Ph12b Class Notes

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Chapter 1

Week 1

1.1 Tuesday 6 Jan 2015

Fine structure constant $\alpha = \frac{e^2}{\hbar c} \approx 1/137$.

More constants $\hbar c = 1973eV \cdot \text{Å} = 197.3MeV \cdot fm$. $m_p \approx m_n \approx 940MeV/c^2$. $m_e = 0.511MeV/c^2$

Blackbody Radiation Ultraviolet catastrophe: Expected that the number of modes (per unit frequency) as a function of frequency increases with frequency, thereby expect that the frequency spectrum will demonstrate an increasing function. Actual blackbody spectrum tapers off at higher frequencies.

Planck hypothesis Energy of radiation is quantised in terms of $\hbar\omega$.

Photoelectric effect Energy of emitted electron depends on frequency of light and not intensity of light. $E_e = \hbar\omega - \phi$, for a fixed work function ϕ that depends on the metal.

Types of light-matter interactions

1. Photoelectric effect: $\gamma e_{bound} \to e_{free}$
2. Compton scattering $\gamma e \to \gamma e$
3. Bremsstrahlung $e \to \gamma e$
4. Pair annihilation $e^+e^- \to \gamma\gamma$
5. Pair production $\gamma\gamma \to e^+e^-$

Compton scattering

$$\Delta\lambda = \lambda_e - \lambda_{inc} = \frac{h}{m_e c}(1 - \cos\theta)$$

Compton wavelength $\frac{h}{m_e c} = 2.43 \times 10^{-12}m$, reduced Compton wavelength has $\hbar$ instead.

Rutherford scattering Differential cross section (as a function of scattered angle): $\frac{d\sigma}{d\theta} \sim \frac{1}{E_\alpha^2} \frac{\sin\theta}{\sin^4(\theta/2)}$.

Atomic stability Why don't accelerating electrons radiate all their energy and fall in? Bohr postulated quantisation using de Broglie wavelength (quantisation of angular momentum $L = n\hbar$). Gives $r_n = n^2 \frac{\hbar^2}{me^2} = n^2 a_0$, $E_n = \frac{-Ry}{n^2}, Ry = \frac{m_e e^4}{2\hbar^2} \approx 13.6eV$. Note CGS. Also $v_n = \frac{e^2}{n\hbar} = \frac{1}{n}\alpha c$ not a very appreciable fraction of the speed of light.

Atomic spectral lines To check Franck-Hertz experiment.

1.2 Lecture 08 Jan 2015

Photoelectric effect $h\nu = w_0 + eV_{stop}$, so plotting V_s against ν gives a slope of $\frac{h}{e}$.

Virial theorem $E = KE + PE = \frac{PE}{2} \implies KE = -\frac{PE}{2}$. Note that this is different from the harmonic oscillator virial theorem (KE=PE) because the potential shape is different.

Hydrogenic atom/ion With Z protons. Modified (semi-classical) formulae:

$$E_n = \frac{-Z^2}{n^2} Ry$$
$$v_n = \frac{Z}{n} \alpha c$$

Classical electron radius Recall $r_e = \frac{e^2}{m_e c^2}$.

Length scales $r_e : \lambda_c : a_0 = 1 : \frac{1}{\alpha} : \frac{1}{\alpha^2}$, where λ_c is the Compton wavelength. Recall that $\alpha = \frac{e^2}{\hbar c}$.

Rydberg atoms Excited atoms with one or more electrons with very high quantum numbers. Since r_n goes as n^2, they have very large atomic radii.

de Broglie wavelength Dispersion relation: $\omega = \frac{\hbar k^2}{2m}, p = \frac{h}{\lambda}$. Note that for a relativistic electron: $E^2 = (pc)^2 + (mc^2)^2$. Replace $E = \hbar c$ and $p = \hbar k$. For $pc >> mc^2$, then $E = pc$.

Bragg Scattering $2d \sin\theta = m\lambda$, d is the spacing between planes and θ is measured with respect to the plane (not the normal to the plane!). Use $\cos\theta$ for the normal to the plane.

Chapter 2

Week 2

2.1 Lecture 13 Jan 2015

Fundamental Wavefunctions $\psi_k(x,t) = Ae^{i(kx-\omega t)} = Ae^{i(px-Et)/\hbar}$. Not normalizable. Has to be superimposed to form a wavepacket.

As a probability $P(x,t) = |\Psi(x,t)|^2$, probability per unit space.

As a travelling wave: $\psi_k(x,t) = \psi_k(x-vt,0)$ where $v = v_p = \frac{\omega}{k} = \frac{p}{2m}$. But the velocity of a classical particle is $\frac{p}{m}$.

Wave Packets as a superposition of de Broglie waves:

$$\Psi(x,t) = \int_{-\infty}^{\infty} A(k)e^{i(kx-\omega t)}dk = \int dkA(k)\psi_k(x,t)$$

Note that $\Psi(x,t)$ can be normalised $\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$.

Group velocity of wave packet Recall that $E = \frac{p^2}{2m} \implies \hbar\omega = \frac{(\hbar\omega)^2}{2m} \implies v_g = \frac{\hbar k}{m} = \frac{p}{m} = v_{classical}$.

As a Fourier transform When $t = 0$, $\Psi(x, t = 0) = \int_{-\infty}^{\infty} dkA(k)e^{ikx}$. Define $\psi_k(x) = \frac{1}{\sqrt{2\pi}}e^{ikx}$, so that $\int_{-\infty}^{\infty} \psi_k(x)\psi_k^*(x)dx = \delta(k-k')$ (delta function normalization). Hence we can write

$$\Psi(x,t=0) = \int_{-\infty}^{\infty} dkA(k)\psi_k(x) \implies A(k) = \int_{-\infty}^{\infty} \Psi(x,t=0)\psi_k^*(x)dx$$

In 3D:

$$\Psi(\vec{r},0) = \iiint d\vec{k}A(\vec{k})\frac{1}{\sqrt{2\pi}}e^{-i\vec{k}\cdot\vec{r}}$$

Gaussian wavepacket

$$A(k) = ce^{-(k-k_0)^2/(2\Delta k)^2}e^{-i(k-k_0)x_0}$$

First term is a Gaussian envelope, second term is the fast oscillation. By normalisation, $c = \frac{1}{\sqrt{\Delta k}(2\pi)^{1/4}}$. Observe that $\Delta k = \sqrt{\langle (k-k_0)^2\rangle} = \sqrt{\langle k^2\rangle - \langle k\rangle^2} = \sqrt{\langle k^2\rangle - k_0^2}$.

In position space, we have:

$$\Psi(x,0) = \int_{-\infty}^{\infty} dkA(k)\frac{e^{ikx}}{\sqrt{2\pi}} = \frac{1}{\sqrt{\Delta x}(2\pi)^{1/4}}e^{-(x-x_0)^2/(2\Delta x)^2}e^{ik_0(x-x_0)}$$

and we also have $\Delta x = \frac{1}{2\Delta k}$.

Uncertainty Apply de Broglie relation to obtain $\Delta k = \frac{\Delta p}{\hbar}$ and combine with previous $\Delta x \Delta k = \frac{1}{2}$ so that:

$$\Delta p \Delta x = \frac{\hbar}{2}$$

Note that after $t = 0$, we have an inequality instead of perfect equality since the wave packet spreads and does not remain a Gaussian.

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

Method of stationary phase Rewrite $\psi_k(x,t) = \frac{1}{\sqrt{2\pi}} e^{i(kx-\omega t)} = \frac{1}{\sqrt{2\pi}} e^{i\phi_k(x,t)}$ and the interference is constructive if ϕ_k does not change very much with $k \implies \frac{\partial \phi}{\partial k}\Big|_{k_0} = 0 \implies \frac{\partial}{\partial k}(kx - \omega t) = 0 \implies x - \frac{\partial \omega}{\partial k}\big|_{k_0} t = 0 \implies x - v_g t = 0$.

Dispersion relations For light:

$$\omega = ck, v_\phi = c, v_g = c$$

For de Broglie waves:

$$\omega = \frac{\hbar k^2}{2m}, v_\phi = \frac{v_{class}}{2}, v_g = v_{class}$$

For Relativistic particles:

$$\omega = \frac{E}{\hbar} = \frac{\sqrt{p^2c^2 + m^2c^4}}{\hbar}, v_\phi = \frac{E}{p} = \sqrt{c^2 + \left(\frac{mc^2}{p}\right)^2} > c, v_g = \frac{dE}{dp} = \frac{pc^2}{E} = \beta c < c$$

Radioactive decay Recall that $N = N_0 e^{-t/\tau}$. The Fourier transform of the exponential is a Lorentzian in frequency space. Then we know that there is a spread in frequency space ($\Delta\omega$) and this leads to an uncertainty in energy.

2.2 Lecture 15 Jan 2015

Momentum operator $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$. Eigenfunctions are $Ae^{i(px)/\hbar}$.

Energy operator $\hat{E} = i\hbar\frac{\partial}{\partial t}$. Eigenfunctions are $Ae^{-iEt/\hbar}$.

Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$.

Position operator $\hat{x}$ is a multiplicative operator. Eigenfunctions of this operator are delta functions $\delta(x - x_0)$.

Chapter 3

Week 3

3.1 Lecture 20 Jan 2015

Angular momentum Particle on a ring. Operator: $\hat{L} = \frac{\hbar}{i}\frac{\partial}{\partial\theta}$. Uncertainty principle: $\Delta\theta\Delta L \geq \frac{\hbar}{2}$. Boundary condition: $\psi(\theta) = \psi(\theta+2\pi)$. Classical variables: $L = MR^2\dot{\theta}, E = \frac{L^2}{2MR^2}$. TDSE: $\hat{H} = \frac{-\hbar^2}{2MR^2}\frac{\partial^2}{\partial\theta^2}$ with solutions $\Psi(\theta,t) = \frac{1}{\sqrt{2\pi}}e^{iL\theta/\hbar}e^{-i\omega t}$. To satisfy boundary conditions, we require that $\frac{L}{\hbar} = m, m \in \mathbb{Z}, m = 0$ is allowed. $m = 0$ indicates that the particle is uniformly likely to be anywhere on the hoop. $m < 0$ is also allowed, and after tacking on time dependence, moves in the opposite direction as $m > 0$. Call m the magnetic quantum number. Then $E_m = \frac{(m\hbar)^2}{2MR^2}$. Note that a single solution has magnitude that is constant everywhere. Localisation is achieved by taking a linear superposition $\Psi(\theta,t) = \sum_{m=0,\pm1,\pm2\ldots} a_m\Psi_m(\theta,t)$.

Expectation for non-normalizable de Broglie "wave functions"

$$\langle p\rangle = \frac{\int_{-\infty}^{\infty}\Psi(x,t)^*\hat{p}\Psi(x,t)}{\int_{-\infty}^{\infty}\Psi(x,t)^*\Psi(x,t)}$$

Expectation for wave packets Let $\Psi(x,t) = \int_{-\infty}^{\infty}dkA(k)\Psi_k(x,t)$. Then $\langle p\rangle = \int_{-\infty}^{\infty}dk|A(k)|^2\hbar k$.

3.2 Lecture 22 Jan 2015

Franck-Hertz Experiment Electrons released through thermionic emission, accelerated to a grid held at positive potential, passes through the grid, flows through a mercury vapour, impinges on a negative potential plate (with associated ammeter back to the positively charged grid). If the electron elastically scatters off the mercury atom or inelastically collides with the mercury atoms (thereby losing some energy), it may not be able to reach the negatively charged collector plate. The question is to verify if energy is transferred (to the mercury atom) in a quantised manner or continuous manner. The measured current drops at regular intervals of accelerating potential when the energy is high enough to transfer a quantum of energy to the mercury atom.

Bra-Ket notation Let $|\psi\rangle$ be the state of a physical system. Then $\psi(x) = \langle x|\psi\rangle$ represents a wave, and $\langle n|\psi\rangle$ is a column vector. Note that the representation is basis-independent.

