Introduction

January 7, 2022 9:44 PM

Energy of light
- Quantized to each photon
- $E = h\nu$, ν is the frequency

Momentum of light
- $p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda}$.

Electron
- Magnetic field acting on electrons generate Lorentz Force on the electrons
- Classical Hall effect
  - Hall coefficient is proportional to magnetic field
- Quantum Hall effect
  - Hall coefficient is quantized

All entities have both particle and wavelike properties
- Waves are distributed displacements of some quantity in space and time
  - Interference, or the superposition of distinct distributed displacements, defines wavelike behavior
- Particle: quantized

The light emitted by lasers doesn't always need to be treated quantum mechanically to understand how it propagates away from the laser

Particle moving in 1 dimension in a time-independent potential V
- Initial speed: 100 m/s
- Start at x=0, t=0
- Uniform electric field exerting a force on the electron of 1N in negative x direction
- Classically
  - $x(t) = 100t - \frac{1}{2m}t^2$.
  - deterministic
- Quantum mechanically
  - Need to solve for the wave function of the electron $\psi(x,t)$ using Schrodinger's equation $i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi$.
  - ψ also gives information on the future dynamics
  - It is probabilistic
  - Note: x in Newton's equation is different from the x in Schrodinger equation.
    - In Newton's equation, x depends on t.
    - In Schrodinger equation, x and t are independent.
  - $\int_a^b |\psi(x,t)|^2 dx$ gives the probability of finding particle between a and b at time t.

Complex numbers
- $z = a + bi = re^{i\phi}$, $i = \sqrt{-1}$.
  - Real part: $Re(z) = a$.
  - Imaginary part: $Im(z) = b$.
  - Complex conjugate: $z^* = a - bi = re^{-i\phi}$.
  - Modulus/magnitude: $r = \sqrt{a^2 + b^2} = \sqrt{z^* z}$.
  - Argument(phase): $\phi = \tan^{-1}\left(\frac{b}{a}\right)$.
- $(a + bi) + (c + di) = (a + c) + (b + d)i$.
- $(a + bi)(c + di) = (ac - bd) + (ad + bc)i$.

Phasor representation of waves

- Euler's formula: $e^{i\phi} = \cos\phi + i\sin\phi$.
- A wave $x(t) = a\cos(\omega t + \phi)$ can be represented as $x(t) = Re\left\{ae^{i(\omega t+\phi)}\right\} = Re\{ae^{i\phi}e^{i\omega t}\}$.
    - Phasor (time-independent): $A = ae^{i\phi}$.

Wave function

January 12, 2022 2:02 PM

Schrodinger's equation $i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi$.

$\int_a^b |\psi(x,t)|^2 dx$ gives the probability of finding particle between a and b at time t.

- Underlying uncertainty in ψ due to phase is missing if only work with ψ^2.
- For any wave function, $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$.
  - The particle must be somewhere. Adding up all the probabilities of finding it must equal 1.

Measurement

- Performing a measurement and finding the particle at location $x = C$ with some uncertainty dx.
- Immediately after a measurement, the wave function collapses to C with dx uncertainty.

Average value/expectation

- $\langle x\rangle = \int_{-\infty}^{\infty} x\,|\psi(x,t_0)|^2 dx$.
- This is the average value we might measure if we had multiple copies of the same wavefunction and measured it several times.
- Or if we had an ensemble of identical wavefunctions and measured them all.
- A state is stationary if $\langle x\rangle = const$.

Standard deviation

- Let $\Delta x = x - \langle x\rangle$, $\langle \Delta x^2\rangle = \int_{-\infty}^{\infty}(x-\langle x\rangle)^2|\psi|^2 dx = \langle x^2\rangle - \langle x\rangle^2$.
- Shows the delocalization/size of the wavefunction

Momentum

- $\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{m}\int \psi^*\frac{\partial\psi}{\partial x}dx$.
- $\langle p\rangle = m\frac{d\langle x\rangle}{dt} = -i\hbar\int \psi^*\frac{\partial\psi}{\partial x}dx = \int \psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\psi dx$.

Operator

- $\hat{x} = x$.
- $\hat{p} = -i\hbar\frac{\partial}{\partial x}$.
- Hamiltonian: $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$.

Bra-ket notation

- $\langle x\rangle = \int \psi^*[x]\psi dx = \langle\psi|\hat{x}|\psi\rangle$.
- $\langle p\rangle = \langle\psi|\hat{p}|\psi\rangle$.

De Broglie equations

- $\lambda = \frac{h}{p}$.
  - $p = \hbar k$, k is the wave factor.
- $f = \frac{E}{h}$.
  - $E = \hbar\omega$.

Uncertainty principle

- The more precise a wave's position is, the less precise is its wavelength (momentum)
- Fourier transform of wavefunction $\psi(x)$ and $\phi(p)$.

    - $\psi(x) = A\int \phi(p)e^{\frac{ipx}{\hbar}}dp.$
    - $\phi(p) = A\int \psi(x)e^{-\frac{ipx}{\hbar}}dx.$
- If a particle is fixed at $x = x_0$
    - $\psi(x) = \delta(x - x_0).$
    - Then $\phi(p) = Ae^{-\frac{ipx_0}{\hbar}}$, $|\phi|^2 = A^2.$
    - p is everywhere, cannot be determined.

Probability densities

- Suppose $P(x)$ is a function describing the probability per unit length of finding a classical particle at a position x
- $P(x)$ is not probability, $P(x)dx$ is the probability of finding the particle in the interval $[x, x + dx]$.

Observables and expectation values

- If $f(x)$ is some observable quantity that depends only on the position x, then the expected average value of $f(x)$ if a number of identical measurements are performed is $\int_\Omega f(x)P(x)dx$, Ω is the support of the probability density P.

Quantum expectation values

- Quantum mechanically, the probability density is $P(x;t) = |\psi(x,t)|^2.$
- Then $P(x \in [a,b];t) = \int_a^b |\psi(x,t)|^2 dx.$
- Observables are associated with operators.
    - Position operator: $\hat{x} = x.$
    - Momentum operator: $\hat{p} = -i\hbar\frac{\partial}{\partial x}.$
- For any observable A, $\langle A\rangle = \int \psi^* \hat{A}\psi dx.$

More about uncertainty principle

- Standard deviation: $\sigma_A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}.$
    - A measure of the precision to which we know the value of an observable quantity
- Quantum mechanically, there is a limit to how precisely certain pairs of observables can be simultaneously known.
    - In general, $\sigma_A\sigma_B \geq \left|\frac{1}{2i}\langle[A,B]\rangle\right|.$
    - For position and momentum $\sigma_x\sigma_p \geq \frac{\hbar}{2}.$

Time-independent Schrodinger

January 12, 2022 2:03 PM

Full (time-dependent) Schrodinger equation

- $i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$.
- To solve it, use separation of variables
  - Let $\psi(x,t) = \psi(x)\phi(t)$
  - Then $\psi_t = \psi\phi_t$, $\psi_{xx} = \psi_{xx}\phi$.
  - $i\hbar\psi\phi_t = -\frac{\hbar^2}{2m}\psi_{xx}\phi + V\psi\phi$.
  - $i\hbar\frac{1}{\phi}\frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V(x)$.
- Setting both sides to equal a constant
  - $\frac{d\phi}{dt} = -\frac{iE\phi}{\hbar}$.
  - $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$.
  - In math, the E value can be any value
  - In physics, $E \sim V(x)$.

Space-independent:

- $\phi(t) = e^{-i\frac{E}{\hbar}t}$.
- Valid for any real E.
- Imaginary E will lead to un-normalizable wavefunction

Time-independent:

- $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi$.
  - E is the energy
- Depending on the potential $V(x)$, there are typically only solutions of the time-independent equation for restricted values of $E = E_n$.
  - E_n is an eigenvalue
  - ψ_n is an eigen function
  - $\langle E\rangle = \langle\psi|\hat{H}|\psi\rangle = \int_{-\infty}^{\infty}\psi_n^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi_n(x)dx = E_n$.
    - When particle is in the nth stationary state.
  - $\langle E^2\rangle = E_n^2$ and $\sigma^2 = 0$.
    - The energy of the particle when it is in a stationary state is precisely E_n.
- For each E_n, we get a specific $\psi_n(x)$.
  - $\psi_n(x,t) = \psi_n(x)e^{-i\frac{E_n}{\hbar}t}$.
  - Each solution is called a stationary state
  - Each $\psi_n(x,t)$ is an orthonormal basis of $\psi(x,t)$.
- Stationary state
  - $\langle\hat{Q}\rangle = \int_{-\infty}^{\infty}\psi_n^*(x)e^{i\frac{E_n}{\hbar}t}\hat{Q}\psi_n(x)e^{-i\frac{E_n}{\hbar}t}dx = \int_{-\infty}^{\infty}\psi_n^*(x)\hat{Q}\psi_n(x)dx$.
  - So $\langle\hat{Q}\rangle$ is time-independent
- Solution set $\{\psi_n(x)\}$ is infinite
  - Each with associated energy $\{E_n\}$.
  - $\psi(x,0) = \sum_{n=1}^{\infty}c_n\psi_n(x)$.
  - The initial state can always be matched with appropriate choice of constants $\{c_n\}$.
  - Then $\psi(x,t) = \sum_{n=1}^{\infty}c_n\psi_n(x)e^{-\frac{iE_nt}{\hbar}} = \sum_{n=1}^{\infty}c_n\psi_n(x,t)$.
    - This means that we only need $\psi(x,0)$ (no need for $\psi_t(x,0)$) to solve for the constant.
- $|c_n|^2$.

