Joe Crandall's PHYS 3167 Principles of Quantum Physics | Used Heavily | Topic | SubTopic | KNOWTHISMATH | Definition/Constant/Operator | Question | break my name is slim shady | Important Quantum Concepts $h = 6.626 \times 10^{-34}$ J s | $\hbar = 1.054 \times 10^{-34}$ J s | $\hbar \equiv \frac{h}{2\pi}$

Quantum Operators operators are used to extract information from the wavefunction **Position**Cartesian component $\hat{x} = x, \hat{y} = y, \hat{z} = z$ General definition $\hat{\vec{r}} = \vec{r}$ units m | **Momentum** Cartesian component General $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$, $\hat{p}_y = -i\hbar\frac{\partial}{\partial y}$,$\hat{p}_z = -i\hbar\frac{\partial}{\partial z}$. General $\hat{p} = -i\hbar\nabla$ units Jsm^{-1} or N s Electromagnetic field $\hat{p}_x = -i\hbar\frac{\partial}{\partial x} - qA_x$, $\hat{p}_y = -i\hbar\frac{\partial}{\partial y} - qA_y$,$\hat{p}_z = -i\hbar\frac{\partial}{\partial z} - qA_z$ Electromagnetic field (uses kinetic momentum $\vec{A}$ = vector potential) $\hat{p} = \hat{P} - q\vec{A} = -i\hbar\nabla - q\vec{A}$ units Jsm^{-1} or N s | **Kinetic energy**Cartesian component Translation $\hat{T}_x = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$, $\hat{T}_y = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}$,$\hat{T}_z = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}$ general definition $\hat{T} = \frac{\hat{p}\cdot\hat{p}}{2m} = \frac{(-\hbar\nabla)\cdot(-\hbar\nabla)}{2m} = \frac{-\hbar^2}{2m}\nabla^2$ Electromagnetic field cartesian component $\hat{T}_x = \frac{1}{2m}(-i\hbar\frac{\partial}{\partial x} - qA_x)^2$, $\hat{T}_x = \frac{1}{2m}(-i\hbar\frac{\partial}{\partial y} - qA_y)^2$, $\hat{T}_z = \frac{1}{2m}(-i\hbar\frac{\partial}{\partial z} - qA_z)^2$ General definition Electromagnetic field $\vec{A}$ = vector potential $\hat{T} = \frac{\hat{p}\cdot\hat{p}}{2m} = \frac{1}{2m}(-i\hbar\nabla - q\vec{A})\cdot(-i\hbar\nabla - q\vec{A}) = \frac{1}{2m}(-i\hbar\nabla - q\vec{A})^2$ unit J Rotation(I=moment of inertia) cartesian component $\hat{T}_{xx} = \frac{\hat{J}_x^2}{2I_{xx}}$, $\hat{T}_{yy} = \frac{\hat{J}_y^2}{2I_{yy}}$, $\hat{T}_{zz} = \frac{\hat{J}_z^2}{2I_{zz}}$ Rotation General definition $\hat{T} = \frac{\hat{J}\cdot\hat{J}}{2I}$ unit J | **Potential energy** general definition $\hat{V} = V(\vec{r},t) = V$ Units J | **Total energy:** general definition $\hat{E} = i\hbar\frac{\partial}{\partial t}$ Time-independent: $\hat{E} = E$ units J | **Hamiltonian:** general definition $\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}\cdot\hat{p}}{2m} + V = \frac{\hat{p}^2}{2m} + V$ Unit J | **Angular momentum operator:** cartesian component $\hat{L}_x = -i\hbar(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y})$, $\hat{L}_y = -i\hbar(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z})$, $\hat{L}_z = -i\hbar(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})$, general definition $\hat{L} = \vec{r}\times -i\hbar\nabla$ Units J s or Nsm^{-1} | **Spin angular momentum** $\hat{S}_x = \frac{\hbar}{2}\sigma_x$ and $\hat{S}_y = \frac{\hbar}{2}\sigma_y$ and $\hat{S}_z = \frac{\hbar}{2}\sigma_z$ where $\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$, $\sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$, $\sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ are the pauli matrices for spin 1/2 particles $\hat{\vec{S}} = \frac{\hbar}{2}\vec{\sigma}$ where $\vec{\sigma}$ is the vector whose components are the pauli matrices J s and Nsm^{-1} | **Total angular momentum**$\hat{J}_x = \hat{L}_x + \hat{S}_x$ and $\hat{J}_y = \hat{L}_y + \hat{S}_y$ and $\hat{J}_z = \hat{L}_z + \hat{S}_z$ general definition $\hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}} = -i\hbar\vec{r}\times\nabla + \frac{\hbar}{2}\vec{\sigma}$ Units Nsm^{-1} | Transition dipole moment (electric) $\hat{d}_x = q\hat{x}$, $\hat{d}_y = q\hat{y}$, $\hat{d}_z = q\hat{z}$, $\hat{d} = q\hat{r}$ units C m

2 Classical Waves **Classical Wave Equation: boundary conditions** head on collision of two identical waves traveling in opposite directions: $f(x,t) = A\sin(kx-\omega t) + A\sin(kx+\omega t) = 2A\sin(kx)\cos(\omega t)$ boundary conditions lead to discrete spectrum $k_n = \frac{n\pi}{L}$ for $n = 1, 2, 3\ldots$ **Classical Wave Equation: uncertainty principle** $f(x,t) = A\cos(k_1x-\omega t) + A\sin(k_2x+\omega t) = 2A\cos[\frac{(k_1+k_2)x}{2}]\cos[\frac{(k_1-k_2)x}{2}]$ | If k_1 and k_2 are close, 'beat' happens: $f(x,t) = 2Acos(kx-\omega t)cos(\Delta kx)$, $k = \frac{k_1+k_2}{2}$, $\Delta k = \frac{k_1-k_2}{2}$, at locations: $x = \frac{(2n+1)\pi}{2\Delta k}$, $\Delta x\Delta k = \pi \geq O(1)$ the degree of localization of a wave packet in space (ΔX) is inversely correlated with the spread in available k values (δk) **Fourier transform** A general function f(x) can be expanded in a continuous integral: $f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} A(k)e^{ikx}dk$ | The "inverse Fourier transform" can be obtained: $A(k) = \frac{1}{\sqrt{2\pi}}\int_{\infty}^{\infty} f(x)e^{-ikx}dx$ | using the Dirac δ-function: $\delta(k-k') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i(k-k')x}dx =$ either 0 for $k \neq k'$ or ∞ for $k = k'$ **Dispersion relation** example: EM wave in plasma: $\omega^2 = (kc)^2 + \omega_p^2$ The need for two velocities, Phase velocity $v_\phi = \frac{\omega}{k}$, group velocity $v_p = \frac{d\omega}{dk}$ **Dirac delta function** $\delta(k-k') = \frac{1}{2\pi}\int_{\infty}^{\infty} e^{i(k-k')x}dx =$ either 0 for $k \neq k'$or$\infty$for$k = k'$ | $\int_{\infty}^{\infty}\delta(k-k')dk = 1$ $\delta_s(k) = \frac{1}{2\pi}\int_{\infty}^{\infty} e^{-\epsilon x^2}e^{i(k-k')x}dx = \frac{1}{2\pi}\sqrt{\frac{\pi}{\epsilon}}e^{-\frac{k^2}{4\epsilon}}$ **The Schrodinger Equation** **Free particle**: operator equation $\hat{E}\psi(x,t) = \frac{\hat{p}}{2m}\psi(x,t)$, $\hat{E} = i\hbar\frac{\partial}{\partial t}$, $\hat{p} = -i\hbar\frac{\partial}{\partial x}$, $i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}$ | **Forced particle**: operator equation $\hat{E}\psi(x,t) = [\frac{\hat{p}^2}{2m} + V(x)]\psi(x,t) \rightarrow i\hbar\frac{\partial\psi(x,t)}{\partial t} = [-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)]\psi(x,t)$ **Free particle: plane - wave solution** $i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}$ | $\psi(x,t) = Ae^{i(px-Et)/\hbar}$ | $e^{i(kx-\omega t)}$, $p = \hbar k$, $E = \hbar\omega$ Quantum mechanically, plane - wave solution has well defined momentum p and energy E, but the particle is everywhere at the same time **Free particle: wave - packet solution** $\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{\infty}^{\infty}\phi(p)e^{i(px-\frac{p^2}{2m\hbar}t)/\hbar}dp = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\phi(p,t)e^{ipx/\hbar}dp$, where $\phi(p,t) = \phi(p)e^{-i\frac{p^2}{2m\hbar}t}$ | $\phi(p,0) = \phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x,0)e^{-ipx/\hbar}dx$

given initial wave - packet $\psi(x,0)$ find $\psi(x,t)$ 1. find initial momentum-space wave packet $\phi(p)$ via inverse Fourier transform 2. find $\phi(p,t)$ via $\phi(p,t) = \phi(p)e^{-i\frac{p^2}{2m\hbar}t}$ 3. find $\psi(x,t)$ by Fourier transform **Free particle: Gaussian wave packet** A free particle is initially located at x_0 and with momentum p_0. It can be modeled by a wave packet: $\psi(x,0) = \frac{1}{\alpha\hbar\sqrt{\pi}}e^{-\frac{(x-x_0)^2}{2\alpha^2\hbar^2}}e^{ip_0(x-x_0)/\hbar}$ **how will it evolve in time $\phi(x,t)$ =?** 1. find its initial momentum - space wave packet via Fourier transform $\phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x,0)e^{-ipx/\hbar}dx = \sqrt{\frac{\alpha}{\sqrt{\pi}}}e^{-\frac{\alpha^2(p-p_0)^2}{2}}e^{-ipx_0/\hbar}$ 2. find $\phi(p,t)$ $\phi(p,t) = \phi(p)e^{-i\frac{p^2}{2m\hbar}t} = \sqrt{\frac{\alpha}{\sqrt{\pi}}}e^{-\frac{\alpha^2(p-p_0)^2}{2}}e^{-i[px_0+\frac{p^2}{2m}t]/\hbar}$ 3. find $\phi(x,t)$, $\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\phi(p,t)e^{ipx/\hbar}dp = \frac{1}{\alpha\hbar\sqrt{F}}e^{-\frac{(x-x_0-\frac{p_0t}{m})^2}{2\alpha^2\hbar^2F}}e^{-i[p_0(x-x_0)-\frac{p_0^2}{2m}t)/\hbar}$ where $F = 1 + i\frac{t}{t_0}$ with $t_0 = m\hbar\alpha^2$ | $|\psi(x,t)|^2 = \frac{1}{\beta_t\sqrt{\pi}}e^{-\frac{(x-x_0-\frac{p_0t}{m})^2}{\beta_t^2}}$ with $\beta_t = \alpha\hbar\sqrt{1+\frac{t^2}{t_0^2}}$