Inner product $\langle\phi|\psi\rangle = \int_{-\infty}^{\infty}\phi^*(x)\psi(x)dx$. Note that $\langle\psi|\psi\rangle = 1$ by normalization.

Expectation value $\langle\hat{A}\rangle \equiv \langle\psi|A|\psi\rangle = \int dx\psi^*(x)\hat{A}\psi(x)$. Note also the conjugate: $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$.

Operators Consider the momentum operator: $\langle p\rangle = \langle\psi|p|\psi\rangle = \langle\psi|p\psi\rangle$ because $\hat{p}|f\rangle = |g\rangle$, the operator acting on a ket gives another ket. Integrating by parts (and ignoring the boundary term), we note that $\langle\psi|p\psi\rangle = \langle p\psi|\psi\rangle = \langle\psi|p\psi\rangle^*$. Hence we have that $\langle\psi|p\psi\rangle$ is purely real.

Hermiticity Operators corresponding to observable quantities are always Hermitian. To each operator $\hat{A}$, there exists a Hermitian conjugate $\hat{A}^\dagger$ such that $\langle\psi|\hat{A}\phi\rangle = \langle\hat{A}^\dagger\psi|\phi\rangle$ for all ψ,ϕ in the Hilbert space corresponding to the physical system in study. A Hermitian operator is such that $\hat{A} = \hat{A}^\dagger$.

Matrix Elements Call $\langle\phi|\psi\rangle$ matrix elements. Note that $\langle n|\hat{A}|m\rangle$ is an off-diagonal matrix element and the diagonal elements have $m = n$. Note further that $(M^*)^T = M^\dagger$. If there are off-diagonal elements, then the state will make transitions

between states over time (off-diagonal elements govern time-evolution and transitions between states).

Time evolution of expectation values

$$\begin{aligned}
\frac{d}{dt}\langle\hat{A}\rangle &= \int dx \left(\partial_t\psi^*\hat{A}\psi + \psi^*\partial_t\hat{A}\psi + \psi^*\hat{A}\partial_t\psi\right) \\
&= \int dx \left(\frac{-(\hat{H}\psi)^*}{i\hbar}\hat{A}\psi + \psi^*\partial_t\hat{A}\psi + \psi^*\hat{A}\frac{\hat{H}\psi}{i\hbar}\right), \quad \text{by TDSE} \\
&= \frac{1}{i\hbar}\left[\langle\psi|\hat{A}\hat{H}|\psi\rangle - \langle\hat{H}\psi|\hat{A}\psi\rangle\right] + \langle\hat{\dot{A}}\rangle \\
&= \frac{1}{i\hbar}\left[\langle\psi|\hat{A}\hat{H}|\psi\rangle - \langle\psi|\hat{H}^\dagger\hat{A}\psi\rangle\right] + \langle\hat{\dot{A}}\rangle \\
&= \frac{1}{i\hbar}\left[\langle\psi|\hat{A}\hat{H}|\psi\rangle - \langle\psi|\hat{H}\hat{A}\psi\rangle\right] + \langle\hat{\dot{A}}\rangle \\
&= \frac{1}{i\hbar}\left[\langle\psi|\hat{A}\hat{H} - \hat{H}\hat{A}|\psi\rangle\right] + \langle\hat{\dot{A}}\rangle \\
&= \frac{1}{i\hbar}\left[\langle\psi|[\hat{A},\hat{H}]|\psi\rangle\right] + \langle\hat{\dot{A}}\rangle \\
&= \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle + \langle\frac{\partial\hat{A}}{\partial t}\rangle
\end{aligned}$$

Canonical Commutation relation Consider $[\hat{x},\hat{p}]$. Consider its operation on a general function. Then we have:

$$[\hat{x},\hat{p}] = i\hbar$$

Note that when operators do not commute, then we have an uncertainty relation.

Ehrenfest's Theorem

$$\frac{d}{dt}\langle\hat{A}\rangle = \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle + \langle\frac{\partial\hat{A}}{\partial t}\rangle$$

Consider the operator $\hat{A} = 1$. It obviously commutes with the Hamiltonian and has zero time derivative. Hence $\langle\hat{A}\rangle = 0$. This means that the normalisation of a wave function does not change in time $\implies$ probability is "conserved".

Consider the Hamiltonian operator. Clearly, it commutes with itself and has no time dependence (for time-invariant potentials). Hence $\langle\hat{H}\rangle = 0$.

Consider the position operator. Note that the commutator is distributive and we can calculate $[\hat{x},V(\hat{x})] = 0, [\hat{x},\hat{H}] = \frac{1}{2m}[\hat{x},\hat{p}^2] = \frac{i\hbar}{m}\hat{p}$ and we have $\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle\hat{p}\rangle$, analogous to classical mechanics.

Consider the momentum operator. Then we have: $[\hat{p},\frac{\hat{p}^2}{2m}] = 0$ but $[\hat{p},V(\hat{x})] \neq 0$ because we know that the momentum does not commute with position. We write:

$$\begin{aligned}
[\hat{p},V(\hat{x})]\psi(x) &= pV\psi - Vp\psi \\
&= \frac{\hbar}{i}\left[V\psi' + V'\psi - V\psi'\right] \\
&= \frac{\hbar}{i}\hat{V}'
\end{aligned}$$

Putting this into Ehrenfest's theorem, we obtain:

$$\frac{d}{dt}\langle p\rangle = -\left\langle\frac{\partial V}{\partial x}\right\rangle$$

Chapter 4

Week 4

4.1 Tuesday 27 Jan 2015

Uncertainty relation from commutators

$$\Delta A \Delta B \geq \frac{1}{2}\left|\left\langle [\hat{A}, \hat{B}] \right\rangle\right|$$

Cauchy-Schwartz inequality

$$|\langle \phi|\psi\rangle| \leq |\psi||\phi| = \sqrt{\langle \psi|\psi\rangle}\sqrt{\langle \phi|\phi\rangle}$$

Spin Uncertainty

$$[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z \implies \Delta S_x \Delta S_y \geq |\langle S_z\rangle| \frac{\hbar}{2}$$

Stationary states If $\hat{H}$ does not have dependence on time, then by Ehrenfest's theorem, $\frac{d}{dt}\langle \hat{H}\rangle = 0$. Also note that $\hat{x}, \hat{p}$ are not explicitly dependent on time, although their expectation values may. Note further that energy eigenstates are stationary in the sense that $|\Psi(\vec{r}, t)|^2$ is time-independent. Hence electrons in atomic wave functions don't accelerate, leading to the stability of atoms.

Parity operator Define $\hat{\mathbb{P}} f(x) = f(-x)$. In 3D, $\hat{\mathbb{P}} f(\vec{r}) = f(-\vec{r})$. In spherical coordinates, the parity operator performs the following operation:

$$\begin{aligned} r &\to r \\ \theta &\to \pi - \theta \\ \phi &\to \phi + \pi \end{aligned}$$

Eigensystem of the Parity operator Note that $\hat{\mathbb{P}}^2|\psi\rangle = p^2|\psi\rangle = |\psi\rangle \implies p^2 = 1 \implies p = \pm 1$. Hence there are two eigenvalues and correspondingly two eigenfunctions. When $p = 1$, $|\psi\rangle$ is unchanged, so call it an even function. For $p = -1$, we have an odd function. Hence the eigenfunctions are even and odd functions of space. Hence we may write:

$$\hat{\mathbb{P}} f_{\pm}(x) = \pm f_{\pm}(x)$$

where f_+ is an even function and f_- is an odd function. Note that any function can be written as a linear superposition of an even and an odd function.

Projectors Consider a projector in parity: $\hat{\Pi}_{\pm} \equiv \frac{1}{2}\left(1 \pm \hat{\mathbb{P}}\right)$. Note that $\hat{\Pi}_{\pm} f(x) = \frac{1}{2}\left(f(x) \pm f(-x)\right) = f_{\pm}(x)$. This operator hence projects out the even or odd operator of a general function. Note that $\hat{\Pi}_{\pm}^2 = f_{\pm}(x)$ as well. Projection operators, when applied multiple times, gives the same answer as if it were applied once:

$$\hat{\Pi}^n = \hat{\Pi}, n \geq 1$$

Application of Projection Operators If the potential is even, then the parity operator commutes with the Hamiltonian.

Proof Let $\phi(x)$ satisfy the TISE: $\hat{H}\phi = E\phi$. Apply the parity operator to both sides: $\hat{\mathbb{P}}\hat{H}\phi = \hat{\mathbb{P}}E\phi = E\hat{\mathbb{P}}\phi$. But note that $\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ is invariant under a change $x \to -x$ if $V(x)$ is even. Hence $\hat{\mathbb{P}}\hat{H}\phi = \hat{H}(\hat{\mathbb{P}}\phi)$. Combining $E\hat{\mathbb{P}}\phi = \hat{H}(\hat{\mathbb{P}}\phi)$. But this is precisely an eigenvalue equation, and we note that $\hat{\mathbb{P}}\phi$ is an eigenstate of $\hat{H}$ with the same eigenvalue E. Note further that any linear combination of ϕ and $\hat{\mathbb{P}}$ will also be an eigenstate of $\hat{H}$ with the same eigenvalue. Hence $\frac{\phi \pm \hat{\mathbb{P}}\phi}{2} = \hat{\Pi}_{\pm}\phi$ also describe eigenfunctions of $\hat{H}$ with the same energy E.

Eigenfunctions of commuting operators If there are two operators that commute, then it is possible to find simultaneous eigenfunctions of both operators. Hence if two (Hermitian?) operators commute, their matrix representations can be simultaneously diagonalised. Mathematically, a set of diagonalisable matrices (of which Hermitian matrices are a subset) commutes iff the set is simultaneously diagonalisable. For example, since the parity operator and Hamiltonian operator commute in the infinite square well case, the energy eigenstates are also parity eigenstates (alternate between even and odd).

Conservation laws Consider a constant zero potential. Then consider the wave function displaced by an amount δx. Write the Taylor expansion:

$$\phi(x + \delta x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{d^n\phi}{dx^n}\right|_{x=0} (\delta x)^n$$

Writing the derivative using the momentum operator, we obtain:

$$\phi(x + \delta x) = \sum_{n=0}^{\infty} \frac{(\delta x)^n}{n!} \left(\frac{i}{\hbar}\hat{p}\right)^n \phi(x) = e^{i\delta x\hat{p}/\hbar}\phi(x)$$

Call $e^{i\delta x\hat{p}/\hbar}$ the displacement operator $\hat{D}(\delta x)$. Then, noting that each power of $\hat{p}$ commutes with the Hamiltonian, $\hat{D}(\delta x)$ also commutes with the Hamiltonian. Then we have:

$$E(\hat{D}\phi) = \hat{H}(\hat{D}\phi)$$

and $\hat{D}\phi$ is also an eigenfunction of $\hat{H}$ with the same energy E. Then this means that we can take the original wave function, displace it in the position axis, and obtain another eigenfunction with the same energy. This corresponds to space-translation invariance (symmetry) and conservation of linear momentum.

$\frac{d}{dt}\hat{H} = 0$ corresponds to time-translational invariance, which is the conservation of energy.

Noether's theorem Correspondence between symmetry and conservation laws. Consider an operator $\hat{A}$ that commutes with the Hamiltonian. Then we can write a unitary displacement operator $D(\delta a) = e^{i\delta a\hat{A}/\hbar}$ applied results in an eigenfunction with the energy unchanged. The unitary time translation operator $\hat{U} = e^{i\delta t\hat{H}/\hbar}$ gives $U\psi(x,t) = \psi(x, t + \delta t)$.

4.2 Recitation 27 Jan 2015

Axioms of QM

1. States: A complete description of a physical system. A ray in a Hilbert space.
2. Observable: A Hermitian operator
3. Time evolution: Governed by the Schrodinger equation.
4. Measurement.

Hilbert space: A vector space over the complex numbers with an inner product, and is complete in the norm.

