3. Principles of QM

Axiomatic principles

State vector axiom: State vector at t is ket $\psi(t)$, or $|\psi\rangle$, bra state.

Probability axiom: Given a system in state $|\psi\rangle$, a measurement will find it in state $|\phi\rangle$ with probability amplitude $\langle\phi|\psi\rangle$.

Hermitian operator axiom: Physical observable is represented by a linear and Hermitian operator.

Measurement axiom: Measurement of a physical observable results in eigenvalue of observable. Observable $\widehat{A}$, we have $\widehat{A}|a\rangle = a|a\rangle$, where a is eigenvalue and $|a\rangle$ is eigenvector. Measurement of the physical quantity represented by $\widehat{A}$ collapses the state $|\psi\rangle$ before measurement into an eigenstate $|a\rangle$ of $\widehat{A}$.

Time evolution axiom: $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \widehat{H}|\psi(t)\rangle$, w/o consider x or p.

Vector space

State vector is neither in position nor momentum space.

Basis vectors: $|0\rangle = \begin{bmatrix}1\\0\\ \vdots\\0\end{bmatrix}, |1\rangle = \begin{bmatrix}0\\1\\ \vdots\\0\end{bmatrix}, |n\rangle = \begin{bmatrix}0\\0\\ \vdots\\1\end{bmatrix}$ (in nth pos).

Linearity : Because the SE is linear, given two states $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$, $|\psi(t)\rangle = c_1|\psi_1(t)\rangle + c_2|\psi_2(t)\rangle$ is also a sol. (c's are complex).

Properties of a vector space

Dual vector space $c|\psi\rangle$ is mapped to $c * \langle\psi|$. Given a vector, $|\psi\rangle = \begin{bmatrix}\vdots\\ \alpha\\ \vdots\end{bmatrix}$, the dual vector is $\langle\psi| = \begin{bmatrix}\cdots & \alpha^* & \cdots\end{bmatrix}$.

Dual basis vectors are $\langle 0| = \begin{bmatrix}1 & 0 & \cdots\end{bmatrix}, \cdots, \langle n| \begin{bmatrix}0 & \cdots & 1\end{bmatrix}$.

Inner product : $\langle\phi|\psi\rangle = c$, where c is complex.

$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^* \rightarrow \langle\psi|\psi\rangle$ is real, positive, and finite for a normalizable ket vector. Can choose $\langle\psi|\psi\rangle = 1$. $\langle\psi_m|\psi_n\rangle = \delta_{mn}$

Operators

A matrix operator $\widehat{A}$ acting on a state vector $|\psi\rangle$ transforms it into another state vector $|\phi\rangle$, $\widehat{A}|\psi\rangle = |\phi\rangle$. It is linear.

Properties of operators

Hermitian conjugate (Hermitian adjoint) operator in the dual space

Hermitian adjoint operator $\widehat{A}^\dagger$ acts on the dual vector $\langle\psi|$ from the right as $\langle\psi|\widehat{A}^\dagger\rangle$, where $\widehat{A}^\dagger = (\widehat{A})^{T*}$.

$$(\widehat{A}|\psi\rangle)^\dagger = |\psi\rangle^\dagger\widehat{A}^\dagger = \langle\psi|\widehat{A}^\dagger \qquad \langle\psi| = |\psi\rangle^\dagger \qquad \langle\psi|^\dagger = |\psi\rangle$$

$$(\widehat{A}\widehat{B})^\dagger = (\widehat{A}\widehat{B})^{T*} = (\widehat{B}^T\widehat{A}^T)^* = \widehat{B}^{T*}\widehat{A}^{T*} = \widehat{B}^\dagger\widehat{A}^\dagger, \quad (c\widehat{A})^\dagger = c^*\widehat{A}^\dagger$$

Outer product operators : $|\psi\rangle\langle\phi| \qquad [|\psi\rangle\langle\phi|]\chi\rangle = |\psi\rangle\langle\phi|\chi\rangle$

Matrix elements of operators

$$\langle\phi|\widehat{A}|\psi\rangle \text{ (complex num)}$$

Hermitian equiv to complex conj $\langle\phi|\widehat{A}|\psi\rangle^\dagger = \langle\psi|\widehat{A}^\dagger|\phi\rangle = \langle\phi|\widehat{A}|\psi\rangle^*$

Hermitian operators : $\widehat{A}^\dagger = \widehat{A}$, so given $\widehat{A}|\phi\rangle$ in the vector space, we have $\langle\psi|\widehat{A}^\dagger = \langle\phi|\widehat{A}$ in the dual vector space.