2.4 Inverting the Fourier transform: the Dirac δ-function $f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A(k)e^{ikx}dk$ | $A(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A(k)e^{-ikx}dk$ | Dirac δ-function $\delta(k-k') = \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i(k-k')x}dx$

4 Interpreting the Schrodinger Equation **Wavefunction $\psi(x,t)$** $i\hbar\frac{\partial\psi(x,t)}{\partial} = [-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)]\psi(x,t)$ | Probability density:$P(x,t) = |\psi(x,t)|^2$: although contact with reality is made through the modulus square $|\psi(x,t)|^2$, the original complex wavefunction $\psi(x,t)$ contains all the information about the particle, more so than $|\psi(x,t)|^2$, in EM, the energy density stored in the electric and magnetic fields is $u = \frac{\epsilon_0}{2}|\vec{E}(\vec{r},t)|^2 + \frac{1}{2\mu_0}|\vec{B}(\vec{r},t)|^2$, E and B are real functions. They have direct consequence on the charge via the Lorentz force: $F = q\vec{E} + q\vec{v}\times\vec{B}$ **Normalization** $|\psi(x,t)|^2dx = 1$ **is the normalization condition time dependent?** $\frac{d}{dt}[\int_{-\infty}^{\infty}|\psi(x,t)|^2dx] \rightarrow 0$ | $\frac{\partial P(x,t)}{\partial t} = \frac{\partial|\psi(x,t)|^2}{\partial t} = \frac{\partial\psi^*(x,t)}{\partial t}\psi(x,t) + \frac{\partial\psi(x,t)}{\partial t}\psi^*(x,t)$ | $i\hbar\frac{\partial\psi(x,t)}{\partial t} = [-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)]\psi(x,t)$ | $i\hbar\frac{\partial\psi^*(x,t)}{\partial t} = [-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V^*(x,t)]\psi^*(x,t)$ | $\frac{\partial P(x,t)}{\partial t} = \frac{i\hbar}{2m}(\frac{\partial^2\psi^*}{\partial x^2}\psi - \frac{\partial^2\psi}{\partial x^2}\psi^*) + \frac{1}{\hbar}(\psi^*\psi)(V^* - V)$ | Assuming the potential is real: $\frac{\partial P(x,t)}{\partial t} = -\frac{\partial j(x,t)}{\partial x}$ (continuity equation) where $j(x,t) = \frac{i\hbar}{2m}(\psi\frac{\partial\psi^2}{\partial x} - \frac{\partial\psi}{\partial x}\psi^2)$ (probability flux) Its a probability conservation | $\int_{-\infty}^{\infty}\frac{\partial P(x,t)}{\partial t}dx = \int_{-\infty}^{\infty}[-\frac{\partial j(x,t)}{\partial x}]dx$ | $\frac{d}{dt}[\int_{-\infty}^{\infty}|\psi(x,t)|^2dx] = -j(\infty,t) + j(-\infty,t) \rightarrow 0$ Normalization is preserved at all times by the Schrodinger equation **Expectation value of position** $\langle x\rangle = \int_{-\infty}^{\infty}x|\psi(x,t)|^2dx$ | $\langle f(x)\rangle = \int_{-\infty}^{\infty}f(x)|\psi(x,t)|^2dx$ | Example: the uncertainty in position for Gaussian wave-packet: $|\psi(x,t)|^2 = \frac{1}{\beta_t\sqrt{\pi}}e^{-(x-x_0-\frac{p_0t}{m})^2/\beta_t^2}$ where $\beta_t = \alpha\hbar\sqrt{1+t^2/t_0^2}$ | $\langle x\rangle x_0 + \frac{p_0t}{m}$ | $\langle x^2\rangle = (x_0 + \frac{p_0t}{m})^2 + \frac{\beta_t^2}{2}$ | $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \frac{\beta_t}{\sqrt{2}}$ **Expectation value of momentum** $\hat{p} \equiv -i\hbar\frac{\partial}{\partial x}$ | $\langle\hat{p}\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)\hat{p}\psi(x,t)dx$ | classically, the trajectory would satisfy $\frac{dx(t)}{dt} = \frac{p(t)}{m}$ This suggests $\frac{d}{dt}\langle x\rangle = \frac{d}{dt}[\int_{-\infty}^{+\infty}x|\psi(x,t)|^2dx] = -\int_{-\infty}^{\infty}x\frac{\partial j(x,t)}{\partial x}dx = -[xj(x,t)]_{-\infty}^{\infty} + \int_{-\infty}^{\infty}j(x,t)dx = \frac{i\hbar}{2m}\int_{\infty}^{\infty}(\phi\frac{\partial\psi^*}{\partial x} - \frac{\partial\psi}{\partial x}\psi^*)dx = \frac{1}{m}\int_{-\infty}^{\infty}\psi^*(-i\hbar\frac{\partial}{\partial x})\psi dx + \frac{i\hbar}{2m}[\psi\psi^*]_{-\infty}^{\infty} = \frac{\langle p\rangle}{m}$ | $\langle\hat{p}\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)(-i\hbar\frac{\partial}{\partial})\psi(x,t)dx$ | $\langle\hat{p}^n\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)(-i\hbar\frac{\partial}{\partial})^n\psi(x,t)dx$ example: the uncertainty in momentum for the free-particle Gaussian wave-packet $\langle\hat{p}\rangle = p_0$, $\langle\hat{p}^2\rangle = p_0^2 + \frac{1}{2\alpha}$, $\Delta p = \sqrt{\langle\hat{p}^2\rangle - \langle\hat{p}^{(2}} = \frac{\hbar}{\sqrt{2}\alpha}$ | Uncertainty principle relation for the Gaussian wave-packet $\Delta x\Delta p = \frac{\hbar}{2}\sqrt{1+\frac{t_0^2}{t^2}}$ **Expectation value of energy** example: the expectation value of energy for the free-particle Gaussian wave-packet $\langle\hat{E}\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)(i\hbar\frac{\partial}{\partial t})\psi(x,t)dx = \frac{1}{2m}(p_0^2 + \frac{1}{2\alpha^2}) = \frac{\langle\hat{p}^2\rangle}{2m}$ **Expectation value of kinetic energy** $\hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ | $\langle\hat{T}\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)\frac{\hat{p}}{2m}\psi(x,t)dx = \frac{-\hbar^2}{2m}\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial^2\psi(x,t)}{\partial x^2}dx = \frac{-\hbar^2}{2m}(\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x})_{-\infty}^{\infty} + \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\frac{\partial\psi^*(x,t)}{\partial x}\frac{\partial\psi(x,t)}{\partial x}dx = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}|\frac{\partial\psi(x,t)}{\partial x}|^2dx$ **Physical interpretation of $\phi(p,t)$** $\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\phi(p,t)e^{ipx/\hbar}dp$ | $\psi(p,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x,t)e^{-ipx/\hbar}dx$ | $|\psi(x,t)|^2dx$ is the probability that a measurement of the position of the particle described by $\psi(x,t)$, at time t, will find it in the region (x,x+dx) | $|\phi(p,t)|^2dx$ is the probability that a measurement of the position of the particle described by $\psi(p,t)$, at time t, will find it in the region (p,p+dp) **Expectation value of momentum in momentum space** $\langle\hat{p}\rangle = \int_{-\infty}^{\infty}\phi^*(x,t)(-i\hbar\frac{\partial}{\partial x})\psi(x,t)dx = \ldots = \int_{-\infty}^{\infty}p|\phi(p,t)|^2dp = \langle p\rangle$ **Expectation value of position in momentum space** $\langle x\rangle = \int_{-\infty}^{\infty}\phi^*(x,t)x\psi(x,t)dx = \ldots = \int_{-\infty}^{\infty}\phi^*(p,t)((-i\hbar\frac{\partial}{\partial p}))\phi(p,t)dp$ | $\hat{x} = i\hbar\frac{\partial}{\partial p}$ **Schrodinger equation in momentum space** Position space: $i\hbar\frac{\partial\psi(x,t)}{\partial t} = [\frac{\hat{p}}{2m} + V(x,t)]\psi(x,t)$, $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ | Momentum space: $i\hbar\frac{\partial\phi(x,t)}{\partial t} = [\frac{p^2}{2m} + V(\hat{x},t)]\phi(p,t)$, $\hat{x} = i\hbar\frac{\partial}{\partial p}$ **example: free particle** zero force, or potential V(x) = 0 $\phi(p,t) = \phi(p,0)e^{\frac{ip^2}{2m\hbar}t}$ **4.4 Real Average Values and Hermitian Operators** the momentum and energy operators $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$ and $\hat{E} = i\hbar\frac{\partial}{\partial t}$ | hermitian operators satisfy $\langle\hat{O}\rangle = \langle\hat{O}\rangle^*$ or $\int_{-\infty}^{\infty}dx\psi^*(x,t)\hat{O}\psi(x,t) = [\int_{-\infty}^{\infty}dx\psi^*(x,t)\hat{O}\psi(x,t)]^*$

4.5 the physical interpretation of $\psi(p)$ position operator $\hat{x} = i\hbar\frac{\partial}{\partial p}$ **4.6 Energy Eigenstates, Stationary States, and the Hamiltonian Operator** In much the same way that Newtons second law relates the time dependence of a particles trajectory to the external force, the time dependent Shrodinger equation dictates the time development of the wavefunction of a particle in the presence of an external potential. $i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t)$ | Hamiltonian operator $\hat{H} \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) = \frac{\hat{p}}{2m} + V(x)$ **4.7 The Schrodinger Equation in Momentum Space** $-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$ **5 The Infinite Well: Physical Aspects**

