a superposition of vectors in the Hilbert space:

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \left(|\vec{p}, \uparrow\rangle_1| - \vec{p}, \downarrow\rangle_2 + |\vec{p}, \downarrow\rangle_1| - \vec{p}, \uparrow\rangle_2 \right) \tag{6.2}$$

Hence if an observation is made on the spin and the first particle yields up, only the first term remains and we immediately know the spin of the second particle.

Two particles Consider two particles described by the eigenstates of a Hermitian operator Ω with eigenvalues ω_j. Then for bosons and fermion eigenstates respectively:

$$|\Psi_B\rangle = |\omega_1, \omega_2, S\rangle = \frac{1}{\sqrt{2}} \left[|\omega_1, \omega_2\rangle + |\omega_2, \omega_1\rangle \right] \tag{6.3}$$

$$|\Psi_F\rangle = |\omega_1, \omega_2, A\rangle = \frac{1}{\sqrt{2}} \left[|\omega_1, \omega_2\rangle - |\omega_2, \omega_1\rangle \right] \tag{6.4}$$

Now consider a general two particle state for a boson. It may be a superposition of eigenstates. Then the probability of obtaining one particle with ω_1 and another with ω_2 is the overlap probability:

$$P_S(\omega_1, \omega_2) = |\langle \omega_1, \omega_2, S | \Psi_{boson} \rangle|^2 \tag{6.5}$$

The normalization condition is the sum over all distinct states:

$$1 = \langle \Psi_{boson} | \Psi_{boson} \rangle = \sum_{\omega_2 = \omega_{min}}^{\omega_{max}} \sum_{\omega_2 = \omega_{min}}^{\omega_2} P_S(\omega_1, \omega_2) \tag{6.6}$$

In the continuous eigenvalue case:

$$1 = \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{x_2} dx_1 P_S(x_1, x_2) \tag{6.7}$$

We can extend the integration to over the whole plane but divide by two because the functions are symmetric about $x_1 \leftrightarrow x_2$:

$$1 = \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dx_1 \frac{P_S(x_1, x_2)}{2} \tag{6.8}$$

This motivates us to introduce the modified wavefunction:

$$\Psi_S(x_1, x_2) = \frac{1}{\sqrt{2}} \langle x_1, x_2, S | \Psi_S \rangle = \frac{1}{2} \left(\langle x_1, x_2 | \Psi_S \rangle + \langle x_2, x_1 | \Psi_S \rangle \right) \tag{6.9}$$

so that the integration is simple:

$$1 = \iint_{-\infty}^{\infty} |\Psi_S(x_1, x_2)|^2 \, dx_1 dx_2 \tag{6.10}$$

but this changes the calculation of individual probabilities:

$$P_S(x_1, x_2) = 2 \, |\Psi_S(x_1, x_2)|^2 \tag{6.11}$$

Example: Harmonic Oscillator Suppose we have a Harmonic oscillator with one particle in the state $n = 3$ and the other in the state $n = 4$. Then the modified wavefunction in the position basis is:

$$\begin{aligned}
\Psi_S(x_1, x_2) &= \frac{1}{\sqrt{2}} \left(\frac{\langle x_1, x_2| + \langle x_2, x_1|}{\sqrt{2}} \right) \left(\frac{|3, 4\rangle + |4, 3\rangle}{\sqrt{2}} \right) \\
&= \frac{1}{2\sqrt{2}} \left(\langle x_1, x_2 | 3, 4 \rangle + \langle x_2, x_1 | 3, 4 \rangle + \langle x_1, x_2 | 4, 3 \rangle + \langle x_2, x_1 | 4, 3 \rangle \right) \\
&= \frac{1}{2\sqrt{2}} \left(\psi_3(x_1)\psi_4(x_2) + \psi_3(x_2)\psi_4(x_1) + \psi_4(x_1)\psi_3(x_2) + \psi_4(x_2)\psi_3(x_1) \right) \\
&= \frac{1}{\sqrt{2}} \left(\psi_3(x_1)\psi_4(x_2) + \psi_3(x_2)\psi_4(x_1) \right)
\end{aligned}$$

Checking normalization:

$$\begin{aligned}
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\Psi_S(x_1, x_2)|^2 \, dx_1 dx_2 &= \frac{1}{2} \int |\psi_3(x_1)\psi_4(x_2) + \psi_3(x_2)\psi_4(x_1)|^2 \, dx_1 dx_2 \\
&= \frac{1}{2}(1 + 1) \\
&= 1
\end{aligned}$$

For the antisymmetric Fermionic case, we proceed similarly. Then the modified wavefunction is:

$$\Psi_A(x_1, x_2) = \frac{1}{\sqrt{2}} \langle x_1, x_2, A | \Psi_A \rangle = \frac{1}{2} \left(\langle x_1, x_2 | \Psi_A \rangle - \langle x_2, x_1 | \Psi_A \rangle \right) \tag{6.12}$$

for the previous example:

$$\Psi_A = \frac{1}{\sqrt{2}} \left(\psi_3(x_1)\psi_4(x_2) - \psi_3(x_2)\psi_4(x_1) \right) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_3(x_1) & \psi_4(x_1) \\ \psi_3(x_2) & \psi_4(x_2) \end{vmatrix} \tag{6.13}$$

and the matrix determinant on the RHS is called the Slater determinant.

Checking normalization for the Fermion wavefunction:

$$\begin{aligned}
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\Psi_S(x_1, x_2)|^2 \, dx_1 dx_2 &= \frac{1}{2} \int |\psi_3(x_1)\psi_4(x_2) - \psi_3(x_2)\psi_4(x_1)|^2 \, dx_1 dx_2 \\
&= \frac{1}{2}(1 + 1) \\
&= 1
\end{aligned}$$

Generalization to N particles First consider $N = 3$. Label the states by quantum numbers n_1, n_2, n_3. Then the state of the system as a whole is:

$$|n_1, n_2, n_3\rangle \tag{6.14}$$

where there are $3! = 6$ permutations. We know that for Bosons, the wavefunction has to be symmetric, and for Fermions, the wavefunction has to be antisymmetric. The bosonic state is easy:

$$|\Psi_S\rangle = |n_1, n_2, n_3, S\rangle = \frac{1}{\sqrt{3!}} \left(|n_1, n_2, n_3\rangle + \ldots\right) \tag{6.15}$$

The fermonic state has to change sign under exchange of any two particle states (for an odd number of permutations, minus sign. for a even number of permutations, plus sign):

$$|\Psi_A\rangle = |n_1, n_2, n_3, A\rangle = \frac{1}{\sqrt{3!}} \left(|n_1, n_2, n_3\rangle - |n_1, n_3, n_2\rangle + |n_3, n_1, n_2\rangle - |n_3, n_2, n_1\rangle + |n_2, n_3, n_1\rangle - |n_2, n_1, n_3\rangle\right) \tag{6.16}$$

which we can write succinctly as:

$$|\Psi_A\rangle = \frac{1}{\sqrt{3!}} \sum_{i \neq j \neq k} \epsilon_{ijk} |n_i, n_j, n_k\rangle \tag{6.17}$$

To compute normalization, we can integrate over all 3D space but need to include an additional factor in each wavefunction.

6.2 Wednesday 4 Nov 2015

Describing identical particle states It will suffice to know the number of particles in each quantum state to fully describe the system. Let the quantum numbers be indexed by $1, 2, \ldots$, and let the number of particles in each quantum number be n_i. The basis for the Hilbert space is just:

$$|n_1, \ldots, n_\infty\rangle \tag{6.18}$$

and normalization requires:

$$\langle n_1, \ldots, n_\infty | n_1', \ldots, n_\infty'\rangle = \delta_{n_1, n_1'} \cdots \delta_{n_\infty, n_\infty'} \tag{6.19}$$

Expanding the Hilbert space: Number operators for Bosons Consider the Hilbert space that does not have a fixed number of particles. Consider an operator on boson states that changes the number of particles in a state. Define the operator b_k with normalization:

$$b_k |n_1, \ldots, n_k, \ldots, n_\infty\rangle = \sqrt{n_k} |n_1, \ldots, n_k - 1, \ldots, n_\infty\rangle \tag{6.20}$$

and the adjoint adds to the state

$$b_k^\dagger |n_1, \ldots, n_k, \ldots, n_\infty\rangle = \sqrt{n_k + 1} |n_1, \ldots, n_k + 1, \ldots, n_\infty\rangle \tag{6.21}$$

Also note that there is a no-particle state $|0, \ldots, 0\rangle$. The commutator of the operator gives:

$$[b_{k'}, b_k] = [b_{k'}^\dagger, b_k] = [b_{k'}^\dagger, b_k^\dagger] = 0, \quad k \neq k' \tag{6.22}$$

$$[b_k, b_k^\dagger] = 1 \tag{6.23}$$

Define the number operator:

$$\hat{N}_k = b_k^\dagger b_k \tag{6.24}$$

which gives the number of particles in the kth quantum number.

Number operators for Fermions Note that the number of particles in each state cannot exceed 1 for Fermionic states. First consider the operator that decreases the number of particles:

$$c_k|n_k = 1\rangle = |n_k = 0\rangle \tag{6.25}$$
$$c_k|n_k = 0\rangle = 0 \tag{6.26}$$
$$c_k^\dagger|n_k = 0\rangle = |n_k = 1\rangle \tag{6.27}$$

But we want to restrict its operation on the filled state:

$$c_k^\dagger|n_k = 1\rangle = 0, \quad c_k^\dagger c_k^\dagger|n_k = 1\rangle = 0 \quad \text{etc.} \tag{6.28}$$

But this means that the anticommutator:

$$\{c_{k'}, c_k^\dagger\} = \delta_{k,k'} \tag{6.29}$$

and for $k \neq k'$,

$$\{c_{k'}, c_k\} = \{c_{k'}^\dagger, c_k^\dagger\} = 0 \tag{6.30}$$

Hence the Fermions obey similar commutation relations except that the anticommutator is used instead of the commutator.

Free Particle solution Consider the Hamiltonian for N particles:

$$H = \sum_{q=1}^{N} T(\vec{x}_q) \tag{6.31}$$

where each kinetic energy operator operates on a single particle:

$$T(\vec{x})\psi_k(\vec{x}) = E_k\psi_k(\vec{x}) \tag{6.32}$$

Note that the Hamiltonian can be written as the number operator and the energy of each quantum state:

$$H = \sum_k E_k N_k = \sum_k E_k b_k^\dagger b_k \tag{6.33}$$

Photon Hamiltonian

$$E_k = \hbar\omega_k \tag{6.34}$$
$$\implies H = \sum_{k,p} \hbar\omega_k b_{k,p}^\dagger b_{k,p} \tag{6.35}$$

Note that we have summed over the two possible polarizations p as well.