Matrix elements of a Hermitian operator

$$\langle\phi|\widehat{A}|\psi\rangle^\dagger = \langle\phi|\widehat{A}|\psi\rangle^* = \langle\psi|\widehat{A}^\dagger|\phi\rangle = \langle\psi|\widehat{A}|\phi\rangle$$

Hermitian operator, real expectation vals: $\langle\psi|\widehat{A}|\phi\rangle^* = \langle\psi|\widehat{A}|\phi\rangle \equiv \langle\widehat{A}\rangle$

Same result whether $\widehat{A}$ acts to right or left: $\langle\phi|\widehat{A}|\psi\rangle = \langle\phi|\widehat{A}^\dagger|\psi\rangle$

Eigenvals and eigenvecs of Hermitian operators : $\widehat{A}|a_n\rangle = a_n|a_n\rangle$

Normalized eigvecs $\langle a_m|a_n\rangle = \delta_{mn}$. Gram-Schmidt, degenerate evec.

Completeness of eigenvector of a Hermitian operator Set $|a_n\rangle$ is complete if $\sum_n |\langle a_n|\psi\rangle|^2 = 1$. $\sum_n |a_n\rangle\langle a_n| = 1$ (identity operator)

Continuous spectra of a Hermitian operator Hermitian operator $\widehat{A}$, $\widehat{A}|a\rangle = a|a\rangle$, where a is continuous.

$\int da'\langle a'|\widehat{A}|a\rangle = a\int da'\langle a'|a\rangle = \int da' a'\langle a'|a\rangle \rightarrow \langle a'|a\rangle = \delta(a'-a)$

Continuous condition: $\int da|a\rangle\langle a| = 1$

Gram-Schmidt orthogonalization procedure Eigval (like energy level) is n-fold degenerate: n states w same eigval.

Orthogonal eigenstates $\rightarrow$ no degeneracy.

1. Normalize each state and define $\alpha_i = \frac{\alpha_i}{\sqrt{\langle\alpha_i|\alpha_i\rangle}}$. 2. $|\alpha_1'\rangle = |\alpha_1\rangle$.

3. $|\alpha_2'\rangle = \frac{|\alpha_2\rangle - |\alpha_1\rangle\langle\alpha_1|\alpha_2\rangle}{\sqrt{\langle\alpha_2|\alpha_2\rangle - \langle\alpha_1|\alpha_2\rangle\langle\alpha_2|\alpha_1\rangle}} = \frac{|\alpha_2\rangle - |\alpha_1\rangle\langle\alpha_1|\alpha_2\rangle}{\sqrt{1 - \langle\alpha_1|\alpha_2\rangle\langle\alpha_2|\alpha_1\rangle}}$

4. Subtract components of $|\alpha_3\rangle$ along $|\alpha_1\rangle$ and $|\alpha_2\rangle$, $|\alpha_3\rangle - |\alpha_1\rangle\langle\alpha_1|\alpha_3\rangle - |\alpha_2\rangle\langle\alpha_2|\alpha_3\rangle$, normalize and promote to $|\alpha_3'\rangle$. ...

Position and momentum representation

$\widehat{\vec r}|\vec r\rangle = \vec r|\vec r\rangle \quad \langle\vec{r'}|\vec r\rangle = \delta^3(\vec{r'}-\vec r), \int d^3\vec r|\vec r\rangle\langle\vec r| = 1, \langle\vec{r'}|\widehat{\vec r}|\vec r\rangle = \vec r\delta^3(\vec{r'}-\vec r)$

$\widehat{\vec p}|\vec p\rangle = \vec p|\vec p\rangle \quad \langle\vec{p'}|\vec p\rangle = \delta^3(\vec{p'}-\vec p), \int d^3\vec p|\vec p\rangle\langle\vec p| = 1$

State vector $|\psi(t)\rangle$ in position space (scalar): $\langle\vec r|\psi(x,t)\rangle \equiv \psi(\vec r, t)$

$\langle\psi|\widehat{\vec p}|\psi\rangle = \frac{d}{dt}\langle\psi|\vec r|\psi\rangle m$

Representation of momentum operator in position space: $\widehat{\vec p} = -i\hbar\vec\nabla$.

$\langle x|\widehat{p}|x'\rangle = -i\hbar\frac{\partial}{\partial x}\delta(x-x') = -i\hbar\frac{\partial}{\partial x}\langle x|x'\rangle$.

$\widehat{p} = -i\hbar\frac{\partial}{\partial x}$ is Hermitian, $\frac{\partial}{\partial x}$ is not.

$\langle x|\widehat{p}|p\rangle = p\langle x|p\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p\rangle$. The solution is $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px}$.

In 3D, $\langle\vec r|\vec p\rangle = \frac{1}{(2\pi\hbar)^{3/2}}e^{\frac{i}{\hbar}\vec p\vec r}$.

We can write the normalized wavefunction of definite position in momentum space, $\langle p|x\rangle = \langle x|p\rangle^*$. So, $\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{i}{\hbar}px}$ (particle moving to the left, or with momentum $-p$, in the momentum space).

Operators and wavefunction in position representation Position and momentum operators in pos space: $\widehat{\vec r} = \vec r$, $\widehat{\vec p} = -i\hbar\vec\nabla$.

$\widehat{\vec r}$ is Hermitian and $\langle\phi|\widehat{\vec r}^\dagger|\psi\rangle = \langle\phi|\widehat{\vec r}|\psi\rangle$.