- The probability that a measurement of the energy would be E_n.
- $\sum_{n=1}^{\infty}|c_n|^2 = 1$.
- Expectation of energy $\langle H\rangle = \sum_{n=1}^{\infty}|c_n|^2 E_n$.
- Energy conservation in quantum mechanics

Infinite well

- $V = \begin{cases} 0, 0 \le x \le a \\ \infty, elsewhere \end{cases}$.
- Boundary conditions: wavefunctions must be continuous at boundary
  - $\psi(x)$ must be continuous and differentiable for Schrodinger equation.
  - $\frac{d\psi}{dx}$ is continuous except the infinity
- Solutions
  - $\psi(x) = \begin{cases} Ae^{i\frac{\sqrt{2m}E}{\hbar}x} + Be^{-i\frac{\sqrt{2m}E}{\hbar}x}, 0 \le x \le a \\ 0, elsewhere \end{cases}$.
  - We also need $\psi(0) = \psi(a) = 0$.
    - This requires $\psi_n(x) = A\sin\left(\frac{n\pi}{a}x\right)$
    - $k_n = \frac{n\pi}{a}$, $E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$, $n = 1,2, \ldots$.
  - Normalization: $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$.
    - They are orthonormal: $\frac{2}{a}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi x}{a}\right)dx = \delta_{mn}$.
- Coefficient c_n.
  - $\psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)e^{-i\frac{n^2\pi^2\hbar}{2ma^2}t}$.
  - If there is only a single non-zero c_n, it is a stationary state, the expectation value of the momentum operator is stationary
  - c_n can be found using Fourier series.
    - $c_n = \sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\psi(x,0)dx$.
    - More generally, $c_n = \int_0^a \psi_n^*(x)\psi(x,t_0)dx$.
      - $\psi(x,t) = \sum_{n=1}^{\infty}\left[\int_0^a \psi_n^*(x)\psi(x,t_0)dx\right]\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)e^{-i\frac{n^2\pi^2\hbar}{2ma^2}(t-t_0)}$ for $t > t_0$.

Orthogonal and orthonormal functions

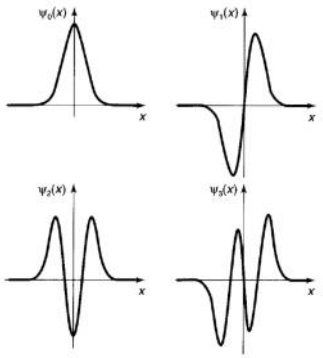
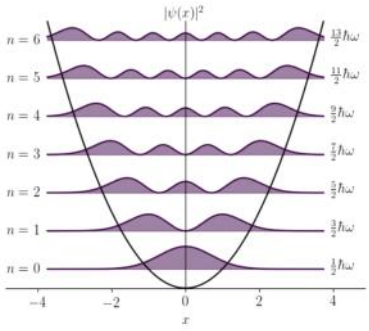
- Orthogonal functions: $\int \psi_m(x)^*\psi_n(x)dx = 0\ (m \ne n)$.
- Orthonormal functions: $\int \psi_m(x)^*\psi_n(x)dx = \delta_{mn}$.
  - Normalized and orthogonal
- A set of functions is complete, if any function $f(x)$ can be approximated by $f(x) = \sum c_n\psi_n(x)$.
  - i.e. this set can provide a Fourier series

Dynamics of an electron in an infinite square well

- Take the initial wavefunction of particle in an infinite square well potential to be an equally weighted superposition of the lowest two stationary states
  - $\psi(x, t=0) = \frac{1}{\sqrt{2}}(\psi_1(x) + \psi_2(x)) = \sqrt{\frac{1}{a}}\left(\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{2\pi x}{a}\right)\right)$.
- $\psi(x,t) = \sqrt{\frac{1}{a}}\left(\sin(kx)\,e^{-i\omega_1 t} + \sin(2kx)\,e^{-i(4\omega_1)t}\right)$.
  - $k = \frac{\pi}{a}$, $\omega_1 = \frac{\pi^2\hbar}{2ma^2}$.
- $\psi(x)$ is valid in $x \in [0, a]$.
- Half period: $\frac{\pi}{3\omega_1}$.
  - $t_0\omega_1 = 4t_0\omega_1 - \pi$.
  - $\psi_2(x)$ is π ahead of $\psi_1(x)$.

- Full period: $\frac{2\pi}{3\omega_1}$.
  - $t_0\omega_1 = 4t_0\omega_1 - 2m\pi$.
  - Overlap again.
- The particle is oscillating in the well (left↔right).
- With $\langle p \rangle = \int_0^a \psi^* \hat{p} \psi dx$, the effective distance travelled is $\Delta x = \int \frac{\langle p \rangle}{m} dt$.

Harmonic oscillator potential

- Potential: $V(x) = \frac{kx^2}{2}$.
- Classically
  - $m\frac{d^2x}{dt^2} = -kx$.
  - General solution: $x(t) = A\sin\sqrt{\frac{k}{m}}t + B\cos\sqrt{\frac{k}{m}}t$.
  - With initial solution $x = -x_0$, $x(t) = -x_0\cos\sqrt{\frac{k}{m}}t$.
- Quantum mechanically
  - $i\hbar\psi_t = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2\right)\psi$, $\omega_0 = \sqrt{\frac{k}{m}}$.
  - If we redefine $\xi = x\sqrt{\frac{m\omega_0}{2\hbar}}$.
    - $\frac{d^2}{d\xi^2}\psi = (\xi^2 - K)\psi$.
    - To solve this, let $\psi = h(\xi)e^{-\frac{\xi^2}{2}}$.
    - And this gives $h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j$, with $a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)}a_j$.
    - Since the wavefunction needs to be 0 at $\pm\infty$, we need some n such that $a_n = 0$.
  - Two implications
    - For the power series to terminate $K = K_n = 2n + 1$, $E_n = \hbar\omega_0\left(n + \frac{1}{2}\right)$.
    - The corresponding eigenfunctions then come in two, odd and even with respect to x, by choosing an n, then using the recurrence relations with the corresponding value of of K_n, starting with either $a_0 = 0$, $a_1 = 1$ for odd solutions, and $a_0 = 1$, $a_1 = 0$ for even solutions
  - 
    
    - Particles have 0 probability at origin for odd n, impossible for classical oscillator.
    - Particles have non-zero probability outside the well.
    - When $n \to \infty$, the eigen states look almost classical
  - Difference between harmonic oscillator and infinite well
    - Energy difference
      - Harmonic oscillator: $\Delta E_n = \hbar\omega$.
      - Infinite square well: $E_n \sim n^2$ (not evenly spaced).
    - Node numbers
      - Harmonic oscillator: nth energy level has n nodes.
      - Infinite square well: nth energy level has $n - 1$ nodes.
    - Nodes
      - Harmonic oscillator: get smaller as we move to the center

        - Infinite square well: periodic
    - Solutions
        - $\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}$.
        - $\psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \sqrt{\frac{2m\omega}{\hbar}} x e^{-\frac{m\omega}{2\hbar}x^2}$.
        - $\psi_n(x) = A_n(\hat{a}_+)^n \psi_0(x) = \frac{1}{\sqrt{n!}}(\widehat{a_+})^n \psi_0$.
        - $\hat{a}_+ \psi_n = \sqrt{n+1}\psi_{n+1}$, $\hat{a}_- \psi_n = \sqrt{n}\psi_{n-1}$.
        - $\widehat{a_\pm} = \frac{1}{\sqrt{2\hbar m\omega}}\left(\mp i\hat{p} + m\omega x\right)$.