Quick derivation of statistical mechanics concepts Recall that the probability of being in a particular state is proportional to its weight:

$$P(n_1, \ldots, n_k, \ldots, n_\infty) \propto \exp\left(-\frac{E - \mu N}{kT}\right) \tag{6.36}$$

where the total energy and number is constrained:

$$E = \sum_l E_l n_l \tag{6.37}$$

$$N = \sum_l n_l \tag{6.38}$$

We can write the product as a sum:

$$P(n_1, \ldots, n_k, \ldots, n_\infty) \propto \prod_l \exp\left(-\frac{n_l(E_l - \mu)}{kT}\right) = \exp\left(\sum_l -\frac{n_l(E_l - \mu)}{kT}\right) \tag{6.39}$$

The average number of particles with a particular quantum number is:

$$\bar{n}_k = \frac{\sum_{n_1,\ldots,n_\infty} n_k P(n_1, \ldots, n_k, \ldots, n_\infty)}{\sum_{n_1,\ldots,n_\infty} P(n_1, \ldots, n_k, \ldots, n_\infty)} \tag{6.40}$$

and substituting the expression for the probability and cancelling common terms,

$$\bar{n}_k = \frac{\sum_{n_k} n_k \exp\left(-\frac{n_k(E_k-\mu)}{kT}\right)}{\sum_{n_k} \exp\left(-\frac{n_k(E_k-\mu)}{kT}\right)} \tag{6.41}$$

$$\implies \bar{n}_k = \frac{\sum_{n=0}^{\infty} n a^n}{\sum_{n=0}^{\infty} a^n}, \quad a \equiv \exp\left(-\frac{E_k - \mu}{kT}\right) \tag{6.42}$$

Summing the geometric series in the denominator:

$$\sum_{n=0}^{\infty} a^n = \frac{1}{1-a} \tag{6.43}$$

$$\sum_{n=0}^{\infty} n a^n = \frac{1}{(1-a)^2} \tag{6.44}$$

$$\implies \bar{n}_k = \frac{a}{1-a} = \frac{1}{\exp\left(\frac{E_k-\mu}{kT}\right) - 1} \tag{6.45}$$

For Fermions, we have the expression:

$$\bar{n}_k = \frac{1}{\exp\left(\frac{E_k-\mu}{kT}\right) + 1} \tag{6.46}$$

6.3 Friday 6 Nov 2015

6.3.1 Symmetries

Transition probability Recall that:

$$P(|\psi\rangle \to |\Psi_1\rangle) = |\langle\Psi_1|\psi\rangle|^2 \tag{6.47}$$

Unitary operators preserve the inner product and hence the probability. Symmetry transformations that are invertible and unitary form a group. We are interested in a group of transformations that are parametrized by a continuous parameter and can be made arbitrary close to the identity transformation. Let the infinitesimal transformation be represented by U_ϵ. We can perform a first order expansion:

$$U_\epsilon = 1 - i\epsilon T + O(\epsilon^2) \tag{6.48}$$

and in this case, T will be Hermitian. This can be shown:

$$U^\dagger U = (1 - \epsilon\epsilon T + O(\epsilon^2)^\dagger (1 - \epsilon\epsilon T + O(\epsilon^2) = (1 + \epsilon\epsilon T^\dagger + O(\epsilon^2)(1 - \epsilon\epsilon T + O(\epsilon^2) = 1 + i\epsilon(T^\dagger - T) + O(\epsilon^2) \tag{6.49}$$

Since we want U to be unitary, we require that $U^\dagger U = 1$, so $T^\dagger = T$ and hence T is Hermitian.

We write $\epsilon = \frac{\theta}{N}$, where $N \to \infty$. Then we can consider the application of the operator N times:

$$\lim_{N\to\infty} \left[1 - \frac{i\theta T}{N}\right]^N = e^{-i\theta T} = U(\theta) \tag{6.50}$$

which is a transformation of θ. T is called the generator of θ transformations.

Symmetry transformations and expectation values Consider an operator O:

$$\langle O \rangle = \langle \psi | O | \psi \rangle \tag{6.51}$$

We make a symmetry transformation U, and want to find the expectation value under this transformation:

$$\langle U\psi | O | U\psi \rangle = \langle \psi U^\dagger O U | \psi \rangle \tag{6.52}$$

Hence we can just take O and perform a similarity transformation on it. To see how this affects the operator, we examine the eigenvalue equation for O:

$$O|o\rangle = o|o\rangle$$

Examine:

$$U^{-1}OU(U^{-1}|o\rangle) = U^{-1}o|o\rangle = oU^{-1}|o\rangle$$

Clearly, $U^{-1}|o\rangle$ is an eigenvector of $U^{-1}OU$.

Now consider the infinitesimal transformation $U_\epsilon = 1 - i\epsilon T$. The associated similarity transformation is:

$$U_\epsilon^{-1} O U_\epsilon = (1 + i\epsilon T)O(1 - i\epsilon T) = O - i\epsilon[O, T] \tag{6.53}$$

where we neglect higher order terms. Hence if the generator T commutes with the operator O, then we have a symmetry of the system.

Spatial Translations The transformation is $\vec{x}_n \to \vec{x}_n + \vec{a}$. So we want the transformation operator to do:

$$U^{-1}(\vec{a})\vec{x}_n U(\vec{a}) = \vec{x}_n + \vec{a} \tag{6.54}$$

Consider an infinitesimal translation:

$$U(\vec{a}) = 1 - i\vec{a} \cdot \frac{\vec{P}}{\hbar} \tag{6.55}$$

so the generator is $\frac{\vec{P}}{\hbar}$. Substituting this into the operator equation, we will require

$$\frac{i}{\hbar}[\vec{a} \cdot \vec{P}, \vec{x}_n] = \vec{a} \tag{6.56}$$

In terms of the components:

$$\frac{i}{\hbar}\sum_{k=1}^{3} a_k[P_k, x_{n,j}] = a_j \tag{6.57}$$

$$\implies [P_k, x_{n,j}] = -i\hbar\delta_{kj} \tag{6.58}$$

but this means that P is the total momentum operator. Hence the generator of translations is:

$$\frac{\vec{P}}{\hbar} = \frac{1}{\hbar}\sum_n \vec{P}_n$$

The full transformation (large step) is given by:

$$U(\vec{a}) = e^{-i\vec{a}\cdot\vec{P}/\hbar} \tag{6.59}$$

The composition of two transformation is given by:

$$U(\vec{a})U(\vec{b}) = U(\vec{a}+\vec{b}) \tag{6.60}$$

6.3.2 Symmetries in Classical Physics

Recall that:

$$\frac{\partial H}{\partial q_i} = -\dot{p}_i \tag{6.61}$$

$$\frac{\partial H}{\partial p_i} = \dot{q}_i \tag{6.62}$$

$$\frac{dH}{dt} = -\frac{\partial L}{\partial t} \tag{6.63}$$

Poisson Bracket Define:

$$\{A, B\}_{PB} = \sum_i \left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}\right) \tag{6.64}$$

Note that:

$$\{B, A\}_{PB} = -\{A, B\}_{PB} \tag{6.65}$$

which has the parallel to the commutator.

Chapter 7

Week 7

7.1 Monday 9 Nov 2015

Poisson bracket with the Hamiltonian For time-independent $A(q_k, p_k)$,

$$\begin{aligned}\{A, H\}_{PB} &= \sum_i \left(\frac{\partial A}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial H}{\partial q_i} \right) \\ &= \sum_i \left(\frac{\partial A}{\partial q_i}\dot{q}_i - \frac{\partial A}{\partial p_i}(-\dot{p}_i) \right) \\ &= \frac{dA}{dt}\end{aligned}$$

Recall that in QM:

$$\langle \frac{-i}{\hbar}[A, H] \rangle = \frac{d}{dt}\langle A \rangle$$

Hence we expect that to transform from CM to QM, we make the replacements:

$$\{A, B\}_{PB} \to \frac{-i}{\hbar}[A, B]$$

Example Consider the Lagrangian:

$$\begin{aligned}L = T - V &= \left(\frac{1}{2}m\dot{x}^2 + k\dot{x}g(x) \right) - V \\ p = \frac{\partial L}{\partial \dot{x}} &= m\dot{x} + kg(x)\end{aligned}$$

The Hamiltonian is:

$$H = p\dot{x} - L = \frac{1}{2m}(p - kg(x))^2 + V$$

Symmetries in CM Consider the infinitesimal transformation:

$$\begin{aligned}q_i &\to q_i + \delta q_i(q, p) \\ p_i &\to p_i + \delta p_i(q, p)\end{aligned}$$

The generator of this transformation written as g, and satisfies the requirements that:

$$\delta q_i = \epsilon \frac{\partial g}{\partial p_i} \tag{7.1}$$

$$\delta p_i = -\epsilon \frac{\partial g}{\partial q_i} \tag{7.2}$$

Consider the first order derivative (which we want to vanish) of the Hamiltonian under the symmetry transformation:

$$0 = \delta H = \sum_i \left(\frac{\partial H}{\partial q_i} \delta q_i + \frac{\partial H}{\partial p_i} \delta p_i \right) \tag{7.3}$$

$$= \epsilon \sum_i \left(\frac{\partial H}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial g}{\partial q_i} \right) \tag{7.4}$$

$$= \epsilon \{H, g\}_{PB} \tag{7.5}$$

But this means that $\frac{dg}{dt} = 0$, so that the g corresponds to the conjugate momentum, which is conserved in time.

The QM analogue is the commutator with the Hamiltonian. An operator that commutes with the Hamiltonian has a basis of energy eigenstates. Hence if it is in one of the energy eigenstates, it will remain in that eigenstate for all time.

Example: Rotationally invariant Hamiltonian Consider:

$$H = \sum_{i=1}^{N} \frac{(\vec{p}_i)^2}{2m_i} + \sum_{i<j} V(|\vec{x}_i - \vec{x}_j|)$$

Consider a displacement of the system in the third axis: $\delta x_1 = \delta x_2 = 0, \delta x_3 = \epsilon$. The generator of this displacement is:

$$g = \epsilon \sum_{i=1}^{N} p_{i,3}$$

which is the sum of the third components of momenta for all the particle. This generator satisfies:

$$\frac{\partial g}{\partial \vec{x}_i} = 0, \quad i = 1, 2, \ldots, N$$
$$\frac{\partial g}{\partial p_{i,3}} = \epsilon, \quad i = 1, 2, \ldots, N$$

This gives:

$$\epsilon \{g, q\}_{PB} = -\delta q$$
$$\epsilon \{g, p\}_{PB} = -\delta p$$

and applying the recipe for introducing commutators

$$\epsilon \frac{i}{\hbar} [G, Q] = \delta Q$$
$$\epsilon \frac{i}{\hbar} [G, P] = \delta P$$

Now if we consider the first order QM unitary operator:

$$U = e^{-i\epsilon T} \approx 1 - i\epsilon T \tag{7.6}$$

and the operator defined by $O' = U^{-1} O U \approx (1 + i\epsilon T) O (1 - i\epsilon T) \approx O + i\epsilon [T, O], \delta O = i\epsilon [T, O]$. Comparing this expression to the CM result, we obtain that:

$$T = \frac{G}{\hbar}$$

Rotations Consider the rotation matrix:

$$\boldsymbol{R} = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}$$

We can compose rotations:

$$\boldsymbol{R}_1\boldsymbol{R}_2 = \boldsymbol{R}_3 \implies \alpha_1 + \alpha_2 = \alpha_3$$

We construct the unitary operator $U[R]$ that implements the rotation. This operator satisfies a similar composition relation:

$$U[R_1]U[R_2] = U[R_3]$$

Expectation Values under rotation Consider a rotation in 2D:

$$\langle\Psi_R|x_i|\Psi_R\rangle = \sum_{j=1}^{2} R_{ij}\langle\Psi|x_j|\Psi\rangle$$

Now consider the two-particle Hilbert space. It will suffice to identify how the unitary operator changes the basis states (assume 2D space):

$$|x_1, x_2\rangle_R = U[R]|x_1, x_2\rangle = |\sum_{j=1}^{2} R_{1j}x_j, \sum_{k=1}^{2} R_{2k}x_k\rangle \tag{7.7}$$

where the third equality corresponds to rotating each of the x terms. It can be shown that:

$$\begin{aligned}
U[R]^\dagger X_i U[R]|x_1, x_2\rangle &= U[R]^\dagger X_i|\sum_j R_{1j}x_j, \sum_k R_{2k}x_k\rangle \\
&= U[R]^\dagger \left(\sum_l R_{il}x_l\right)|\sum_j R_{1j}x_j, \sum_k R_{2k}x_k\rangle \\
&= \left(\sum_l R_{il}x_l\right) U[R]^\dagger|\sum_j R_{1j}x_j, \sum_k R_{2k}x_k\rangle \\
&= \left(\sum_l R_{il}x_l\right)|x_1, x_2\rangle \\
&= \sum_l R_{il}X_l|x_1, x_2\rangle, \quad \text{states are eigenstates of } X_l \\
\implies U[R]^\dagger X_i U[R] &= \sum_l R_{il}X_l
\end{aligned}$$