$\widehat{O}(\widehat{\vec r}, \widehat{\vec p}) = \widehat{O}(\vec r, -i\hbar\vec\nabla)$

The expectation val of the observable should be indep of representation. In state $\psi(t)$, $\langle\widehat{O}\rangle = \langle\psi(t)|\widehat{O}|\psi(t)\rangle$.

Insert $\int d^2\vec r|\vec r\rangle\langle\vec r| = 1$ to get $\langle\widehat{O}\rangle = \int d^2\vec r\langle\psi(t)|\vec r\rangle\langle\vec r|\widehat{O}|\psi(t)\rangle$

$\psi(\vec r, t) = \langle\vec r|\psi(t)\rangle, \qquad \psi(\vec r, t)^* = \langle\vec r|\psi(t)\rangle^* = \langle\psi(t)|\vec r\rangle$,

$\langle\vec r|\widehat{O}|\psi(t)\rangle = \widehat{O}(\vec r, -i\hbar\vec\nabla)\psi(\vec r, t), \langle\widehat{O}\rangle = \int d^3\vec r\psi(\vec r, t)^*\widehat{O}(\vec r, -i\hbar\vec\nabla)\psi(\vec r, t)$

Operators and wavefunction in momentum representation $\widehat{\vec r} = i\hbar\vec\nabla_{\vec p}$, or in 1D, $\widehat{x} = i\hbar\frac{\partial}{\partial p}$, $\widehat{\vec p} = \vec p$, where $\vec p^* = \vec p$.

$\widehat{O}(\widehat{\vec r}, \widehat{\vec p}) = \widehat{O}(i\hbar\vec\nabla_{\vec p}, \vec p)$

$\langle\widehat{O}\rangle = \langle\psi(t)|\widehat{O}|\psi(t)\rangle \rightarrow \langle\widehat{O}\rangle = \int d^2\vec p\langle\psi(t)|\vec p\rangle\langle\vec p|\widehat{O}|\psi(t)\rangle$.

$\psi(\vec p, t) = \langle\vec p|\psi(t)\rangle, \qquad \psi(\vec p, t)^* = \langle\vec p\psi(t)\rangle^* = \langle\psi(t)|\vec p\rangle$

$\langle\vec p|\widehat{O}|\psi(t)\rangle = \widehat{O}(i\hbar\vec\nabla_{\vec p}, \vec p), \langle\widehat{O}\rangle = \int d^3\vec p\psi(\vec p, t)^*\widehat{O}(i\hbar\vec\nabla_{\vec p}, \vec p)\psi(\vec p, t)$.

$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \widehat{H}|\psi(t)\rangle$, where $\widehat{H} = \frac{\widehat{\vec p}^2}{2m} + V(\widehat{\vec r}, t)$ becomes

$i\hbar\frac{\partial\psi(\vec r, t)}{\partial t} = -\frac{\hbar^2}{2m}\vec\nabla^2\psi(\vec r, t) + V(\vec r, t)\psi(\vec r, t)$

Commuting operators

If $[\widehat{A}, \widehat{B}] = 0$ and the states are nondegenerate, $|\psi\rangle$ is a simultaneous eigenstate of $\widehat{A}$ and $\widehat{B}$.

$|\psi\rangle = |ab\rangle$, and $\widehat{A}|ab\rangle = a|ab\rangle$, $\widehat{B}|ab\rangle = b|ab\rangle$

Non-commuting operators and the general uncertainty principle

$(\Delta A)^2(\Delta B)^2 \geq (\frac{1}{2i}\langle[\widehat{A}, \widehat{B}]\rangle)^2$

Cannot construct simulatneous eigenstates (which correspond to definite eigenvalues) of non-commuting observables.

Time evolution of expectation value of an operator and Ehrenfest's theorem

Ehrenfest's theorem: how observable $\widehat{O}$'s expectation value in state $|\psi(t)\rangle$ evolves in time, $\frac{d}{dt}\langle\widehat{O}\rangle = \langle\frac{\partial\widehat{O}}{\partial t}\rangle + \frac{i}{\hbar}\langle[\widehat{H}, \widehat{O}]\rangle$

For $\widehat{O} = \widehat{\vec p}$ and a Hamiltonian that is TI, $\frac{d}{dt}\langle\widehat{\vec p}\rangle = -\langle\vec\nabla V(\widehat{\vec r})\rangle$, which is just Newton's Second Law! $\rightarrow$ QM contains all of classical mech.

The simple harmonic oscillator

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

Raising and lowering operators Lowering op: $\widehat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\widehat{x} + \frac{i}{m\omega}\widehat{p})$, Raising op: $\widehat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\widehat{x} - \frac{i}{m\omega}\widehat{p})$.