Energy Eigenstates and stationary states $i\hbar\frac{\partial\psi(x,t)}{\partial} = \hat{H}\psi(x,t)$ where $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)$ If the potential is independent of time V(x,t) = v(x) we can try a solution by separation of variables: $\psi(x,t) = \psi(x)T(t)$ | $i\hbar\frac{dT(t)}{T(t)dt} = \frac{\hat{H}\psi(x)}{\psi(x)} = E(constant)$ | $i\hbar\frac{dT(t)}{T(t)dt} = E$ | $\hat{H}\psi_E(x) = E\psi_E(x)$ | $T(t) = e^{-iEt/\hbar}$ | $\psi(x,t) = \psi_E(x)e^{-iEt\hbar}$ | **instead of solving** $i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t)$ | $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ **solve eigenvalue problem first** $\hat{H}\psi_E(x) = E\psi_e(x)$ the the final solution is $\psi(x,t) = \psi_E(x)e^{-iEt/\hbar}$ 1. Energy eigenstate = energy eigenvalue E and eigenfunction $\psi_E(x)$. $\hat{E}\psi(x,t) = (i\hbar\frac{\partial}{\partial t})\psi(x,t) = E\psi(x,t)$ | $\langle\hat{E}\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)(i\hbar\frac{\partial}{\partial t})\psi(x,t)dx = E$ | $\langle\hat{E}^2\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)(i\hbar\frac{\partial}{\partial t})^2\psi(x,t)dx = E^2$ | $\Delta E = \sqrt{\langle\hat{E}^2\rangle - \langle\hat{E}\rangle^2} = 0$ 2. Probability density is independent of time for eigenstates. $P(x,t) = |\psi(x,t)|^2 = |\psi_E(x)|^2$ 3. Expectation value of operators in such states is also independent of time $\langle\hat{O}\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)\hat{O}\psi(x,t)dx = \int_{-\infty}^{\infty}\psi_E^*(x)\hat{O}\psi_E(x)dx$ for these reasons, energy eigenstates are called stationary states 4. a general quantum state can be expressed as a linear combination of energy eigenstates (principle of superposition) $\psi(x,t) = \sum_E a_E\psi_E(x)e^{-iEt/\hbar}$ | $P|\psi(x,t)|^2$ is no longer time independent due to cross-term interference. **Example: free particle V(x)=0** $[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}]\psi_E(x) = E\psi_E(x)$ | $\frac{d^2\psi_E(x)}{dx^2} = -k^2\psi_E(x)$ where $k = \sqrt{\frac{2mE}{\hbar^2}}$ | $\psi_E(x) = e^{ikx}$ or e^{-ikx} | $E = \frac{\hbar^2k^2}{2m} = \frac{p^2}{2m}$ s | Stationary states (plane waves): $\psi(x,t) = \psi_E(x)e^{-iEt/\hbar} = e^{i(px-Et)/\hbar}$(traveling +x direction) or $= e^{i(-px-Et)/\hbar}$(traveling -x direction) **The infinite well: classically** $m\frac{d^2x(t)}{dt^2} = -\frac{\partial V(x,t)}{\partial x}$, $V(x) = 0$ for $0, x, L$ or ∞ for $x < 0$ or $x > L$ | Constant Energy E, or speed $v_0 = sqrt2E/m$, or momentum $p_0 = mv_0 = \sqrt{2mE}$, elastic collisions with the walls, periodic motion $\tau = 2L/v_0$ **The infinite well: classical probabilities** **Position space:** $P_{CL}(x)dx = \frac{dx}{\tau/2} = \frac{2}{\tau v}dx \rightarrow P_{CL}(x) = \frac{2}{\tau v} = \frac{1}{L}$ | $\langle x\rangle = \int_0^L xP_{CL}(x)dx = \frac{L}{2}$, $\langle x\rangle^2 = \int_0^L x^2P_{CL}(x)dx = \frac{L^2}{3}$, $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \frac{L}{\sqrt{12}} = 0.29L$ **Momentum space:** $P_{Cl}(p) = \frac{1}{2}[\delta(p-p_0) + \delta(p+p_0)]$, $\langle p\rangle = \int_{-\infty}^{\infty}pP_{Cl}(p)dp = \frac{1}{2}[p_0 + (-p_0)] = 0$, $\langle p^2\rangle = \int_{-\infty}^{\infty}p^2P_{Cl}(p)dp = \frac{1}{2}[p_0^2 + (-p_0)^2] = p_0^2$, $\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = p_0$ | "Classical uncertainty relation": $\Delta x\Delta p = \frac{L}{\sqrt{12}}p_0$ can be made to vanish ($p_0 = mv_0 = 0$) **The infinite well: quantum solution** $[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)]\psi_E(x) = E\psi_E(x)$ | $\psi(x,t) = \psi_E(x)e^{-iEt/\hbar}$ | $V(x) =$ either 0for$0 < x < L$ or ∞ for $x < 0$ or $x > L$ | **Inside:** $[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}]\psi_E(x) = E\psi_E(x)$, $\frac{d^2\psi_E(x)}{dx^2} = -k^2\psi_E(x)$0 where $k = \sqrt{\frac{2mE}{\hbar^2}}$, $\psi_E(x) = A\sin(kx) + B\cos(kx)$ | **Outside:** $\psi_E(x) = 0$ | Matching $\psi_E(x)$ at boundaries $x = 0$ and $x = L$, $A\sin(0) + B\cos(0) = 0$, $A\sin(kL) + B\cos(kL) = 0$ | Solution: $B = 0$ and $\sin(kL) = 0$ | $k_n = \frac{n\pi}{L}$ for $n = 1, 2, 3, \ldots$, $E_n = \frac{(\hbar k_n)^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2}$, $\psi_n(x) = A\sin\left(\frac{n\pi x}{L}\right)$ | Fix A by normalization: $|A|^2\int_0^L\sin^2(\frac{n\pi x}{L})dx = 1$, $|A|^2\frac{L}{2} = 1$, $\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ **Particle in a box: Classical vs. Quantum** $P_{CL} = \frac{1}{L}$, $P_Q = |\psi(x)|^2 = \frac{2}{L}\sin^2(\frac{n\pi x}{L})$ (many oscillations average out to 1/L for quantum) Correspondence principle **The infinite well: expectation values** $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$, $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$, where $n = 1, 2, 3, \ldots$ | $\langle x\rangle = \int_0^a x|\psi_n(x)|^2dx = \frac{a}{2}$ (same as classical) | $\langle x^2\rangle = \int_0^a x^2|\psi_n(x)|^2dx = \frac{a^2}{3}(1 - \frac{3}{s(\pi n)^2}) = [0.283a^2, 0.321a^2, \ldots, 0.333a^2]$ (agrees with classical for large n) | $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \frac{a}{\sqrt{12}}\sqrt{1 - \frac{6}{(n\pi)^2}} = [0.181a, 0.266a, \ldots 0.289a]$ (agrees with classical for large n) | $\langle\hat{p}\rangle = \int_{-\infty}^{\infty}\psi_n^*(x)(-i\hbar\frac{\partial}{\partial x})\psi_n(x)dx = \frac{2}{a}(-i\hbar\frac{n\pi}{a})\int_0^a\sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{n\pi x}{a}\right)dx = 0$ same as classical | $\langle\hat{p}^2\rangle = \frac{2(-\hbar^2)}{a}(\frac{n\pi}{a})^2(-1)\int_0^a\sin^2(\frac{n\pi x}{a})dx = (\frac{\hbar k\pi}{a})^2 = \hbar^2k_n^2$ quantized | Uncertainty principle relation: $\Delta x\Delta p = \frac{\hbar}{\sqrt{12}}\sqrt{(n\pi)^2 - 6} = [0.568\hbar, 1.670\hbar, 2.623\hbar, \ldots]$, $\Delta x\Delta p \geq \hbar/2$

The infinite well: momentum space $\phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi_n(x)e^{-ipx/\hbar}dx$ | $\Delta p = \frac{2\hbar}{a}$ | $\phi_n(p) = \frac{-i}{\sqrt{2\pi\hbar}p}e^{ip/\Delta p}\{e^{+in\pi/2}(\frac{\sin[(p_n+p)/\Delta p]}{(p_n+p)/\Delta p}) - e^{-in\pi/2}(\frac{\sin[(p_n+p)/\Delta p]}{(p_n+p)/\Delta p})\}$ | $|\phi_n(p)|^2 = \frac{\pi n^2\hbar^2}{a^3}\frac{1-\cos[(p-p_n)a/\hbar]}{(p^2-p_n^2)^2}$ | $|\phi_n(-p)|^2 = |\phi_n(+p)|^2$ | In the limit $\Delta p \rightarrow 0$(either$\hbar \rightarrow 0$ or $a \rightarrow \infty$) | $P_{QM} = \lim_{\Delta p\rightarrow 0}|\phi_n(p)|^2 = \frac{1}{2}[\delta(p-p_0) + \delta(p+p_0)] = P_{Cl}$ Results in momentum space are consistent wth classical expectations **Symmetric infinite well, emergence of even and odd solutions, parity** $V(x) =$ either 0 for $|x| < a$ or ∞ for $|x| > a$, **Inside:**$\psi_E(x) = A\sin(kx) + B\cos(kx)$, **Outside:**$\psi_E(x) = 0$ | The only difference is boundary conditions: $A\sin(ka) + B\cos(ka) = 0$, Solution: $A\sin(ka) = 0$ and $B\cos(ka) = 0$, $A\sin(-ka) + B\cos(-ka) = 0$, Two possibilites: $A = 0$ or $B = 0$ (Both A=B=0 is trivial, | **Even solutions:** $A = 0$ and $\cos(ka) = 0$, $k_n^+ = \frac{(n-1/2)\pi}{a}$ with $n = 1, 2, 3\ldots$, $E_n^+ = \frac{(\hbar k_n)^2}{2m} = \frac{(2n-1)^2\pi^2\hbar^2}{8ma^2}$, $\psi_n^+ = \frac{1}{\sqrt{a}}\cos\left(\frac{(n-1/2)\pi x}{a}\right)$ | **Odd solutions:** $B = 0$ and $\sin(ka) = 0$, $k_n^- = \frac{n\pi}{a}$ with $n = 1, 2, 3\ldots$, $E_n^- = \frac{(\hbar k_n^-)^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$, $\psi_n^- = \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi x}{a}\right)$

Standard infinite well **Translation: a to 2a, and x to x-a** $k_n = \frac{n\pi}{a}$ with $n = 1, 2, 3\ldots$, $E_n = \frac{(\hbar k_n)^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$, $\psi_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$ | $k_n = \frac{n\pi}{a}$ with $n = 1, 2, 3\ldots$, $E_n = \frac{(\hbar k_n)^2}{2m} = \frac{n^2\pi^2\hbar^2}{8ma^2}$, $\psi_n = \sqrt{\frac{1}{a}}\sin\left(\frac{n\pi(x-a}{2a}\right)$