7.2 Wednesday, 11 Nov 2015

Wavefunction of rotated state Note that in the position basis:

$$\begin{aligned}
\Psi(x_1, x_2) &= \langle x_1, x_2|\Psi\rangle && (7.8)\\
\Psi_R(x_1, x_2) &= \langle x_1, x_2|\Psi_R\rangle && (7.9)\\
&= \langle x_1, x_2|U[R]\Psi\rangle && (7.10)\\
&= \langle U[R]^{-1}x_1, x_2|\Psi\rangle && (7.11)\\
&= \langle U[R^{-1}]x_1, x_2|\Psi\rangle && (7.12)\\
&= \Psi\left(\sum_k R_{1k}^{-1}x_k, \sum_k R_{2k}^{-1}x_k\right) && (7.13)\\
&= \Psi\left(R^{-1}\vec{x}\right) && (7.14)\\
\implies \Psi_R(R\vec{x}) &= \Psi(\vec{x}) && (7.15)
\end{aligned}$$

Infinitesimal rotations Recall that we can write the infinitesimal rotation to first order as:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\epsilon & -\sin\epsilon \\ \sin\epsilon & \cos\epsilon \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \tag{7.16}$$

$$\implies \begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 1 & -\epsilon \\ \epsilon & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \tag{7.17}$$

$$R_\epsilon \equiv \begin{pmatrix} 1 & -\epsilon \\ \epsilon & 1 \end{pmatrix} \tag{7.18}$$

Hence (using the inverse $R_\epsilon^{-1} = \begin{pmatrix} 1 & \epsilon \\ -\epsilon & 1 \end{pmatrix}$, determinant is unity to first order):

$$\Psi_R(x_1, x_2) = \Psi(x + \epsilon y, y - \epsilon x) \tag{7.19}$$

$$\approx \Psi(x,y) + \epsilon \left[y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y} \right] \Psi(x,y) \tag{7.20}$$

$$= \Psi(x,y) - \frac{i\epsilon}{\hbar} L_z \Psi(x,y) \tag{7.21}$$

Hence we have the first order operator:

$$U[R(\epsilon\hat{z})] = 1 - \frac{i\epsilon L_z}{\hbar} \tag{7.22}$$

where we indicate that the rotation was about the z axis. Hence the generator of rotations is L_z. The rotation for large angles is the exponential:

$$U[R(\theta\hat{z})] = \lim_{N\to\infty} \left(1 - \frac{i\theta}{N}\frac{L_z}{\hbar}\right)^N = e^{-i\theta L_z/\hbar} \tag{7.23}$$

We can write the angular momentum operator in polar coordinates:

$$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \sim -i\hbar\frac{\partial}{\partial\phi} \tag{7.24}$$

and hence the unitary rotation operator in polar coordinates is:

$$U[R(\theta\hat{z})] = e^{-\theta\frac{\partial}{\partial\phi}} \tag{7.25}$$

Its operation on a wavefunction in polar coordinates is given by:

$$U[R(\theta\hat{z})]\psi(\rho,\phi) = \sum_{n=0}^{\infty} \frac{(-\theta)^n}{n!}\frac{\partial^n}{\partial\phi^n}\psi(r,\phi) = \psi(r,\phi-\theta) \tag{7.26}$$

where the last equality holds by Taylor expansion in ϕ. Note that if the system has rotational invariance, then the rotation operator commutes with the Hamiltonian and hence we can simultaneously diagonalize both this rotation operator and the Hamiltonian.

Eigenstates of rotation operator Write the PDE:

$$L_z|l_z\rangle = l_z|l_z\rangle \tag{7.27}$$

$$\implies -i\hbar\frac{\partial}{\partial\phi}\Psi_{l_z}(\rho,\phi) = l_z\Psi_{l_z}(\rho,\phi) \tag{7.28}$$

$$\implies \Psi_{l_z}(\rho,\phi) = R(\rho)e^{il_z\phi/\hbar} \tag{7.29}$$

We demand that the system be single-valued in ϕ:

$$\Psi_{l_z}(\rho, 0) = \Psi_{l_z}(\rho, 2\pi) \tag{7.30}$$
$$\implies l_z = n\hbar, \quad n = 0, \pm 1, \pm 2, \ldots \tag{7.31}$$

We can verify Hermiticity: $\langle \Psi_1 | U \Psi_2 \rangle = \langle U \Psi_1 | \Psi_2 \rangle$.

We may define the normalized eigenstates:

$$\Phi_m(\phi) = \frac{e^{im\phi}}{\sqrt{2\pi}}, \quad m = 0, \pm 1, \pm 2, \ldots \tag{7.32}$$
$$\implies L_z \Phi_m(\phi) = m\hbar \Phi_m(\phi) \tag{7.33}$$
$$\int_0^{2\pi} d\phi \Phi_m^*(\phi) \Phi_n(\phi) = \delta_{nm} \tag{7.34}$$

3D rotations A general rotation in 3D can be written as rotations in each of the axes:

$$R = R(\alpha_1 \hat{x}) R(\alpha_2 \hat{y}) R(\alpha_3 \hat{z}) \tag{7.35}$$

and each of the matrices in 3D can be :

$$R(\alpha_1 \hat{x}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha_1 & -\sin\alpha_1 \\ 0 & \sin\alpha_1 & \cos\alpha_1 \end{pmatrix} \tag{7.36}$$
$$R(\alpha_2 \hat{y}) = \begin{pmatrix} \cos\alpha_2 & 0 & -\sin\alpha_2 \\ 0 & 1 & 0 \\ \sin\alpha_2 & 0 & \cos\alpha_2 \end{pmatrix} \tag{7.37}$$
$$R(\alpha_3 \hat{z}) = \begin{pmatrix} \cos\alpha_3 & -\sin\alpha_3 & 0 \\ \sin\alpha_3 & \cos\alpha_3 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{7.38}$$

Note that the angular momentum operators in each direction are:

$$L_x = YP_z - ZP_y \tag{7.39}$$
$$L_y = ZP_x - XP_z \tag{7.40}$$
$$L_z = XP_x - YP_x \tag{7.41}$$

The unitary operator for this 3D rotation is the product of 3 operators:

$$U[R_1 R_2 R_3] = U[R(\alpha_1 \hat{x})] U[R(\alpha_2 \hat{y})] U[R(\alpha_3 \hat{z})] \tag{7.42}$$

Note that we cannot write the unitary operator as a single exponential since the individual momentum operators do not commute with each other.

We can write the rotation through an angle α about the axis $\hat{n}$ as:

$$U[\alpha \hat{n}] = e^{-i\alpha \hat{n} \cdot \vec{L}/\hbar} \tag{7.43}$$

Commutation relations between angular momentum operators

$$[L_x, L_y] = [YP_z - ZP_y, ZP_x - XP_z] \tag{7.44}$$
$$= [YP_z, ZP_x] + [ZP_y, XP_z] \tag{7.45}$$
$$= Y[P_z, Z]P_x + X[Z, P_z]P_y \tag{7.46}$$
$$= i\hbar L_z \tag{7.47}$$

We can write all the commutation relations in the compact form:

$$[L_i, L_j] = i\hbar \sum_k \epsilon_{ijk} L_k \tag{7.48}$$

7.3 Friday, 13 Nov 2015

Total angular momentum Define $L^2 = L_x^2 + L_y^2 + L_z^2$. The commutation relations are:

$$[L^2, L_i] = 0, \quad i = 1, 2, 3 \tag{7.49}$$

Hence for a rotationally invariant system, the complete set of commuting operators are H, L^2, L_j, where $j = 1, 2$ or 3. Index the eigenvalues by n, l, m respectively.

Consider the action of the angular momentum operators:

$$L^2|\alpha, \beta\rangle = \alpha|\alpha, \beta\rangle \tag{7.50}$$
$$L_z|\alpha, \beta\rangle = \beta|\alpha, \beta\rangle \tag{7.51}$$

We want to construct raising and lowering operators for each of these operators:

$$L_\pm = L_x \pm iL_y \tag{7.52}$$
$$L_+^\dagger = L_- \tag{7.53}$$
$$[L_z, L_\pm] = \pm\hbar L_\pm \tag{7.54}$$

Hence:

$$L_z L_+|\alpha, \beta\rangle = (L_+ L_z + [L_z, L_+])|\alpha, \beta\rangle = (\beta + \hbar)L_+|\alpha, \beta\rangle \tag{7.55}$$

Hence $L_+|\alpha, \beta\rangle$ is an eigenstate of L_z with eigenvalue $\beta + \hbar$. Note further that:

$$L^2 L_+|\alpha, \beta\rangle = L_+ L^2|\alpha, \beta\rangle \tag{7.56}$$

because L^2 commutes with each of the L_x and L_y components of L_+. Hence we write the action of $L_\pm$ as:

$$L_\pm = C_\pm(\alpha, \beta)|\alpha, \beta \pm \hbar\rangle \tag{7.57}$$

Limits on m and l Consider:

$$\langle\alpha, \beta|L_x^2 + L_y^2|\alpha, \beta\rangle \tag{7.58}$$

is positive because we can write this as:

$$\langle L_x(\alpha, \beta)|L_x(\alpha, \beta)\rangle + \langle L_y(\alpha, \beta)|L_y(\alpha, \beta)\rangle \tag{7.59}$$

Hence,

$$\langle\alpha, \beta|L^2 - L_z^2|\alpha, \beta\rangle = \alpha - \beta^2 > 0 \tag{7.60}$$

We also know that $\alpha > 0$, hence it provides a bound for β^2. Hence there exists some β_{max} and β_{min} such that:

$$L_+|\alpha, \beta_{max}\rangle = 0 \tag{7.61}$$
$$L_-|\alpha, \beta_{min}\rangle = 0 \tag{7.62}$$

Note that:

$$L_- L_+ = L^2 - L_z^2 - \hbar L_z \tag{7.63}$$

so that when operating on the limiting eigenstates:

$$L_- L_+ |\alpha, \beta_{max}\rangle = (\alpha - \beta_{max}^2 - \hbar\beta_{max}|\alpha, \beta_{\max}\rangle = 0 \tag{7.64}$$

$$\implies \alpha = \beta_{max}(\beta_{max} + \hbar) \tag{7.65}$$

Similarly, for β_{min}:

$$\alpha = \beta_{min}(\beta_{min} - \hbar) \tag{7.66}$$

Comparing these two expressions for α, we hence obtain that:

$$\beta_{min} = -\beta_{max} \tag{7.67}$$

$$\beta_{max} - \beta_{min} = 2\beta_{max} = \hbar k \tag{7.68}$$

where we define k accordingly. We also let $\beta = \hbar m$, so that m is dimensionless.

If we write $\alpha = \hbar^2 j(j+1)$, then we can write:

$$\hbar^2 j(j+1) = \hbar^2 m_{max}(m_{max}+1) \implies j = m_{max} \tag{7.69}$$

Hence the allowed values of m are $-j, -j+1, \ldots, j$.

Note that if k is even, then m is integer-valued. If k is odd, then m is half-integer valued.