$[\widehat{a}, \widehat{a}^\dagger] = 1 \qquad \widehat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\widehat{a}^\dagger + \widehat{a})$, $\widehat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(\widehat{a}^\dagger - \widehat{a})$

$\widehat{H} = (\widehat{N} + \frac{1}{2})\hbar\omega$, where $\widehat{N} = \widehat{a}^\dagger\widehat{a}$. Now $\widehat{N}$ is Hermitian, and $\widehat{N}|n\rangle = n|n\rangle$

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

$\widehat{N}(\widehat{a}|n\rangle) = (n-1)(\widehat{a}|n\rangle)$, $\widehat{N}(\widehat{a}^\dagger|n\rangle) = (n+1)(\widehat{a}^\dagger|n\rangle)$

Normalized number state vectors Energy levels are not degenerate, so $|n-1\rangle = c_n\widehat{a}|n\rangle \rightarrow c_n = \frac{1}{\sqrt{n}} \rightarrow \widehat{a}|n\rangle = \sqrt{n}|n-1\rangle$.

$|n+1\rangle = d_n\widehat{a}^\dagger|n\rangle \rightarrow d_n = \frac{1}{\sqrt{n+1}} \rightarrow \widehat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$

Ground state: $|0\rangle$, excited state: $|n\rangle = \frac{(\widehat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle$, $n = 0, 1, 2, \ldots$

$\langle n'|\widehat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle n'|(\widehat{a}^\dagger + \widehat{a})|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1})$

$\langle n'|\widehat{p}|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}\langle n'|(\widehat{a}^\dagger - \widehat{a})|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}(\sqrt{n+1}\delta_{n',n+1} - \sqrt{n}\delta_{n',n-1})$

Wavefunctions in position representation $E_n = (n + \frac{1}{2})\hbar\omega$, $n = 0, 1, 2, \ldots$

The stationary wavefunctions of definite energy: $\psi_n(x) = \langle x|n\rangle$

$\langle x'|\widehat{a}^\dagger|x''\rangle = \delta(x'-x'')\frac{1}{\sqrt{2}\sigma}(x'' - \sigma^2\frac{\partial}{\partial x''})$, where $\sigma \equiv \sqrt{\frac{\hbar}{m\omega}}$

$\xi = \frac{x}{\sigma}, \qquad \langle x|n\rangle = \frac{1}{\sqrt{\sqrt{\pi}n!2^n\sigma}}(\xi - \frac{\partial}{\partial\xi})^n e^{-\frac{1}{2}\xi^2}$

$\langle x|0\rangle = (\frac{m\omega}{\pi\hbar})^{1/4}e^{-\frac{m\omega}{2\hbar}x^2}, \qquad \langle x|1\rangle = \sqrt{2}(\frac{m^3\omega^3}{\pi\hbar^3})^{1/4}xe^{-\frac{m\omega}{2\hbar}x^2}$

Classical simple harmonic oscillator Hamiltonian of a simple harmonic is $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2. \qquad \dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}, \qquad \dot{p} = -\frac{\partial H}{\partial x} = -m\omega^2 x$

Define $\sqrt{\hbar\omega}\alpha = \sqrt{\frac{m\omega^2}{2}}x + \frac{i}{\sqrt{2m}}p$, so $x = \sqrt{\frac{2\hbar}{m\omega}}\alpha_R$ and $p = \sqrt{2m\hbar\omega}\alpha_I$

Rewrite Hamiltonian, $H = \hbar\omega|\alpha|^2, \qquad \dot\alpha = -i\omega\alpha$. The sol is $\alpha = \alpha_0 e^{-i\omega t}$.

The quantum simple harmonic oscillator and coherent state Coherent state, superpos of stat states $|n\rangle$: $|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^\infty \frac{\alpha^n}{\sqrt{n!}}|n\rangle$

$P(n) = |\langle n|\alpha\rangle|^2 = |\alpha_n|^2 = \frac{\langle n\rangle^n e^{-\langle n\rangle}}{n!}$, where $\langle n\rangle = \langle\alpha|a^\dagger a|\alpha\rangle = |\alpha|^2$.

4. Three-dimensional systems

Three-dimensional infinite square well

$-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})\psi(x, y, z) = E\psi(x, y, z)$ for $0 \leq x \leq l_x, \ldots$ while $\psi(x, y, z) = 0$ outside.

Separation of vars: $\psi(x, y, z) = \psi_1(x)\psi_2(y)\psi_3(z)$

$\rightarrow$ SE becomes $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_1(x) = E_1\psi_1(x), \ldots$, where $E = E_1 + E_2 + E_3$.

$\psi_{n_xn_yn_z}(x, y, z) = \sqrt{\frac{8}{l_xl_yl_z}}\sin\left(\frac{n_x\pi}{l_x}x\right)\sin\left(\frac{n_y\pi}{l_y}z\right)\sin\left(\frac{n_z\pi}{l_z}z\right)$

$E_{n_xn_yn_z} = \frac{\hbar^2\pi^2}{2m}(\frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_y^2} + \frac{n_z^2}{l_z^2})$, with $n_x, n_y, n_z = 1, 2, \ldots$.