Ray: Equivalence class of vectors. Define a vector multiplied by a complex constant to be equivalent to the vector itself.
Identity

$$|\phi\rangle = \sum_i |i\rangle\langle i|\phi\rangle$$

4.3 Thursday 29 Jan 2015

Symmetries and Commutators Recall we may write the TDSE as

$$|\Psi(t+dt)\rangle = e^{idt\hat{H}/\hbar}|\Psi(t)\rangle$$

The evolution operator $\hat{U} = e^{idt\hat{H}/\hbar}$ is unitary in the sense that it preserves normalisation. Note that we can write the operator in Taylor expansion form to obtain that $[\hat{U}, \hat{H}] = 0$, giving time-translation invariance symmetry.

Momentum Note that $[\hat{p}, \hat{H}] = 0$ under the assumption that $V(x) =$ constant. The eigenstates are de Broglie waves, and by Ehrenfest's theorem, we have $\frac{d}{dt}\langle p\rangle = 0$. In this case, the position displacement operator can be written as $\hat{D} = e^{idx\hat{p}/\hbar}$, which commutes with the Hamiltonian as well. When applied to the wave function,

$$|\Psi(x+dx)\rangle = e^{idx\hat{p}/\hbar}|\Psi(x)\rangle$$

This indicates spatial displacement invariance (homogeneity).

Angular momentum Consider $[\hat{L}, \hat{H}] = 0$. Then we can get simultaneous energy and angular momentum eigenstates. Now consider the Hamiltonian: $\hat{H} = \frac{\hat{p}^2}{2m} + V(\vec{r})$. The first term in the Hamiltonian has a dot product of $\hat{p}$ and hence is invariant under rotations. If we insist that $V(\vec{r})$ is independent of angle, then we will get that $\frac{d}{dt}\langle\vec{L}\rangle = 0$, and angular momentum is conserved. Hence symmetry under rotations implies conservation of angular momentum. Define the angular displacement operator $\hat{R} = e^{id\vec{\theta}\cdot\vec{L}/\hbar}$. Then $[\hat{R}, \hat{H}] = 0$, which is a condition of isotropy in space.

Parity The parity operator commutes with the Hamiltonian $[\hat{P}, \hat{H}] = 0$. The associated conservation law is that parity is conserved. A system in a particular state of parity will remain in that state of parity under time evolution.

Types of symmetries Time, linear space, angular space are continuous symmetries (and conservation laws) of nature. However, parity is a discrete symmetry.

Relativistic systems Recall that we can perform Lorentz boosts that preserve the dot products between four-vectors. Under this symmetry, there exists a set of Lorentz invariant quantities (such as mass). The boost operator commutes with the Hamiltonian.

More discrete symmetries Time direction, charge conjugation (particles to antiparticles and vice versa).

TISE solutions in 1D Define $U(x) = \frac{2m}{\hbar^2}V(x), \mathcal{E} = \frac{2mE}{\hbar^2}$. Then we have the ODE:

$$\phi'' + [\mathcal{E} - U(x)]\phi = 0$$

Case 1a: Uniform potential $\mathcal{E} > U_0$, classically allowed, and $U(x) = U_0$ everywhere. Then $\phi(x) = Ae^{ikx} + Be^{-ikx}, k^2 = \mathcal{E} - U_0$.

Case 1b: Uniform potential $\mathcal{E} < U_0$, classically disallowed, $U(x) = U_0$ everywhere. Then $\phi(x) = Ae^{\kappa x} + Be^{-\kappa x}, \kappa^2 = U_0 - \mathcal{E}$. Observe that all $\phi(x)$ cannot be normalised. Hence there is no quantum state.

Case 2: Potential step Let $U(x) = U_0\theta(x)$ where θ is the Heaviside step function. The boundary conditions ensure that the exponentially growing solution is zero and the only wave function in the $x > 0$ region is the exponentially decaying wave function. Then we require that both the $\phi(x)$ and $\phi'(x)$ functions are continuous everywhere. Note that in the classically forbidden region, we will only have one exponential term (the one that does not blow up at the infinities). The wave will be reflected in such a way that the boundary condition at the interface allows for exactly the single exponential term alone (this is quantisation!). We can use the WKB solution to write $\phi = e^{\int \kappa(x)dx}$ or $\phi = e^{-\int \kappa(x)dx}$ in the classically disallowed region.

Chapter 5

Week 5

5.1 Lecture 03 Feb 2015

Quantum Harmonic Oscillator

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

Dimensionless version Define $E = \hbar\omega = \mathcal{E}$, where $\mathcal{E}$ is a unitless "energy". Define $x = \sqrt{\frac{\hbar}{m\omega}}z$ where z is the unitless "length". Define $t = \frac{\tau}{\omega}$, where τ is a dimensionless "time". Then we have:

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial z^2} + \frac{1}{2}z^2\right)\psi(z) = \mathcal{E}\psi(z)$$
$$\psi''(z) = (z^2 - 2\mathcal{E})\psi(z)$$

Asymptotic solutions at $x \to \pm\infty$. Observe that at large z, $\psi'' = z^2\psi$. This has solution $\psi(z) = e^{-z^2/2}$. Then we make the ansatz: $\psi(z) = e^{-z^2/2}\sum_{n=0}^{\infty} a_n z^n$. Substituting this into the ODE, we obtain:

$$\sum_{n=0}^{\infty}\left[n(n-1)a_n z^{n-2} - 2na_n z^n + (2\mathcal{E}-1)a_n z^n\right] = 0$$

Re-indexing,

$$\sum_{n=0}^{\infty}\left[(n+2)(n+1)a_{n+2}z^n - 2na_n z^n + (2\mathcal{E}-1)a_n z^n\right] = 0$$

Then we obtain the recursion relation:

$$(n+2)(n+1)a_{n+2} - 2na_n + (2\mathcal{E}-1)a_n = 0, n \geq 0$$
$$\implies a_{n+2} = \frac{2n+1-2\mathcal{E}}{(n+2)(n+1)}a_n$$

But we want normalizable solutions. Hence we need to cut the polynomial off for some n. Then we require $2n+1-2\mathcal{E} = 0$ for some n. Otherwise, we note that for large n,

$$\frac{a_{n+2}}{a_n} = \frac{2}{n}$$

which forms an infinite series that increases as e^{z^2}, which, hence multiplied by e^{-z^2}, reaches infinity at $z \to \pm\infty$.

The polynomials for $\mathcal{E} = p + \frac{1}{2}, p \in \mathbb{Z}, p \geq 0$ described by the recursion relation are the Hermite polynomials. Then we have solutions that look like:

$$\psi_n = C_n H_n\left(\frac{x}{b}\right) e^{-x^2/2b^2}, b = \sqrt{\frac{\hbar}{m\omega}}$$

where C_n is there to normalise the wave function. Note that these are Hamiltonian eigenstates (by construction) and are also parity eigenstates (Hermite polynomials are either even or odd). In fact, $\hat{\mathbb{P}}\psi_n(x) = (-1)^n\psi_n(x)$.

Normalizing,

$$|C_n|^2 = \frac{1}{2^n n!\sqrt{\pi}}$$

Wavepackets in the QHO Note that the QHO wave packets disperse as they propagate from one end to another but they collect back to the initial position (reflected in the position axis), then bounce back to the original position and shape. These are called coherent states and are unique to the quantum harmonic oscillator.

Alternative solution to QHO Recall that the TDSE can be written as $\hat{H}\psi(x) = E\psi(x)$. Then write the Hamiltonian as $\hat{H} = H\hbar\omega$, where H is a dimensionless operator. Define the generalised particle position operator $\hat{Q} = \sqrt{\frac{m\omega}{\hbar}}\hat{x}$ and the generalized momentum operator: $\hat{P} = \frac{\hat{p}}{\sqrt{m\omega\hbar}}$. Then we can write: $H = \frac{1}{2}(P^2 + Q^2)$. Note that all these are Hermitian operators. Also, we have the canonical commutation relationship: $[Q, P] = i$, which can be re-written as $P = -i\frac{\partial}{\partial Q}$. Define the operator $a = \frac{1}{\sqrt{2}}(Q + iP)$ and the adjoint $a^\dagger = \frac{1}{\sqrt{2}}(Q - iP)$. These operators are not Hermitian. Expressing Q and P in terms of a,

$$Q = \frac{1}{\sqrt{2}}(a + a^\dagger)$$
$$P = \frac{-i}{\sqrt{2}}(a - a^\dagger)$$

Then the Hamiltonian is:

$$H = \frac{1}{2}(aa^\dagger + a^\dagger a)$$

The commutator for a and $a^\dagger$ is:

$$[a, a^\dagger] = 1$$

So the Hamiltonian is:

$$H = \frac{1}{2} + a^\dagger a$$

Define the operator $\hat{N} = a^\dagger a$. We want to find the eigenvalues and eigenstates of $\hat{N}$, and by extension we have the eigensystem for the Hamiltonian.

Note that $\langle H\rangle = \frac{1}{2}\langle P^2\rangle + \frac{1}{2}\langle Q^2\rangle \geq 0$. We also note that:

$$\langle\psi|N|\psi\rangle = \langle\psi|a^\dagger a|\psi\rangle = \langle a\psi|a\psi\rangle \geq 0$$

Hence the expectation value of $\hat{N}$ is non-negative. Now to examine the eigenvalue equation:

$$N|n\rangle = n|n\rangle$$

where $|n\rangle$ is the eigenstate labelled by n (shorthand). Note that

$$Na|n\rangle = a^\dagger aa|n\rangle = (aa^\dagger - 1)a|n\rangle = a(a^\dagger a - 1)|n\rangle = a(n-1)|n\rangle$$

Hence we observe that $a|n\rangle$ is an eigenstate of N with eigenvalue $n-1$. Hence it must be proportional to the eigenstate $|n-1\rangle$. It can also be shown that $a^\dagger|n\rangle = c'_n|n+1\rangle$.

Now by repeated application of a, we can reduce the eigenvalue. But we note that this cannot continue indefinitely because the expectation value of N is non-negative. Let the lowest state be $|n_0\rangle$. Then $a|n_0\rangle = 0$. Hence $n_0 = 0$. Then the allowed values of n are non-negative integers.

Let c_n be such that $|n\rangle$ is normalized. Then $\langle n|a^\dagger a|n\rangle = n\langle n|n\rangle = |c_n|^2\langle n-1|n-1\rangle \implies c_n = \sqrt{n}$. Hence:

$$\begin{gathered} a|n\rangle = \sqrt{n}|n-1\rangle \\ a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \\ N|n\rangle = n|n\rangle \end{gathered}$$

Returning to the Hamiltonian,

$$\hat{H}\psi_n = (\hat{N} + \frac{1}{2})\hbar\omega\psi_n$$

Hence the eigenvalues of the Hamiltonian are $E_n = (n+\frac{1}{2})\hbar\omega$, and the eigenstates are $|\psi(t)\rangle = |n\rangle e^{-i(n+\frac{1}{2})\omega t}$.

5.2 Recitation 03 Feb 2015

Noether's theorem Define a symmetry as an operation that does not change the things we observe about it (i.e. the eigenvalues of Hermitian operators). Note that the operation $|\psi\rangle \to |\psi'\rangle$ can be represented by the operation of a unitary operator: $|\psi'\rangle = U|\psi\rangle, UU^\dagger = \mathbb{I}$. Consider a unitary matrix implementing symmetry R_1 and another of R_2. Then we have $U(R_1)U(R_2) = U(R_2 \circ R_1)$. Note that the time evolution of a unitary operator is given by $U(R)e^{-i\hat{H}t/\hbar}$, which can also be written as $e^{-it\hat{H}/\hbar}U(R)$. This is the requirement that the unitary operator commutes with the Hamiltonian. If the symmetry is continuous, U can be expanded in the form $U = e^{i\epsilon Q}$ where we call Q the charge. Q commutes with the Hamiltonian, and Q is the conserved quantity. Consider momentum. It commutes with the Hamiltonian (clearly, since it commutes with itself). Then we define the operator $U = e^{iap} = e^{a\hbar(\partial/\partial x)}$. Note that when operating on a wave function, we can expand the operator in a Taylor series to obtain $U(p)\psi(x) = \psi(x + a\hbar)$.