Free particle ($V(x) = 0$)

- Similar to infinite well
- General form: $\psi(x) = Ae^{ikx} + Be^{-ikx}$.
    - $k = \frac{\sqrt{2mE}}{\hbar}$.
    - No restriction, can take any positive energy.
- Note: if $E < V$ or $E < 0$, $\psi(\pm\infty)$ diverges and cannot be normalized.
    - To normalize, we must have $\psi(\pm\infty) = 0$.
    - Current ψ cannot directly normalized
- Take the time dependence, we get $\psi(x,t) = Ae^{ik\left(x - \frac{\hbar k}{2m}t\right)} + Be^{-ik\left(x + \frac{\hbar k}{2m}t\right)}$.
    - The real and imaginary parts differ by a phase
    - Any function $x \pm vt$ represents a wave of unchanging shape, traveling in the direction $\mp x$ at speed v.
    - Fixed point: a fixed value of argument such that $x \pm vt = const$. Or $x = \mp vt + const.$.
- $k = \pm\frac{\sqrt{2mE}}{\hbar}$, with $\begin{cases} k > 0, traveling\ to\ the\ right \\ k < 0, traveling\ to\ the\ left \end{cases}$.
- Phase velocity of a harmonic wave $e^{i(kx-\omega t)}$.
    - $\phi = kx - \omega t = const.$.
    - For fixed points, $0 = \frac{d\phi}{dt} = k\frac{dx}{dt} - \omega$, so $\frac{dx}{dt} = \frac{\omega}{k}$.
    - $v_p = \frac{\omega}{k} = \frac{\hbar|k|}{2m} = \sqrt{\frac{E}{2m}}$.
    - It can take two values $\pm\sqrt{\frac{E}{2m}}$.
- Difference to infinite square well and harmonic oscillator
    - Eigenstates and eigenvalues
        - In infinite square well and harmonic oscillator, each E_n corresponds to one ψ_n.
        - In free particles, each E corresponds to 2 waves (one moving left, one moving right).
    - Energy values
        - In infinite square well and harmonic oscillator, E_n are discrete, can only be certain numbers. (energy is quantized)
        - In free particle, energy $E > 0$ is a continuous spectrum.
- Expectation values.
    - With a finite interval $[-L, L]$, we have $\langle v\rangle = \frac{1}{m}\langle p\rangle = \frac{\hbar k}{m} = 2v_p$.
- A free particle cannot exist in a stationary state
    - There is no such thing as a free particle with a definite energy
- The eigen functions won't change for any positive constant $V = V_0$.
    - Only $k = \pm\frac{\sqrt{2m(E-V)}}{\hbar}$ changes.

Wave packet

- Real case for the free particle
- $\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}dk$.
    - It is a superposition of waves.

- Superposition of 1D plane waves can sum to form a quantum Gaussian wave packet that propagates to left/right while spreading
- 1st dynamic: Central group velocity ($\frac{d\omega}{dk}$) ≈ 2 phase velocity ($\frac{\omega}{k}$)
    - Group velocity: velocity of the wave packet
    - Phase velocity: velocity of the individual waves
- 2nd dynamic: Dispersion
    - Without dispersion, shape of the wave packet doesn't change
    - With dispersion, the wave packet itself gets dispersed overtime

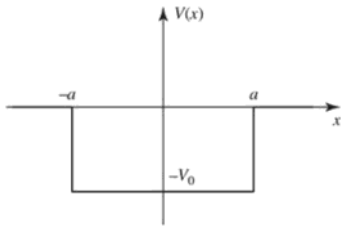
Fourier transform

- How to determine $\phi(k)$ to match the initial wave function $\psi(x,0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{ikx}dk$.
- Plancherel's theorem
    - $f(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}F(k)e^{ikx}dk \Leftrightarrow F(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x)e^{ikx}dx$.
- So $\phi(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x,0)e^{ikx}dx$.

Gaussian wave packet

- Dispersion only: $\psi(x,t)=\frac{1}{\sqrt{2\pi}}\left(\frac{2}{\pi}\right)^{1/4}\sqrt{\sigma}\sqrt{4\pi}\sqrt{\frac{m}{2}}\frac{1}{\sqrt{2m\sigma^2+i\hbar t}}e^{-\frac{1}{2}\left(\frac{m}{2m\sigma^2+i\hbar t}\right)\left(x-x_0\right)^2}$.
- Adding center of mass velocity $\psi(x,0)=\left(\frac{1}{\sqrt{2\pi}\sigma}\right)^{\frac{1}{2}}e^{-\frac{\left(x-x_0\right)^2}{4\sigma^2}}e^{ik_0x}$.
    - $\phi(k)=\left(\frac{2}{\pi}\right)^{\frac{1}{4}}\sqrt{\sigma}e^{-\sigma^2\left(k-k_0\right)^2}$.
    - With Taylor expansion $\psi(x,t)=\frac{1}{\sqrt{2\pi}}\left(\frac{2}{\pi}\right)^{1/4}\sqrt{\sigma}\sqrt{4\pi}\sqrt{\frac{m}{2}}\frac{1}{2m\sigma^2}e^{-\frac{\left(x-\frac{\hbar k_0}{m}t\right)^2}{4\sigma^2}}e^{i\left(k_0x-\frac{\hbar k_0^2}{2m}t\right)}$.
        - $\psi^*\psi=\frac{1}{\sqrt{2\pi}}\frac{1}{\sigma}e^{-\frac{\left(x-\frac{\hbar k_0}{m}t\right)^2}{2\sigma^2}}$ doesn't disperse.
    - Otherwise, $\psi(x,t)=\frac{1}{\sqrt{2\pi}}\left(\frac{2}{\pi}\right)^{\frac{1}{4}}\sqrt{\sigma}e^{-\sigma^2k_0^2}\int_{-\infty}^{\infty}e^{-\sigma^2k^2}e^{-i\frac{\hbar k^2}{2m}t}e^{ik\left(x-x_0\right)+k2\sigma^2k_0}dk$.
        - $\psi^*\psi=\sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{\sigma^2+\frac{\hbar^2t^2}{4m^2\sigma^2}}}e^{-\frac{\left(x-\frac{\hbar k_0}{m}t\right)^2}{2\left(\sigma^2+\frac{\hbar^2t^2}{4m^2\sigma^2}\right)}}$.
- Group velocity: $v_g=\sqrt{\frac{2E}{m}}=\sqrt{\frac{2\hbar\omega}{m}}=\frac{d\omega}{dk}=\frac{\hbar k_0}{m}$.
- Wavelength: $\lambda=\frac{2\pi}{k}$.
- Phase velocity: $\frac{\omega}{k}=\frac{v_g}{2}$.
- When the original size (dispersion) is small, it collapses fast.
- When the original dispersion is large, it collapses slowly
- Classical analogy
    - Water drop
    - Entropy
- Net wave packet = envelope + carrier
    - Envelope: $e^{-\left(\frac{x-x_0-\frac{\hbar k_0}{m}t}{2\sigma}\right)^2}$.
    - Carrier: $e^{i\left(k_0x-\frac{\hbar^2x_0^2t}{2m}\right)}$.

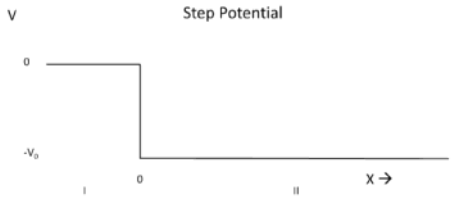
Finite potential well

- 

- Negative energy is just a reference number
- Bound states ($0 > E > -V_0$)
  - The particle is trapped in the well
  - In the well, $\psi(x) = C\sin lx + D\cos lx$ $(-a \le x \le a)$.
    - $l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$.
  - Outside the well, $\psi(x) = Fe^{-\kappa x} + Ge^{\kappa x}$ $(x < -a, x > a)$.
    - $\kappa = \frac{\sqrt{-2mE}}{\hbar}$.
  - Even solution
    - $\psi(x) = \begin{cases} Fe^{-\kappa x}, x > a \\ D\cos(lx), 0 < x < a. \\ \psi(-x), x < 0 \end{cases}$
    - For continuity ($\psi(x)$ and $\frac{d\psi}{dx}$), we need $\kappa = l\tan la$.
    - Let $z = la$, $z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$.
    - Energy eigenstates are solutions to $\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$.
      - Wide, deep well: If z_0 is large, $z_n \approx \frac{n\pi}{2}$ (n odd), $E_n + V_0 \approx \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$.
      - Shallow, narrow well: if z_0 is small (close to 0), only one bound state for $z_0 < \frac{\pi}{2}$.
  - Odd solution
    - Replace $\cos lx$ with $\sin lx$.
- Scattering states ($E > 0$)
  - Two eigen solutions
  - Transmission/tunneling effect
  - $\psi(x) = Ae^{ikx} + Be^{-ikx}$ $(x < -a)$, $\psi(x) = Fe^{-ikx}(x > a)$.
    - $k = \frac{\sqrt{2mE}}{\hbar}$.
  - In the well, $\psi(x) = C\sin lx + D\cos lx$ $(-a \le x \le a)$.
    - $l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$.
  - With continuity requirements
    - $ik\left(Ae^{-ika} - Be^{ika}\right) = l(C\cos la + D\sin la)$.
    - $C\sin la + D\cos la = Fe^{-ika}$.
    - $l\,(C\cos la - D\sin la) = ikFe^{ika}$.
    - Then, $B = \frac{i\sin 2la}{2kl}\left(l^2 - k^2\right)F$, $F = \frac{e^{-2ika}A}{\cos 2la - i\frac{k^2+l^2}{2kl}\sin 2la}$.
  - Transmission coefficient
    - $T = \frac{|F|^2}{|A|^2}$.
    - $T^{-1} = 1 + \frac{V_0^2}{4E\,(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)$.
  - Perfect transmission
    - $T = 1$ when $\frac{2a}{\hbar}\sqrt{2m(E_n+V_0)} = n\pi$.
    - $E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$.
  - Reflection coefficient
    - $R = \frac{|B|^2}{|A|^2}$.

- $T + R = 1$.