Wave vector: $\vec k = (k_x, k_y, k_z) = (\frac{n_x\pi}{l_x}, \frac{n_y\pi}{l_y}, \frac{n_z\pi}{l_z})$

The Schrödinger equation in spherical coordinates

$i\hbar\frac{\partial\psi(\vec r, t)}{\partial t} = -\frac{\hbar^2}{2m}\vec\nabla^2\psi(\vec r, t) + V(\vec r)\psi(\vec r, t)$, where $\vec r = (r, \theta, \phi)$, $\psi(\vec r, t) = \psi(r, \theta, \phi, t)$ and $\vec\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$ is Laplacian operator.

For a TI and central potential, potential depends only on r, $V(\vec r) = V(r)$.

$\frac{1}{R(r)}[\frac{d}{dr} - \frac{2mr^2}{\hbar^2}(V(r) - E)] = -\frac{1}{Y(\theta, \phi)}[\frac{1}{\sin\theta}\frac{d}{d\theta} + \frac{1}{\sin^2\theta}\frac{d^2Y(\theta, \phi)}{d\phi^2}]$

Each side must be constant and equal.

$\frac{1}{\sin\theta}\frac{d}{d\theta} + \frac{1}{\sin^2\theta}\frac{d^2Y(\theta, \phi)}{d\phi^2} = -l(l+1)Y(\theta, \phi)$

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

Orbital angular momentum $[\widehat{L}_i, \widehat{L}_j] = i\hbar\epsilon_{ijk}\widehat{L}_k$, with $i = 1, 2, 3$ representing the x, y, and z components, and the epsilon tensor is $\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1$, which is -1 for odd perms of indicies, and vanishes when repeated.
$\widehat{L}^2 = \widehat{L}_x^2 + \widehat{L}_y^2 + \widehat{L}_z^2$, $[\widehat{L^2}, \widehat{L}_i] = 0$
In pos rep, $\widehat{L} = \widehat{r} \times \widehat{p} = -i\hbar\vec{r} \times \vec{\nabla}$
In sph coords,
$\widehat{L} = -i\hbar r\widehat{r} \times (\frac{\partial}{\partial r}\widehat{r} + \frac{1}{r}\frac{\partial}{\partial\theta}\widehat{\theta} + \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\widehat{\phi} = -i\hbar(\widehat{\phi}\frac{\partial}{\partial\theta} - \widehat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi})$
Components along cartesian unit vectors:
$\widehat{r} = \sin\theta\cos\psi\widehat{x} + \sin\theta\sin\phi\widehat{y} + \cos\theta\widehat{z}$
$\widehat{\theta} = \cos\theta\cos\phi\widehat{x} + \cos\theta\sin\phi\widehat{y} - \sin\theta\widehat{z}$
$\widehat{\phi} = -\sin\phi\widehat{x} - \cos\phi\widehat{y}$
$\widehat{L}_x = i\hbar(\sin\theta\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi})$ $\widehat{L}_y = i\hbar(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi})$
$\widehat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$ $\widehat{L}^2 = -\hbar^2[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}]$
$\widehat{L}Y(\theta,\phi) = l(l+1)\hbar^2 Y(\theta,\phi)$
$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r} - V_{\text{eff}}(r)R(r) = ER(r)$, $V_{\text{eff}}(r) = V(r) + \frac{l(l+1)\hbar^2}{2mr^2}$
Spherical harmonics Find the sols to the angular eqn. Use sep of vars $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$.
$\frac{1}{\Theta}[\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta} + l(l+1)\sin^2\theta = -\frac{1}{\Theta}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2} = constant = m^2$