7.3.1 Spin

The total angular momentum has two components:

$$\vec{J} = \vec{L} + \vec{S} \tag{7.70}$$

and the spin operators commute with the other angular momentum operators:

$$[S_i, L_j] = 0 \tag{7.71}$$

and satisfy similar commutation relations:

$$[S_i, S_j] = i\hbar \sum_k \epsilon_{ijk} S_k \tag{7.72}$$

Hence the total angular momentum also satisfies the commutation relations:

$$[J_i, J_j] = i\hbar \sum_k \epsilon_{ijk} J_k \tag{7.73}$$

A rotation in the system rotates the total angular momentum:

$$U[R(\vec{n})] = e^{-i\vec{n}\cdot\vec{J}/\hbar} \tag{7.74}$$

The eigenvalues of the total spin S^2 can be indexed by $\hbar^2 s(s+1)$ so that $S^2|s, m_s\rangle = \hbar^2 s(s+1)|s, m_s\rangle$. The total spin is not changed by experiments. We can, however, change the component of the spin along a particular direction m_s. Note that a general vector in the Hilbert space can be written as a tensor product $|x, y, z\rangle|s, m_s\rangle$. The dimensionality of $|s, m_s\rangle$ for a fixed s is $2s+1$ since there are $2s+1$ possible values for m_s.

The operation of the total angular momentum is:

$$J_z|x,y,z\rangle|s,m_s\rangle = (L_z|x,y,z\rangle|s,m_s\rangle) + \hbar m_s|x,y,z\rangle|s,m_s\rangle \tag{7.75}$$

Spin Half particles There are two eigenstates of the spin component $|s,m_s\rangle = |1/2,\pm 1/2\rangle$. Hence we may write each of these states as a vector:

$$|1/2,1/2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{7.76}$$

$$|1/2,-1/2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{7.77}$$

Hence the matrix form of the operators in this basis is:

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}S_3 \tag{7.78}$$

Similarly, we can show that $S_x = \frac{\hbar}{2}\sigma_1, S_y = \frac{\hbar}{2}\sigma_2$. We may hence write the total spin as:

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma} \tag{7.79}$$

We may also write the wavefunction of the state as a vector:

$$\Psi_{1/2}(x,y,z) = \begin{pmatrix} \psi_+(x,y,z) \\ \psi_-(x,y,z) \end{pmatrix} \tag{7.80}$$

The momentum of this state is:

$$P\Psi_{1/2}(x,y,z) = -i\hbar\nabla\Psi(x,y,z) = \begin{pmatrix} -i\hbar\nabla\psi_+(x,y,z) \\ -i\hbar\nabla\psi_-(x,y,z) \end{pmatrix} \tag{7.81}$$

because the momentum commutes with the spin operators.

Chapter 8

Week 8

8.1 Monday 16 Nov 2015

Matrix representation of rotations Define the $2j+1 \times 2j+1$ matrix:

$$D^{(j)}_{m'm}(R) = \langle j, m'|U[R]|j, m\rangle$$

Polar coordinate representation of Angular Momentum Eigenstates Recall the coordinate transform:

$$\begin{aligned} x &= R\sin\theta\cos\phi \\ y &= R\sin\theta\sin\phi \\ z &= R\cos\theta \end{aligned}$$

Then the z-component of the angular momentum is:

$$L_z = -i\hbar\frac{\partial}{\partial\phi}$$

The eigenfunctions are the spherical harmonics:

$$\begin{aligned} L^2 Y^m_l(\theta,\phi) &= \hbar^2 l(l+1)Y^m_l(\theta,\phi) \\ L_z Y^m_l(\theta,\phi) &= \hbar m Y^m_l(\theta,\phi) \end{aligned}$$

We can solve for the spherical harmonics by noting that the ϕ dependence must be contained in the term $e^{im\phi}$. Hence we write:

$$Y^m_l(\theta,\phi) = e^{im\phi} f_{l,m}(\theta)$$

and substituting into the polar coordinate representation of the L^2 operator, we have a differential equation for $f_{l,m}(\theta)$:

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} - \frac{m^2}{\sin^2\theta}\right) f_{l,m}(\theta) = -l(l+1)f_{l,m}(\theta)$$

The normalization condition for the spherical harmonics is:

$$\int d\Omega Y^{m'}_{l'}(\theta,\phi)Y^l_m(\theta,\phi) = \delta_{l'l}\delta^{m'm}$$

The subscript/superscript in the Kronecker deltas are just by convention. An additional identity is:

$$Y^{-m}_l = (-1)^m (Y^m_l)^*$$

where the $*$ represents complex conjugation.

Spin-half particles Consider the column vector representation:

$$\Psi = \begin{pmatrix} f_+(r)Y_l^m(\theta,\phi) \\ f_-(r)Y_l^m(\theta,\phi) \end{pmatrix}$$
$$L^2\Psi = \hbar^2 l(l+1)\Psi$$
$$S_z\Psi = \frac{\hbar}{2}\sigma_3 = \hbar \begin{pmatrix} \frac{1}{2}f_+(r)Y_l^m(\theta,\phi) \\ -\frac{1}{2}f_-(r)Y_l^m(\theta,\phi) \end{pmatrix}$$

Note that the operation of S_z on Ψ does not result in a vector that is proportional to Ψ, since Ψ is usually not an eigenstate of S_z.

Total angular momentum Recall:

$$J^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle$$
$$J_z|j,m\rangle = \hbar m|j,m\rangle$$

and the raising and lowering operators were:

$$J_-|j,m\rangle = c_-(j,m)|j,m-1\rangle$$
$$J_+|j,m\rangle = c_+(j,m)|j,m+1\rangle$$

We can calculate the coefficients by implementing the normalization condition:

$$\langle j,m|J_-J_+|j,m\rangle = \langle J_+j,m|J_+j,m\rangle = |c_+(j,m)|^2$$

But we also knew that $J_-J_+ = J^2 - J_z^2 - \hbar J_z$. But $|j,m\rangle$ is an eigenstate of J^2 and J_z, so it is also an eigenstate of J_-J_+. We may hence write:

$$J_-J_+|j,m\rangle = \hbar^2[j(j+1) - m^2 - m]|j,m\rangle$$

But this means that:

$$|c_+(j,m)|^2 = \hbar^2[j(j+1) - m^2 - m]$$

The convention for the sign is:

$$c_+(j,m) = \hbar\sqrt{(j-m)(j+m+1)}$$

Similar calculations yield:

$$c_-(j,m) = \hbar\sqrt{(j+m)(j-m+1)}$$

We may hence write the combined expression:

$$J_\pm|j,m\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}|j,m\pm 1\rangle$$

Other directions to measure angular momentum

$$J_x = \frac{J_+ + J_-}{2}$$
$$J_y = \frac{J_+ - J_-}{2i}$$

Rotation operator matrix representation Recall that:

$$U[R] = \exp\left(-\frac{i\vec{n}\cdot\vec{S}}{\hbar}\right)$$

Consider the spin-half case. Then the rotation operator is:

$$D^{(1/2)}(\vec{n}) = \exp\left(-\frac{i\vec{n}\cdot\vec{\sigma}}{2}\right)$$

But we knew how to exponentiate the Pauli matrix vector:

$$\begin{aligned} D^{(1/2)}(\vec{n}) &= \cos\frac{n}{2} - i\hat{n}\cdot\vec{\sigma}\sin\frac{n}{2}, \quad n = |\vec{n}| \\ &= \cos\frac{n}{2}\boldsymbol{I} - i\sin\frac{n}{2}\frac{(n_x\boldsymbol{\sigma}_1 + n_y\boldsymbol{\sigma}_2 + n_z\boldsymbol{\sigma}_3)}{\sqrt{n_x^2+n_y^2+n_z^2}} \end{aligned}$$

Spin along another axis (not z)
Define the eigenstates for the angular momentum along an arbitrary direction:

$$(\hat{n}\cdot\vec{J})|\hat{n},\pm\rangle = \pm\frac{\hbar}{2}|\hat{n},\pm\rangle$$

where the $\hat{n}$ vector is defined by:

$$\begin{aligned} \hat{n}_x &= \sin\theta\cos\phi \\ \hat{n}_y &= \sin\theta\sin\phi \\ \hat{n}_z &= \cos\theta \end{aligned}$$

Then for the spin-half particle:

$$\hat{n}\cdot\vec{J}^{(1/2)} = \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}$$

8.2 Wednesday 18 Nov 2015

Spherically symmetric systems Consider the Schrodinger equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(|\vec{x}|)\right]\psi_E(\vec{x}) = E\psi_E(\vec{x}) \tag{8.1}$$

In spherical coordinates,

$$\left[-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{\vec{L}^2}{\hbar^2 r^2}\right) + V(r)\right]\psi_E(r,\theta,\phi) = E\psi_E(r,\theta,\phi) \tag{8.2}$$

Writing the solution in separable form:

$$\psi_E(r,\theta,\phi) = R_{E,l}(r)Y_l^m(\theta,\phi) \tag{8.3}$$

The radial differential equation is:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right) + V(r)\right]R_{E,l}(r) = ER_{E,l}(r) \tag{8.4}$$

Note that m does not feature in the differential equation. Make the substitution:

$$R_{E,l}(r) = \frac{U_{E,l}(r)}{r} \tag{8.5}$$

Hence the differential equation for U is:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right) + V(r)\right] U_{E,l}(r) = E U_{E,l}(r) \tag{8.6}$$

First examine the behavior for $r \to 0$. We ignore the potential since the $\frac{1}{r^2}$ will dominate any $V(r)$ we will use. We also take the RHS to be zero:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right)\right] U_{E,l}(r) = 0 \tag{8.7}$$

We make the ansatz: $U_{E,l}(r) = r^p$. Then the characteristic equation is:

$$p(p-1) - l(l+1) = 0 \implies p = l+1, p = -l \tag{8.8}$$

Note that if $p = -l$, then the wavefunction goes as $|\psi(r)|^2 = \frac{1}{r^{2l+2}}$. For $l = 0$, the wavefunction is normalizable. For $l > 0$, the wavefunction is not normalizable. $l = 0$ corresponds to the s wave. Consider for $l = 0$. Then:

$$R_{E,0}(r) \sim \frac{a}{r} + b \tag{8.9}$$

Note that we cannot allow the $\frac{1}{r}$ term because the Laplacian will give a delta function.

$$\nabla^2\left(\frac{1}{r}\right) = 4\pi\delta(\vec{r}) \tag{8.10}$$

Probability current and flux Consider the probability current dotted into the radial direction. This will give us the probability "flowing out" of the origin.

$$\hat{r}\cdot\vec{j} = \frac{\hbar}{2mi}\left(\psi^*\frac{\partial}{\partial r}\psi - \psi\frac{\partial}{\partial r}\psi^*\right) \tag{8.11}$$

$$= \frac{\hbar}{2mi}\left(\left(\frac{a^*}{r} + b^*\right)\left(-\frac{a}{r^2}\right) - \left(\frac{a}{r} + b\right)\left(-\frac{a^*}{r^2}\right)\right) \tag{8.12}$$

$$= -\frac{\hbar}{2mi}\frac{b^*a - a^*b}{r^2} \tag{8.13}$$

$$= \frac{\Im(ab^*)\hbar}{mr^2} \tag{8.14}$$

The integral over the ball centered at the origin is:

$$\int_{S_{B(0)}} \vec{j}\cdot d\vec{a} = \frac{4\pi\Im(ab^*)\hbar}{m} \tag{8.15}$$

which holds for all positive ball radii. This means that for an arbitrarily small ball centered at the radius, there is a finite probability flux through that ball. This is not physical. We hence cannot admit $\frac{a}{r}$ as part of the radial solution.

Note further that $\frac{a}{r}$ cannot solve the Schrodinger equation since its second derivative is the delta function. We hence throw out the $\frac{a}{r}$ solution for $s = 0$. We hence ignore all $p = -l$ and only consider $p = l + 1$.