5.3 Lecture 05 Feb 2015

Summary Recall the QHO solution in "number" space:

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

with the generalised coordinates and momenta:

$$\begin{gathered} \hat{Q} = \sqrt{\frac{m\omega}{\hbar}}\hat{x} \\ \hat{P} = \frac{\hat{p}}{\sqrt{m\omega\hbar}} \\ \implies \hat{H} = \frac{1}{2}(\hat{Q}^2 + \hat{P}^2) \\ [\hat{Q}, \hat{P}] = i \end{gathered}$$

and defined the creation and annihilation operators:

$$Q = \frac{1}{\sqrt{2}}(a + a^\dagger)$$
$$P = \frac{-i}{\sqrt{2}}(a - a^\dagger)$$
$$\implies a = \frac{1}{\sqrt{2}}(Q + iP)$$
$$\implies a^\dagger = \frac{1}{\sqrt{2}}(Q - iP)$$
$$\implies [a, a^\dagger] = 1$$

Hence we may write the hamiltonian as:

$$\hat{H} = \hbar\omega(a^\dagger a + \frac{1}{2})$$

and define the number operator:

$$N = a^\dagger a$$
$$\implies H = \hbar\omega(N + \frac{1}{2})$$

with associated eigenstates:

$$N|n\rangle = n|n\rangle$$

such that the hamiltonian eigenstates are

$$H|n\rangle = \hbar\omega(n + \frac{1}{2})|n\rangle$$

Now we note the effect of the individual raising or lowering a operators:

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

We require a ground state with an expectation value that is non-negative $\langle N\rangle \geq 0$, and such that the annihilation operator operating on it gives the zero element:

$$a|a_0\rangle = 0$$

Call the ground state $n = 0$. Then $|n\rangle$ are the QHO eigenstates, and are stationary states. Call this a state of n quanta.

QHO wave packets Recall that a travelling wave packet starting from one end of the quadratic potential well coheres back at the other end even though it disperses in the middle. We examine this phenomena in number space. Write the general wave packet as a linear superposition of energy eigenstates:

$$|\phi_0(t = 0)\rangle = \sum_m a_m|m\rangle$$

Note that in coordinate space, we can write: $\psi_m(x) = c_m H_m(x)e^{-x^2/2b^2}, b = \sqrt{\frac{\hbar}{m\omega}}$, but we do not need to know this explicitly.

We then apply the bra on both sides:

$$\langle n|\phi_0\rangle = \sum_m a_m\langle n|m\rangle$$

The eigenstates are orthonormal by construction, hence we have that the sum is just a_n. Hence we can write:

$$|\phi_0\rangle = \sum_m |m\rangle\langle m|\phi_0\rangle$$

Recall that $\langle m|\psi_0\rangle$ is just a number:

$$\langle m|\psi_0\rangle = \int_{-\infty}^{\infty} dx \psi_m^*(x)\phi_0(x, t=0)$$

Then we have the identity:

$$\sum_m |m\rangle\langle m| = \mathbb{I}$$

We can also insert the time dependence:

$$|\phi_0(t)\rangle = \sum_m |m\rangle e^{-iE_m t/\hbar}\langle m|\phi_0(t=0)\rangle = e^{-i\tau/2}\sum_m |m\rangle e^{-im\tau}\langle m|\phi_0(t=0)\rangle, \tau = \omega t$$

where we let τ be the unitless time. We pick times where $\tau = p\pi, p \in \mathbb{Z}$. Then $e^{-im\tau} = e^{-imp\pi} = 1$ if p is an even integer. Then at those times, the wave function is back to the initial conditions. Hence the motion is periodic. If p is an odd integer, and m is odd, then $e^{-ipm\pi} = -1$. Then all the odd m terms have their sign flipped. But the eigenstates of the Hamiltonian are also parity eigenstates with parity eigenvalue $(-1)^m$. Hence if m is odd, then the eigenstate is an odd function. Hence if we flip the sign of all the odd functions and not touch the even functions, we will get $\phi(x, \tau = p\pi) = \phi(-x, t = 0)$. Hence we will have a wave packet that is flipped in the x-axis.

Charged particle Consider the EM radiation emitted by a particle in QHO well. Recall that the power of an oscillating dipole is given as:

$$P = \frac{2}{3c^2}|\ddot{d}|^2, d = qx, \ddot{d} = q\ddot{x}$$

In QM, we construct the operator corresponding to $\langle\ddot{d}\rangle$ to be $q\frac{d^2}{dt^2}\langle x\rangle$. Note that if the wave function is a parity wave function like in the QHO eigenstates, then $\langle x\rangle = \int \psi^*(x)x\psi(x)dx = 0$ because the magnitude squared will always be even. Hence there will not be any radiation if the charge distribution is symmetric.

On the other hand, if the particle is not in an energy eigenstate, it may have a non-zero dipole moment:

$$P = \frac{2q^2}{3c^3}\frac{d^2}{dt^2}|\langle\psi|x|\psi\rangle|^2, |\psi\rangle = \sum_n c_n|n\rangle$$

Hence:

$$\langle\psi|x|\psi\rangle = \sum_{n,m} c_n c_m^*\langle m|x|n\rangle e^{-i(E_n - E_m)t/\hbar}$$

We can split this into the diagonal and non-diagonal term, and note that the matrix is going to be symmetric under the inversion $m \leftrightarrow n$.

$$\sum_n |c_n|^2\langle n|x|n\rangle + 2\sum_{n>m}\langle m|x|n\rangle\left[\Re(c_n c_m^*)\cos\left[(E_n - E_m)t/\hbar\right] + \Im(c_n c_m^*)\sin\left[(E_n - E_m)t/\hbar\right]\right]$$

Clearly, the diagonal terms are going to be zero under the time derivative. But the diagonal terms have non-zero derivative because of the time dependence. Observe that $\langle m|x|n\rangle$ is a transition from $|n\rangle$ to $|m\rangle$ with $\Delta E = E_n - E_m$. It will emit or absorb a photon of the energy difference. Write using the raising and lowering operator (recalling that $Q = \frac{x}{b}$):

$$\langle m|Q|n\rangle = \frac{1}{\sqrt{2}}\langle m|a + a^\dagger|n\rangle = \frac{1}{\sqrt{2}}\left[\langle m|a|n\rangle + \langle m|a^\dagger|n\rangle\right] = \frac{1}{\sqrt{2}}\left[\sqrt{n}\langle m|n-1\rangle + \sqrt{n+1}\langle m|n+1\rangle\right]$$
$$= \frac{1}{\sqrt{2}}\left[\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right]$$

Note that for $\langle m|x|n\rangle$ to be non-zero, m is either $n-1$ or $n+1$. Hence changes must be changes in ± 1. The parity hence changes in such a transition. This is called the **Parity Selection Rule**.

Now consider the dipole operator: $d = qbQ$. We can write the operator as a matrix:

$$\langle m|Q|n\rangle = Q_{mn}$$
$$Q_{mn} = \frac{1}{\sqrt{2}}\left[\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right]$$

This is the operator in number basis space. Note that the matrix is symmetric and the elements are real. Recall that the Hermitian conjugate of a matrix is the conjugate transpose. Hence a real symmetric matrix is Hermitian.

Chapter 6

Week 6

6.1 Tuesday Lecture 10 Feb 2015

Zero-point energy All binding potentials have a zero-point energy.

Total energy in EM field:

$$E = \int d\vec{k} \left(n + \frac{1}{2} \right) \hbar\omega(\vec{k})$$

where we treat n to be the number of photons occupying each mode (the occupation number). Hence at the ground state, $T = 0$, the energy becomes the integral of the zero point energy (clearly diverges).

Relation between infinite square well and QHO Note that the ground state energy of the square well is $\frac{\hbar^2\pi^2}{2mL^2}$. The characteristic oscillator length is $b = \sqrt{\frac{\hbar}{m\omega}}$. Then we can replace $L = b$.

Coulomb potential Wavefunctions vanish at $r = 0$.

6.2 Tuesday Recitation 10 Feb 2015

Symmetries and conservation laws Consider a unitary operator $U : |\psi\rangle \to |\psi'\rangle$, $UU^\dagger = \mathbb{I}$.

Time symmetry: Should not matter if I do the operation and then wait time t, or wait time t and do the operation.

$$Ue^{-it\hat{H}/\hbar}|\psi\rangle = e^{-it\hat{H}/\hbar}U|\psi\rangle$$

which only holds when $[\hat{H}, \hat{U}] = 0$. For continuous symmetries, we can perform a first order approximation to write:

$$U = \mathbb{I} - i\epsilon\hat{Q} + O(\epsilon^2) \implies U = e^{-i\Theta\hat{Q}/\hbar}$$

Then for Q to be a conserved quantity, $[H, Q] = 0$. Then Q is a conserved quantity that generates a symmetry.

Conversely, if an operator $\hat{Q}$ commutes with the Hamiltonian, then the operator generates a symmetry. Write $U = e^{-i\Theta\hat{Q}/\hbar}$.

Translational invariance Consider a free particle with the Hamiltonian $\hat{H} = \frac{p^2}{2m}$. Then $[\hat{p}, \hat{H}] = 0$. Hence we can define the unitary operator for the symmetry $U(a) = e^{-ia\hat{p}/\hbar}$. This operator becomes a translation in space. Hence we have translational invariance.

Time translation The Hamiltonian commutes with itself. Then we write the operator that generates the symmetry $U = e^{-i\hat{H}t/\hbar}$ which translates the wave function in time.

Change of basis Recall that $\psi(x) = \langle x|\psi\rangle$. Then we can write $|\psi\rangle = \int dx\psi(x)|x\rangle$. To find the components, $\langle x'|\psi\rangle = \int dx'\psi(x)\langle x'|x\rangle = \psi(x')$.

In momentum eigenstates Let the identity be written in momentum eigenstates:

$$\mathbb{I} = \int dp|p\rangle\langle p|$$

Then,

$$|\psi\rangle = \int dx\psi(x) \int dp|p\rangle\langle p|x\rangle$$

We can obtain the inner product for the momentum and position:

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-i\hat{p}\hat{x}/\hbar}$$

which comes from solving the differential equation:

$$-i\hbar\frac{\partial}{\partial x}\langle x|p\rangle = \hat{p}\langle x|p\rangle$$

Hence we can write:

$$|\psi\rangle = \int dp \left(\int \frac{dx}{\sqrt{2\pi\hbar}} e^{-i\hat{p}\hat{x}/\hbar}\psi(x) \right) |p\rangle = \int dp\mathcal{F}(p)|p\rangle$$

where we define the Fourier transform:

$$\mathcal{F}(p) = \int \frac{dx}{\sqrt{2\pi\hbar}} e^{-i\hat{p}\hat{x}/\hbar}\psi(x)$$

Quantum Harmonic Oscillator Recall the Hamiltonian: $\hat{H} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$ and the ladder operators:

$$a = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{i}{m\omega}\hat{p})$$
$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{i}{m\omega}\hat{p})$$

which can also be written as:

$$\hat{x} = \sqrt{\frac{\hbar}{m\omega}}(a + a^\dagger)$$
$$\hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a)$$

The commutator $[a, a^\dagger] = 1$. So the Hamiltonian becomes:

$$\hat{H} = \hbar\omega(a^\dagger a + \frac{1}{2})$$

We can show that

$$\hat{H}(\hat{a}|\psi\rangle) = (-\hbar\omega + E)\hat{a}|\psi\rangle$$

where $\hat{H}|\psi\rangle = E|\psi\rangle$. Then we see that $\hat{a}$ is a lowering operator.

Similarly,

$$\hat{H}(\hat{a}^\dagger|\psi) = (\hbar\omega + E)\hat{a}^\dagger|\psi\rangle$$

Chapter 7

Week 7

7.1 Tuesday 17 Feb 2015

Hilbert space

- Linear: If $|f\rangle, |g\rangle$ are states in the Hilbert space, then $a|f\rangle + b|f\rangle$ is also a state in Hilbert space.
- Dual space. For every $|f\rangle$ there exists a dual $\langle f|$ that defines an inner product $\langle f|f\rangle \in \mathbb{C}$.
- Norm. We can define the norm of a state $\langle f|f\rangle = \int dx \langle f|x\rangle\langle x|f\rangle$. Recall that $f(x) = \langle x|f\rangle$, so $\langle f|x\rangle = f^*(x)$. We can write it in momentum space as well: $\int dk \langle f|k\rangle\langle k|f\rangle$.
- Completeness: $\int dx|x\rangle\langle x| = \mathbb{I}, \int dk|k\rangle\langle k| = \mathbb{I}$.