$\Psi(\psi) = e^{im\psi}$
$\Psi(\psi)$ is periodic in ψ w period 2π gives the constraint $m = 0, \pm1, \pm2, \cdots$
The eq for $\Theta(\theta)$ can be written in terms of $x \equiv \cos\theta$
$(1-x^2)\frac{\mathrm{d}^2P(x)}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}P(x)}{\mathrm{d}x} + (l(l+1) - \frac{m^2}{1-x^2})P(x) = 0$
Associated Legendre functions: $P_l^{m_l}(x) = (1-x^2)^{|m_l|/2}(\frac{\mathrm{d}}{\mathrm{d}x})^{|m_l|}P_l(x)$, where $P_l(x)$ is the l^{th} Legendre polynomial given by the Rodrigues formula $P_l(x) = \frac{1}{2^l l!}(\frac{\mathrm{d}}{\mathrm{d}x})^l(x^2-1)^l$, with l taking values $l = 0, 1, 2, \ldots$
and for each l, m_l takes $2l+1$ values $m_l = -l, -l+1, \ldots, l-1, l$.
Spherical harmonics, normalized angular wave functions:
$Y_l^m(\theta,\phi) = \epsilon\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}e^{im\phi}P_l^m(\cos\theta)$, where $\epsilon = (-1)^m$ for $m \geq 0$ and $\epsilon = 1$ for $m \leq 0$.
The Legendre polynomials are normalized s.t. they satisfy the ortho relation $\int_{-1}1 P_{l'}P_l(x)dx = \int_0^\pi P_{l'}(\theta)P_l(\theta)\sin\theta d\theta = \frac{2}{2l+1}\delta_{l'l}$
First few associated Legendre functions:
$P_0^0(x) = 1, P_1^1(x) = \sqrt{1-x^2}, P_1^0(x) = x, P_2^2(x) = 3(1-x^2), P_2^1(x) = 3x\sqrt{1-x^2}, P_2^0 = \frac{1}{2}(3x^2-1)$
$P_0^0(\theta) = 1, P_1^1(\theta) = \sin\theta, P_1^0(\theta) = \cos\theta, P_2^2(\theta) = 3\sin^2\theta, P_2^1(\theta) = 3\cos\theta\sin\theta, P_2^0(\theta) = \frac{1}{2}(3\cos^2\theta - 1)$
with $P_l^{-m_l}(x) = P_l^{m_l}(x)$
$\int_{-1}^1 P_{l'}^{m_l'}(x)P_l^{m_l}(x)dx = \int_0^\pi P_{l'}^{m_l'}(\theta)P_l^{m_l}(\theta)\sin\theta d\theta = \frac{(l+m_l)!}{(2l+1)(l-m_l)!}\delta_{l'l}\delta_{m_l',m_l}$
First few spherical harmonics:
$Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}}, Y_1^{\pm1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}, Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta$
The spherical harmonics satisfy the orthogonality relation
$\int_0^{2\pi}d\phi\int_0^\pi d\theta\sin\theta Y_{l'}^{m_l'*}(\theta,\phi)Y_l^{m_l}(\theta,\phi) = \delta_{l'l}\delta_{m_l'm_l}$
$\widehat{L}^2|lm_l\rangle = l(l+1)\hbar^2|lm_l\rangle$, $\widehat{L}_z|lm_l\rangle = m\hbar|lm_l\rangle$
The spherical harmonics are the wavefunctions in pos rep, $Y_l^{m_l}(\theta,\phi) = \langle\vec{r}|lm_l\rangle$
Parity of the spherical harmonics Cartesian coords:
$\widehat{P}\psi(x,y,z) = \psi(-x,-y,-z)$
Spherical coords: $\widehat{P}\psi(r,\theta,\phi) = \psi(r,\pi-\theta,\phi+\theta)$
For the Legendre polynomials, $\widehat{P}P_l^{m_l}(\theta) = (-1)^{l-|m_l|}P_l^{m_l}(\theta) \to$ even for $l+|m_l|$ even and odd for $l+|m_l|$ odd.
Azimuthal part of the wavefunction, $\widehat{P}e^{im_l\phi} = e^{im_l(\phi+\pi)} = (-1)^{m_l}e^{im_l\phi}$.
The spherical harmonics are products of two, and
$\widehat{P}Y_l^{m_l}(\theta,\phi) = Y_l^{m_l}(\pi-\theta,\phi+\pi) = (-1)^{l-|m_l|+m_l}Y_l^{m_l}(\theta,\phi) = (-1)^l Y_l^{m_l}(\theta,\phi)$