Step potential

- 

- left to right
  - Left: $\psi_1 = Ae^{i\frac{\sqrt{2m}E}{\hbar}x} + Be^{-i\frac{\sqrt{2m}E}{\hbar}x}$.
    - A: incident
    - B: reflection
  - Right: $\psi_2 = Ce^{i\frac{\sqrt{2m(E+V_0)}}{\hbar}x}$.
    - C: transmission
  - Reflectivity: $\frac{|B|^2}{|A|^2}$.
  - Transmission: $\frac{|C|^2}{|A|^2}$.
- right to left
  - Left: $\psi = Ce^{-i\frac{\sqrt{2m}E}{\hbar}x}$
    - Transmission
  - Right: $\psi = Ae^{-ik'x} + Be^{ik'x}$
    - A: Incident
    - B: Reflection

For bound states, energies are discrete. For scatter states, energies can be continuous.

Formalism

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Bra-ket notation:

- Dot product of r and r': $\langle r'|r\rangle = x'x + y'y$.
- If $\langle i|r'\rangle = x'$ and $\langle j|r'\rangle = y'$, then $|r'\rangle = \begin{pmatrix} x' \\ y' \end{pmatrix}$.
- Bra (transpose + conjugate): $\langle r| = |r\rangle^\dagger = (x^*, y^*)$.
  - Transpose: $\tilde{a}$.
  - Conjugate: a^*.
- $|r\rangle = (|i\rangle\langle i| + |j\rangle\langle j|)|r\rangle$.
  - $|i\rangle\langle i| + |j\rangle\langle j|$ is a unity operator.
  - $|i\rangle\langle i|$ and $|j\rangle\langle j|$ are projection operators
- Matrix: $\sum_{i=1}^n |\alpha_i\rangle\langle\alpha_i|$.
  - $\langle W|r'\rangle|r\rangle = \langle r'|W^\dagger|r\rangle$.
  - Linear transformation to a set of basis vectors: $T_{ij} = \langle e_i|T|e_j\rangle = \sum_{i=1}^n T_{ij}|j\rangle$.
  - Matrix multiplication: $AB_{ij} = \langle i|AB|j\rangle = \sum_k \langle i|A|k\rangle\langle k|B|j\rangle = \sum_k A_{ik}B_{kj}$.
- If $|\alpha_i\rangle$ are orthonormal.
  - Orthonormality: $\langle \alpha_i|\alpha_j\rangle = \delta_{ij}$.
  - Completeness: $\sum_{i=1}^n |\alpha_i\rangle\langle\alpha_i| = I$.
- A complete inner product has properties
  - $\langle u|v\rangle = \langle v|u\rangle^*$.
  - $\langle u|v\rangle \geq 0$, equality if and only if $u = 0$.
  - Linearity:
    - $\langle u|c_1v_1 + c_2v_2\rangle = c_1\langle u|v_1\rangle + c_2\langle u|v_2\rangle$.
    - $\langle c_1u_1 + c_2u_2|v\rangle = c_1^*\langle u_1|v\rangle + c_2^*\langle u_2|v\rangle$.

Hilbert space

- For $a = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$, $b = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$, $\langle a|b\rangle = a_1^*b_1 + a_2^*b_2$.
- Complex functions: $f(x), g(x) \in \mathbb{C}, L^2(\mathbb{R})$.
  - $\langle f|g\rangle = \langle g|f\rangle^* = \int_{-\infty}^{\infty} f^* g dx$.
- Series of functions
  - $\langle f_n|f_m\rangle = \delta_{mn}$.
  - $f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$.
  - $c_n = \langle f_n|f\rangle$.

Operators

- Operators are objects $O: V \to V$, $O(|v\rangle) = O|v\rangle$.
  - O is naturally written as $O = |u\rangle\langle v|$.
  - $O = \sum_{i,j} |i\rangle\langle i|O|j\rangle\langle j|$.
  - Since $\langle u|O|v\rangle^* = \langle v|O^\dagger|u\rangle$, if we choose u, v as orthonormal basis vectors
    - $\langle i|O^\dagger|j\rangle = \langle j|O|i\rangle$.
    - $O_{ij}^\dagger = O_{ji}$.
    - $\langle f|O = (O^\dagger|f\rangle)^\dagger$.
  - If $O = |a\rangle\langle b|$, then $O^\dagger = |b\rangle\langle a|$.
  - $\langle O^\dagger u|v\rangle = \langle u|Ov\rangle$.
- Rotation operator:
  - $R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$.

- $\hat{R}^{\dagger}(\theta) = \hat{R}^{T}(\theta) = R(-\theta)$.
- Operators for functions
  - $\langle O^{\dagger} f | g \rangle = \int (O^{\dagger} f)^{*} g dx = \int f^{*} O g dx.$
  - If $O = \frac{d}{dx'}$, then $O^{\dagger} = -\frac{d}{dx}$. (not Hermitian)
  - $p = -i\hbar \frac{d}{dx'}$, $p^{\dagger} = p$. (Hermitian)
- Hermitian operators
  - $O^{\dagger} = O$.
  - Operators with real expectation values for any arbitrary state must be Hermitian
    - $\langle O \rangle = \langle O \rangle^{*}$.
    - $\langle f | Of \rangle = \langle Of | f \rangle$.
  - Eigen states that have zero variance in their expectation values (determinate states) for Hermitian operators must be eigen states of those Hermitian operators
    - If the variance of an observable is identically 0 in a particle state for an operator Q, the state under consideration is an eigenstate of Q with eigen value $\langle Q \rangle$.
    - $\sigma^2 = 0 = \left\langle (Q-q)^2 \right\rangle = \left\langle \psi \left| (Q-q)^2 \right| \psi \right\rangle = \left| (Q-q)|\psi\rangle \right|^2$.

Discrete & continuous eigen spectrum

- When the eigen spectrum is discrete for Hermitian operators,
  - Reality: the eigenvalues must be real,
    - $Q|f_n\rangle = q|f_n\rangle$, so $\langle f|Qf\rangle = \langle Qf|f\rangle$, $q\langle f|f\rangle = q^{*}\langle f|f\rangle$.
  - Orthonormality: the eigen states corresponding to different eigen values are orthogonal,
    - $Q|f_{n'}\rangle = q'|f_{n'}\rangle$, $\langle f_{n'}|Qf_n\rangle = \langle Qf_{n'}|f_n\rangle$, $q\langle f_{n'}|f_n\rangle = q'\langle f_{n'}|f_n\rangle$.
  - Completeness: a complete orthonormal basis that spans the relevant state space can be formed from the eigen states
  - e.g. infinity quantum well, harmonic oscillators
- When the eigen spectrum is continuous,
  - Reality, orthonormality, completeness still hold.
  - e.g. free particles
  - Eigen states of the position operator
    - $x g_y(x) = y g_y(x)$ with eigen state $g_y(x)$, eigen value y can be any real numbers.
    - $g_y(x) = A\delta(x-y)$.
    - $\langle g_{y'} | g_y \rangle = |A|^2 \int \delta(x-y')\delta(x-y)dx = |A|^2 \delta(y-y')$.
    - Following the notation, $f_{x'}(x) = \delta(x-x')$, $\langle f_{x''} | f_{x'} \rangle = \delta(x''-x')$.
  - Eigen states of the momentum operator
    - $-i\hbar \frac{d}{dx} f_p(x) = p f_p(x)$, with eigen state $f_p(x)$.
    - $f_p(x) = Ae^{\frac{ipx}{\hbar}}$.
      - Note: If we replace $p = k\hbar$, it is the free particle general solution.
    - p can be any real value.
    - $\langle f_{p'}(x) | f_p(x) \rangle = |A|^2 \int_{-\infty}^{\infty} \exp\left(\frac{i(p-p')x}{\hbar}\right) dx = |A|^2 \, 2\pi\hbar\delta(p-p')$.
      - Let $|A| = \frac{1}{\sqrt{2\pi\hbar}}$, then $\langle f_{p'}(x) | f_p(x) \rangle = \delta(p-p')$.
    - So $f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}}$.
  - Dirac orthonormality
    - $\langle f_{p'}(x) | f_p(x) \rangle = \delta(p-p')$.

Transform of basis

- $f(x) = \int C_p f_p(x) dp$ converts from momentum space to position space.
  - $C(p) = \langle f_p(x) | f(x) \rangle = \int \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{ipx}{\hbar}} \psi(x,t) dx = \phi(p,t)$.

- Position space wave function $\psi(x,t)$, with basis $|x\rangle$.
  - $\psi(x,t) = \int \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}} \phi(p,t) dp$.
- Momentum space wave function $\phi(p,t)$, with basis $|p\rangle$.
  - $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}}$.
- Energy space wave function $Z(E_n,t)$, with basis $|E_n\rangle$.
  - $\langle x|E_n\rangle = \psi_n(x)$.
  - $\langle E_n|x\rangle = \psi_n^*(x)$.