Levi-Civita tensor

$$\epsilon_{ink} = \begin{cases} 0, & i = j, j = k, i = k \\ +1, & i, j, k = (1,2,3), (2,3,1), (3,1,2) \\ -1, & i, j, k = (1,3,2), (2,1,3), (3,2,1) \end{cases}$$

Photon spatial wave function For one photon, write $\Psi(\vec{r}) = Ne^{i\vec{k}\cdot\vec{r}} = N\langle x|k_x\rangle\langle x|k_y\rangle\langle z|k_z\rangle$. For a linear superposition (i.e. wavepacket), $\Psi = \int d\vec{k} f(\vec{k}) e^{i\vec{k}\cdot\vec{r}}$. Ψ for a wavepacket lives in a Tensor Product Hilbert Space, which is spanned by $\sum (|x\rangle\langle x|) \otimes (|y\rangle\langle y|) \otimes (|z\rangle\langle z|) = \sum_{i,j,k}^{1,2,3} |x_i x_j x_k\rangle\langle x_i x_j x_k|$ where $|xyz\rangle = |x\rangle|y\rangle|z\rangle$.

Polarisation Direction of the electric field in vacuum is transverse to the direction of motion, which comes from the $\nabla \cdot \vec{E} = 0 \implies \vec{k} \cdot \vec{E} = 0 \implies \vec{E} \perp \vec{k}$. Now write the polarisation of the wave function as a function multiplying the spatial wave function. Note that the polarisation is not a spatial wave function since it does not depend on position. Then the wave function of a single photon travelling in the z direction is:

$$\Psi = \Psi_{pol}\Psi_{spatial} = (a|x\rangle + b|y\rangle)Ne^{ik_z z}$$

Polarization space

$$\text{Right circular polarisation: } \frac{1}{\sqrt{2}}(|x\rangle + i|y\rangle)$$
$$\text{Left circular polarisation: } \frac{1}{\sqrt{2}}(|x\rangle - i|y\rangle)$$
$$\text{Longitudinal polarisation: } |z\rangle$$

Spin and Angular Momentum For spin-1 particles like the photon, the right handed circular polarisation $\frac{1}{\sqrt{2}}(|x\rangle + i|y\rangle)$ is an eigenstate of the angular momentum operator with $l = 1, m = +1$ and $L_z = \hbar$. Left handed circular polarisation is an eigenstate of the angular momentum operator with $l = 1, m = -1, L_z = -\hbar$. Longitudinal polarisation corresponds to $l = 1, m = 0, L_z = 0$.

For spin-1/2 particles like the electron and proton, $\Psi_{electron} = \Psi_{spin}\Psi_{spatial}$. We write Ψ_{spin} as a linear superposition of $|l = 1/2, m = +1/2\rangle, |l = 1/2, m = -1/2\rangle$, which we call spinors.

In general, for N particles, the wave function (include polarisation), lives in $(\mathbb{R}^3 S_3)^N$ space, where the $\mathbb{R}^3$ refers to the polarisation state and the S_3 is the spatial wave function.

7.2 Recitation

Tensor product Consider 2x2 matrices A and B:

$$A \otimes B = \begin{pmatrix} \mathbf{A}B_{11} & \mathbf{A}B_{12} \\ \mathbf{A}B_{21} & \mathbf{A}B_{22} \end{pmatrix}$$

So you get a 4x4 matrix.

Multiple qubits Consider a quit, which has two states: up and down. Let the first Hilbert space have a basis $span\mathcal{H}_1 = \{|\uparrow_1\rangle, |\downarrow_1\rangle\}$ and a second Hilbert space be $span\mathcal{H}_2 = \{|\uparrow_2\rangle, |\downarrow_2\rangle\}$. Hence the tensor product of these two spaces is all possible products:

$$\mathcal{H}_1 \otimes \mathcal{H}_2 = \{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$$

where the double kets indicate the tensor product of the individual kets.

Entanglement When the Hilbert space cannot be written as a tensor product of individual Hilbert spaces.

Approximations using QHO Given a particular Hamiltonian with a particular potential with a minimum at x_0.

$$V(x) = V(x_0) + (x - x_0)V'(x_0) + (x - x_0)^2 \frac{1}{2!}V''(x_0) + \dots$$

at the minimum, we are only interested in the coefficient of the second derivative:

$$m\omega^2 = \left.\frac{\partial^2 V}{\partial x^2}\right|_{x=x_0}$$

so we can write: $V(x) = \frac{1}{2}m\omega^2(x - x_0)^2$ for small oscillations.

Dimensional analysis Note that the wave function has units $1/\sqrt{L}$. A philosophical comment: Nothing physical can depend on something with dimensions. For example, the raising and lowering operators do not have dimension.

7.3 Thursday 19 Feb 2015

Operators as combinations of bra-kets Note that we can write $\hat{A} = \sum_n |a_n\rangle a_n \langle a_n|$, a linear combination of eigenkets, eigenbras and eigenvalues.

Postulates of quantum mechanics

1. A physical system has observables and to each observable we can assign an operator. This gives an eigenvalue equation: $\hat{A}|a_n\rangle = a_n|a_n\rangle$, which gives a set of eigenvalues and associated eigenstates.
2. The state of any physical system can be written as a linear superposition of eigenstates of any observable operator. $|\psi\rangle = \sum_n c_n|a_n\rangle$. The eigenstates of the operator define a Hilbert space in which the physical system wavefunction lives, and the eigenstates span that space. **Corollary:** In general, there will be several such observables in the physical system. Consider the operators that commute with the Hamiltonian. Then we can obtain a complete set of commuting observables (CSCO) - this includes the Hamiltonian itself $\{\hat{H}, \hat{A}, \hat{B}, \dots\}$ - which commute pairwise with each other. The spectrum of the CSCO can be written as a linear combination of kets $\{|E_n, a_m, b_l, \dots\rangle\}$ which will completely span the Hilbert space of the system $|\psi\rangle$. Note further that different states may be associated with same values of E_n (i.e. a_m, b_l are different), and we call these degenerate states. Once we specify the eigenvalues of every one of the CSCO, then there is no more degeneracy, and the state is unique.

3. In between measurements, the wavefunction evolves predictably according to the time-dependent Schrodinger Equation: $i\hbar\frac{\partial|\Psi\rangle}{\partial t} = \hat{H}|\Psi\rangle$. Then if $|\Psi(0)\rangle = \sum_n c_n|E_n, a_m, b_l, \ldots\rangle$, then $|\Psi(t)\rangle = \sum_n c_n|E_n, a_m, b_l, \ldots\rangle e^{-iE_nt/\hbar}$. A perfect measurement will give a result which is one of the eigenvalues associated with the operator, and the probability of obtaining this measurement is $|c_n|^2$ (this is the Born probability hypothesis).

Collapse of wavefunction Suppose we have two observables: $\hat{H}|n\rangle = E_n|n\rangle, \hat{A}|a_n\rangle = a_n|a_n\rangle$. Then after a measurement of the energy, obtaining an eigenvalue E_n, the state of the system is $|\psi\rangle = |n\rangle$. If $[\hat{H}, \hat{A}] = 0$, then the operators can share the same set of eigenstates (i.e. they can be simultaneously diagonalized).

Proof that two operators can share eigenstates if they commute Consider $\hat{A}|a_n\rangle = a_n|a_n\rangle$. Operate on both sides with $\hat{B}$, a commuting operator. Then we have that:

$$\hat{B}\hat{A}|a_n\rangle = \hat{B}a_n|a_n\rangle$$
$$\hat{A}\hat{B}|a_n\rangle = \hat{B}a_n|a_n\rangle \quad \text{since they commute}$$

hence we see that $\hat{B}|a_n\rangle$ is an eigenket of $\hat{A}$ with eigenvalue a_n. Now assume there are no degeneracies. Then it follows that $\hat{B}|a_n\rangle$ must be proportional to $|a_n\rangle$. Call the proportionality constant b_m. Then we see that $\hat{B}|a_n\rangle = b_m|a_n\rangle$, so $|a_n\rangle$ is also an eigenket of $\hat{B}$ with eigenvalue b_m.

Non-commuting observables If $[\hat{A}, \hat{B}] \neq 0$, then we need to write the eigenkets of each operator as a linear superposition of the eigenkets of the other operator: $|b_m\rangle = \sum_n c_n|a_n\rangle$. Hence when an observation is made, the system collapses into a linear superposition of eigenkets of the other operator, thereby perturbing the system, and hence the order of observables matters.

Hamiltonian in momentum basis Consider $\hat{H} = i\hbar\frac{\partial}{\partial t}$. In position space, $\hat{x} = x, \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$. In momentum space, $\hat{p} = p, \hat{x} = \frac{\hbar}{i}\frac{\partial}{\partial p}$, and the wavefunction in the momentum basis is $\langle p|\psi\rangle$. Hence $\hat{H}$ in momentum space can be written as:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}$$

now we need to write $\hat{V}$ in momentum space. Recall in coordinate space, $\langle x|\hat{H}|\psi\rangle = \langle x|\frac{p^2}{2m} + V(x)|\psi\rangle = \langle x|\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}|\psi\rangle + V(x)\langle x|\psi\rangle = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\langle x|\psi\rangle + V(x)\langle x|\psi\rangle$. Now in momentum space,

$$\begin{aligned}
\langle k|\hat{H}|\psi\rangle &= \langle k|\frac{p^2}{2m} + V(x)|\psi\rangle \\
&= \langle k|\frac{p^2}{2m} + \mathbb{I}V(x)\mathbb{I}|\psi\rangle \\
&= \langle k|\frac{p^2}{2m} + \left(\int dk''|k''\rangle\langle k''|\right)V(x)\left(\int dk'|k'\rangle\langle k'|\right)|\psi\rangle \\
&= \langle k|\frac{p^2}{2m}|\psi\rangle + \int dk''dk'\langle k|k''\rangle\langle k''|V(x)|k'\rangle\langle k'|\psi\rangle \\
&= \langle k|\frac{p^2}{2m}|\psi\rangle + \int dk''dk'\delta(k'-k'')\langle k''|V(x)|k'\rangle\psi(k') \\
&= \langle k|\frac{p^2}{2m}|\psi\rangle + \int dk'\langle k|V(x)|k'\rangle\psi(k') \\
&= \langle k|\frac{p^2}{2m}|\psi\rangle + \int dk'dxdx'\langle k|x\rangle\langle x|V(x)|x'\rangle\langle x'|k'\rangle\psi(k') \quad \text{using the same identity trick above} \\
&= \langle k|\frac{p^2}{2m}|\psi\rangle + \int dk'dxdx'\langle k|x\rangle V(x)\delta(x-x')\langle x'|k'\rangle\psi(k')
\end{aligned}$$

Now note that $\langle x'|k'\rangle = \frac{1}{\sqrt{2\pi}}e^{ik'x'}$ and $\langle k|x\rangle = \frac{1}{\sqrt{2\pi}}e^{-ikx}$, which is either the position or momentum space representation of a de-Broglie wave. Hence we may write (after performing the x' integral by noting that there was a delta function):

$$\begin{aligned}
\langle k|\hat{H}|\psi\rangle &= \langle k|\frac{p^2}{2m}|\psi\rangle + \frac{1}{\sqrt{2\pi}}\int dk'dxe^{-ikx}V(x)e^{ik'x}\psi(k') \\
&= \frac{\hbar^2k^2}{2m} + \int\frac{dk'}{\sqrt{2\pi}}V(k-k')\psi(k')
\end{aligned}$$

Matrix mechanics Given $|\psi\rangle = \sum_n c_n|n\rangle$ or $\int dkc(k)|k\rangle$, then the coefficients are: $c_n = \langle n|\psi\rangle, c(k) = \langle k|\psi\rangle$, which is the representation of $|\psi\rangle$ in a basis. We may hence represent the state using a column vector (for the discrete case):

$$\begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \\ \vdots \\ \langle n_{max}|\psi\rangle \end{pmatrix}$$

Note that we may also use a column vector to represent an operator with infinite (continuous) spectra.