Note that for $l = 1, 2, \ldots$, the solution goes as $U_{E,l} \sim r^{l+1}$ only, since the other solution will be singular and not normalizable.

Free particle wavefunction in spherical coordinates Note that we can write the energy in terms of the wavenumber $E = \frac{\hbar^2 k^2}{2m}$. Make the change of variables $\rho = kr$. Then the differential equation becomes:

$$\left(\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + 1\right) U_{E,l}(\rho) = 0 \tag{8.16}$$

The solutions are spherical Bessel functions with asymptotic behavior at $r \to \infty$:

$$J_l(\rho) \to \frac{1}{\rho} \sin\left(\rho - \frac{l\pi}{2}\right) \tag{8.17}$$

$$\eta_l(\rho) \to \frac{1}{\rho} \cos\left(\rho - \frac{l\pi}{2}\right) \tag{8.18}$$

and asymptotic behavior at $r \to 0$:

$$J_l(\rho) \to \frac{\rho^l}{(2l+1)!!} \tag{8.19}$$

$$\eta_l(\rho) \to \frac{(2l+1)!!}{\rho^{l+1}} \tag{8.20}$$

Observe that the η_l solutions are singular at the origin.

The eigenfunctions of the free particle are not normalizable and can be written as:

$$\psi_{E,l,m}(r,\theta,\phi) = j_l(kr) Y_l^m(\theta,\phi) \tag{8.21}$$

Legendre polynomial expansion of exponential Consider the plane-wave eigenfunction of the position operator $\psi \propto e^{i\vec{p}\cdot\vec{x}/\hbar} = e^{i\vec{k}\cdot\vec{x}} = e^{ikr\cos\theta}$ where we measure θ with respect to $\vec{k}$.

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) j_l(rk) \tag{8.22}$$

We relate these to the spherical harmonics using:

$$Y_l^0(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta) \tag{8.23}$$

8.3 Harmonic Oscillator in 3D

Write the Hamiltonian:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2(X^2+Y^2+Z^2) \tag{8.24}$$

The wavefunctions are:

$$\psi_{E,l,m}(r,\theta,\phi) = \frac{U_{E,l}(r)}{r} Y_l^m(\theta,\phi) \tag{8.25}$$

Introduce the dimensionless variables:

$$\lambda = \frac{E}{\hbar\omega} \tag{8.26}$$

$$y = \sqrt{\frac{m\omega}{\hbar}} r \tag{8.27}$$

This gives the differential equation:

$$\left[\frac{d^2}{dy^2} + 2\lambda - y^2 - \frac{l(l+1)}{y^2}\right] U_{E,l}(y) = 0 \tag{8.28}$$

In the limit where $y \to \infty$, we have the differential equation:

$$\left(\frac{d^2}{dy^2} - y^2\right) U_{E,l} = 0 \implies U_{E,l} \sim e^{-y^2/2} \tag{8.29}$$

We hence make the ansatz $U_{E,l}(y) = v_{E,l}(y)e^{y^2/2}$ and make the power series substitution:

$$v = y^{l+1} \sum_{j=0}^{\infty} c_j y^j \tag{8.30}$$

We obtain the energies by requiring that the series terminate to get a normalizable solution. The conditions are hence:

$$c_{j+2} = -c_j \frac{2\lambda - 1 - 2(j+l+1)}{(j+l+3)(j+l+2) - l(l+1)} \tag{8.31}$$

$$c_0(l(l+1) - l(l+1)) = 0 \implies c_0 \text{ is arbitrary} \tag{8.32}$$

$$c_1((l+2)(l+1) - l(l+1)) = 0 \implies c_1 = 0 \tag{8.33}$$

$$\lambda = 2k + l + \frac{3}{2}, \quad j = 2k \tag{8.34}$$

We hence have the energies:

$$E = \hbar\omega \left(2k + l + \frac{3}{2}\right) \tag{8.35}$$

We introduce the principal quantum number $n = 2k + l$. Then the energies are:

$$E = \hbar\omega \left(n + \frac{3}{2}\right) \tag{8.36}$$

and the allowed values of l are $l = n - 2k = n, n-2, n-4, \ldots, 0$.

For $n = 0, l = 0$ only. For $n = 1, l = 1, m = \pm 1, 0$.

8.4 Wednesday Evening, 18 Nov 2015

Bound state problems The standard method of attack is:

- Write down Schrodinger equation and non-dimensionalize.
- Examine large r behavior and define $U_{E,l}(r) = v(r)F(r)$ where $F(r)$ solves the asymptotic behavior for large r.

Huthen Potential

$$V_H(r) = -\frac{e^2\alpha e^{-\alpha r}}{1 - e^{-\alpha r}} \tag{8.37}$$

Note that in the limit $r \to 0$, $V_H \to -\frac{e^2\alpha}{\alpha r} = -\frac{e^2}{r}$. In the limit $r \to \infty$, $V_H \to -e^2\alpha e^{-\alpha r}$.

8.4.1 Hydrogen Atom

Consider the Hamiltonian:

$$\left[\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}\left[E + \frac{e^2}{r} - \frac{l(l+1)\hbar^2}{2mr^2}\right]\right] U_{E,l}(r) = 0 \tag{8.38}$$

Introduce the dimensionless parameters for bound states $E < 0$:

$$\rho = \left(-\frac{2mE}{\hbar^2}\right)^{1/2} r \tag{8.39}$$

$$\lambda = \sqrt{-\frac{2m}{E\hbar^2}} \tag{8.40}$$

The differential equation becomes:

$$\left[\frac{d^2}{d\rho^2} - 1 + \frac{\lambda e^2}{\rho} - \frac{l(l+1)}{\rho^2}\right] U_{E,l}(\rho) = 0 \tag{8.41}$$

At large ρ,

$$\left(\frac{d^2}{d\rho^2} - 1\right) U_{E,l}(\rho) = 0 \tag{8.42}$$

$$\implies U_{E,l} = e^{\pm\rho} \tag{8.43}$$

Hence we pick the normalizable solution and write $U_{E,l}(\rho) = v_{E,l}(\rho)e^{-\rho}$. The differential equation for v is:

$$v'' + -2v' + \left(\frac{e^2\lambda}{\rho} - \frac{l(l+1)}{\rho^2}\right) v = 0 \tag{8.44}$$

We try a power series solution:

$$v = \rho^{l+1} \sum_{k=0}^{\infty} c_k \rho_k \tag{8.45}$$

The recursion relation is:

$$c_{k+1} = -c_k \frac{e^2\lambda - 2(k+l+1)}{(k+l+2)(k+l+1) - l(l+1)} \tag{8.46}$$

$$c_0 \text{ arbitrary} \tag{8.47}$$

The possible values of the energy (to ensure the series terminates) are:

$$E = -\frac{me^4}{2\hbar^2(k+l+1)^2} \tag{8.48}$$

Pick the principal quantum number $n = k+l+1$. Note that the smallest value of n is 1. $l = n-k-1 = n-1, n-2, \ldots, 0$. Then the energies are:

$$E = -\frac{me^4}{2\hbar^2 n^2} \tag{8.49}$$

8.5 Friday, 20 Nov 2015

8.5.1 Hydrogen Atom

Consider the hydrogen atom model parameters:

$$V(r) = -\frac{e^2}{r} \tag{8.50}$$

$$\mu = \frac{m_e m_p}{m_e + m_p} \approx m_e \tag{8.51}$$

$$\lambda = \sqrt{\frac{2m}{-E\hbar}} \tag{8.52}$$

$$\rho = \sqrt{\frac{-2mE}{\hbar^2}} r \tag{8.53}$$

and the energies are quantized:

$$e^2\lambda = 2(k+l+1) \implies E = -\frac{me^4}{2\hbar^2(k+l+1)^2}, \quad k = 0,1,2,\ldots, l = 0,1,2,\ldots \tag{8.54}$$

We defined the principal quantum number:

$$n = k + l + 1, \quad n = 1,2,3,\ldots \tag{8.55}$$

$$E_n = -\frac{m_e e^4}{2\hbar^2 n^2} \equiv -\frac{Ry}{n^2} \tag{8.56}$$

Define the dimensionless quantities:

$$\frac{e^2}{\hbar c} \equiv \alpha \approx \frac{1}{137} \tag{8.57}$$

Note further that the dimensionless length can be written as:

$$\rho = \frac{r}{na_0} \quad a_0 \equiv \frac{\hbar^2}{m_e e^2} \tag{8.58}$$

where a_0 is the Bohr radius.

Degeneracies in the Hydrogen Atom For $n = 1$, $l = 0$ only. For $n = 2, l = 0, l = 1$. When $l = 1$, then $m = \pm 1, 0$. Not including spin degeneracy, the number of degenerate states as a function of n goes as $\sum_{l=0}^{n-1}(2l+1) = n^2$ because there are $2l+1$ values of m for each value of l.

Ground state of hydrogen atom

$$\psi_{100} = \sqrt{\frac{1}{\pi a_0^3}} e^{-r/a_0} \tag{8.59}$$

where we index states based on nlm.

Yukawa potential Note that the exponential dependence of ψ_{nlm} goes as e^{-r/na_0} so that an approximate size of the state is na_0. The Yukawa potential goes as:

$$V = -\frac{e^2}{r} e^{-r/\lambda} \tag{8.60}$$

Hence a first approximation for bound states is $na_0 < \lambda$. Hence the Yukawa potential has a finite number of bound states.

Hulthen Potential Recall that:

$$V_H(r) = -\frac{\alpha e^2 e^{-\alpha n}}{1 - e^{-\alpha n}} \tag{8.61}$$

The Schrodinger equation for the s wave $l = 0$ is:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{e^2\alpha e^{-\alpha n}}{1 - e^{-\alpha n}} - E\right] U_{E,0}(r) = 0 \tag{8.62}$$

Introduce the dimensionless variables z, ϵ:

$$r = a_0 z \tag{8.63}$$

$$E = -\left(\frac{e^4 m \delta^2}{2\hbar^2}\right)\epsilon^2 \tag{8.64}$$

$$\delta = \alpha a_0 \tag{8.65}$$

The updated differential equation is:

$$\frac{1}{2}\frac{d^2 U_{E,0}(z)}{dz^2} + \frac{\delta e^{-\delta z}}{1 - e^{-\delta z}} U_{E,0}(z) - \frac{\epsilon^2}{2}\delta^2 U_{E,0}(z) = 0 \tag{8.66}$$

First examine the long-range behavior $z \to \infty$.

$$\frac{1}{2}\frac{d^2 U_{E,0}(z)}{dz^2} - \frac{\epsilon^2}{2}\delta^2 U_{E,0}(z) = 0 \tag{8.67}$$

$$\implies U_{E,0}(z) \to e^{-\epsilon\delta z}, \epsilon > 0 \tag{8.68}$$

Then introduce the function: $U_{E,0}(z) = \phi_E(z)e^{-\epsilon\delta z}$. The differential equation of ϕ_E is (coefficients may include some $\frac{1}{2}$ terms:

$$\phi_E'' - \epsilon\delta\phi_E' + \frac{\delta e^{-\delta z}}{1 - e^{-\delta z}}\phi_E = 0 \tag{8.69}$$

Perform another change of variables $y = 1 - e^{-\delta z}$. Then the differential equation becomes:

$$y(1-y)\frac{d^2\phi_E}{dy^2} - y\frac{d\phi_E}{dy}(1 + 2\epsilon) + \frac{2}{\delta}\phi_E = 0 \tag{8.70}$$

Then make the power series substitution (since we pick the s wave, we have $l = 0$):

$$\phi_E(y) = \sum_{n=0}^{\infty} c_k y^{k+1} \tag{8.71}$$

The condition for the termination of the series is:

$$\epsilon = \frac{1}{\delta(k+1)} - \frac{k+1}{2} \tag{8.72}$$

and the quantized energies are:

$$E = -\frac{e^4 m}{2\hbar^2}\left(\frac{1}{k+1} - \frac{(k+1)\delta}{2}\right)^2 \tag{8.73}$$

Note that as $\delta \to 0, \alpha \to 0$, so the Yukawa potential approximates the Coulomb potential. Note that the energy does indeed approach the Coulomb energy as $\delta \to 0$.