The hydrogen atom

Coulomb's law, $\widehat{V} = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$
Let $u(r) \equiv rR(r)$, Radial eq: $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2u}{\mathrm{d}r^2} + [-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}]u = Eu$
The radial wave function $\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$
$\frac{1}{\kappa^2}\frac{\mathrm{d}^2u}{\mathrm{d}r^2} = [1 - \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}\frac{1}{(\kappa r)} + \frac{l(l+1)}{(\kappa r)^2}]u$
Introduce $\rho \equiv \kappa r$, $\rho_0 \equiv \frac{me^2}{2\pi\epsilon\hbar^2\kappa}$, $\frac{\mathrm{d}^2u}{\mathrm{d}\rho^2} = [1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}]u$
As $\rho \to \infty$, the constant term in the brackets dominates, so $\frac{\mathrm{d}^2u}{\mathrm{d}\rho^2} = u$.
General sol is $u(\rho) = Ae^{-\rho} + Be^{\rho}$, but $B = 0 \to u(\rho) \approx e^{-\rho}$ for large ρ.
As $\rho \to 0$, centriugal term dominates, $\frac{\mathrm{d}^2u}{\mathrm{d}\rho^2} = \frac{l(l+1)}{\rho^2}u$
The general sol is $u(\rho) = C\rho^{l+1} + D\rho^{-l}$, but ρ^{-l} blows up as $\rho \to 0$, so $D = 0$. Thus, $u(\rho) \approx C\rho^{l+1}$ for small ρ.
Peel off the asymptotic behavior, $u(\rho) = \rho^{l+1}e^{-\rho}v(\rho)$
Radial eq in terms of $v(\rho)$, $\rho\frac{\mathrm{d}^2v}{\mathrm{d}\rho^2} + 2(l+1-\rho)\frac{\mathrm{d}v}{\mathrm{d}\rho} + [\rho_0 - 2(l+1)]v = 0$
Assume the solution, $v(p)$, can be expressed as a power series in ρ:
$v(\rho) = \sum_{j=0}^\infty c_j\rho^j$.
$c_{j+1} = \frac{2(j+l+1)-\rho_0}{(j+1)(j+2l+2)}c_j$
For large j (corresponding to large ρ), $c_{j+1} = \frac{2j}{j(j+1)}c_j = \frac{2}{j+1}c_j$
If this were exact, $c_j = \frac{2^j}{j!}c_0$, $v(\rho) = c_0\sum_{j=0}^\infty\frac{2^j}{j!}\rho^j = c_0e^{2\rho}$, and hence $u(\rho) = c_0\rho^{l+1}e^{\rho}$, which blows up at large ρ
Must exist $c_{j_{\max}+1} = 0$, beyond which all coefficients vanish automatically.
Define principle quantum number, $n \equiv j_{\max} + l + 1$, $\rho_0 = 2n$
$E = -\frac{\hbar^2\kappa^2}{2m} = -\frac{me^3}{8\pi^2\epsilon_0^2\hbar^2\rho_0^2}$
Bohr formula: $E_n = -[\frac{m}{2\hbar^2}(\frac{e^2}{4\pi\epsilon}^2]\frac{1}{n^2} = \frac{E_1}{n^2} = \frac{-13.6\text{ eV}}{n^2}$, $n = 1, 2, 3, \ldots$
$\kappa = (\frac{me^2}{4\pi\epsilon_0\hbar^2})\frac{1}{n} = \frac{1}{an}$, Bohr radius: $a \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10}\text{m}$
$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_l^m(\theta,\phi)$
$\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi a^3}}e^{-r/a}$
For arbitrary n, $l = 0, 1, 2, \ldots, n-1$, so $d(n) = \sum_{l=0}^{n-1}(2l+1) = n^2$
$v(\rho) = L_{n-l-1}^{2l+1}(2\rho)$, where $L_{q-p}^p(x) \equiv (-1)^p(\frac{\mathrm{d}}{\mathrm{d}x})^pL_q(x)$ is an associated Laguerre polynomial. $L_q(x) \equiv e^x(\frac{\mathrm{d}}{\mathrm{d}x})^q(e^{-x}x^q)$ is the qth Laguerre polynomial.
The normalized hydrogen wavefunctions are:

$$\psi_{nlm} = \sqrt{(\frac{2}{na})^3\frac{(n-l-1)!}{2n[(n+1)!]^3}}e^{-r/na}(\frac{2r}{na})^l[L_{n-l-1}^{2l+1}(2r/na)Y_l^m(\theta,\phi)$$

Wavefunctions are mutually orthogonal.
Spectrum Transitions: $E_\gamma = E_i - E_f = -13.6eV(\frac{1}{n_i^2} - \frac{1}{n_f^2})$
Planck formula, $E_\gamma = h\nu$, wavefunction is $\lambda = c/\nu$.
Rydberg formula: $\frac{1}{\lambda} = R(\frac{1}{n_f^2} - \frac{1}{n_i^2})$
Rydberg constant: $R \equiv \frac{m}{4\pi c\hbar^3}(\frac{e^2}{4\pi\epsilon_0})^2 = 1.097 \times 10^7\ \text{m}^{-1}$

General angular momentum

$\widehat{J} = (\widehat{J}_x, \widehat{J}_y, \widehat{J}_z) = (\widehat{J}_1, \widehat{J}_2, \widehat{J}_3)$
$\widehat{J}^2 = \widehat{J}_x^2 + \widehat{J}_y^2 + \widehat{J}_z^2$
The commutation relations are $[\widehat{J}_i, \widehat{J}_j] = i\hbar\epsilon_{ijk}\widehat{J}_k$, $[\widehat{J}^2, J_i] = 0$
Take the commuting set to be $\widehat{J}^2$ and $\widehat{J}_z$. Now suppose we trade $\widehat{J}_x$ and $\widehat{J}_y$ for $\widehat{J}_\pm = \widehat{J}_x \pm i\widehat{J}_y$
The commutation relations become $[\widehat{J}_+, \widehat{J}_-] = 2\hbar\widehat{J}_z$ and $[\widehat{J}_z, \widehat{J}_\pm] = \pm\hbar\widehat{J}_\pm$ and $[\widehat{J}^2, \widehat{J}_\pm] = 0$
Because $\widehat{J}^2$ and $\widehat{J}_z$ commute, we can simulaneously diagonalize them. Let the simultaneous eigenstate be $|ab\rangle$ s.t. $\widehat{J}^2|ab\rangle = a|ab\rangle$, $\widehat{J}_z|ab\rangle = b|ab\rangle$
$\widehat{J}^2(\widehat{J}_\pm|ab\rangle) = a(\widehat{J}_\pm|ab\rangle)$, so $\widehat{J}_\pm|ab\rangle$
$\widehat{J}_z(\widehat{J}_\pm|ab\rangle) = (b \pm \hbar)(\widehat{J}_\pm|ab\rangle)$
Thus, $\widehat{J}_+$ raises and $\widehat{J}_-$ lowers the eigenvalue b of $\widehat{J}_z$. Therefore, assuming $|ab\rangle$ is normalized, $\widehat{J}_\pm|ab\rangle = c_\pm|ab \pm \hbar\rangle$, where $c_\pm$ are normalization constants.
Define $j = \frac{n}{2}$, then $a = b_{\max}^2 + \hbar b_{\max} = j^2\hbar^2 + \hbar^2 j = j(j+1)\hbar^2$
$\widehat{J}_\pm|jm_j\rangle = \hbar\sqrt{(j \mp m_j)(j \pm m_j + 1)}|jm_j \pm 1\rangle$
The matrix elements of $\widehat{J}_\pm$ are
$\langle j'm_j'|\widehat{J}_\pm|jm_j\rangle = \hbar\sqrt{(j \mp m_j)(j \pm m_j + 1)}\langle j'm_j'|jm_j \pm 1\rangle = \hbar\sqrt{(j \mp m_j)(j \pm m_j + 1)}\delta_{j'j}\delta_{m_j'm_j\pm1}$