Two-state systems Consider a physical system with only two eigenstates (e.g. spin-1/2 particle in a magnetic field): $|1\rangle, |2\rangle$. The magnetic moment of the electron in given by $\vec{\mu} = 2\mu_B\vec{S}$, where $\vec{S}$ is the spin. Then the Hamiltonian is given by $\hat{H} = -\vec{\mu}\cdot\vec{B}$. Consider an operator $\hat{A}$ that does not commute with the Hamiltonian. This operator has a set of eigenstates that differs from the energy eigenstates. Define the energy eigenstates as $|1\rangle, |2\rangle$ with energy eigenvalues E_1 and E_2. We can write the eigenstate of $\hat{A}$ as a linear combination of energy eigenstates

$$\begin{aligned} |a_1\rangle &= T_{11}|1\rangle + T_{12}|2\rangle \\ |a_2\rangle &= T_{21}|1\rangle + T_{22}|2\rangle \end{aligned}$$

We write this in matrix form with linear operator T:

$$T = \begin{pmatrix} |a_1\rangle\langle 1| & |a_1\rangle\langle 2| \\ |a_2\rangle\langle 1| & |a_2\rangle\langle 2| \end{pmatrix}$$

In the energy eigenbasis, the energy eigenstates are, by definition:

$$\begin{aligned} |1\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ |2\rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned}$$

We may also write $\hat{A}$ in its eigenbasis:

$$\begin{pmatrix} \langle a_1|A|a_1\rangle & \langle a_1|A|a_2\rangle \\ \langle a_2|A|a_1\rangle & \langle a_2|A|a_2\rangle \end{pmatrix}$$

but in the energy eigenbasis, $\hat{A}$ looks different:

$$\begin{aligned} \hat{A} &= \left(\sum_{i=1}^{2}|i\rangle\langle i|\right) A \left(\sum_{i=1}^{2}|i\rangle\langle i|\right) \\ &= |1\rangle\langle 1|A|1\rangle\langle 1| + |1\rangle\langle 1|A|2\rangle\langle 2| + |2\rangle\langle 2|A|1\rangle\langle 1| + |2\rangle\langle 2|A|2\rangle\langle 2| \end{aligned}$$

Now bras are row vectors:

$$|\psi\rangle = \begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \end{pmatrix} \iff \langle\psi| = \begin{pmatrix} (\langle\psi|1\rangle)^* & (\langle\psi|2\rangle)^* \end{pmatrix}$$

Expectation Values Consider:

$$\langle\phi|\hat{A}|\psi\rangle = \begin{pmatrix} \langle\phi|1\rangle & \langle\phi|2\rangle \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \end{pmatrix}$$

where $A_{ij} = \langle i|A|j\rangle$.

Chapter 8

Week 8

8.1 Tuesday 24 Feb 2015

Spectral representation of operator $\hat{A} = \sum_{n=1}^{N} |a_n\rangle a_n \langle a_n|$.

Change of basis Consider the energy eigenbasis $\{|n\rangle\}$. Then the representation of operator A in the energy eigenbasis is:

$$\begin{aligned}\hat{A} &= \sum_{n'=1}^{N} |n'\rangle\langle n'| \sum_{n=1}^{N} |a_n\rangle a_n \langle a_n| \sum_{n''=1}^{N} |n''\rangle\langle n''| \\ &= \sum_{n',n''} |n'\rangle \left(\sum_{n=1}^{N} \langle n'|a_n\rangle a_n \langle a_n|n''\rangle \right) \langle n''| \\ &= \sum_{n',n''} |n'\rangle A_{n',n''} \langle n''|\end{aligned}$$

where we define the transformation matrix:

$$A_{n',n''} = \sum_{n=1}^{N} T_{nn'} a_n T^{\dagger}_{nn''} = TAT^{\dagger}, T_{nn'} = \langle n'|a_n\rangle$$

8.2 Tuesday 24 Feb 2015

Observables Note that Hermitian and self-adjoint are not the same thing in infinite dimensional Hilbert space. We require the operator to be self-adjoint and bounded to be Hermitian. An operator is represented by a Hermitian operator. All the eigenvalues are real, but if there degenerate eigenvalues, then we need to find an orthonormal basis for the degenerate subspace.

Spectral Decomposition Write the identity as $\mathbb{I} = \sum |\alpha\rangle\langle\alpha| = \sum_{\alpha} \mathbb{P}_{\alpha}$ in terms of the orthonormal basis of some Hermitian operator. The projection operator is defined to be $|\alpha\rangle\langle\alpha|$. The projection operator is idempotent: $\mathbb{P}_{\alpha}^2 = \mathbb{P}_{\alpha}$. Hence we can write the operator $\hat{A}$ as a diagonal matrix $\hat{A} = \sum |\alpha\rangle\alpha\langle\alpha|$ which is diagonal in its eigenbasis. This statement is only true iff A has no degenerate eigenvalues. More generally,

$$A = \sum_{\alpha} \alpha \mathbb{P}_{\alpha}$$

The projection operator usually projects onto a 1D subspace, but if there are degenerate eigenvalues ,then the projection operator projects onto the larger dimensional subspace.

Operators that commute are simultaneously diagonalizable. More rigorously, if $\hat{A}|\alpha\rangle = \alpha|\alpha\rangle$ and $[\hat{A}, \hat{B}] = 0$, then $\hat{A}(\hat{B}|\alpha\rangle) = \alpha(\hat{B}|\alpha\rangle)$. If α is a non-degenerate eigenvalue of A, then $|\alpha\rangle$ must be proportional to $\hat{B}|\alpha\rangle$ so $|\alpha\rangle$ is also an eigenvector of $\hat{B}$. But if α is degenerate, then $\hat{B}|\alpha\rangle$ lies in the higher dimensional subspace.

Complete Set of Commuting Observables In 1D, $\hat{x}$ is a complete set of commuting observables because it never has degenerate eigenvalues. Note that we need a CSCO so that the degeneracies in one observable can be distinguished using another operator. It allows us to specify an orthonormal basis of the Hilbert space by eigenvalues. If we have an operator with a completely non-degenerate spectrum, then it is a CSCO by itself (like the particle on the line with $\hat{x}$).

Note about unitary operators A unitary operator can be thought of as a change of basis. Consider a Hilbert space with two orthonormal bases: $\{|n\rangle\}$ and $\{|m\rangle\}$. Then the operator $\hat{W}|n\rangle = |m\rangle$ that maps one basis element to the other is a unitary operator. Using bras, $\langle n|W^\dagger = \langle m|$. Then we examine:

$$\begin{aligned} WW^\dagger &= \left(\sum_{n_1} W|n_1\rangle\langle n_1|\right)\left(\sum_{n_2} |n_2\rangle\langle n_2|W^\dagger\right) \\ &= \sum_{i,j} m_i\rangle\langle n_i|n_j\rangle\langle m_j| = \sum_i |m_i\rangle\langle m_i| = \mathbb{I} \end{aligned}$$

by orthonormality so $\langle n_i|n_j\rangle$ is the Kronecker delta. Hence W is a unitary operator, and we can always find a basis in which a Hermitian is diagonal.

Measurement Measurement corresponds to obtaining an eigenvalue of a Hermitian operator. Measurement collapses the wavefunction into the eigenfunction of that eigenvalue. The probability of obtaining the eigenvalue a is (given initial state $|\Psi\rangle$):

$$P(a;\Psi) = \langle\Psi|\mathbb{P}_a|\Psi\rangle$$

If a is non-degenerate, then the projection operator can be written as $|a\rangle\langle a|$, so $P(a;\Psi) = |\langle\Psi|a\rangle|^2$. Hence upon measurement, the state becomes the eigenstate (appropriately normalised):

$$|\Psi\rangle \to \frac{1}{\sqrt{\langle\Psi|\mathbb{P}_a|\Psi\rangle}}\mathbb{P}_a|\Psi\rangle$$

and if a is non-degenerate, then:

$$|\Psi\rangle \to |\alpha\rangle$$

Composition of observables The sum of observables is not necessarily and observable. But the product of observables is not necessarily and observable. If they commute, then they are an observable and we can measure the two observables simultaneously since the order does not matter.

8.3 Thursday 26 Feb 2015

Centre of Mass coordinates Consider the Hamiltonian for a two-body central-potential system:

$$\hat{H} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + V(|\vec{r}_1 - \vec{r}_2|)$$

Then we have the eigenvalue problem in the TISE:

$$\hat{H}\Psi(\vec{r}_1,\vec{r}_2) = E\Psi(\vec{r}_1,\vec{r}_2)$$

Now we enter centre of mass coordinates in one dimension. Then let x be the position. Define $x = x_1 - x_2$, the relative position, $X = \frac{m_1x_1+m_2x_2}{m_1+m_2}$, the position of the CM. Define $M = m_1 + m_2$. Also define similar quantities for the momentum: $p = \frac{m_2p_1-m_1p_2}{m_1+m_2}$, $P = p_1 + p_2$. Then we have the inverse relations:

$$\begin{aligned} x_1 &= \frac{m_2x}{M} + X \\ x_2 &= \frac{-m_1x}{M} + X \end{aligned}$$

Recall that the momentum operator can be written $p_1 = \frac{\hbar}{i}\frac{\partial}{\partial x_1}$. Hence, replacing x_1 with its representation in x and X using the chain rule:

$$\frac{\partial}{\partial x_1} = \frac{\partial x}{\partial x_1}\frac{\partial}{\partial x} + \frac{\partial X}{\partial x_1}\frac{\partial}{\partial X}$$

We can write the Hamiltonian in terms of the centre of mass coordinates:

$$\hat{H} = \frac{-\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2M}\frac{\partial^2}{\partial X^2}, \quad \frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

Hence we want to solve the new eigenvalue equation in CM coordinates:

$$\hat{H}\Psi = \left[\frac{-\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2M}\frac{\partial^2}{\partial X^2} + V(x)\right]\Psi(x, X) = E\Psi(x, X)$$

Define:

$$\hat{H}_x = \frac{-\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + V(x)$$
$$\hat{H}_X = \frac{-\hbar^2}{2M}\frac{\partial^2}{\partial X^2}$$

Now, noting the structure of the Hamiltonian, we claim that we can write the wavefunction as a product: $\Psi(x, X) = \psi(x)\Phi(X)$.

Substituting this ansatz into the CM hamiltonian equation:

$$\frac{1}{\psi(x)}\hat{H}_x\psi(x) = \mathcal{E}$$
$$\frac{1}{\Phi(X)}\hat{H}_X\Phi(X) = E - \mathcal{E}$$

Now note that $E - \mathcal{E}$ is the kinetic energy of the centre of mass. Hence we write $E - \mathcal{E} = \frac{\hbar^2 k^2}{2M}$. Now we note that the centre of mass equation is simply the TISE for the free particle, which has solutions which are de Broglie waves:

$$\Phi(X) = Ce^{ikX}e^{-i\Omega t}, \Omega = \frac{\hbar k^2}{2M}$$

as for the relative motion, we have the equation:

$$\left[\frac{-\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = \mathcal{E}\psi(x)$$

which is equivalent to a single particle with the reduced mass in a fixed potential.

Asymptotic states Consider wave functions far away from the interface.