Spin and magnetic field Consider a particle in a vector potential: $\vec{B} = \nabla \times \vec{A}$ and scalar potential $\phi = 0$ so that there are no electrical influences. Then the Hamiltonian is:

$$H = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 \tag{8.74}$$

Considering the non-relativistic case, we take the first order approximation:

$$H \approx \frac{p^2}{2m} - \frac{q}{2mc}(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}) \tag{8.75}$$

We move into quantum mechanics by promoting $p \to P$. Note that in the position basis:

$$\vec{P}\cdot\vec{A}\Psi(\vec{x}) = -i\hbar\nabla\cdot(\vec{A}(\vec{x})\Psi(\vec{x})) = -i\hbar\left((\nabla\cdot\vec{A})\Psi + \vec{A}\cdot\nabla\Psi(\vec{x})\right) \tag{8.76}$$

Align the z-axis with the magnetic field.

Chapter 9

Week 9

9.1 Monday, 23 Nov 2015

9.1.1 Spin dynamics in magnetic field

Consider a magnetic field $\nabla \times \vec{A}$ and no electric field. Then the non-relativistic Hamiltonian, where we throw away terms that go as $\frac{1}{c^2}$, is:

$$H = \frac{P^2}{2m} - \frac{q}{2mc}\left(\vec{P}\cdot\vec{A} + \vec{A}\cdot\vec{P}\right) \tag{9.1}$$

Consider a constant magnetic field. WLOG, point the z-axis along the B field. Then in the Cartesian coordinate system,

$$\vec{A} = \frac{B_0}{2}\left(-y\hat{x} + x\hat{y}\right) \tag{9.2}$$

which allows us to note that $\vec{P}\cdot\vec{A} = 0$ (vector potential has been chosen to have zero divergence), and hence:

$$H = \frac{P^2}{2m} - \frac{qB}{2mc}L_z \tag{9.3}$$

Define the magnetic moment:

$$\vec{\mu} = \frac{q}{2mc}\vec{L} \tag{9.4}$$

and hence the Hamiltonian can be written as:

$$H = \frac{P^2}{2m} - \vec{\mu}\cdot\vec{B} \tag{9.5}$$

Now spin angular momentum also contribute to the magnetic moment. Call the magnetic moment due to spin:

$$\vec{\mu} = \gamma\vec{S} \tag{9.6}$$

where γ is a constant of proportionality. Typical values of γ are:

$$\gamma_e = g\left(\frac{-e}{2m_e c}\right), \quad g = 2\left[1 + \frac{\alpha}{2\pi} + \ldots\right] \tag{9.7}$$

$$\gamma_p = 5.6\left(\frac{e}{2m_p c}\right) \tag{9.8}$$

$$\gamma_n = -3.8\left(\frac{e}{2m_n c}\right) \tag{9.9}$$

Time evolution Construct the propagator, ignoring all other degrees of freedom except the spin degree of freedom. Since the Hamiltonian is independent of time:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{9.10}$$
$$= e^{-iHt/\hbar}|\psi(0)\rangle \tag{9.11}$$
$$= e^{i\gamma\vec{S}\cdot\vec{B}t/\hbar}|\psi(0)\rangle \tag{9.12}$$

Observe that this is simply a rotation by an angle $-\gamma|\vec{B}|t$ along an axis in the direction $\hat{B}$. Then the angular velocity of this rotation is simply $\omega_0 = \gamma|\vec{B}|$. If we orient $\vec{B}$ along the z-axis, then we can write:

$$U(t) = \exp\left(\frac{i\omega_0\sigma_z t}{2}\right) = \begin{pmatrix} e^{i\omega_0 t/2} & 0 \\ 0 & e^{-i\omega_0 t/2} \end{pmatrix} \tag{9.13}$$

Let the spin of the particle be initially aligned along an arbitrary direction $\hat{n}$. Let $\hat{n}$ have polar angle θ and azimuthal angle ϕ.

$$|\psi(0)\rangle = \begin{pmatrix} \cos\frac{\theta}{2}e^{-i\phi/2} \\ \sin\frac{\theta}{2}e^{i\phi/2} \end{pmatrix} \tag{9.14}$$
$$\implies |\psi(t)\rangle = \begin{pmatrix} \cos\frac{\theta}{2}e^{-i(\phi-\omega_0 t)/2} \\ \sin\frac{\theta}{2}e^{i(\phi-\omega_0 t)/2} \end{pmatrix} \tag{9.15}$$

Time-dependent magnetic field Consider a uniform magnetic field along the vertical z-axis. Let there be a time-dependent magnetic field in the xy plane rotating with angular frequency ω. Then we write:

$$\vec{B} = (0, 0, B) + B'(\cos\omega t, -\sin\omega t, 0) \tag{9.16}$$

The interaction Hamiltonian (ignoring the other degrees of freedom) is hence (using the Pauli matrices):

$$H = -\gamma\vec{B}\cdot\vec{S} = -\frac{\gamma\hbar}{2}\begin{pmatrix} B & B'(\cos\omega t + i\sin\omega t) \\ B'(\cos\omega t - i\sin\omega t) & -B \end{pmatrix} \tag{9.17}$$
$$\implies H = -\frac{\gamma\hbar}{2}\begin{pmatrix} B & B'e^{i\omega t} \\ B'e^{-i\omega t} & -B \end{pmatrix} \tag{9.18}$$

We substitute this into Schrodinger's equation:

$$\Psi(t) = \begin{pmatrix} \psi_+(t) \\ \psi_-(t) \end{pmatrix} \tag{9.19}$$
$$i\hbar\frac{d}{dt}\Psi = H\Psi \implies \begin{cases} i\frac{d\psi_+}{dt} = -\frac{\gamma B}{2}\psi_+ - \frac{\gamma B'e^{i\omega t}}{2}\psi_- \\ i\frac{d\psi_-}{dt} = -\frac{\gamma B'e^{-i\omega t}}{2}\psi_+ + \frac{\gamma B}{2}\psi_- \end{cases} \tag{9.20}$$

We make the substitution:

$$\psi_+(t) = e^{i\omega t/2}C_+(t) \tag{9.21}$$
$$\psi_-(t) = e^{-i\omega t/2}C_-(t) \tag{9.22}$$

Then the coupled differential equations are:

$$i\dot{C}_+ = \left(-\frac{\gamma B}{2} + \frac{\omega}{2}\right)C_+ - \frac{\gamma B'}{2}C_- \tag{9.23}$$
$$i\dot{C}_- = -\frac{\gamma B'}{2}C_+ + \left(\frac{\gamma B}{2} - \frac{\omega}{2}\right)C_- \tag{9.24}$$

We proceed to find the normal modes:

$$\begin{pmatrix} C_+ \\ C_- \end{pmatrix} = e^{i\alpha t} \begin{pmatrix} a_+ \\ a_- \end{pmatrix} \tag{9.25}$$

We pick $a_+ = 1$ for convenience. The eigenfrequencies are:

$$\alpha_\pm = \pm\frac{1}{2}\sqrt{(\gamma B - \omega)^2 + \gamma^2 (B')^2} \tag{9.26}$$

and the second coefficient of each eigenvector is:

$$a_2^\pm = \frac{\alpha_\pm - \frac{\gamma B}{2} - \frac{\omega}{2}}{\gamma B'/2} \tag{9.27}$$

To obtain the general state vector, we superimpose the solutions due to each normal mode:

$$|\psi(t)\rangle = \begin{pmatrix} e^{i\omega t/2} e^{i\alpha_+ t} \\ e^{-i\omega t/2} e^{i\alpha_+ t} a_2^+ \end{pmatrix} A + \begin{pmatrix} e^{i\omega t/2} e^{i\alpha_- t} \\ e^{-i\omega t/2} e^{i\alpha_- t} a_2^- \end{pmatrix} B \tag{9.28}$$

9.2 Wednesday, 25 Nov 2015

9.2.1 More spin dynamics in magnetic fields

Interaction Hamiltonian Recall that we wrote $H_{int} = -\vec{\mu} \cdot \vec{B}$. For orbital angular momentum, $\vec{\mu} = \frac{q\vec{L}}{2mc}$ which holds for both spatially varying and constant magnetic fields. For spin angular momentum, we wrote $\vec{\mu} = \gamma \vec{S}$. The state evolves in time as:

$$|\psi(t)\rangle = e^{i\gamma \vec{S} \cdot \vec{B} t/\hbar} |\psi(0)\rangle \tag{9.29}$$

which we noted is just a rotation in space around the $\vec{B}$ axis. For the time-varying magnetic field, we considered the special case where the xy magnetic field rotated with constant angular velocity:

$$\vec{B}(t) = (0, 0, B) + B'(\cos \omega t, -\sin \omega t, 0) \tag{9.30}$$

The solutions were superpositions of two normal modes:

$$|\psi(t)\rangle = \begin{pmatrix} e^{i\omega t/2} e^{i\alpha_+ t} \\ e^{-i\omega t/2} e^{i\alpha_+ t} a_2^+ \end{pmatrix} A + \begin{pmatrix} e^{i\omega t/2} e^{i\alpha_- t} \\ e^{-i\omega t/2} e^{i\alpha_- t} a_2^- \end{pmatrix} B \tag{9.31}$$

Consider an initial wavefunction $\psi(0) = (1, 0)^T$. The transition probability as a function of time is $|\psi_-(t)|^2$. To obtain this, we solve for A and B given the initial conditions, then time evolve the state and find the required probability component. The answer is:

$$P(\uparrow \to \downarrow, t) = \frac{\gamma^2 (B')^2}{(\omega - \gamma B)^2 + \gamma^2 (B')^2} \sin^2 \left(\frac{t}{2} \sqrt{(\omega - \gamma B)^2 + \gamma^2 (B')^2} \right) \tag{9.32}$$

Hence the times when the flip probability is maximized are:

$$t_{flip} = \frac{(2n+1)\pi}{\sqrt{(\omega - \gamma B)^2 + \gamma^2 (B')^2}}, \quad n \in \mathbb{Z} \tag{9.33}$$

9.3 Angular momentum and other degrees of freedom

Uncoupled Hamiltonian Consider an additive Hamiltonian:

$$H = H_0 + H_{spin} \tag{9.34}$$

Then we can write the wavefunction as a product:

$$|\psi\rangle = |\psi_0\rangle|\psi_{spin}\rangle \tag{9.35}$$

where the individual kets are the eigenstates of each of the additive components of the Hamiltonian with energy eigenvalues E_0 and E_{spin} respectively. Then $|\psi\rangle$ has energy eigenvalue $E = E_0 + E_{spin}$.

Coulomb Problem Consider the Hamiltonian with the Coulomb Hamiltonian and both orbital and spin angular momentum with a magnetic field in the z-direction:

$$H = H_{coulomb} - \left(\frac{-eB}{2m_e c}\right) L_z - 2\left(\frac{-eB}{2m_e c}\right) S_z \tag{9.36}$$

Note that we only included the contribution from the electron. The proton also has spin, but since its mass is much larger than that of the electron, we can ignore it. Now we knew that the eigenstate of the Coulomb Hamiltonian was indexed by the quantum numbers n, lm. Then we can write the basis of the combined Hamiltonian as (noting that the eigenvalues of L_z are determined by m):

$$|n, l, m, m_s\rangle \tag{9.37}$$

where $m_s\hbar$ is the eigenvalue of the spin eigenstate.