Asymmetric infinite well $[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)]\psi_E(x) = E\psi_E(x)$ $V(x) =$ either 0 for $-L < x < 0$ or V_0 for $0 < x < L$ or ∞ for $|x| > L$ **Left side** $(-L < x < 0)$: $\frac{d^2\psi_E(x)}{dx^2} = -k^2\psi_E(x)$ where $k = \sqrt{\frac{2mE}{\hbar^2}}$ | $\psi_E(x) = A\sin(kx) + B\cos(kx)$ | Right side $(0 < x < L)$, we have to consider two possibilities: $E > V_0$ case: $\frac{d^2\psi_E(x)}{dx^2} = -q^2\psi_E(x)$ where $q = \sqrt{\frac{2m(E-V_0}{\hbar^2}}$, $\psi_E(x) = C\sin(qx) + D\cos(qx)$ | $0 < E < V_0$ case: $\frac{d^2\psi_E(x)}{dx^2} = +q^2\psi_E(x)$ where $q = \sqrt{\frac{2m(V_0-E}{\hbar^2}}$, $\psi_E(x) = C'e^{+qx} + D'e^{-qx}$ | **Outside (—x— ¿ L):**$\psi_E(x) = 0$ | Matching$\psi_*(x)$ and $d\psi_E(x)/dx$ at the boundaries (x=-L, x = 0, x = L) leads to solutions, including the quantization of energyt | Penetration of classically forbidden region, characterized by $d = \sqrt{\frac{\hbar^2}{2m(V_0-E}}$

Two-state system in the symmetric infinite well (time dependence) $\psi(x,t) = \frac{1}{\sqrt{2}}[\psi_1^+(x)e^{-iE_1^+t/\hbar} + \psi_1^-(x)e^{-iE_1^-t/\hbar}]$ | $|\psi(x,t)|^2 = \frac{1}{2}[|\psi_1^+(x)|^2 + |\psi_1^-(x)|^2 + 2\psi_1^+(x)\psi_1^-(x)\cos\left(\frac{\Delta Et}{\hbar}\right)$ | where $\Delta E = E_1^- - E_1^+$ | $\langle x\rangle = \int_{-a}^{+a} x|\psi(x,t)|^2dx = a(\frac{32}{9\pi^2})\cos\left(\frac{\Delta Et}{\hbar}\right)$ | $\langle p\rangle = m\frac{d\langle x\rangle}{dt}$ | $\langle p\rangle = \int_{-a}^{+a}\psi^*(x,t)(-u\hbar\frac{\partial}{\partial x})\psi(x,t)dx = -(\frac{4\hbar}{3a})\sin\left(\frac{\Delta Et}{\hbar}\right)$ | $j(x,t) = \frac{i\hbar}{2m}(\psi\frac{\partial\phi^*}{\partial x} - \frac{\partial\psi}{\partial x}\psi^*) = F_{2s}(x)\sin\left(\frac{\Delta Et}{\hbar}\right)$ | $\phi(p,t) = \frac{1}{\sqrt{2}}[\phi_1^+(p)e^{-iE_1^+t/\hbar} + \phi_1^-(p)e^{-iE_1^-t/\hbar_+}]$ |

Quantum revival in the standard infinite well $T_{rev} = \frac{4mL^2}{h\pi}$ | $\psi(x,t+T_{rev}) = \sum_{n=1}^{\infty} a_n u_n(x)e^{-iE_n(t+T_{rev})/\hbar} = \sum_{n=1}^{\infty} a_n u_n(x)e^{-iE_n t/\hbar}e^{-2\pi in^2} = \psi(x,t)$(because $e^{-2\pi in^2} = 1$ for all n

5.2 Stationary States for the Infinite Well quantized energies $E_n = \frac{\hbar^2k^2}{2m} = \frac{\hbar^2n^2\pi^2}{2ma^2}$ (standard infinite well) | Stationary state wave functions written in the form $\psi(x) = u_n(x)$ must satisfy the normalization condition $1 = \int P_{QM}(x)dx = \int_0^a |u_n(x)|^2dx = 1$ | $u_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$ (standard infinite well)

6 The Infinite Well: Formal Quantum Mechanics Aspects **Dirac braket notation** $\langle\psi|\psi\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)dx = 1$ | $\angle\psi|\psi\rangle = 1$ | $\langle\psi_1|\psi_2\rangle = \int_{-\infty}^{\infty}\psi_1^*(x,t)\psi_2(x,t)dx$ | $\langle\psi_1|\psi_2\rangle^* = \langle\psi_2|\psi_1\rangle$ | $\langle\phi_1|\phi_2\rangle = \int_{-\infty}^{\infty}\phi_1^*(p,t)\phi_2(p,t)dp$ | $\langle\phi_1|\phi_2\rangle = \langle\psi_1|\psi_2\rangle$ | $\langle\hat{O}\rangle = \langle\psi|\hat{O}|\psi\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)\hat{O}\psi(x,t)dt$

Hermitian operator $\langle\hat{O}\rangle = \langle\hat{O}\rangle^*$ or $\langle\psi|\hat{O}|\psi\rangle = \langle\psi|\hat{O}|\psi\rangle^*$ In other words: operators whose expectation values are real or more generally: $\langle\psi_1|\hat{O}|\psi_2\rangle^* = \langle\psi_2|\hat{O}|\psi_1\langle$ Extension of the concepts of realness of numbers of numbers to operators

Hermitian conjugation $\langle\psi|\hat{O}^\dagger|\psi\rangle \equiv \langle\hat{O}\psi|\psi\rangle$ An operator is hermitian if it is equal to its hermitian conjugation: $\hat{O}^\dagger = \hat{O}$ |Proof $\langle\psi|\hat{O}|\psi\rangle = \langle\psi|\hat{O}\psi\rangle^* = \langle\hat{O}\psi|\psi\rangle = \langle\psi|\hat{O}^\dagger|\psi\rangle = \langle\psi|\hat{O}|\psi\rangle$| Extension of the concept of complex conjugation of numbers to operators | Example 1: What is the Hermitian conjugation of a complex number c? $\langle\psi|c^\dagger|\psi\langle = \int\psi^*c^\dagger\psi dx = \int(c\psi)^*\psi dx = \int\psi^*c^*\psi dx = \langle\psi|c^*|\psi\rangle$ Hermitian conjugation of complex numbers it its complex conjugation: $c^\dagger = c^*$ | Example 2: What is the hermitian conjugation of the differential operator d/dx? $\int\psi^*(\frac{d}{dx})^\dagger\psi dx \equiv \int(\frac{d}{dx}\psi)^*\psi dx = (\psi^*\psi)_{x=-\infty}^{x=+\infty} - \int\psi^*\frac{d\psi}{dx}dx = \int\psi^*(-\frac{d}{dx})\psi dx$ | $(\frac{d}{dx})^\dagger = -\frac{d}{dx}$ | Properties $(\hat{O}^\dagger)^\dagger = \hat{O}$, $f(\hat{O})^\dagger = f(\hat{O}^\dagger)$, $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$ | If an operator is represented by a matrix, then the Hermitian conjugation is its transpose and complex conjugation | $\hat{O}^\dagger = \hat{O}^{T*}$, $(\hat{O}^\dagger)_{mn} = \hat{O}^*_{mn}$

What good is Hermitian Hermitian operators naturally correspond to physical observables Position operator, in momentum space $\hat{x} = i\hbar\frac{d}{dp}$, Momentum operator, $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ Potential Energy U Operator $U(x)$ Total Energy Operator $\hat{E} = i\hbar\frac{\partial}{\partial t}$ Kinetic energy operator in position space $\hat{K} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ Hamiltonian Operator $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)$ | $\langle\hat{O}\rangle = \int_{-\infty}^{\infty}\psi^*\hat{O}\psi dx$

Properties of Hermitian Operators **1. Hermitian operators have real eigenvalues** $\hat{A}\psi_a(x) = a\psi_a(x)$, $\langle\hat{A}\rangle = \angle\psi_a|\hat{A}|\psi_a\rangle = \int_{-\infty}^{\infty}\psi_a^*(x)\hat{A}\psi_a(x)dc = \int_{-\infty}^{\infty}\psi_a^*(x)a\psi_a(x)dx = a\langle\psi_a|\psi_a\rangle$, $a = \frac{\langle\psi_a|\hat{A}|\psi_a\rangle}{\langle\psi_a|\psi_a\rangle}$ **2 The eigenfunctions of a hermitian operator corresponding to different eigenvalues are orthogonal** Example: standard well $\langle u_n|u_m\rangle = \delta_{mn}$ Same is true for the symmetric infinite well: $\langle u_n^+|u_m^-\rangle = 0$ for all m and n $\langle u_n^+|u_m^+\rangle = \delta_{mn}$ $\langle u_n^-|u_m^-\rangle = \delta_{mn}$ Same is true in momentum space, if the eigenfunctions are also normalized $\langle u_n|u_n\rangle = 1$ we sat they from an orthonormal set | the orthogonality is not limited to energy eigenstates, example: eigenstates of the momentum operator in position space $\hat{p}\psi_p(x) = p\psi_p(x)$, $-i\hbar\frac{d\psi_p(x)}{dx} = p\psi_p(x)$, $\psi_p(x) = \frac{1}{\sqrt{s\pi\hbar}}e^{ipx/\hbar}$, $\langle\psi_p|\psi_{p'}\langle = \int_{-\infty}^{\infty}(\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar})^*(\frac{1}{\sqrt{2\pi\hbar}}e^{ip'x/\hbar})dx = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}e^{i(p'-p)x/\hbar}dx = \delta(p'-p)$ This is an example of an orthonormal set of eigenfunctions in the continuum (eigenstates of momentum operator in position space) **The eigenfunctions of a hermitian operator corresponding to different eigenvalues are orthogonal, if there's a degeneracy (there are more than one eigenfunction for the same eigenvalue), the set of such eigenfunctions are generally not orthogonal, but can be made so by hand**

Expansion in energy eigenstates example: standard infinite well $\psi(x,t) = \sum_{n=1}^{\infty}a_n u_n(x)e^{-iE_n t/\hbar}$ $\langle\psi|\psi\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)dx = \int_{-\infty}^{\infty}(\sum_{n=1}^{\infty}a_n u_n(x)e^{-iE_n t/\hbar})^*(\sum_{m=1}^{\infty}a_m u_m(x)e^{-iE_m t/\hbar})dx = \sum_{n=1}^{\infty}\sum_{n=1}^{\infty}a_n^*a_m e^{-i(E_m-E_n)t/\hbar}\int_0^L u_n^*(x)u_m(x)dx = \sum_{n=1}^{\infty}|a_n|^2$, $\langle\psi|\psi\rangle = 1$ means $\sum_{n=1}^{\infty}|a_n|^2 = 1$ For $\psi(x,t)$ to be normalized, all the expansion coefficients $|a_n|^2$ must sum to unity

What about energy expectation values $\phi(x,t) = \sum_{n=1}^{\infty}a_n u_n(x)e^{-iE_n t/\hbar}$ | $\langle\hat{E}\rangle =\rangle = \langle\psi|\hat{E}|\psi\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)\hat{E}\psi(x,t)dx = \int_{\infty}^{\infty}(\sum_{n=1}^{\infty}a_n u_n(x)e^{-E_n t/\hbar})^*(i\hbar\frac{\partial}{\partial t})(\sum_{m=1}^{\infty}a_m u_m(x)e^{-iE_m t/\hbar})dx = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}a_n^*a_m E_m e^{-i(E_m-E_n)t/\hbar}\int_0^L u_n^*(x)u_m(x)dx = \sum_{n=1}^{\infty}|a_n|^2E_n$ | $\langle\hat{E}^k\rangle = \sum_{n-1}^{\infty}|a_n|^2E_n^k$ | A general state will have | $\Delta E = \sqrt{\langle\hat{E}^2\rangle - \langle\hat{E}\rangle^2} \neq 0$ unless it is an energy eigenstate.