Review: Classical EM Consider a charge distribution ρ, charge flux $\vec{J}$. Then the total charge in a region is:

$$Q = \iiint \rho dV$$
$$\frac{dQ}{dt} = -\iint \vec{J}\cdot d\vec{n} = -\iiint (\nabla\cdot\vec{J})dV \implies \frac{\partial\rho}{\partial t} + \nabla\cdot\vec{J} = 0$$

Conservation of Probability Consider the $\Psi^* \times TDSE - (TDSE)^* \Psi$:

$$i\hbar\Psi^* \frac{\partial}{\partial t}\Psi + i\hbar\left(\frac{\partial}{\partial t}\Psi^*\right)\Psi = -\frac{\hbar^2}{2m}\left[\Psi^* \frac{\partial^2}{\partial x^2}\Psi - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right]$$
$$\implies i\hbar\frac{\partial}{\partial t}|\Psi|^2 = \frac{-\hbar^2}{2m}\frac{\partial}{\partial x}\left[\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right]$$

Define the probability flux:

$$J(x) = \frac{\hbar}{2mi}\left[\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right] = \frac{\hbar}{m}\Im\left(\Psi^*\frac{\partial}{\partial x}\Psi\right)$$

Note that for a deBroglie wave, $\Psi = e^{ikx}e^{-i\omega t}$, $J(x) = \frac{\hbar k}{m}|\Psi|^2$. Hence we see that the flux is the probability multiplied by some velocity ($\hbar k$ is the momentum). Combining with the previous relation, we obtain:

$$\frac{\partial\rho}{\partial t} + \frac{\partial J}{\partial x} = 0, \rho(x) = |\Psi(x)|^2$$

In 3D,

$$\vec{J} = \frac{\hbar}{2mi}\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) = \frac{\hbar}{m}\Im\left(\Psi^*\nabla\Psi\right)$$

and the 3D conservation:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{J} = 0$$

Effect of phase on flux Write the complex wavefunction in exponential form:

$$\Psi(x,t) = |\Psi(x,t)|^2 e^{i\phi(x,t)}, \phi(x,t) = \arg\Psi(x,t)$$

If we substitute the exponential form into the flux, we obtain that the flux arises from a changing phase $\phi(x,t)$ in position.

Potential step boundary conditions

$$J_i + J_r = J_t$$
$$R = \left|\frac{J_r}{J_i}\right|, T = \left|\frac{J_t}{J_i}\right|$$
$$\implies 1 - R = T$$

Tunnelling Consider a potential barrier of height V_0 and width L:

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)}\sinh^2\kappa L}, \frac{\hbar^2\kappa^2}{2m} = V_0 - E > 0$$

In the limit of a tall barrier $V_0 >> E, T = \frac{1}{\frac{V_0}{4E}\sinh^2\kappa L}$. In the limit of a wide barrier, $\kappa L >> 1$, $T = 16\frac{E}{V_0}e^{-2\kappa L}$.

Note further that if $E > V_0$, then κ is imaginary, and the denominator of T oscillators as E is varied. The peaks in $T(E)$ are Lorentzians and demonstrate resonant behaviour.

Chapter 9

Week 9

9.1 Tuesday 3 Mar 2015

3D QM Hamiltonian:

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})$$

Consider positions $\vec{r}$ in the CM frame of reference.

QHO in 3D Consider $V(\vec{r}) = V(|r|) = \frac{1}{2}m\omega^2 r^2 = \frac{1}{2}m\omega^2(x^2+y^2+z^2)$. Then the system is symmetrical in permutations of x, y, z. Since for a single dimension $E_x = \hbar\omega\left(n_x + \frac{1}{2}\right)$, then for the 3D case, $E_{n_x,n_y,n_z} = \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right)$ and we have a degeneracy possibility.

Central potentials and spherical coordinates Consider $V(\vec{r}) = V(r)$.

Spherical. $d\mathbf{l} = dr\,\hat{\mathbf{r}} + r\,d\theta\,\hat{\boldsymbol{\theta}} + r\sin\theta\,d\phi\,\hat{\boldsymbol{\phi}}; \quad d\tau = r^2\sin\theta\,dr\,d\theta\,d\phi$

Gradient :
$$\nabla t = \frac{\partial t}{\partial r}\hat{\mathbf{r}} + \frac{1}{r}\frac{\partial t}{\partial \theta}\hat{\boldsymbol{\theta}} + \frac{1}{r\sin\theta}\frac{\partial t}{\partial \phi}\hat{\boldsymbol{\phi}}$$

Divergence :
$$\nabla \cdot \mathbf{v} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 v_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}(\sin\theta\, v_\theta) + \frac{1}{r\sin\theta}\frac{\partial v_\phi}{\partial \phi}$$

Curl :
$$\nabla \times \mathbf{v} = \frac{1}{r\sin\theta}\left[\frac{\partial}{\partial\theta}(\sin\theta\, v_\phi) - \frac{\partial v_\theta}{\partial \phi}\right]\hat{\mathbf{r}} + \frac{1}{r}\left[\frac{1}{\sin\theta}\frac{\partial v_r}{\partial \phi} - \frac{\partial}{\partial r}(r v_\phi)\right]\hat{\boldsymbol{\theta}} + \frac{1}{r}\left[\frac{\partial}{\partial r}(r v_\theta) - \frac{\partial v_r}{\partial \theta}\right]\hat{\boldsymbol{\phi}}$$

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

Momentum and Angular Momentum Write $\vec{p} = \vec{p}_r + \vec{P}_\perp$. Define the angular momentum $\vec{L} = \vec{r}\times\vec{p} = r\vec{p}_\perp$. Hence $p^2 = p_r^2 + \frac{L^2}{r^2} \implies \frac{p^2}{2m} = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2}$.

The radial momentum operator can be symmetrized to become Hermitian:

$$p_r = \frac{1}{2}\left[\frac{\vec{r}}{|r|}\cdot\vec{p} + \vec{p}\cdot\frac{\vec{r}}{|r|}\right]$$

Applying the chain rule to the Cartesian momentum operator:

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial x}\frac{\partial}{\partial\phi} \quad \text{etc.}$$

Hence we have the radial momentum operator in spherical coordinates:

$$\hat{p}_r = \frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r}r$$

It is hermitian: $\hat{p}_r^\dagger = \hat{p}_r$, and commutes in the following manner:

$$\begin{aligned}
[\hat{r}, \hat{p}_r] &= i\hbar \\
[\hat{\theta}, \hat{p}_r] &= 0 \\
[\hat{\phi}, \hat{p}_r] &= 0 \\
[\hat{p}_\theta, \hat{p}_r] &= 0 \\
[\hat{p}_\phi, \hat{p}_r] &= 0
\end{aligned}$$

Angular momentum operator Note that $\vec{L} = \vec{r} \times \vec{p}$ is already Hermitian. The commutators are the following:

$$[L_x, L_y] = i\hbar L_z$$

Index the position coordinates with $1, 2, 3$ for x, y, z respectively. Then we can write the completely antisymmetric Levi-Civita Tensor:

$$L_i = \sum_{j,k} \mathcal{E}_{i,j,k} r_j p_k$$

$$\varepsilon_{ijk} = \begin{cases} +1 & \text{if } (i,j,k) \text{ is } (1,2,3), (2,3,1) \text{ or } (3,1,2), \\ -1 & \text{if } (i,j,k) \text{ is } (3,2,1), (1,3,2) \text{ or } (2,1,3), \\ 0 & \text{if } i = j \text{ or } j = k \text{ or } k = i \end{cases}$$

The square $L^2 = (\vec{r} \times \vec{p}) \cdot (\vec{r} \times \vec{p}) = (\mathcal{E}_{i,j,k} r_j p_k)(\mathcal{E}_{i,j,k} r_j p_k)$ where we use the implied Einstein summation convention (sum across repeated indices). Note that the Levi-Civita symbol has an identity:

$$\mathcal{E}_{ijk}\mathcal{E}_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$$

After much painful algebra, we have:

$$\begin{aligned}
L_x &= i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right) \\
L_y &= i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) \\
L_z &= \frac{\hbar}{i}\frac{\partial}{\partial\phi} \\
L^2 = L_x^2 + L_y^2 + L_z^2 &= -\hbar^2\frac{1}{\sin^2\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{\partial^2}{\partial\phi^2}\right]
\end{aligned}$$

Hence we have that L^2 depends only on θ, ϕ and p_r depends only on r.

Hamiltonian in spherical coordinates for central force

$$\hat{H} = \left[\frac{p_r^2}{2m} + V(r)\right] + \frac{L^2}{2mr^2}$$

and we note that we can write the TISE solution as a separation of variables:

$$\psi(\vec{r}) = R(\vec{r})Y(\theta,\phi)$$
$$\implies \frac{2mr^2}{R}\left[\frac{\hat{p}_r R}{2m} + (V-E)R\right] = \lambda\hbar^2, \frac{L^2 Y}{Y} = \lambda\hbar^2$$

for some dimensionless λ. We consider the angular part, which does not require us to know $V(r)$.

$$L^2 Y(\theta,\phi) = \lambda\hbar^2 Y(\theta,\phi)$$

we perform separation of variables again:

$$Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$$

to obtain the decoupled equations:

$$\frac{\Phi''}{\Phi} = -m^2, \quad \frac{-\sin^2\theta}{\Theta(\theta)}\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \lambda\Theta\right] = -m^2$$
$$\implies \Phi(\phi) = e^{im\phi}$$

for constant m, the magnetic quantum number. We note that $m\hbar$ is an eigenvalue for L_z since $L_z\Phi(\phi) = m\hbar\Phi(\phi)$. Since L_z is hermitian, $m\hbar$ is real, hence $-m^2$ is negative. Now impose the boundary condition: $\Psi(r,\theta,\phi)$ is single-valued: $\Psi(r,\theta,\phi+2\pi) = \Psi(r,\theta,\phi) \implies m \in \mathbb{Z}$.

For the θ differential equation, make the change of variables $x = \cos\theta, dx = -\sin\theta d\theta$:

$$\frac{d}{dx}\left[(1-x^2)\frac{d\Theta(x)}{dx}\right] + \left(\lambda - \frac{m^2}{1-x^2}\right)\Theta(x) = 0$$

which is Legendre's differential equation. The solutions are Legendre polynomials. We obtain convergent solutions only when $\lambda = l(l+1), l \in \mathbb{Z}, l \geq 0$, where l is the number of half-oscillations in the domain $\theta \in [0,\pi]$ and $m = -l, -l+1, \ldots, 0, \ldots, +l$. For a given value of l, there will be $2l+m$ values of m. The solutions will be standing waves in θ.

Spin angular momentum has that m is half-integer. We cannot represent the spin angular momentum in coordinate space, since it will not be single-valued.

9.2 Thursday 5 Mar 2015

Hamiltonian under central force Recall the TISE for central forces:

$$\hat{H} = \left(\frac{p_r^2}{2m} + \frac{L^2}{2mr^2} + V(r)\right)\psi = E\psi$$

with separable solutions $\psi = R(r)Y(\theta,\phi)$.

Orbital angular momentum eigenequation

$$L^2 Y_{lm}(\theta,\phi) = l(l+1)\hbar Y_{lm}(\theta,\phi), \quad l = 0.1, 2, \ldots$$

where l is the order of the Legendre polynomial. $Y_{lm} = P_{lm}(\cos\theta)e^{im\phi}$ is written in terms of the Legendre function (not the same as the Legendre polynomial) with parameters l, m where $m = -l, -l+1, \ldots, 0, +l$. The first few functions are:

$$P_{00} = 1$$
$$P_{10} = \frac{z}{r} = \cos\theta$$
$$P_{1,\pm1} = \mp\sin\theta = \sqrt{1-\cos^2\theta}$$
$$P_{20} = \frac{1}{2}(3\cos^2\theta - 1)$$
$$P_{2,\pm1} = \mp\frac{1}{2}\sin\theta\cos\theta$$
$$P_{22} = \sin^2\theta$$

Azimuthal angular momentum

$$L_z Y_{lm}(\theta,\phi) = \frac{\hbar}{i}\frac{\partial}{\partial\phi}Y_{lm}(\theta,\phi) = m\hbar Y_{lm}(\theta,\phi)$$

Angular eigenfunctions are orthonormal Note that the azimuthal angular momentum eigenfunctions are the same as that of the total orbital angular momentum, indicating that the operators can be simultaneously diagonalized and commute.

$$\int_S d\Omega Y^*_{lm}(\theta,\phi)Y_{l',m'}(\theta,\phi) = \delta_{l,l'}\delta_{m,m'}$$

where we integrate over the surface of the sphere S. $d\Omega$ is the differential solid angle $d\Omega = d(\cos\theta)d\phi$ such that $\int d\Omega = 4\pi$. Hence we may use completeness to obtain the coefficients of a linear combination:

$$f(\theta,\phi) = \sum_{l,m} a_{lm}Y_{lm}(\theta,\phi) \iff a_{lm} = \int d\Omega Y^*_{lm}(\theta,\phi)f(\theta,\phi)$$

Parity operator Note that $Y_{lm}(\theta,\phi)$ is also a parity eigenstate. Under parity, $\vec{r}\to\vec{r}, r\to r, \theta\to\pi-\theta, \phi\to\phi+\pi$. Then:

$$\hat{\mathbb{P}}Y_{lm}(\theta,\phi) = (-1)^l Y_{lm}(\theta,\phi)$$

hence even l corresponds to even parity, and odd l corresponds to odd parity.