Then we write the Hamiltonian as:

$$H|n, l, m, m_s\rangle = \left[-\frac{Ry}{n^2} + \frac{eB\hbar}{2m_e c}(m_e + 2m_s)\right]|n, l, m, m_s\rangle \tag{9.38}$$

Observe that the spin and orbital angular momentum hence change the energy of the system by $\frac{eB\hbar}{2m_e c}(m_e + 2m_s)$.

Stern-Gerlach Experiment Consider a beam of particles moving in the $\hat{y}$ direction. Let a magnetic field point in the $-\hat{z}$ direction. The interaction Hamiltonian is $H_{int} = -\vec{\mu} \cdot \vec{B}$. Let the magnetic field be non-uniform. The force on the particles is $\vec{F} = -\nabla H_{int}$. Since we specified that the magnetic field only points in the $\hat{z}$ direction, we can write the force as:

$$\vec{F} = \mu_z \frac{\partial B_z}{\partial z}\hat{z} \tag{9.39}$$

Let the initial state of the particles be written as:

$$\psi_{initial} = \psi_y(\vec{x}_{CM})\psi_{100}(\vec{r}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{9.40}$$

which moves in the $\hat{y}$ direction and depends on the center of mass position and only consists of hydrogen atoms in the ground state with spin up. For convenience, let $\frac{\partial B_z}{\partial z} < 0$.

Now after the particles pass through the magnetic field, the wavefunction is given by:

$$\psi_{out} = \psi_{y(\hat{z})}(\vec{x}_{CM})\psi_{100}(\vec{r}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{9.41}$$

because the spin-up is an eigenstate of the spin operator in the Hamiltonian. Note that we wrote $\psi_y(\hat{z})$ to indicate that these particles are deflected in the $\hat{z}$ direction. On the other hand, spin-down particles will be deflected in the opposite direction $\psi_{y(-\hat{z})}(\vec{x}_{CM})\psi_{100}(\vec{r}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Hence if we write the arbitrary incoming wave as:

$$\psi_{initial} = \psi_y(\vec{x}_{CM})\psi_{100}(\vec{r}) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{9.42}$$

then the outgoing wave is:

$$\psi_{out} = \psi_{y(+\hat{z})}(\vec{x}_{CM})\psi_{100}(\vec{r}) \begin{pmatrix} \alpha \\ 0 \end{pmatrix} + \psi_{y(-\hat{z})}(\vec{x}_{CM})\psi_{100}(\vec{r}) \begin{pmatrix} 0 \\ \beta \end{pmatrix} \tag{9.43}$$

9.4 Addition of Angular momentum

Consider two particles. Let the states be written as:

$$|s_1, m_1\rangle, \quad |s_2, m_2\rangle \tag{9.44}$$

The combined state is:

$$|s_1, m_1\rangle|s_2, m_2\rangle = |s_1, m_1, s_2, m_2\rangle \tag{9.45}$$

Note that this is not the only basis that we can describe the system in. We can consider the total spin $\vec{S} = \vec{S}_1 + \vec{S}_2$ and index the states by the total spin numbers s, m_s. These two bases are related by a unitary transformation with dimension $(2s_1 + 1)(2s_2 + 1)$.

Chapter 10

Week 10

10.1 Monday, 30 Nov 2015

10.1.1 Addition of angular momentum

Setup Suppose we have two particles with angular momenta $|j_1, m_1\rangle, |j_2, m_2\rangle$ respectively. We can write the total angular momentum as $\vec{J} = \vec{J}_1 + \vec{J}_2$. Note that we can also perform this with $\vec{S}$ instead of $\vec{J}$.

Example Consider spin-half particles $|1/2, m_1\rangle|1/2, m_2\rangle$. Since $m_1, m_2 \in \{-1/2, 1/2\}$, we write the combined state using $|\pm, \pm\rangle$ where we only refer to the sign of the spin. Then the total spin is $\vec{S} = \vec{S}_1 + \vec{S}_2$. Then, the operators on the individual spaces act as:

$$S_{1z}|-,+\rangle = -\frac{\hbar}{2}|-,+\rangle \tag{10.1}$$

$$S_2^2|-,+\rangle = \frac{1}{2}(\frac{1}{2}+1)\hbar^2|-,+\rangle \tag{10.2}$$

while the operators on the combined Hilbert space act as:

$$S_z|+,+\rangle = \hbar\left(\frac{1}{2}+\frac{1}{2}\right)|+,+\rangle \tag{10.3}$$

$$S_z|+,-\rangle = 0 \tag{10.4}$$

$$S_z|-,-\rangle = -\hbar|-,-\rangle \tag{10.5}$$

Now consider the combined total spin:

$$\vec{S}^2 = (\vec{S}_1 + \vec{S}_2)\cdot(\vec{S}_1 + \vec{S}_2) = \vec{S}_1^2 + \vec{S}_2^2 + 2\vec{S}_1\cdot\vec{S}_2 \tag{10.6}$$

where we note that the spin operators for different particles commute. The cross term can be written as:

$$\vec{S}_1\cdot\vec{S}_2 = S_{1z}S_{2z} + \frac{1}{2}\left(S_{1+}S_{2-} + S_{1-}S_{2+}\right) \tag{10.7}$$

where we use the raising and lowering operators in each of the spaces to express the x and y components.

Recall that the raising and lowering operators are:

$$J_\pm = J_x \pm iJ_y \tag{10.8}$$

and their operations are:

$$J_\pm|j,m\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}|j, m\pm 1\rangle \tag{10.9}$$

Hence we can treat the total spin operator:

$$\vec{S}^2 = \frac{3}{2}\hbar^2 + 2S_{1z}S_{2z} + (S_{1+}S_{2-} + S_{1-}S_{2+}) \tag{10.10}$$

Note that the operation of the raising and lowering operators on the eigenstates are:

$$S_{1+}S_{2-}|+,+\rangle = 0 \tag{10.11}$$
$$S_{1+}S_{2-}|-,-\rangle = 0 \tag{10.12}$$
$$S_{1-}S_{2+}|+,+\rangle = 0 \tag{10.13}$$
$$S_{1-}S_{2+}|-,-\rangle = 0 \tag{10.14}$$
$$S_{1+}S_{2-}|-,+\rangle = \hbar^2|+,-\rangle \tag{10.15}$$
$$S_{1-}S_{2+}|+,-\rangle = \hbar^2|-,+\rangle \tag{10.16}$$

all other eigenstates give zero. We hence have:

$$S^2|+,+\rangle = \hbar^2\left(\frac{3}{2}+\frac{1}{2}\right)|+,+\rangle = \hbar^2\cdot 1(1+1)|+,+\rangle \tag{10.17}$$
$$S^2|-,-\rangle = \hbar^2(3/2-1/2)|-,-\rangle \tag{10.18}$$
$$S^2|+,-\rangle = \hbar^2(3/2-1/2)|+,-\rangle + \hbar^2|-,+\rangle \tag{10.19}$$
$$S^2|-,+\rangle = \hbar^2|-,+\rangle + \hbar^2|+,-\rangle \tag{10.20}$$

Observe that the $|+,-\rangle$ and $|-,+\rangle$ states are not eigenstates of the S^2 operator, hence they get mixed up. However, linear combinations of the states are eigenstates:

$$S^2\frac{1}{\sqrt{2}}\left[|+,-\rangle + |-,+\rangle\right] = \hbar^2 2\frac{1}{\sqrt{2}}\left[|+,-\rangle + |-,+\rangle\right] \tag{10.21}$$
$$S^2\frac{1}{\sqrt{2}}\left[|+,-\rangle - |-,+\rangle\right] = \hbar^2 0\cdot\frac{1}{\sqrt{2}}\left[|+,-\rangle - |-,+\rangle\right] = 0 \tag{10.22}$$

Hence we have the eigenstates for $s = 1$:

$$|+,+\rangle, \quad \frac{1}{\sqrt{2}}\left[|+,-\rangle + |-,+\rangle\right], \quad |-,-\rangle \tag{10.23}$$

and exactly one eigenstate for $s = 0$:

$$\frac{1}{\sqrt{2}}\left[|+,-\rangle - |-,+\rangle\right] \tag{10.24}$$

There are a total of 4 eigenstates of S^2, corresponding to the dimensionality of the direct product space 2×2.

Now consider the operation of the total z-component of the angular momentum:

$$J_z|j_1,m_1,j_2,m_2\rangle = \hbar(m_1+m_2)|j_1,m_1,j_2,m_2\rangle \tag{10.25}$$

Clearly, the maximum value of the z-component is $\hbar(j_1+j_2)$. The allowed values of the total J_z is:

$$j_1+j_2, j_1+j_2-1, \ldots, j_1-j_2 \tag{10.26}$$

and the total number of states is:

$$\sum_{j=j_1-j_2}^{j_1+j_2}(2j+1) \tag{10.27}$$

Possible states organized by total J

$J = j_1 + j_2$	$J = j_1 + j_2 - 1$	$\cdots$	$J = j_1 - j_2$
$\lvert j_1 + j_2, j_1 + j_2\rangle$	$\lvert j_1 + j_2 - 1, j_1 + j_2 - 1\rangle$	$\cdots$	$\lvert j_1 - j_2, j_1 - j_2\rangle$
$\lvert j_1 + j_2, j_1 + j_2 - 1\rangle$	$\lvert j_1 + j_2 - 1, j_1 + j_2 - 2\rangle$	$\cdots$	$\lvert j_1 - j_2, j_1 - j_2 - 1\rangle$
$\vdots$	$\vdots$	$\ddots$	$\vdots$
$\lvert j_1 + j_2, -(j_1 + j_2)\rangle$	$\lvert j_1 + j_2 - 1, -(j_1 + j_2 - 1)\rangle$	$\cdots$	$\lvert j_1 - j_2, -(j_1 - j_2)\rangle$

(10.28)

Observe that the maximum J_z corresponds to only one state:

$$|j_1 + j_2, j_1 + j_2\rangle = |j_1, j_1, j_2, j_2\rangle \tag{10.29}$$

We obtain the other states by using the raising and lowering operators defined over the combined space:

$$J_- = J_{1-} + J_{2-} \tag{10.30}$$
$$J_+ = J_{1+} + J_{2+} \tag{10.31}$$

$$J_-|j_1 + j_2, j_1 + j_2\rangle = \hbar\sqrt{2(j_1 + j_2)}|j_1 + j_2, j_1 + j_2 - 1\rangle \tag{10.32}$$

which we can also write as:

$$(J_{1-} + J_{2-})|j_1, j_1, j_2, j_2\rangle = \hbar\sqrt{2j_1}|j_1, j_1 - 1, j_2, j_2\rangle + \hbar\sqrt{2j_2}|j_1, j_1, j_2, j_2 - 1\rangle \tag{10.33}$$

and equating the two expressions,

$$|j_1 + j_2, j_1 + j_2 - 1\rangle = \sqrt{\frac{j_1}{j_1 + j_2}}|j_1, j_1 - 1, j_2, j_2\rangle + \sqrt{\frac{j_2}{j_1 + j_2}}|j_1, j_1, j_2, j_2 - 1\rangle \tag{10.34}$$

This gives us the expressions for the individual particles for all states with $J_z = j_1 + j_2$ by using the lowering operator because we knew the first state.