Eigen states
- Immutable state that represents the essence of a quantum mechanical particle's temporal evolution, subject to some potential
- The state can be fully described using any number of expansions in distinct bases that each span the more general Hilbert state space of the problem
- Let $|S(t)\rangle$ be an arbitrary quantum state.
  - Identity: $I = \sum_n |\alpha_i\rangle\langle\alpha_i| = \int |s\rangle\langle s|$,
    - $|S(t)\rangle = \sum_n \langle O_n|S(t)\rangle |O_n\rangle = (\sum_n |O_n\rangle\langle O_n|)|S(t)\rangle$.
  - $\psi(x,t) = \langle x|S(t)\rangle$.
    - Let $|O_n\rangle \to |x_n\rangle \to |x\rangle$, $|S(t)\rangle = \int |x\rangle\langle x||S(t)\rangle dx = \langle x|S(t)\rangle$.
    - Projection of the immutable state of the particle at any time onto eigen states of the immutable position operator with eigen values x'.
    - $\hat{x}|x\rangle = x|x\rangle$.
    - Can think of any $\psi(x,t)$ as projection of $|S(t)\rangle$ onto each abstract eigen state of the $\hat{x}$ operator with real eigen values x, eigenvector $|x\rangle$.
    - $\psi_{|x\rangle}(x') = \langle x'|x\rangle = \delta(x-x')$.
      - It is the projection of $|x\rangle$ onto the basis $|x'\rangle$.
      - $\langle x'|S(t)\rangle = \psi_{|S(t)\rangle}(x',t) = \int \psi_{|S(t)\rangle}(x,t)\langle x'|x\rangle dx$.
  - $\phi(p,t) = \langle p|S(t)\rangle$.
  - $Z(E_n,t) = \langle E_n|S(t)\rangle$.

Eigen states and eigen functions
- Ket is the state ($|p\rangle$, $|x\rangle$)
- Bra is the basis we want to project to ($\langle x|$).
- Position operator
  - Eigen state: $|x\rangle$.
  - Eigen function in the position space: $f_{x'}(x) = \delta(x-x') = \langle x'|x\rangle$.
- Momentum operator
  - Eigen state: $|p\rangle$.
  - Eigen function in the position space: $\langle x|p\rangle = f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}}$.
  - Note: $\langle x|p\rangle^* = \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{ipx}{\hbar}}$.
  - $\langle p'|p\rangle = \delta(p-p')$.
- Abstract state at time t.
  - Eigen state: $|S(t)\rangle$.
  - Eigen function: $\langle x|S(t)\rangle$.
  - Eigen function is the projection of the abstract state at time t in Hilbert space onto the eigens tates of the position operator in abstract Hilbert space

Given the eigen value equation for the position operator $\hat{x}|\zeta\rangle = \zeta|\zeta\rangle$.
- Project onto the position basis $\langle x'|\hat{x}|\zeta\rangle = \langle x'|\zeta|\zeta\rangle$.
  - RHS: $\langle x'|\zeta|\zeta\rangle = \zeta\langle x'|\zeta\rangle = \zeta f(x')$.
  - LHS: $\langle x'|\hat{x}|\zeta\rangle = \langle \hat{x}^\dagger|x'\rangle|\zeta\rangle = x'\langle x'|\zeta\rangle = x' f(x')$.
- So $x' f(x') = \zeta f(x')$.

Expectation value

- $\langle\hat{x}\rangle|_{S(t)} = \langle S(t)|\hat{x}|S(t)\rangle$.
- Convert into expectation values using wavefunctions.
  - $\langle\hat{x}\rangle|_{S(t)} = \left\langle S(t)\left|\int|x'\rangle\langle x'|dx'\,\hat{x}\int|x''\rangle\langle x''|dx''\right|S(t)\right\rangle$.
  - $= \int dx'dx''\,\langle S(t)|x'\rangle\langle x'|\hat{x}|x''\rangle\langle x''|S(t)\rangle$.
  - $= \sum_n\sum_m\langle S(t)|x_m\rangle\langle x_m|\hat{x}|x_n\rangle\langle x_n|S(t)\rangle$.
  - Note $\langle S(t)|x'\rangle = \psi_s^*(x',t)$, $\langle x''|S(t)\rangle = \psi_s(x'',t)$, $\langle x'|\hat{x}|x''\rangle = x''\langle x'|x''\rangle = x''\delta(x'-x'')$.
  - So, we get $\langle\hat{x}\rangle|_{S(t)} = \int dx'dx''\psi_s^*(x',t)\delta(x'-x'')\psi_s(x'',t) = \int dx'\psi_s^*\psi_s$.
- Expand $|S(t)\rangle$ in momentum basis.
  - $|S(t)\rangle = \int|p\rangle\langle p|dp\,|S(t)\rangle = \int dp\langle p|S(t)\rangle|p\rangle$.
  - $= \int dp\left(\int dx'\,\langle p|x'\rangle\langle x'|S(t)\rangle\right)|p\rangle$.
  - Now, use $\langle p|x'\rangle = \langle x'|p\rangle^*$ and $\langle x'|p\rangle = f_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx'}{\hbar}}$.
  - We get $|S(t)\rangle = \int dp\left(\int dx'\frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{ipx'}{\hbar}}\psi_s(x',t)\right)|p\rangle = \int dp\,\phi(p,t)|p\rangle$.

Important techniques

- All QM equations can be represented in Dirac notation, wavefunctions + differential operators, matrices.
- Insertion of unity operator $I = \int d\zeta|\zeta\rangle\langle\zeta|$, expanding in terms of the complete set of eigenstates of any observable $\{|\zeta\rangle\}$.
- Decompose a state $|S(t)\rangle$ into a specific basis associated with a dynamic variable ζ, determine the wavefunction in that basis $\psi_s(\zeta,t) = \langle\zeta|S(t)\rangle$.
- $\langle a|b\rangle = \langle b|a\rangle^*$.
- Common expressions
  - $|S(t)\rangle = \int dx\langle x|S(t)\rangle|x\rangle$.
    - $\hat{x}|x\rangle = x|x\rangle$.
  - $|S(t)\rangle = \int dp\langle p|S(t)\rangle|p\rangle$.
    - $\hat{p}|p\rangle = p|p\rangle$.
  - $|S(t)\rangle = \sum_{n=0}^{\infty}\langle E_n|S(t)\rangle|E_n\rangle$.
    - $\hat{E}|E_n\rangle = E_n|E_n\rangle$.
    - $\langle x|E_n\rangle = \psi_n(x)$.

Examples

- Manipulations
  - If $|S(t)\rangle = \int dx\langle x|S(t)\rangle|x\rangle$, then $\langle x'|S(t)\rangle = \int dx\langle x|S(t)\rangle\langle x'|x\rangle = \int dx\psi_S(x,t)\delta(x-x')$,
  - If $|S(t)\rangle = \int dp\langle p|S(t)\rangle|p\rangle$, then $\langle x'|S(t)\rangle = \int dp\phi(p,t)\frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx'}{\hbar}}$.
  - If $|S(t)\rangle = \sum_{n=0}^{\infty}\langle E_n|S(t)\rangle|E_n\rangle$, then $\langle x'|S(t)\rangle = \sum_{n=0}^{\infty}\langle E_n|S(t)\rangle\langle x'|E_n\rangle = \sum_n^{\infty}\psi(E,t)\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^n n!}}\,H_n\left(\sqrt{\frac{m\omega}{\hbar}}x'\right)e^{-\frac{m\omega x'^2}{2\hbar}}$.
- Relevance of wavefunctions in different bases
  - Write the expression for the expectation value of M for a particle in an arbitrary state $|S(t)\rangle$, working in an arbitrary basis defined by Q with eigen states $|q_n\rangle$ and corresponding eigen values q_n .
  - $\langle M\rangle|_{S(t)} = \langle S(t)|M|S(t)\rangle = \sum\sum\langle S(t)|q_n\rangle\langle q_n|M|q_m\rangle\langle q_m|S(t)\rangle$.
  - If $Q = M$, $\langle M\rangle|_{S(t)} = \sum|\psi(M_n,t)|^2 M_n$.

Operator in different basis

- In position space
  - $\hat{x} = x$.

    - $\hat{p} = -i\hbar\frac{\partial}{\partial x}$.
    - $\langle x|\hat{x}|S(t)\rangle = x\psi(x,t)$.
    - $\langle x|\hat{p}|S(t)\rangle = -i\hbar\frac{\partial}{\partial x}\psi(x,t)$. (project both p and $|S(t)\rangle$ onto $\langle x|$)
- In momentum space
    - $\hat{x} = i\hbar\frac{\partial}{\partial p}$.
    - $\hat{p} = p$.
    - $\langle p|\hat{x}|S(t)\rangle = i\hbar\frac{\partial}{\partial p}\phi(p,t)$.
    - $\langle p|\hat{p}|S(t)\rangle = p\phi(p,t)$.