Diatomic molecule has both rotational (angular) and vibrational (radial) degrees of freedom. The rotational motions are excited at lower energies.

We can associate the classical moment of inertia with the molecule:

$$I = \sum_i m_i d_i^2$$

where d_i is the perpendicular distance to the axis of rotation. We may also write the energies associated with the different types of motion:

$$\text{Centre of mass motion, kinetic energy:} \quad KE = \frac{\hbar^2 k^2_{CMS}}{2m_{tot}}$$
$$\text{Rotational:} \quad \frac{L^2}{2I}$$
$$\text{Vibrational:} \quad \left(n+\frac{1}{2}\right)\hbar\omega$$

Rigid rotator Ignore CM motion and vibrational motion. Then the eigenstate of the rotator will be $Y_{lm}(\theta,\phi)$ with associated energy $E_{rot} = \frac{l(l+1)\hbar^2}{2I}$. Transitions between rotational eigenstates require the emission or absorption of a photon of energy.

Rotational states are named $l = 0, 1, 2, 3$ are s,p,d,f respectively.

Radial solutions for central potential Consider the hamiltonian after substituting the angular solution:

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

Define another radial function: $R(r) = \frac{u_l(r)}{r}$, which depends on l. Then the ODE becomes:

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)}{2mr^2} + V(r)\right]u_l(r) = Eu_l(r)$$

The central term $\frac{l(l+1)}{2mr^2}$ is called the centrifugal barrier, which can be added to the central potential to give a new effective central potential function.

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dr^2} + V_{eff,l}(r)\right]u_l(r) = Eu_l(r)$$

Define the integer parameter n_r to be the number of nodes in r over the infinite interval $[0,\infty)$. Then the solutions for u_l can be characterized by n_r. Then we can write the full wavefunction to be:

$$\psi(\vec{r}) = \frac{u_{n_r,l}(r)}{r}Y_{lm}(\theta,\phi)$$

and we can label the state using the eigenvalues as:

$$\psi(\vec{r}) = \langle\vec{r}|n_r, l, m\rangle$$

Note that the number of nodes in angular space is $l - m$.

Note that for the eigenfunction to be defined for all r, we require $u_{nr,l}$ to vanish at $r = 0$ faster or as fast as $\frac{1}{r}$ so that the pole from $\frac{1}{r}$ does not blow up. Note that $\frac{u(r)}{r}$ can be finite as $r \to 0$. Also at infinity, we require the eigenfunction to vanish as $r \to \infty$ (obtain a bound state).

Normalization of wavefunction Since we have defined $Y_{ml}(\theta,\phi)$ such that it is normalised on the surface of a sphere, we just require that:

$$\int |\psi(\vec{r})|^2 d\vec{r} = 1, \quad d\vec{r} = r^2 dr d\Omega = d^3r$$

$$\int_S |Y_{ml}(\theta,\phi)|^2 d\Omega = 1$$

$$\implies \int_0^\infty |R|^2 r^2 dr = 1 \implies \int_0^\infty |u(r)|^2 dr = 1$$

Coulomb potential Define $V(r) = \frac{-e^2}{r}$. Let l be non-zero. Since l is non-negative, we have that the centrifugal part of the effective potential is always positive. Then we will have a value of r such that the value of $V_{eff,l}$ is minimized.

Energies In the absence of an external magnetic field, the energy is only a function of n_r and l, not on m.

Spherical box Consider potential function $V(r) = \begin{cases} 0, r < a \\ \infty, r > a \end{cases}$. Hence for $r < a$, the effective potential only contains the centrifugal barrier. We write the TISE:

$$\frac{-\hbar^2}{2m}u''(r) + \frac{l(l+1)\hbar^2}{2mr^2}u = Eu$$

with boundary conditions:

$$u(a) = 0$$
$$u(0) < \infty$$

In the regime of small r, we neglect the Eu term and obtain the Euler equation:

$$u'' = \frac{-l(l+1)}{r^2}u$$

which has solutions:

$$u = c_1 r^{l+1}, u = c_2 r^{-l}$$

but the latter solution is singular at $r = 0$, hence we require only the first solution.

In the other regime where $l = 0$ or $E >> \frac{l(l+1)\hbar^2}{2mr^2}$, we want to solve the ODE:

$$u'' + k^2 u = 0, \quad E = -\frac{\hbar^2 k^2}{2m}$$

This is just a trigonometric function, and hence implementing the boundary condition at $r = a$, we obtain the quantisation law $k = \frac{n_r \pi}{a}$. Hence the approximate form of the radial function is:

$$R = \frac{u}{r} = Cr^l \sin\frac{n_r \pi r}{a}$$

More precisely, if we do not make the approximations, we have the Bessel ODE:

$$u'' - \frac{l(l+1)}{r^2}u + k^2 u = 0$$

which have solutions that are linear combinations of functions:

$$R = \frac{u}{r} = Aj_l(kr) + Bn_l(kr)$$

the cosine-line functions n_l will vanish when we implement the boundary conditions (they are singular at $r = 0$).

Principal Quantum Number Note that in the Coulomb potential, the energy is given by $E = \frac{-Ry}{(n_r+l+1)^2}$. Note that we have degeneracy when $n_r + l$ can remain the same when they individually change. Hence we define the principal quantum number $n = n_r + l + 1$. Hence $E_{n_r,l,m} = E_n = \frac{-Ry}{n^2}$. Since n_r is nonnegative and n is positive, the maximum value of l is $n - 1$. Hence the total energy degeneracy is: $\sum_{l=0}^{n-1}(2l+1)(2) = 2n^2$ where we include the 2 to account for spin.

Chapter 10

Week 10

10.1 Tuesday 10 Mar 2015

Hydrogen Atom Write the Hamiltonian as:

$$\hat{H} = \frac{p_N^2}{2m_N} + \frac{p_e^2}{2m_e} - \frac{Ze^2}{|\vec{r}_e \cdot \vec{r}_n|}$$

Move into the CM frame:

$$\begin{gathered}\vec{r} \equiv \vec{r}_e - \vec{r}_N \\ M_{tot} = m_n + m_e \approx m_n \\ \mu = \frac{m_e m_N}{m_e + m_N} \approx m_e\end{gathered}$$

Write the wavefunction in separable form:

$$\Psi(\vec{R}, \vec{r}, t) = \Psi_{CM}(\vec{R}, t)\Psi_{rel}(\vec{r}, t)$$

where $\Psi_{CM}(\vec{R}, t)$ is the solution to the free particle wave packet with $E_{CM} = \frac{\hbar^2 k^2}{2m_{tot}}$. Then we have the ODE for the relative wavefunction:

$$\left(\frac{-\hbar^2 \nabla_{rel}^2}{2\mu} - \frac{Ze^2}{r}\right)\Psi(\vec{r}, t) = E_r \Psi(\vec{r}, t)$$

Separating variables and solving for the time aspect (for the spatial eigenfunctions):

$$\Psi_{rel}(\vec{r}, t) = \psi(\vec{r})e^{-iE_r t/\hbar}$$

Factor the eigenfunction further into the angular and radial coordinates:

$$\psi(\vec{r}) = R_{n_r,l}(r)Y_{l,m}(\theta, \phi) = \frac{u(r)}{r}Y_{l,m}(\theta, \phi)$$

where we impose the normalisation condition:

$$\begin{gathered}\int_S |Y_{l,m}(\theta, \phi)|^2 d\Omega = 1 \\ \int_0^\infty |u(r)|^2 dr = 1\end{gathered}$$

then $u(r)$ satisfies the ODE:

$$\left[\frac{-\hbar^2}{2\mu}\frac{d}{dr^2} - \frac{Ze^2}{r} + \frac{l(l+1)\hbar^2}{2mr^2}\right] u_{n_r,l}(r) = E_r u_{n_r,l}(r)$$

Now define:

$$\frac{\hbar^2 k^2}{2\mu} = |E_r|$$

where E_r is the binding energy which is negative for bound states. Also define dimensionless coordinate $\rho = kr$. Then the ODE can be written in the dimensionless form:

$$u'' - \frac{l(l+1)}{\rho^2}u + \left(\frac{\lambda}{\rho} - 1\right)u = 0, \lambda = \frac{2\mu Z e^2}{\hbar^2 k}$$

where the derivatives are taken with respect to ρ instead of r. This is a Laguerre equation. The solution looks like:

$$u(\rho) = e^{-\rho}\rho^{l+1}\sum_{j=0}^{\infty} a_j \rho_j$$

where the summation is a polynomial. In general, the solution will blow up as $\rho \to \infty$ unless we cut off the polynomial at some finite number j_{max}:

$$u(\rho) = e^{-\rho}\rho^{l+1}\sum_{j=0}^{j_{max}} a_j \rho_j$$

Then the energies will depend on j_{max}, which is some non-negative integer. Note that $u(\rho)$ will have j_{max} nodes between $(0, \infty)$ (does not include the node at zero). We also have a constraint for λ:

$$\frac{2\mu Z e^2}{\hbar^2 k} = 2(n_r + l + 1)$$

and hence the energy is:

$$E_r = \frac{-\hbar^2 k^2}{2\mu} = \frac{-\mu Z^2 e^4}{2\hbar^2(n_r + l + 1)^2} = \frac{-Z^2 Ry}{n^2}, n \equiv n_r + l + 1$$

where n is the number of radial nodes plus the number of angular nodes plus one. We can write the Rydberg as:

$$\frac{\mu e^4}{2\hbar^2} = \frac{1}{2}(\mu c^2)\frac{e^4}{\hbar^2 c^2} = Ry$$

where $\alpha = \frac{e^2}{\hbar^2 c^2}$.

Dirac Equation For relativistic particles:

$$\hat{H}\Psi = \hat{p}c\Psi = E\Psi$$

where $\hat{p} = \sqrt{(pc)^2 + (mc^2)^2}$.

Spin The eigenvalue equation is

$$\hat{S}^2|s, m_s\rangle = s(s+1)\hbar^2|s, m_s\rangle$$

it also commutes with the z-component of the angular momentum and hence share the same eigenstates:

$$S_z|s, m_s\rangle = m_s\hbar|s, m_s\rangle$$

where $m_s \in [-s, s]$ in integral units. Hence there are $2s + 1$ possible values of s. Note that s can be integral or half-integral.

Dirac notation $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$. Do proof.

$$\begin{aligned}\langle x|\hat{p}|p\rangle &= p\langle x|p\rangle \\ &= \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|p\rangle\end{aligned}$$

Equate and solve.

Commutator relations $[p, f(\hat{x})] = \frac{\hbar}{i} f'(x)$.

Delta function $\delta(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx e^{ikx}$.

Virial Theorem $2\langle T\rangle = \langle \mathbf{r}\cdot\nabla V\rangle$.

Delta function potential in infinite square well Consider a potential well of length $2a$, centred at the origin, with a delta function $w\delta(x)$ at the origin.

Note that all the odd solutions have a wavefunction value of zero at the origin, and hence there is no discontinuity in the first derivative there. The odd solutions are just the solutions to the infinity square well.

Gamma function $\Gamma(n+1) = \int_0^{\infty} dx x^n e^{-x} = n!, n \in \mathbb{Z}$.