The parity operator **Definition:** $\hat{P}\psi(x) \equiv \psi(-x)$ **Eigenvalues:** $\hat{P}\psi(x) \equiv \lambda_p\psi(x)$, $\hat{P}^2\psi(x) \equiv \lambda_p\hat{P}\psi(x) = \lambda_p^2\psi(x) = \psi(x)$, $\lambda_p^2 = 1$ or $\lambda_p = \pm 1$ **Eigenfunctions:** $\hat{P}\psi_E(x) \equiv +\psi_E(x)$, $\hat{P}\psi_O(x) \equiv +-psi_o(x)$ Any wavefunction can be decomposed into and even and odd parts: $\psi(x) = \frac{\psi(x)+\psi(-x)}{2} + \frac{\psi(x)-\psi(-x)}{2} = \psi_E(x) + \psi_o(x) = C_E\tilde{\phi}_E(x) + c_o\tilde{\phi}_o(x)$ for normalized $\tilde{\phi}_E(x)$ $\tilde{\phi}_o(x)$ They are naturally orthogonal: $\langle\psi_E|\psi_o\langle = \int_{-\infty}^{\infty}\psi_E^*(x)\phi_0(x)dx = 0$ Te modulus squares of the coefficients, $|c_E|^2$ and $|c_o|^2$, are the probabilities of finding the state with even (positive) or odd (negative) parity.

Commutator $[\hat{x},\hat{p}] \equiv \hat{x}\hat{p} - \hat{p}\hat{x}$ | $(\hat{x}\hat{p} - \hat{p}\hat{x})\phi(x) = x(-i\hbar\frac{d}{dx})\phi(x) - (-i\hbar\frac{d}{dx}[x\psi(x)] = i\hbar\psi(x)$ | $[\hat{x},\hat{p}] = i\hbar$ In quantum mechanics, if two operators do not commute, then there exists an uncertainty prince associated with them for example $[\hat{x},\hat{p}] = i\hbar$, $\Delta x\Delta p \leq \hbar/2$ In other words, they cannot be determined to arbitrary precision simultaneously. In quantum mechanics, if two operators commute, then there exists simultaneous eigenfunctions between them. For example, in the symmetric infinite well, the parity operator commutes with the hamiltonian operator: $[\hat{P},\hat{H}] = 0$ The wavefunctions $u_n^+(x)$ and $u_n^-(x)$ are simultaneous eigenfunctions to energy and parity: $\hat{H}u_n^+(x) = E_n^+u_n^+(x)$, $\hat{H}u_n^-(x) = E_n^-u_n^-(x)$, $\hat{P}u_n^+(x) = (+1)u_n^+(x)$, $\hat{P}u_n^-(x) = (-1)u_n^-(x)$, In other words, they can be determined to arbitrary precision simultaneously. In quantum mechanics, we always seek the largest set of commuting operators in a given problem.

The expansion postulate The eigenfunctions of a Hermitian operator form a complete set: any admissible wave function can be expanded in such eigenfunctions given $\psi(x,0)$ find $\psi(x,t)$ $\psi(x,0) = \sum_{n=1}^{\infty}a_n u_n(x)$ Invert it to find the coefficients: $a_n = \int_0^L\psi(x,0)u_n(x)dx$ The solution is then $\psi(x,t) = \sum_{n=1}^{\infty}a_n u_n(x)e^{-iE_n t/\hbar}$

6.6 Parity parity operator $\hat{P}f(x) \equiv f(-x)$

6.7 Simultaneous Eigenfunctions Two hermitian operators $\hat{A}$ and $\hat{B}$ can have simultaneous eigenfunctions if and only if they commute with each other, that is, $[\hat{A},\hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} = 0$

Symmetric infinite well

$$V(x) = \begin{cases} 0 \text{ for } 0 < x < a \\ +\infty \text{ for } x < 0 \text{ or } +a < x \end{cases}$$

Inside: $\psi_E(x) = A\sin(kx) + B\cos(kx)$ | Outside: $\psi_E(x) = 0$ | The only difference is boundary conditions: $A\sin(ka) + B\cos(ka) = 0$ | $A\sin(-ka) + B\cos(-ka) = 0$ | Solution: $A\sin(ka) = 0$and$B\cos(ka) = 0$ | Two possibilities: A=0 or B=0 (Both A=B=0 is trivial) | Even solutions:$A = 0$ and $\cos(ka) = 0$ | $k_n^+ = \frac{(n-1/2)\pi}{a}$ with $n = 1, 2, 3\ldots$ | $E_n^+ = \frac{(\hbar k_n)^2}{2m} = \frac{(2n-1)^2\pi^2\hbar^2}{8ma^2}$ | $\psi_n^+(x) = \frac{1}{\sqrt{a}}\cos\left(\frac{(n-1/2)\pi x}{a}\right)$ | Odd solutions:$B = 0$ and $\sin(ka) = 0$ | $k_n^- = \frac{n\pi}{a}$ with $n = 1, 2, 3\ldots$ | $E_n^- = \frac{(\hbar k_n^-)^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$ | $\psi_n^-(x) = \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi x}{a}\right)$ | The emergence of even and odd solutions is called parity

Normalization $\int_{-\infty}^{\infty}P(x,t)dx = \int_{-\infty}^{\infty}|\psi(x,t)|^2dx = \int_{-\infty}^{\infty}\psi^*(x,0)\psi(x,0)dx = 1$

6.6 Parity $\hat{P}f(x) \equiv f(-x)$ |

8 Other one-dimensional potentials $i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t)$ | Hamiltonian operator $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)$ | If the potential is independent of time $V(x,t) = V(x)$, we seek stationary states: $\psi(x,t) = \psi_E(x)e^{-iEt/\hbar}$ | by solving the eigenvalue problem: $\hat{H}\psi_E(x) = E\psi_E(x)$ (time-independent schrodinger equation)

The symmetric finite square well: classically $m\frac{d^2x(t)}{dt^2} = -\frac{\partial V(x,t)}{\partial x}$ | $V(x) = -V_0 for - a < x < +a, 0$ otherwise , If total energy $E < 0$, speed $v_0 = \sqrt{2|E|/m}$, momentum $p_0 = mv_0 = \sqrt{2m|E|}$, elastic collisions with the walls (forbidden to go inside the walls), periodic motion $\tau = 2a/v_0$ | If total energy $E > 0$, -unbound motion, motion speeds up across the well (T = E-V)

The symmetric finite square well: quantum - mechanically $[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)]\psi_E(x) = E\psi_E(x)$ | $V(x) = -V_0 for - a < x < +a, 0$ otherwise We seek bound states (Ei0) Unbound states (E¿0) will be considered later in scattering problems | For bound states ($E < 0$) 1. Potential is symmetric → expect even and odd solutions(eigenfunctions of parity), same as in infinite well 2. Finite well → finite number of bound states, depending on depth (V_0) and width (a), vs. infinite number of states in the infinite well 3. Penetration of classically forbidden region vs no penetration in classical well | Inside ($|x| < a$) : $\frac{d^2\psi_E(x)}{dx^2} = -q^2\psi_E(x)$ where $q = \sqrt{\frac{2m(V_0-|E|)}{\hbar}}$ | Outside ($|x| > a$) : $\frac{d^2\psi_E(x)}{dx^2} = +k\psi_E(x)$ where $k = \sqrt{\frac{2m|E|}{\hbar}}$ | Even solutions: $\psi^{(+)}(-x) = \psi^{(+)}(x)$ | $\psi^{(+)}(x) = Ce^{+kx}$ for $x \leq -a$, $A\cos(qx)$ for $-a \leq x \leq +a$, Ce^{-kx} for $+a \geq x$ | Match $\psi^{(+)}$ at $x = +a$: $A\cos(qa) = Ce^{-ka}$, Match $\frac{d\psi^{(+)}}{dx}$ at $x = +a$: $-qA\sin(qa) = -kCe^{-ka}$, Matching at X = -a yields the same conditions | Odd solutions: $\psi^{(-)}(-x) = -\psi^{(-)}(x)$ | $\psi^{(-)}(x) = -Ce^{+kx}$ for $x \leq -a$, $B\sin(qx)$ for $-a \leq x \leq +a$, $+Ce^{-kx}$ for $+a \geq x$ | Match $\psi^{(-)}$ at $x = +a$: $B\sin(qa) = Ce^{-ka}$, Match $\frac{d\psi^{(-)}}{dx}$ at $x = +a$: $qB\sin(qa) = -kCe^{-ka}$, Matching at X = -a yields the same conditions | Even eigenvalue condition: $q\tan(qa) = k$, Odd eigenvalue condition: $-q\cot(qa) = k$ | Even eigenvalue condition: $\sqrt{R^2 - y^2} = +y\tan(y)$, Odd eigenvalue condition $\sqrt{R^2 - y^2} = +y\cot(y)$, where $y = qa$ and $R = \sqrt{\frac{2mV_0a^2}{\hbar^2}}$ The number of bound states is finite, but increases with depth (V_0) and width (a), for fixed width, as $V_0 \to \infty$, $y \to (n-1/2)\pi$, implying $\frac{(n-1/2)^2\hbar^2\pi^2}{2ma^2} \to E_n^{(+)}$ | There is always at least one bound state (even parity) no matter how narrow or shallow the well. Odd-parity states appear only if $R \geq \pi/2$, there will be $(n+1)$ even bound states if $n\pi < R < (n+1)\pi$, the will be n odd bound states if $(n-1/2)\pi < R < (n+1/2)\pi$