Generalized statistical interpretation

- $\left|\psi_{|S(t)\rangle}(M_n,t)\right|^2$ is the probability distribution function of finding the particle with some eigenvalue M_n of the observable operator $\widehat{M}$, when that particle is in the state $|S(t)\rangle$ that is a solution of the Schrodinger equation.
    - In momentum space, $P(a \le p \le b) = \int_a^b |\phi(p,t)|^2 dp$.
- $\psi_{|S(t)\rangle}(M_n,t) = \langle M_n|S(t)\rangle$, $|M_n\rangle$ is an eigenstate of the observable operator $\widehat{M}$, $\widehat{M}|M_n\rangle = M_n|M_n\rangle$ with eigenvalue M_n.
- Physical interpretation
    - If we carry out a measurement of any observable with the particle in some state at time t with sufficient resolution, we must measure one of the eigenvalues of the observable and the state will be collapsed immediately after the measurement to the corresponding eigen state
    - The probability of measuring any one eigenvalue is given by the squared magnitude of the wavefunction of $|S(t)\rangle$ in the basis of the observable being measured.
- Preparing a state with zero variance in some observable A.
    - Eigenstate or determinate state.
    - Measure any state with observable A.
- Take another measurement immediately for another observable B.
    - If A, B shares an eigenstate, we get that eigenstate.
    - Otherwise, depends on the probability measure.

Generalized uncertainty relation

- If two operators $\hat{A}, \hat{B}$ satisfy $AB = BA$.
    - A, B must share a common set of eigenstates, $A(B\psi_n) = B(A\psi_n) = A_n(B\psi_n)$.
        - i.e. $B\psi_n$ is also an eigenstate of A with eigenvalue A_n.
- $[A,B] = AB - BA$ is the commutator of A and B.
    - $[\hat{x},\hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x}$.
    - $(\hat{x}\hat{p} - \hat{p}\hat{x})f(x) = -xi\hbar\frac{\partial}{\partial x}f(x) + i\hbar\frac{\partial}{\partial x}(xf(x))$.
    - $= -xi\hbar\frac{\partial}{\partial x}f(x) + i\hbar f(x) + xi\hbar\frac{\partial}{\partial x}f(x) = i\hbar\, f(x)$.
    - So $[\hat{x},\hat{p}] = i\hbar$, x and p are incompatible (non-commuting).
        - They cannot share the same eigenstates
    - $[A,B,C] = A[B,C] + [A,C]B$.
- Standard deviation with which we could measure the observables when the particle is in one of their shared eigenstates
- $\sigma_A^2\sigma_B^2 \ge \left(\frac{1}{2i}\langle S|[A,B]|S\rangle\right)^2$.
    - $\sigma_x\sigma_p \ge \frac{\hbar}{2}$.
- Uncertainty principal between energy and momentum for a free particle
    - It is possible (not necessarily) for variances of both to be arbitrarily close to zero (sharing eigen bases)
    - Momentum conserved, $[p,H] = 0$, $\frac{d\langle p\rangle}{dt} = 0$.
    - $\sigma_p^2\sigma_H^2 \ge 0$
- Uncertainty principal between energy and momentum for a harmonic oscillator

- Momentum not conserved, $[p, H] \neq 0, \frac{d\langle p \rangle}{dt} \neq 0$.
- $H = \frac{p^2}{2m} + \frac{kx^2}{2} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{k}{2}x^2$.
- $[p, H] = -i\hbar kx$.
- $\sigma_p^2 \sigma_H^2 \geq \frac{\hbar^2}{4} k^2 \langle x \rangle^2$.
- Product of variance is state dependent, and in general not equal to zero (not sharing common eigen states)
- Since it is state dependent, it is time-dependent

- Constraint on the product of variance one would deduce by making several measurements of the exact same state $|S(t)\rangle$ at some time $t = t_0$. Firstly in one observable, and then in another (or randomly measuring one of the two variables many time)
  - If two operators do not commute, and their commutator is state-independent, if we try to manufacture a state that has very small variance in one of the observables, then as we decrease the variance, the minimum possible variance of the other observable must increase.
  - It does not imply anything about the product of these variances at any other time
  - It does not imply anything about what happens if we try to measure two quantities at the same time
- Minimum uncertainty state
  - Gaussian wave packet: $\psi(x) = Ae^{-\frac{a(x-\langle x \rangle)^2}{2\hbar}} e^{\frac{i\langle p \rangle x}{\hbar}}$.
- Energy and time uncertainty.
  - $\hat{H}$: total energy operator.
  - $\hat{Q}$: any time-independent operator with $\left\langle \frac{\partial}{\partial t}\hat{Q} \right\rangle = 0$.
    - Note: $\frac{d}{dt}\langle \hat{Q} \rangle \neq \left\langle \frac{\partial}{\partial t}\hat{Q} \right\rangle$.
  - $\frac{d}{dt}\langle Q \rangle = \frac{i}{\hbar}\langle [H, Q] \rangle + \left\langle \frac{\partial Q}{\partial t} \right\rangle$.
  - $\sigma_H \sigma_Q \geq \frac{\hbar}{2}\left|\frac{d}{dt}\langle Q \rangle\right|$.
  - $\sigma_H \Delta t_Q \geq \frac{\hbar}{2}$, or $\Delta E \Delta t_Q \geq \frac{\hbar}{2}$.
  - Direct connection between the generalized uncertainty relation and the energy-time uncertainty relation is through the proportionality of the product of the variances of the energy operator and any other Hermitian operator, with the rate of change of the expectation value of the Hermitian operator of interest
  - The variance in the energy of some state at any given time must be greater than or equal to the normalized rate of change of any Hermitian observable in that state

3D Quantum

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Dynamical variables changes

- Position $\vec{r}$
- Momentum $\vec{p}$
- More degree of freedom

New observable

- Angular momentum $r \times p$.

Total energy in 3D

- Classical equation: $\frac{\vec{p}^2}{2m} + V(\vec{r})$.
- Hamiltonian operator: $\frac{\hat{p}^2}{2m} + V(\hat{r})$.
- Change to position basis:
  - Need to choose the basis (Cartesian, cylindrical or spherical)
  - Cartesian:
    - $p_x = -i\hbar\frac{\partial}{\partial x}, p_y = -i\hbar\frac{\partial}{\partial y}, p_z = -i\hbar\frac{\partial}{\partial z}$.
    - Define $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$, $\hat{p} = -i\hbar\nabla$.
    - $\frac{\hat{p}^2}{i^2\hbar^2} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2$ (Laplacian).
    - Then $-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\psi_t = E\psi$.

Algorithm for finding time dependent wavefunction

- $\psi_n(\vec{r}, t = 0) = \psi_n(\vec{r})$.
- $\psi_n(\vec{r}, t) = \psi_n(\vec{r})e^{-\frac{iE_n t}{\hbar}}$.
- $\psi(\vec{r}, t) = \sum_n c_n\psi_n(\vec{r})e^{-\frac{iE_n t}{\hbar}}$.
- Same as 1D.
- Probability density: $|\psi(r,t)|^2$.
  - $\int_V |\psi|^2 dV = 1$.

Infinite potential well

- $V = \begin{cases} 0, (x,y,z) \in [0,a]^3 \\ \infty, elsewhere \end{cases}$.
- Separate into three different equations
  - $-\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\psi(x) + V\psi(x) = E_x\psi(x)$.
  - $-\frac{\hbar^2}{2m}\frac{\partial}{\partial y}\psi(y) + V\psi(y) = E_y\psi(y)$.
  - $-\frac{\hbar^2}{2m}\frac{\partial}{\partial z}\psi(z) + V\psi(z) = E_z\psi(z)$.
  - $\psi(r) = \psi(x)\psi(y)\psi(z)$.
- So $\psi_{n_x,x_y,n_z}(x,y,z) = \left(\frac{2}{a}\right)^{\frac{3}{2}}\sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{a}y\right)\sin\left(\frac{n_z\pi}{a}z\right)$.
- $E = E_x + E_y + E_z = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2\left(n_x^2 + n_y^2 + n_z^2\right)$.
- Physical interpretation of n_x, n_y, n_z.
  - Number of nodes in each direction.
- Lowest energy state: $n_x = n_y = n_z$.
- There are 3 states that have an energy equal to twice the lowest possible energy
  - $(1,1,2), (1,2,1), (2,1,1)$.