Spin

Classical orbital and spinning motion Infinitesimal classical angular momentum corresponding to an infinite linear momentum $d\vec{p} = dm\vec{v}$ at position $\vec{r}$ from the axis of rotation is $d\vec{L} = \vec{r} \times d\vec{p}$
The total angular momentum is $\vec{L} = \int\vec{r} \times d\vec{p} = \int\vec{r} \times dm\vec{v}$
Point particle of mass m at radius r spinning w constant angular velocity ω about the z-axis, $\vec{L} = I\omega\widehat{z} = m\omega r^2\widehat{z}$
Considering a particle of mass m and charge q rotating with angular velocity ω at radius r about the z-axis, the angular momentum $\vec{L}$ and the momentum dipole momentum $\vec{\mu}$ are given by $\vec{L} = m\omega r^2\widehat{z}$, $\vec{\mu} = \frac{q}{2}\omega r^2\widehat{z}$, where we used $\mu = I\pi r^2$ with current $I = \frac{q}{2\pi/\omega} = \frac{q\omega}{2\pi}$. Thus, $\vec{\mu} = \frac{q}{2m}\vec{L}$
Spin
Basis vectors are $|\frac{1}{2},\frac{1}{2}\rangle \equiv |1\rangle = \begin{bmatrix}1\\0\end{bmatrix}$, $|\frac{1}{2},\frac{1}{2}\rangle \equiv |1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$
Construct the matrices for $\widehat{S}_x$, $\widehat{S}_y$, $\widehat{S}_z$, and $\widehat{S}^2$.
The matrices $\widehat{S}_z$ and $\widehat{S}^2$ are diagonal, since they are the ones that are simultaneously diagonalized. The matrix elements are
$\langle s'm_s'|\widehat{S}^2|sm_s\rangle = s(s+1)\hbar^2\delta_{s's}\delta_{m_s'm_s}$,
$\langle s'm_s'|\widehat{S}_z|sm_s\rangle = m_s\hbar\delta_{s's}\delta_{m_s'm_s}$
In matrix form, $\widehat{S}^2 = \frac{3}{4}\hbar^2\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$, $\widehat{S}_z = \frac{\hbar}{2}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$
$\widehat{S}_+ = \hbar\begin{bmatrix}0 & 1\\0 & 0\end{bmatrix}$, $\widehat{S}_- = \frac{\hbar}{2}\begin{bmatrix}1 & 0\\0-1\end{bmatrix}$
$\widehat{S}_x = \frac{1}{2}(\widehat{S}_+ + \widehat{S}_-)$ and $\widehat{S}_x = \frac{1}{2i}(\widehat{S}_+ - \widehat{S}_-)$, we have $\widehat{S}_x = \frac{\hbar}{2}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$,
$\widehat{S}_y = \frac{\hbar}{2}\begin{bmatrix}0 & -i\\i & 0\end{bmatrix}$
Spin angular momentum: $\vec{S} = \frac{\vec{\sigma}}{2}$
where the components of $\vec{\sigma}$ are called the Pauli matrices, and given by $\sigma_x = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$, $\sigma_y = \begin{bmatrix}0 & -i\\i & 0\end{bmatrix}$, $\sigma_z = \begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$
Observe that $[\widehat{S}_i, \widehat{S}_j] = i\hbar\epsilon_{ijk}\widehat{S}_k$ and $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$
A general state of a spin-half system is given by a spinor,
$|\chi\rangle = \alpha|\frac{1}{2},\frac{1}{2}\rangle + \beta|\frac{1}{2},\frac{1}{2}\rangle = \begin{bmatrix}\alpha\\\beta\end{bmatrix}$, where α and β are complex constants.
Magnetic moment of the electron
Electron in a magnetic field
The Stern-Gerlach experiment

Addition of angular momentum

Triplet and singlet states of a system of two spin-halves
Addition of general angular momentum