9 The Harmonic Oscillator

Harmonic oscillator classically $m\frac{d^2x(t)}{dt^2} = F = \frac{\partial V(x,t)}{\partial x}$ | $V(x) = \frac{1}{2}Kx^2 = \frac{1}{2}m\omega^2x^2$ | $F = -Kx$ | $\omega = \sqrt{K/m}$ | $x(t) = C_1\sin(\omega t) + C_2\cos(\omega t)$ | Total energy $E = 0.5mv^2 + 0.5Kx^2$ is conserved | All kinetic energy at equilibrium position (x=0) | Periodic motion $\tau = \frac{2\pi}{\omega}$

Unstable classic harmonic oscillator $V(x) = -\frac{1}{2}Kx^2 = -\frac{1}{2}m\omega^2x^2$ | $F = -Kx$ | $\frac{d^2x(t)}{dt^2} = +\omega^2(x)$ | $x(t) = C_1e^{\omega t} + C_2e^{-\omega t}$

Harmonic oscillator: quantum solution $[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2]\psi(x) = E\psi(x)$ | $\psi(x,t) = \psi(x)e^{-iEt/\hbar}$ | Change variable: $x = \rho y$ | We seek bound states ($E > 0$) Expect even and odd solutions | $\frac{d^2\psi(y)}{dy^2} - \frac{m^2\omega^2\rho^4}{\hbar^2}y^2\psi(y) = -\frac{2m\rho^2E}{\hbar^2}\psi(y)$ | Dimentionless diff. eq: $\frac{d^2\psi(y)}{dy^2} - y^2\psi(y) = -\epsilon\psi(y)$ | $\rho = \sqrt{\frac{\hbar}{m\omega}}$ | $\epsilon = \frac{2E}{\hbar\omega}$ | Large y behavior: $\frac{d^2\psi(y)}{dy^2} \approx y^2\psi(y)$ | which has approx. solution $\psi(y) \sim e^{\pm y^2/2}$ | Try solution: $\psi(y) = h(y)e^{-y^2/2}$ | $\frac{d^2h(y)}{dy^2} - 2y\frac{dh(y)}{dy} + (\epsilon-1)h(y) = 0$

Harmonic oscillator: quantum even-party solution $\frac{d^2h(y)}{dy^2} - 2y\frac{dh(y)}{dy} + (\epsilon-1)h(y) = 0$ | Try even solution: $h^{(+)}(y) = \sum_0^{\infty}a_sy^{2s}$ | $\sum_{s=0}^{\infty}2s(2s-1)a_sy^{2s-2} + \sum_{s=0}^{\infty}(\epsilon-1-4s)a_sy^{2s} = 0$ | $\sum_{s=0}^{\infty}2(s+1)(2s+1)a_{s+1} + (\epsilon-1-4s)a_sy^{2s} = \sum_0^{\infty}B_sy^{2s} = 0$ | $B_s = 0$ leads to recurrence relation: $a_{s+1} = a_s[\frac{4s+1-\epsilon}{2(s+1)(2s+1)}]$ | For large s and fixed y: $\frac{a_{s+1}y^{2(s+1)}}{a_sy^{2s}} \to \frac{y^2}{s}$ | Same behavior as: $e^{y^2} = \sum_{s=0}^{\infty}\frac{1}{s!}(y^2)^s$ | $h^{(+)}(y) = a_0 + a_1y^2 + a_2y^4 + \ldots \to e^{y^2}$ | $\psi^{(+)}(y) = h^{(+)}(y)e^{-y^2/2} \to e^{y^2/2} \to \infty$ for large y | Boundary condition: we want $\psi(x)$ to be finite at large y. This mean that $h^{(+)}$ series must terminate to a polynomial at some order n, given by: $4n+1-\epsilon = 0$ | $a_{s+1} = a_2[\frac{4s+1-\epsilon}{2(s+1)(2s+1)}]$ | Even solution: $E_n^{(+)} = (2n+\frac{1}{2})\hbar\omega$ | $\psi_n^{(+)}(y) = h_n^{(+)}(y)e^{-y^2/2}$ | $n = 0, 1, 2\ldots$ | $\epsilon = \frac{2E}{\hbar\omega} = 4n+1$: must be an integer (quantized) | $E_0^{(+)} = \frac{1}{2}\hbar\omega$, $\psi_0^{(+)}(y) = a_0e^{-y^2/2}$ | $E_1^{(+)} = \frac{5}{9}\hbar\omega$, $\psi_1^{(+)}(y) = a_0(1-2y^2)e^{-y^2/2}$ | $E_2^{(+)} = \frac{9}{2}\hbar\omega$, $\psi_2^{(+)}(y) = a_0(1-4y^2+4y^4/3)e^{-y^2/2}$

Harmonic oscillator: quantum odd-party solution $\frac{d^2h(y)}{dy^2} - 2y\frac{dh(y)}{dy} + (\epsilon-1)h(y) = 0$ | Try odd solution: $h^{(-)}(y) = \sum_0^{\infty}b_sy^{2s+1}$ | $\sum_{s=0}^{\infty}2s(2s-1)b_sy^{2s-1} + \sum_{s=0}^{\infty}(\epsilon-1-2(2s+1))b_sy^{2s+1} = 0$ | which leads to recurrence relation: $b_{s+1} = b_s[\frac{4s+3-\epsilon}{2(s+1)(2s+3)}]$ | Series must terminate: $4n+3-\epsilon = 0$ | $\epsilon = \frac{2E}{\hbar\omega} = 4n+3$ | Odd solution: $E_n^{(-)} = (2n+\frac{3}{2})\hbar\omega$ | $\psi_n^{(-)}(y) = h_n^{(-)}(y)e^{-y^2/2}$ | $n = 0, 1, 2\ldots$ | $E_0^{(-)} = \frac{3}{2}\hbar\omega$, $\frac{7}{2}\hbar\omega$, $\frac{11}{2}\hbar\omega$, $\ldots$

Harmonic oscillator: combined solution $E_n = (n+\frac{1}{2})\hbar\omega$ | $n = 0, 1, 2\ldots$ | $\psi_n(x) = C_nH_n(y)e^{-y^2/2}$ | $y = x/\rho$, $\rho \equiv \sqrt{\frac{\hbar}{m\omega}}$ | $C_n = \frac{1}{\sqrt{\rho\sqrt{\pi}2^nn!}}$

Hermite polynomials $H_n(y) = \sum_{s=0}^{n}a_sy^2$ Solutions to the differential equation: $\frac{d^2H_n(y)}{dy^2} - 2y\frac{dH_n(y)}{dy} + 2nH_n(y) = 0$ | Orthogonality: $\int_{-\infty}^{\infty}H_m(y)H_n(y)e^{-y^2}dy = 2^nn!\sqrt{\pi}\delta_{mn}$ | Parity: $H_n(-y) = (-1)^nH_n(y)$ | Recurrence relation: $H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1}(y)$ | Derivative: $H_n'(y) = 2nH_{n-1}(y)$ | Special values:

$$H_n(O) = \begin{cases} 0 \text{ if n odd} \\ (-1)^{n/2}2^{n/2}(n-1)! \text{ if n even} \end{cases}$$

Can be generated by: $H_n(y) = (-1)^ne^{y^2}\frac{d^n}{dy^n}(e^{-y^2})$ | $H_0(y) = 1$ | $H_1(y) = 2y$ | $H_2(y) = 4y^2 - 2$ | $H_3(y) = 8y^3 - 12y$ | $H_4(y) = 16y^4 - 48y^2 + 12$ | $H_5(y) = 32y^5 - 160y^3 + 120y$

Harmonic oscillator: comments $V(x) = \frac{1}{2}Kx^2 = \frac{1}{2}m\omega^2x^2$ | Eigenenergies: $E_n = (n+\frac{1}{2})\hbar\omega$, $n = 0, 1, 2\ldots$ | Eigenfunctions: $\psi_n(x) = C_nH_n(y)e^{-y^2/2}$, $y = x/\rho$, $\rho \equiv \sqrt{\frac{\hbar}{m\omega}}$, $C_n = \frac{1}{\sqrt{\rho\sqrt{\pi}2^nn!}}$ | Orthogonality: $\langle\psi_n|\psi_k\rangle = \int_{-\infty}^{\infty}\psi_n(x)\psi_k(x)dx = \delta_{n,k}$ | Parity:$\psi_n(-x) = (-1)^n\psi_n(x)$ (even if n even, odd if n odd) | Useful integrals (matrix elements): $\langle\psi_n|x|\psi_k\rangle = \sqrt{\frac{\hbar}{m\omega}}(\delta_{n,k-1}\sqrt{k} + \delta_{n,k+1}\sqrt{k+1})$ | $\langle\psi_n|\hat{p}|\psi_k\rangle = -i\sqrt{\frac{m\omega\hbar}{2}}(\delta_{n,k-1}\sqrt{k} + \delta_{n,k+1}\sqrt{k+1})$ | $\langle\psi_n|x^2|\psi_k\rangle = \frac{\hbar}{m\omega}(n+\frac{1}{2})$ | $\langle\psi_n|\hat{p}^2|\psi_k\rangle = m\hbar\omega(n+\frac{1}{2})$ | $\langle\psi_n|\hat{x}^4|\psi_k\rangle = \frac{3}{4}(\frac{\hbar}{m\omega})^2(2n^2+2n_1)$ | $\langle\psi_n|\hat{p}^4|\psi_k\rangle = \frac{3}{4}(m\hbar\omega)^2(2n^2+2n_1)$ | 1) Energy levels are evenly spaced, with a spacing of $\hbar\omega$, 2) Alternating in parity, with the lowest state even, 3) Zero-point energy | Eigenfunctions from a complete set: $\psi(x,t) = \sum_{n=0}^{\infty}a_n\psi_n(x)e^{-iE_nt/\hbar}$

Harmonic oscillator: uncertainty principle $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\frac{\hbar}{m\omega}(n+\frac{1}{2})}$ | $\Delta p = \sqrt{\langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2} = \sqrt{m\hbar\omega(n+\frac{1}{2})}$ | $\Delta x\Delta p = (n+\frac{1}{2})\hbar \geq \frac{\hbar}{2}$ | The minimum allowed by the uncertainty principle is satisfied by the ground state of the harmonic oscillator | Ground-state energy: $E_0 = \frac{\hbar\omega}{2}$ | Ground-state wavefunction is Gaussian: $\psi_0(x) = \frac{1}{\sqrt{\rho\sqrt{\pi}}}e^{-\frac{1}{2}\frac{x^2}{2\rho^2}}$, where $\rho \equiv \sqrt{\frac{\hbar}{m\omega}}$