Degenerate states

- Linked to symmetry properties of $V(\vec{r})$.
- Level spacing (energy difference $E_{i+1} - E_i$) will be different in 1D and 3D
- Any superposition of degenerate stationary solutions of the Schrodinger equation with the same eigen energy

Central potentials and spherical coordinates

- Used for atoms
- For hydrogen atom
  - $V = \frac{e^2}{4\pi\epsilon_0 r}$.
  - $H = KE(e^-) + V(r) + KE(proton)$ ($KE(proton) \approx 0$).
- Let r be the radiu, θ be the polar angle (from positive z), ϕ be the azimuthal angle (angle in xy plane).
  - $\theta \in [0, \pi]$, $\phi \in [0, 2\pi)$.
- Spherical Laplacian: $\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\left(\frac{\partial^2}{\partial \phi^2}\right)$.
- Spherical Schrodinger: $i\hbar \frac{\partial}{\partial t}\psi(r,\theta,\phi,t) = -\frac{\hbar^2}{2m}\nabla^2\psi(r,\theta,\phi,t) + V(r)\psi(r,\theta,\phi,t)$.
  - $-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)\right) + V\psi = E\psi$.
  - Let $\psi = R(r)Y(\theta,\phi)$.
    - $\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V(r) - E) = l(l+1)$.
    - $\frac{1}{Y}\left(\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\left(\frac{\partial^2 Y}{\partial\phi^2}\right)\right) = -l(l+1)$ (Angular equation).
  - Let $Y = \Theta(\theta)\Phi(\phi)$.
    - $\frac{1}{\Theta}\left(\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)\right) + l(l+1)\sin^2\theta = m^2$.
    - $\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2$.
  - Solution
    - $\Phi(\phi) = e^{im\phi}$, $m = 0, \pm1, \pm2, \ldots$.
      - $\Phi(\phi + 2\pi) = \Phi(\phi)$.
    - $\Theta(\theta) = A\,P_l^m(\cos\theta)$, $l \geq 0$, $l \in \mathbb{Z}$.
      - $P_l^m(x) = (1-x^2)^{\frac{|m|}{2}}\left(\frac{d}{dx}\right)^{|m|} P_l(x)$ is the associated Legendre function.
      - In $P_l^m(\cos\theta)$, there are $l - |m|$ nodes between $0 < \theta < \pi$.
$P_0^0 = 1$	$P_2^0 = \frac{1}{2}(3\cos^2\theta - 1)$
$P_1^1 = -\sin\theta$	$P_3^3 = -15\sin\theta(1-\cos^2\theta)$
$P_1^0 = \cos\theta$	$P_3^2 = 15\sin^2\theta\cos\theta$
$P_2^2 = 3\sin^2\theta$	$P_3^1 = -\frac{3}{2}\sin\theta(5\cos^2\theta - 1)$
$P_2^1 = -3\sin\theta\cos\theta$	$P_3^0 = \frac{1}{2}(5\cos^3\theta - 3\cos\theta)$
      - $P_l(x) = \frac{1}{2^l\, l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l$.
      - l must be a non-negative integer
      - Also, $|m| \leq l$, otherwise, the derivative doesn't work.
    - $Y_l^m(\theta,\phi) = \epsilon\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}\, e^{im\phi}P_l^m(\cos\theta)$.
      - $\epsilon = (-1)^m$ for $m \geq 0$, $\epsilon = 1$ for $m < 0$.

- $\int_0^{2\pi}\int_0^{\pi}\left(Y_l^m\right)^*\left(Y_{l'}^{m'}\right)\sin\theta\, d\theta\, d\phi = \delta_{ll'}\delta_{mm'}$.
- $Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$ $\quad Y_2^{\pm2} = \left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta e^{\pm2i\phi}$
- $Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$ $\quad Y_3^0 = \left(\frac{7}{16\pi}\right)^{1/2}(5\cos^3\theta - 3\cos\theta)$
- $Y_1^{\pm1} = \mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta e^{\pm i\phi}$ $\quad Y_3^{\pm1} = \mp\left(\frac{21}{64\pi}\right)^{1/2}\sin\theta(5\cos^2\theta - 1)e^{\pm i\phi}$
- $Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta - 1)$ $\quad Y_3^{\pm2} = \left(\frac{105}{32\pi}\right)^{1/2}\sin^2\theta\cos\theta e^{\pm2i\phi}$
- $Y_2^{\pm1} = \mp\left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta e^{\pm i\phi}$ $\quad Y_3^{\pm3} = \mp\left(\frac{35}{64\pi}\right)^{1/2}\sin^3\theta e^{\pm3i\phi}$
- l defines the s,p,d,f,g,h,i orbits.
- m defines the orientation.
- The total number of nodes, split between the θ and ϕ degrees of freedom is l, and the number of nodes in the ϕ degree of freedom is $|m|$.

- Note: the solutions' θ and ϕ dependence is constrianed to functions with shapes that depend only on two integers l and m, where for any $l \geq 1$, there are $2l+1$ allowed values of m, $|m| \leq l$.
- Radial part ($R(r)$)
  - Let $u(r) = rR(r)$, $-\frac{\hbar^2}{2m}u_{rr} + \left(V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right)u = Eu$.
    - $V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$ is the effective potential
  - For hydrogen atom $V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$.
  - Let $k = \frac{\sqrt{-2mE}}{\hbar}$
  - Bound states $E < 0$
  - Let $\rho = kr$, $\rho_0 = \frac{me^2}{2\pi\epsilon_0\hbar^2 k}$, $\frac{d^2u}{d\rho^2} = \left(1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right)u$.
  - As $\rho \to \infty$, $u(\rho) \sim Ae^{-\rho}$.
  - As $\rho \to 0$, $u(\rho) \sim C\rho^{l+1}$.
  - This gives a differential equation $u(\rho) = \rho^{l+1}e^{-\rho}v(\rho)$.
  - So $v(\rho) = \sum_{j=0}^{\infty} a_j\rho^j$, $a_{j+1} = \frac{2(j+l-1)-\rho_0}{(j+1)(j+2l+2)}a_j$.
    - There must be an N, such that $a_N = 0$, $a_{N-1} \neq 0$.
    - $2(N+l) - \rho_0 = 0$.
    - Define $n = N + l$, then
      - $N \geq 1$ and $n \geq l + 1$.
      - For any n, the condition $2n = \rho_0$ defines the allowed values of ρ_0 that terminate the polynomial for any l.
  - $E = -\frac{\hbar^2k^2}{2m} = -\frac{me^4}{8\pi^2\epsilon_0^2\hbar^2\rho_0^2}$.
  - $E_n = -\left(\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right)\frac{1}{n^2} = \frac{E_1}{n^2}$, $n = 1,2,3,\ldots$.
  - Bohr radius: $a = \frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10}m$.
  - Node number $n - l - 1$.
- Full solution
  - $\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_l^m(\theta,\phi)$.
  - $R_{nl}(r) = \frac{1}{r}\rho^{l+1}e^{-\rho}v(\rho)$, $v(\rho) = \sum_{j=0}^{\infty} a_j\rho^j$, $a_{j+1} = \frac{2(j+1+l-n)}{(j+1)(j+2l+2)}a_j$.
    - $\rho = \frac{r}{na}$.
    - ρ_0 can be assumed to be 0.
  - $\int \psi'_{nlm}\psi_{n'l'm'}r^2\sin\theta\, dr d\theta d\phi = \delta_{nn'}\delta_{ll'}\delta_{mm'}$.
    - $r \in (0,\infty)$.
    - $\theta \in (0,\pi)$.
    - $\phi \in (0,2\pi)$.
  - The normalization has to be determined for each eigenstate by adjusting a_0.

- $\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}} e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right) Y_l^m(\theta, \phi)$.
  - Y_l^m is valid for any potential that has no θ, ϕ dependence.
    - l nodal planes.
  - $P_l^m(\cos\theta)$ has $l - |m|$ nodal planes in θ.
  - $R_{n,l}(r)$ is specific to the $-\frac{1}{r}$ hydrogen potential.
    - $n - l - 1$ nodal planes.
- Nodes: number of nodes associated with the radial, polar and azimuthal contributes to the full 3D eigenstates
- Degeneracy
  - There are n^2 degenerate states with different l, m, for each value of n.
  - For each n, there are $2l + 1$ states of different m values, for each $l \in [0, n - 1]$.

Angular momentum

- e^{ikx} represents a particle with linear momentum
- Classical
  - Linear momentum $p = m\frac{dx}{dt}$.
  - Equivalent angular momentum $L = r \times p$.
  - In 2D, $L = rmv_\perp = rmv\sin\theta$.
  - In terms of angular velocity, $L = I\frac{d\phi}{dt}$.
    - I is the angluar inertia.
- Hydrogen atom
  - $e^{im\phi}$ are the eigenfunctions directly related to angular momentum.
  - It is associated with L_z.

Angular momentum operators in position basis

- $L_x = yp_z - zp_y$.
- $L_y = zp_x - xp_z$.
- $L_z = xp_y - yp_x$.
- $L = r \times (-i\hbar\nabla)$.
- $L^2 = L \cdot L = L_x^2 + L_y^2 + L_z^2$.
- Commutations relationship
  - $\left[L_x, L_y\right] = i\hbar L_z$.
  - $\left[L_y, L_z\right] = i\hbar L_x$.
  - $\left[L_z, L_x\right] = i\hbar L_y$.
  - $\left[L^2, L_x\right] = 0$.
  - $\left[L^2, L_y\right] = 0$.
  - $\left[L^2, L_z\right] = 0$.
- Shared eigenstates
  - $L^2 f = \lambda f$, $L_z^2 f = \mu f$.
  - Since L_x, L_y, L_z do not commute, they don't share the same set of eigen functions.
- Ladder operators
  - $L_+ = L_x + iL_y$.
  - $L_- = L_x - iL_y$.
  - $\left[L_z, L_\pm\right] = \left[L_z, L_x\right] \pm i\left[L_z, L_y\right] = i\hbar L_y \mp \hbar L_x = \pm\hbar L_\pm$.
  - $\left[L^2, L_\pm\right] = \left[L^2, L_x\right] \pm i\left[L^2, L_y\right] = 0$.
- Eigen spectrum of L^2 and L_z.
  - $L^2(L_\pm f) = L_\pm(L^2 f) = \lambda(L_\pm f)$.
  - $L_z(L_\pm f) = \left(\left[L_z, L_\pm\right] + L_\pm L_z\right)f = \left(\pm\hbar L_\pm + L_\pm L_z\right)f = (\pm\hbar + \mu)(L_\pm f)$.
    - Apply multiple times, we get $(\mu \pm n\hbar)(L_\pm f)$.
    - However, $|\mu|^2 \leq \lambda$, because $|L_z| \leq |L^2|$.