Now consider states with $J = j_1 + j_2 - 1$. The highest J_z state is:

$$|j_1 + j_2 - 1, j_1 + j_2 - 1\rangle = \alpha|j_1, j_1 - 1, j_2, j_2\rangle + \beta|j_1, j_1, j_2, j_2 - 1\rangle \tag{10.35}$$

where we noted that it must be a linear combination of two possible states. We want to solve for $\frac{\alpha}{\beta}$. Note that this state must be orthogonal to $|j_1 + j_2, j_1 + j_2 - 1\rangle$, which we had already expressed as a linear combination of these states. But this means that we can dot the expressions into each other and set it to zero to obtain the constraint on α, β:

$$\alpha\sqrt{\frac{j_1}{j_1 + j_2}} + \beta\sqrt{\frac{j_2}{j_1 + j_2}} = 0 \tag{10.36}$$

and solving for α/β, we hence have:

$$|j_1 + j_2 - 1, j_1 + j_2 - 1\rangle = -\sqrt{\frac{j_2}{j_1 + j_2}}|j_1, j_1 - 1, j_2, j_2\rangle + \sqrt{\frac{j_1}{j_1 + j_2}}|j_1, j_1, j_2, j_2 - 1\rangle \tag{10.37}$$

Note that we have a phase ambiguity because α and β can be complex. The particular way we wrote the state is just one convention.

Now we have the top state of the second column of the table with $J = j_1 + j_2 - 1$, so we can obtain all the other states as a linear combination of the individual states by using the lowering operator.

General Form - Clebsch-Gordan coefficients Note that we have written the combined state as a linear combination of the individual states:

$$|j, m\rangle = \sum_{m_1, m_2} |j_1, m_1, j_2, m_2\rangle\langle j_1, m_1, j_2, m_2|j, m\rangle \tag{10.38}$$

Hence the coefficients we have determined are $\langle j_1, m_1, j_2, m_2|j, m\rangle$, which are called the Clebsch-Gordan coefficients.

10.2 Wednesday, 2 Dec 2015

About spin Note that orbital angular momentum is always an integer multiple of $\hbar$. Spin, on the other hand, can be half-integer as well. Hence the fundamental particles with half-integer spin cannot be thought of as composite systems with the angular momentum coming from hidden orbital angular momentum.

Addition of angular momentum - orbital and spin Consider a bound electron to a nucleus with orbital angular momentum l and spin $\frac{1}{2}$. Hence the total angular momentum is: $l \pm \frac{1}{2}$. We can write the state using the $(2l+1) \times (2s+1)$ dimension vector:

$$|l, m, s, m_s\rangle \tag{10.39}$$

and we can also write this using the total angular momentum operators J^2, J_z. The state is hence parametrized by (to check this in Shankar):

$$|j = l \pm \frac{1}{2}, m\rangle = \pm\sqrt{\frac{l + 1/2 \pm m}{2l+1}}|l, m - \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\rangle + \sqrt{\frac{l + 1/2 \mp m}{2l+1}}|l, m + \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\rangle \tag{10.40}$$

Relativistic correction We need to include the L dot S coupling:

$$\Delta H = g\vec{L} \cdot \vec{S} \tag{10.41}$$

and this contributes to the Hamiltonian. Observe that the dot product can be written as:

$$\vec{L} \cdot \vec{S} = \frac{\vec{J}^2 - \vec{L}^2 - \vec{S}^2}{2}, \quad \vec{J} = \vec{L} + \vec{S} \tag{10.42}$$

We hence want to move into the total angular momentum basis:

$$\vec{L} \cdot \vec{S}|j = l \pm 1/2, m\rangle = \frac{\hbar^2}{2}\left[j(j+1) - l(l+1) - s(s+1)\right]|j = l \pm 1/2, m\rangle, \quad s = \frac{1}{2} \tag{10.43}$$

$$= \frac{\hbar^2}{2}\left[j(j+1) - l(l+1) - \frac{3}{4}\right]|j = l \pm 1/2, m\rangle \tag{10.44}$$

Spectroscopic notation We can write the state as ${}^{2s+1}l_J$, where l is the s,p,d,f designation.

Discrete transformations Consider the parity transformation $(x, y, z) \to (-x, -y, -z)$. Observe that two parity transformations composed is the identity. Note that the operator can be written as:

$$\Pi|x, y, z\rangle = |-x, -y, -z\rangle \tag{10.45}$$

Then in the 1D position basis:

$$\langle x'|\Pi x\rangle = \delta(x' + x) = \langle \Pi x'|x\rangle \tag{10.46}$$

Clearly, Π is Hermitian. Its allowed eigenvalues are ± 1. The parity operation on a momentum eigenstate is:

$$\Pi|p\rangle = \Pi \int d^3x|x\rangle\langle x|p\rangle = \int d^3x|-x\rangle\langle x|p\rangle = \int d^3u|u\rangle e^{-ip\cdot u/\hbar}\frac{1}{(2\pi\hbar)^{3/2}} = \int d^3u|u\rangle\langle u|-p\rangle = |-p\rangle \tag{10.47}$$

and its operation on an operator is:

$$\Pi^\dagger\Omega(X, P)\Pi = \Pi\Omega(X, P)\Pi = \Omega(-X, -P) \tag{10.48}$$

Parity of Hydrogen atom eigenstates To find: $\Pi|n, l, m\rangle$.

10.2.1 Perturbation Theory

Classes Time-independent and time-dependent.

Setup Suppose we have a Hamiltonian $H^{(0)}$ and we have solved the eigenstate problem:

$$H^{(0)}|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle \tag{10.49}$$

Then we write a new Hamiltonian $H = H^{(0)} + H^{(1)}$ where $H^{(1)}$ is "small". Let $H^{(1)}$ be proportional to a small dimensionless quantity ϵ. Suppose we can write E_n and $|n\rangle$ as a power series in ϵ, where the superscript indicates the powers in ϵ:

$$E_n = E_n^{(0)} + E_n^{(1)} + \dots \tag{10.50}$$

$$|n\rangle = |n^{(0)}\rangle + |n^{(1)}\rangle + \dots \tag{10.51}$$

Then we want to solve:

$$(H^{(0)} + H^{(1)})(|n^{(0)}\rangle + |n^{(1)}\rangle + \dots) = (E_n^{(0)} + E_n^{(1)} + \dots)(|n^{(0)}\rangle + |n^{(1)}\rangle + \dots) \tag{10.52}$$

Then organizing the terms by order:

$$H^{(0)}|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle \quad \text{zeroth order} \tag{10.53}$$

$$H^{(0)}|n^{(1)}\rangle + H^{(1)}|n^{(0)}\rangle = E_n^{(0)}|n^{(1)}\rangle + E_n^{(1)}|n^{(0)}\rangle \quad \text{first order} \tag{10.54}$$

$$H^{(0)}|n^{(2)}\rangle + H^{(1)}|n^{(1)}\rangle = E_n^{(2)}|n^{(0)}\rangle + E_n^{(1)}|n^{(1)}\rangle + E_n^{(0)}|n^{(2)}\rangle \quad \text{second order} \tag{10.55}$$

The zeroth order equation is already solved. Hence we can obtain $|n^{(1)}\rangle$ and $E^{(1)}$ from the first order equation using the zeroth order solution. First take the inner product of the first order equation with $|n^{(0)}\rangle$.

$$\langle n^{(0)}|H^{(0)}|n^{(1)}\rangle + \langle n^{(0)}|H^{(1)}|n^{(0)}\rangle = E_n^{(0)}\langle n^{(0)}|n^{(1)}\rangle + E_n^{(1)} \tag{10.56}$$

$$\implies \langle n^{(0)}|H^{(1)}|n^{(0)}\rangle = E_n^{(1)} \tag{10.57}$$

where we note that the energies are real numbers $E_n^{(0)} = (E_n^{(0)})^*$. Hence we immediately obtain the first order energy shift. Now consider taking the inner product with another vector $|m^{(0)}\rangle$ where $m \neq n$. Then:

$$\langle m^{(0)}|H^{(0)}|n^{(1)}\rangle + \langle m^{(0)}|H^{(1)}|n^{(0)}\rangle = E_n^{(0)}\langle m^{(0)}|n^{(1)}\rangle + E_n^{(1)}\langle m^{(0)}|n^{(0)}\rangle \tag{10.58}$$

$$\implies \langle m^{(0)}|H^{(0)}|n^{(1)}\rangle + \langle m^{(0)}|H^{(1)}|n^{(0)}\rangle = E_n^{(0)}\langle m^{(0)}|n^{(1)}\rangle \tag{10.59}$$

$$\implies E_m^{(0)}\langle m^{(0)}|n^{(1)}\rangle + \langle m^{(0)}|H^{(1)}|n^{(0)}\rangle = E_n^{(0)}\langle m^{(0)}|n^{(1)}\rangle \tag{10.60}$$

$$\implies \langle m^{(0)}|n^{(1)}\rangle = \frac{\langle m^{(0)}|H^{(1)}|n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \tag{10.61}$$

Hence reconstructing the unknown $|n^{(1)}\rangle$:

$$|n\rangle = |n^{(0)}\rangle(1 + c\epsilon) + \sum_{m\neq n} |m^{(0)}\rangle \frac{\langle m^{(0)}|H^{(1)}|n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \tag{10.62}$$

The constant c can be fixed by using a normalization convention at order ϵ:

$$1 = \langle n|n\rangle \tag{10.63}$$

$$= \langle n^{(0)}|n^{(0)}\rangle|1 + c\epsilon|^2 + O(\epsilon^2) \tag{10.64}$$

$$\approx 1 + 2\epsilon\Re(c) \tag{10.65}$$

$$= 1 + 2\epsilon\Re(ic_I) \tag{10.66}$$

Hence we can require:

$$|n\rangle = e^{iC_i\epsilon}\left(|n^{(0)}\rangle + \sum_{m\neq n}|m^{(0)}\rangle\frac{\langle m^{(0)}|H^{(1)}|n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}}\right) \tag{10.67}$$

where we can multiply the exponential into the sum because the sum just contains terms of order ϵ^2 and higher. Then C_I behaves as an overall phase, and we can use a phase convention to set it to zero. Hence:

$$|n\rangle = |n^{(0)}\rangle + \sum_{m\neq n}|m^{(0)}\rangle\frac{\langle m^{(0)}|H^{(1)}|n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}} \tag{10.68}$$

$$\implies |n^{(1)}\rangle = \sum_{m\neq n}|m^{(0)}\rangle\frac{\langle m^{(0)}|H^{(1)}|n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}} \tag{10.69}$$

Example Consider a screened Coulomb Yukawa potential:

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}e^{-\lambda r} \tag{10.70}$$

This is close to the Coulomb theory when $\lambda << 1$. We can calculate the energy shift using perturbation theory. We expand the Hamiltonian in λ:

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} + \lambda e^2 - \lambda^2\frac{r}{2} + O(\lambda^3) \tag{10.71}$$

Hence we have the Hamiltonians:

$$H^{(0)} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} + \lambda e^2 \tag{10.72}$$

$$H^{(1)} = -\lambda^2\frac{r}{2}e^2 \tag{10.73}$$

We can calculate the energy shift of the ground state. The ground state wavefunction in the position basis is:

$$\psi_{100} = \sqrt{\frac{1}{\pi a_0^3}}e^{-r/a_0}, \quad a_0 = \frac{\hbar^2}{me^2}, \quad E_0 = -Ry + \lambda e^2 \tag{10.74}$$

Hence we evaluate the perturbed energy:

$$E_{100}^{(1)} = -\frac{e^2\lambda^2}{2}\frac{1}{\pi a_0^3}4\pi\int_0^\infty dr r^3 e^{-2r/a_0} \tag{10.75}$$

$$= -\frac{3}{4}\frac{\lambda^2\hbar^2}{m^2} \tag{10.76}$$