- $L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z$.
  - This gives $\lambda = 0 + \hbar^2 l^2 + \hbar\hbar l$.
- For a given eigenvalue $\lambda = \hbar^2 l(l+1)$ there must be a maximum L_z eigenvalue of $\mu^t = \hbar l$ and a minimum L_z eigenvalue of $\mu^b = -\hbar l$, there must be an integer N such that $N = 2l$.
  - l must be an integer or a half integer.
  - The shared eigen states of L^2 and L_z come in distinct sets labeled by any non-zero integer or half integer l. Each of the $2l+1$ in number shared eigenstates for any given l have the same eigenvalue $\hbar^2 l(l+1)$ for the L^2 operator, and eigenvalues $m\hbar$ with $m \in [-l, l]$ for the L_z operator.
- Eigenfunctions (in spherical coordinates)
  - $L_x = -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right)$.
  - $L_y = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right)$.
  - $L_\pm = \pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right)$.
  - $L_z = -i\hbar\frac{\partial}{\partial\phi}$.
    - $L_z f_l^m = m\hbar f_l^m$.
    - $f_l^m = Y_l^m$.
  - $L^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$.
    - $L^2 f_l^m = \hbar^2 l(l+1) f_l^m$.
    - $f_l^m = Y_l^m$.
  - Spherical harmonics Y_l^m are nothing other than the common eigenfunctions of the L^2 and the L_z operators in the position basis, in spherical coordinates, but only including non-negative integer, not half-integer values of l.
  - Restriction to integer l.
    - We forced the associated wavefunctions in the position basis to be single-valued at all positions. (in particular all values of ϕ, at a period of 2π)
    - But this doesn't mean the hydrogen atom half-integer values are invalid

Matrices of angular momentum

- $l = 1, m = 0, \pm 1$ (three states).
  - Define $|1,1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix}$, $|1,0\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix}$, $|1,-1\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}$.
- $\langle lm'|L_z|lm\rangle = m\hbar\delta_{m'm}$.
  - Note that $L_z|lm\rangle = m\hbar|lm\rangle$.
- $\langle lm'|L_\pm|lm\rangle = \sqrt{l(l+1) - m(m\pm1)}\hbar\delta_{m'(m\pm1)}$.
  - $L_+|lm\rangle = \hbar\sqrt{l(l+1) - m(m+1)}|l, m+1\rangle$.
- $L_x = \frac{1}{2}(L_+ + L_-) = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}$.
- $L_y = \frac{1}{2i}(L_+ - L_-) = \frac{\hbar}{\sqrt{2}i}\begin{pmatrix}0&1&0\\-1&0&1\\0&-1&0\end{pmatrix}$.
- $L_z = \hbar\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}$.

Measuring angular momentum

- If we measure the magnitude of the angular momentum, and then measure the z component of the angular momentum, another measurement of the magnitude would yield the same result.
  - Firstly, measure magnitude, $l = 1$, don't know m_z.

- Secondly, measure z, fixed $m_z = -1,0,1$, collapsed state to eigenstate of L_z.
- The third measurement will only be $l = 1$.

- If we measure the magnitude of the angular momentum, and then measure the z component of the angular momentum, another measurement of the x component would yield some value that cannot be precisely predicted.
  - Consider $L_x|1,1\rangle$.
  - L_x has three eigenstates: $\frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix}, \frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\\1\end{pmatrix}$ with eigenvalues $\hbar, 0, -\hbar$.
  - Expand $|1,1\rangle$ in eigenstates.
  - Probability: $P(L_x = \pm 1) = \frac{1}{4}$, $P(L_x = 0) = \frac{1}{2}$.

Electron spin

- If we send a beam of hydrogen atoms in the ψ_{100} state through an apparatus with magnetic field, there are two spots on the screen corresponding to an upward and downward deflection one would expect for a particle having an additional angular momentum of $\pm\frac{\hbar}{2}$.
- Point-like particle possesses intrinsic angular momentum quantized in units of $\frac{\hbar}{2}$ independent of position, linear or angular orbital momentum of the electron.
- Using index s instead of l, s is fixed.
  - Electron: $\frac{1}{2}$.
  - Photon: 1.
- Two possible eigenvalues of a cartesian component of angular momentum $m = \pm\frac{\hbar}{2}$.
- Spin operator S.
  - Only operates on the intrinsic spin of the electron
  - Same commutation relations as the angular momentum
  - $[S_x, S_y] = i\hbar S_z$, $[S_y, S_z] = i\hbar S_x$, $[S_z, S_x] = i\hbar S_y$.
  - $[S^2, S_x] = [S^2, S_y] = [S^2, S_z] = 0$.
  - $[S_z, S_\pm] = \pm\hbar S_\pm$, $[S^2, S_\pm] = 0$ where $S_\pm = S_x \pm iS_y$.
  - S^2, S_z share a common set of eigenstates.
    - $s = \frac{1}{2}$, $m = m_z = \pm\frac{1}{2}$, $\left|\frac{1}{2}, \frac{1}{2}\right\rangle$ and $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$.
    - $S^2\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle = \hbar^2 s(s+1)\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle = \frac{3}{4}\hbar\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle$.
    - $S_z\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle = \hbar m\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle = \pm\frac{1}{2}\hbar\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle$.
    - $S_\pm\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle = \hbar\sqrt{s(s+1) - m(m\pm 1)}\left|\frac{1}{2}, \frac{1}{2} \pm 1\right\rangle$.
  - Note:
    - S_+ cannot operate on $\left|\frac{1}{2}, \frac{1}{2}\right\rangle$ (there is no $\frac{3}{2}$ states).
    - S_- cannot operate on $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$ (there is no $-\frac{3}{2}$ states).
- State vector
  - An arbitrary state in the spin Hilbert space can be written as $|\chi(t)\rangle = a(t)\left|\frac{1}{2}, \frac{1}{2}\right\rangle + b(t)\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$.
  - Use vector representation
    - $\left|\frac{1}{2}, \frac{1}{2}\right\rangle = \begin{pmatrix}1\\0\end{pmatrix}$.
    - $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle = \begin{pmatrix}0\\1\end{pmatrix}$.
    - $|\chi(t)\rangle = \begin{pmatrix}a(t)\\b(t)\end{pmatrix}$.
    - $a = \left\langle\frac{1}{2}, \frac{1}{2}\middle|\chi\right\rangle$.

- Matrix representation of spin operators
  - $S^2_{i,j} = \left\langle \frac{1}{2}, i \middle| S^2 \middle| \frac{1}{2}, j \right\rangle$, $S^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.
  - $S_{zi,j} = \left\langle \frac{1}{2}, i \middle| S_z \middle| \frac{1}{2}, j \right\rangle$, $S_z = \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.
  - $S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$.
- Pauli spin matrices
  - $S_i = \frac{\hbar}{2}\sigma_i$, $i = x, y, z$.
  - $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.
  - $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$.
  - $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.
- Measurement $S_x = \frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
  - $\frac{\hbar}{2}: \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, $-\frac{\hbar}{2}: \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$.
  - $\begin{pmatrix} a \\ b \end{pmatrix} = \frac{a+b}{\sqrt{2}} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} + \frac{a-b}{\sqrt{2}} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$.

Two spins

- Four states: ↑↑, ↑↓, ↓↑, ↓↓.
  - First arrow refers to the electron, second arrow refers to the proton.
- Operators
  - $S = S^{(1)} + S^{(2)}$.
  - $S^2 = \left(S^{(1)} + S^{(2)}\right)\left(S^{(1)} + S^{(2)}\right)$.
  - $S^{(1)}$ acts only on χ_1, $S^{(2)}$ acts only on χ_2.
  - $S_{z\chi_1\chi_2} = \left(S_z^{(1)} + S_z^{(2)}\right)\chi_1\chi_2 = \hbar\left(m_1 + m_2\right)\chi_1\chi_2$.
    - ↑↑: $m = m_1 + m_2 = 1$.
    - ↑↓: $m = m_1 + m_2 = 0$.
    - ↓↑: $m = m_1 + m_2 = 0$.
    - ↓↓: $m = m_1 + m_2 = -1$.
- Lowering operator
  - $S_- = S_-^{(1)} + S_-^{(2)}$.
  - $S_-(\uparrow\uparrow) = \hbar(\downarrow\uparrow + \uparrow\downarrow)$.
  - With $s = 1$. ($|sm\rangle$)
    - $|11\rangle = \uparrow\uparrow$.
    - $|10\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$.
    - $|1-1\rangle = \downarrow\downarrow$.
  - $m = 0$ carries $s = 0$.
    - $|00\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$.