9.2 Solutions for the Simple Harmonic Oscillator SHO potential $V(x) = \frac{Kx^2}{2} = \frac{m\omega^2x^2}{2}$ | time-independent Schrodinger equation $\frac{-\hbar}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{m\omega^2x^2}{2}\psi(x) = E\psi(x)$

Exam 11

Chap11 Scattering from 1d potentials 30 points

Scattering in 1d Incident + Reflected. free-particle $V(x) = 0$ | $[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}]\psi(x) = E\psi(x) = E\psi(x)$ | $\psi_{inc}(x,t) = Ie^{i(px-Et)\hbar}$ | $\psi_{ref}(x,t) = Re^{i(-px-Et)/\hbar}$ | $E = \frac{\hbar^2k^2}{2m} = \frac{p^2}{2m}$ **Interaction region** $V(x)$ | $[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)]\psi(x) = E\psi(x)$ | $\psi_{int}(x)$ | **Transmitted "free-particle"(step** V_0) $[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}]\psi(x) = (E-V_0)\psi(x)$ | $\psi_{tran}(x,t) = Te^{I(qx-E_qt)/\hbar}$ | $E_q - V_0 = \frac{\hbar^2q^2}{2m}$ | The wavefunctions are scattering states (not bound states), The wave functions in the 3 regions must match up smoothly (ψ and ψ'), For plane-waves, we can drop the time dependence for convenience | In scattering, the entity that naturally corresponds to experiments is not the wave function, but the probability flux: $j(x,t) = \frac{\hbar}{2mi}(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}) = \frac{1}{2m}(\psi^*\hat{p}\psi - \psi\hat{p}\psi^*)$ | For plane-waves traveling in either directions $\psi(x,t) = Ae^{i(\pm px-Et)/\hbar}$ | $j(x,t) = \pm\frac{p}{m}|A|^2 \equiv= \pm v|A|^2$ | The flux carries information on the veocity and intensity of the wave particle. It could be thought of as "number of particles passing through per unit time". If the number of particles is conserved in te process (called elastic scattering), then we expect flux conservatoin:

$|j_i| = |j_r| + |j_T|$ **Scattering from a potential step** $[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}]\psi(x) = (E)\psi(x)$ | $V(x) = 0$ when $x < 0$ and V_0 when $x > 0$ | $E > V_0 > 0$ | $\psi(x) = Ie^{+ikx} + Re^{-ikx}$ for $x < 0$ where $k = \sqrt{2mE\hbar^2}$ and Te^{iqx} for $x > 0$ where $q = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ | Match $\psi(x)$ at $x = 0$: $I + R = T$ | Match $\psi'(x)$ at $x = 0$: $ikI - ikR = iqT$ | $R = I(\frac{k-q}{k+q})$ and $T = I(\frac{2k}{k+q})$ | Reflection coefficient $= \left|\frac{j_r}{j_I}\right| = \frac{(\hbar k/m)|R|^2}{(\hbar k/m)|I|^2} = \frac{|R|^2}{|I|^2} = (\frac{k-q}{k+q})^2 = (\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}})^2$ | transmission coefficient $= \left|\frac{j_T}{j_I}\right| = \frac{(\hbar q/m)|T|^2}{(\hbar k/m)|I|^2} = \frac{q|R|^2}{k|I|^2} = \frac{2kq}{(k+q)^2} = \frac{2\sqrt{E(E-V_0)}}{(\sqrt{E}+\sqrt{E-V_0})^2}$ | Check flux conservation $\left|\frac{j_R}{j_I}\right| + \left|\frac{j_T}{j_I}\right| = 1$ | for Case $E > V_0$ change sign of V_0 | wave functions with shorter period are faster | Case $0 < E < V_0$l, now $E - V_0$ in q is negative | $q = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} = i\sqrt{\frac{2m(V_0-E)}{\hbar^2}} = ik$ | $\psi(x) = Ie^{+ikx} + Re^{-ikx}$ for $x < 0$ where $k = \sqrt{\frac{2mE}{\hbar^2}}$ and Te^{-Kx} for $x > 0$ where $K = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$ | $R = I(\frac{k-iK}{k+iK})$ and $T = I(\frac{2k}{k+iK})$ | Reflection coefficient $= \left|\frac{j_R}{j_I}\right| = \frac{(\hbar k/m)|R|^2}{(\hbar k/m)|I|^2} = \frac{|R|^2}{|I|^2} = (\frac{k-iK}{k+iK})^2 = 1$ | transmission coefficient $= \left|\frac{j_T}{j_I}\right| = \frac{0}{(\hbar k/m)|I|^2} = 0$ | Observations: All reflection, no transmission, consistent with classical physics, the particle ventures into the classically-forbidden region. How much it does so depends on the difference $V_0 - E$ One can define penetration depth $\frac{1}{K}$, Phase shift on reflection, the bigger $(V_0 - E)$ the more shift **Scattering from the finite square well** $[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)]\psi(x) = (E)\psi(x)$ | $V(x) = -V_0$ when $-a < x < a$ and 0 otherwise | $\psi(x) = Ie^{+ikx} + Re^{-ikx}$ for $x \leq -a$ and $Ge^{+iqx} + Fe^{-iqx}$ for $-a \leq x \leq a$ and Te^{ikx} for $a \leq x$ where $k = \sqrt{\frac{2mE}{\hbar^2}}$ and $q = \sqrt{\frac{2m(E+V_0}{\hbar^2}}$ | Match ψ at $x = -a$: $Ie^{-ika} + Re^{ika} = Ge^{-iqa} + Fe^{iqa}$ and at $x = +a$: $Ie^{ika} + Re^{-ika} = Te^{iqx}$ | Match ψ' at $x = -a$: $ik(Ie^{-ika} - Re^{ika}) = iq(Ge^{-iqa} + Fe^{iqa})$ and at $x = +a$: $ik(Ie^{ika} - Re^{-ika}) = iq(Te^{iqx})$ | Flux conservation in 3 regions $|j_I| - |j_R| = |j_w ell| = |j_T|$ | $\left|\frac{T}{I}\right|^2 = \frac{1}{1+(\frac{k^2-q^2}{2kq})^2 \sin^2(2qa)}$ | $\left|\frac{R}{I}\right|^2 = 1 - \left|\frac{T}{I}\right|^2$ | Observations A classical particle speeds up (shorter wavelength) over the well, the reflection is purely quantum, when $E >> V_0$ little reflection, another purely quantum phenomenonL there are special vlaues of E for which there's no reflection, corresponding to transmission resonances. Conditions are $sin(2qa) = 0$, for $n = 1, 2, 3\ldots$ **Scattering from finite square barrier** Case $E > V_0$ reverse sign of V_0 from finite square well | Case $E < V_0$ | $\psi(x) = Ie^{+ikx} + Re^{-ikx}$ for $x \leq a$ and $Ee^{-Kx} + Fe^{Kx}$ for $-a \leq x \leq a$ and Te^{ikx} for $x > 0$ where $k = \sqrt{2m\hbar^2}$ $K = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$ | **Quantum tunneling probability** $\left|\frac{T}{I}\right|^2 = \frac{1}{1+(\frac{k^2+\kappa^2}{2k\kappa})^2 \sinh^2(2Ka)}$ **Chap12 More formal aspects 30points** **Fynman-Hellman theorem** Suppose the hamiltonian of a system has an explicit dependence on a parameter λ, with its energy eigenvalues and eigenfunctions: $\hat{H}(\lambda)\psi(\lambda) = E(\lambda)\psi(\lambda)$ then the following relation holds $\frac{\partial E(\lambda)}{\partial\lambda} = \langle \frac{\partial\hat{H}(\lambda)}{\partial\lambda} \rangle = \left\langle \psi(\lambda)\middle|\frac{\partial\hat{H}(\lambda)}{\partial\lambda}\middle|\psi(\lambda)\right\rangle \left|\psi(\lambda)\right| \left\langle\frac{\partial\hat{H}(\lambda)}{\partial\lambda}\middle|\psi(\lambda)\right\rangle$ In words: the derivative of the expectation value of energy with respect to a parameter on which it may depend, can be computed from the explicit dependence in the hamiltonian operator only, disregarding the implicit one. | Example: harmonic oscilator, $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2$, $E_n = (n + \frac{1}{2})\hbar\omega$, Choosing $\hbar$ as parameter, we have $\frac{\partial\hat{H}(\hbar)}{\partial\hbar} = -\frac{\hbar}{m}\frac{d^2}{dx^2}$ and $\frac{\partial E(\hbar)}{\partial}$ and $\frac{\partial E(\hbar)}{\partial\hbar} = (n + \frac{1}{2})\omega$ | $\frac{\partial E(\hbar)}{\partial\hbar} = \left\langle\frac{\partial\hat{H}(\hbar)}{\partial\hbar}\middle|\frac{\partial\hat{H}(\hbar)}{\partial\hbar}\right\rangle$ leads to $(n + \frac{1}{2})\omega = \left\langle -\frac{\hbar}{m}\frac{d^2}{dx^2}\middle|-\frac{\hbar}{m}\frac{d^2}{dx^2}\right\rangle$ Or $\langle T|T\rangle = \left\langle -\frac{\hbar}{2m}\frac{d^2}{dx^2}\middle|-\frac{\hbar}{2m}\frac{d^2}{dx^2}\right\rangle = \frac{E_n}{2}$ A result obtained before by relying on the integral $\left\langle\psi|\hat{p}^2|\psi\middle|\psi|\hat{p}^2|\psi\right\rangle$. The Feynman-Hellman theorem achieved it by simply derivatives, without going through the wavefunction explicitly. **Virial theorem** In classical mechanics, the virial theorem provides a general relation between the time average of the kinetic energy and potential energy of the system. $\langle T|T\rangle = \frac{1}{2}\left\langle x\frac{dV(x)}{dx}\middle|x\frac{dV(x)}{dx}\right\rangle$ (one-dimensional) $\langle T|T\rangle = \frac{1}{2}\langle\vec{r}\cdot\nabla V(\vec{r})|\vec{r}\cdot\nabla V(\vec{r})\rangle$ (three-dimensional) The quantum version has the same form, except $\langle\ldots|\ldots\rangle$ now means expectation values in the eigenstates of the Hamiltonian of the system $\hat{H} = \hat{T} + V$, $\hat{H}\psi = E\psi$ It quickly establishes how energy is shared in the system with little calculation. hIl Example: harmonic oscilator, $\hat{H} = \hat{T} + V = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2$, $\langle T|T\rangle = \frac{1}{2}\left\langle x\frac{dV(x)}{dx}\middle|x\frac{dV(x)}{dx}\right\rangle = \frac{1}{2}m\omega^2\left\langle x^2\middle|x^2\right\rangle = \langle V|V\rangle = \frac{E}{2}$ So the energy is shared half and half in the harmonic oscillator system | **Geometric structures of quantum mechanics** Hilbert space (infinite-dimentional) | State: ket $|\psi\rangle$ and bra $\langle\psi|$ | Complex functions | Inner product of a bra and a ket: $\langle\psi|\chi|\psi|\chi\rangle$ | Normalization: $\langle\psi|\psi|\psi|\psi\rangle = 1$ | Expansion in eigenstates: $|\psi\rangle = \sum_{n=1}^{\infty} a_n|u_n\rangle$ | Complete and orthonormal basis: $\left\langle u_i\middle|u_j\middle|u_i\middle|u_j\right\rangle = \delta_{ij}$ | Different representations | Position space $\psi(x)$ | Momentum Space $\phi(p)$ | Expansions coefficients:$\{a_n\}$ | Hilbert space is closed: linear combinations of states are still states. Same is true of Euclidean space: linear combinations of vectors are still vectors. We deal exclusively with linear operators on Hilbert space: $\hat{O}(\alpha\psi_a + \beta\psi_b) = \alpha\hat{O}\psi_a + \beta\hat{O}\psi_b$ Hence the close connection between linear algebra and quantum mechanics | **Unitary operators** A class of operators in Hilbert space that preserve the inner products of bras and kets | if $|\psi'\rangle = \hat{U}|\psi\rangle$, then $\langle\psi_a|\psi_b|\psi_a|\psi_b\rangle = \left\langle\psi'_a\middle|\psi'_b\middle|\psi'_a\middle|\psi'_b\right\rangle = \left\langle\hat{U}\psi_a|hatU\psi_b\middle|\hat{U}\psi_a|hatU\psi_b\right\rangle = \left\langle\psi_a|\hat{U}^\dagger\hat{U}|\psi_b\middle|\psi_a|\hat{U}^\dagger\hat{U}|\psi_b\right\rangle$ | $\hat{U}^\dagger\hat{U} = I$ (Definition of unitary operator) | $U^{T*}U = I$ or $\sum_k (U^{T*})_{ik}U_{kj} = \delta_{ij}$ | Example1: rotation of two-dimensional vectors as unitary transformations. $\vec{x}' = R\vec{x}$ or $\begin{pmatrix}x'\\y'\end{pmatrix} = \begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}x\\y\end{pmatrix}$ | $R^\dagger R = \begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix} = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix} = I$ | Example2: Fourier transform as a unitary transformation $\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\phi(p)e^{ipx/\hbar}dp = \int_{-\infty}^{\infty}(\frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}})\phi(p)dp = \int_{-\infty}^{\infty}U_{px}\phi(p)dp$ | $U_{px} = \frac{e^{ipx/\hbar}}{\sqrt{x\pi\hbar}}$ | $\int_{-\infty}^{\infty}(U^{T*})_{x'p}U_{px}\phi(p)dp = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{ip(x-x')/\hbar}dp = \delta(x-x')$ Similarly for the inverse Fourier transform | **Example 3: Expansion in a complete set of eigenstates** $\psi(x) = \sum_n a_n u_n(x) = \sum_n U_{xn}a_n$ | $\int_{-\infty}^{\infty}(U^{T*})_n xU_{xm}dx = \int_{-\infty}^{\infty}u_n^*(x)u_m(x)dx = \delta_{nm}$ (orthogonality) | or $\sum_n (U^{T*})_{x'n}U_{nx} = \sum_n u_n^+(x')u_n(x) = \delta(x-x')$ (completeness) **More on commutators** $\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$ | $\left[c,\hat{A}\right] = 0$ | $\left[\hat{A},\hat{A}\right] = 0$ | $\left[\hat{A},\hat{B}\right] = -\left[\hat{B},\hat{A}\right]$ | $\left[\alpha\hat{A}+\beta\hat{B},\hat{C}\right] = \alpha\left[\hat{A},\hat{C}\right] + \beta\left[\hat{B},\hat{C}\right]$ | $\left[\hat{A}\hat{B},\hat{C}\right] = \hat{A}\left[\hat{B},\hat{C}\right] + \left[\hat{A},\hat{C}\right]\hat{B}$ | $\left[\hat{A},\hat{B}\hat{C}\right] = \hat{B}\left[\hat{A},\hat{C}\right] + \left[\hat{A},\hat{B}\right]\hat{C}$ | $\left[\hat{x}^2,\hat{p}\right] = \hat{x}[\hat{x},\hat{p}] + [\hat{x},\hat{p}]\hat{x} = 2i\hbar\hat{x}$ | $\left[\hat{x},\hat{p}^2\right] = \hat{p}[\hat{x},\hat{p}] + [\hat{x},\hat{p}]\hat{p} = 2i\hbar\hat{p}$ | $[\hat{x},f(\hat{p})] = i\hbar\frac{df(\hat{p})}{dp}$ | $[\hat{p},f(x)] = -i\hbar\frac{df(x)}{dx}$ | **Vector equivalent** $\vec{A}\times\vec{A} = 0$ | $\vec{A}\times\vec{B} = -\vec{B}\times\vec{A}$ | $(\alpha\vec{A}+\beta\vec{B})\times\vec{C} = \alpha\vec{A}\times\vec{C} + \beta\vec{B}\times\vec{C}$ | $\vec{A}\times\vec{B}\times\vec{C} = (\vec{A}\cdot\vec{C})\vec{B} - (\vec{A}\cdot\vec{B})\vec{C}$ **Simultaneous eigenfunctions** Two hermitian operators, A and B, can have simultaneous eigenfunctions if and only if they commute with each other | Proof: Let's first assume that $\hat{A}$ and $\hat{B}$ commute, and that we have found the eigenstates of $\hat{A}$ by: $\hat{A}\psi_a = a\psi_a$ | then we note: $\hat{A}(\hat{B}\psi_a) = \hat{B}\hat{A}\psi_a = a(\hat{B}\psi_a)$ | So $\hat{B}\psi_a$ must be the same as ψ_a up to multiplicative constant: $\hat{B}\psi_a = b\psi_a$ | Next we assume that we have found the simultaneous eigenfunctions of $\hat{A}$ and $\hat{B}$ | $\hat{A}\psi_a = a\psi_a$ and $\hat{B}\psi_b$ | Then we note: $\left[\hat{A},\hat{b}\right]\psi_a^b = (\hat{A}\hat{B} - \hat{B}\hat{A})\psi_a^b = (ab - ba)\psi_a^b = 0$ | So $\hat{A}$ and $\hat{B}$ commute: $\left[\hat{A},\hat{B}\right] = 0$ | This is true of any state which can be expanded in the complete set $\psi\sum_{a,b}c_a^b\psi_a^b$ which implies $\left[\hat{A},\hat{B}\right]\psi = \psi\sum_{a,b}c_a^b(\hat{A}\hat{B} - \hat{B}\hat{A})\psi_a^b = \psi\sum_{a,b}c_a^b * 0 = 0$ | In quantum mechanics, we always seek the largest set of commuting Hermitian operators in a given problem **Uncertainty principle: general derivation** Two operators, $\hat{A}$ and $\hat{B}$, are Hermitian, but may not commute with each other. What general constraint can be imposed on the product of their 'uncertainties', $\Delta A \cdot \Delta B$ | $\Delta A^2 = \langle\psi|(\hat{A} - \left\langle\hat{A}\right\rangle)^2|\psi\rangle$ where $\left\langle\hat{A}\right\rangle = \langle\psi|\hat{A}|\psi\rangle$ | $\Delta B^2 = \langle\psi|(\hat{B} - \left\langle\hat{B}\right\rangle)^2|\psi\rangle$ where $\left\langle\hat{B}\right\rangle = \langle\psi|\hat{B}|\psi\rangle$ | Consider ket $|\zeta\rangle = (\hat{A} - \left\langle\hat{A}\right\rangle)|\psi\rangle + i\lambda(\hat{B} - \left\langle\hat{B}\right\rangle)|\psi\rangle$ where λ is a real number | ket $\langle\zeta| = \left\langle(\hat{A} - \left\langle\hat{A}\right\rangle)\psi\middle| - i\lambda\left\langle(\hat{B} - \left\langle\hat{B}\right\rangle)\psi\right|$ | $0 \leq \langle\zeta|\zeta\rangle \equiv I(\lambda) \equiv \left\langle(\hat{A} - \left\langle\hat{A}\right\rangle)\psi\middle|(\hat{A} - \left\langle\hat{A}\right\rangle)\psi\right\rangle + \lambda^2\left\langle(\hat{B} - \left\langle\hat{B}\right\rangle)\psi\middle|(\hat{B} - \left\langle\hat{B}\right\rangle)\psi\right\rangle + i\lambda\left\langle(\hat{A} - \left\langle\hat{A}\right\rangle)\psi\middle|(\hat{B} - \left\langle\hat{B}\right\rangle)\psi\right\rangle - \left\langle(\hat{B} - \left\langle\hat{B}\right\rangle)\psi\middle|(\hat{A} - \left\langle\hat{A}\right\rangle)\psi\right\rangle$ | $I(\lambda) = \langle\psi|(\hat{A} - \left\langle\hat{A}\right\rangle)^2|\psi\rangle + \lambda^2\langle\psi|(\hat{B} - \left\langle\hat{B}\right\rangle)^2|\psi\rangle + i\lambda\langle\psi|(\hat{A} - \left\langle\hat{A}\right\rangle)(\hat{B} - \left\langle\hat{B}\right\rangle) - (\hat{B} - \left\langle\hat{B}\right\rangle)(\hat{A} - \left\langle\hat{A}\right\rangle)|\psi\rangle$ | $I(\lambda) = (\Delta A)^2 + \lambda^2(\Delta B)^2 + \lambda\langle\psi|\hat{F}|\psi\rangle \geq 0$ where $\hat{F} = i\left[\hat{A},\hat{B}\right]$ | True for all λ, including the minimum λ given by $0 = \frac{I(\lambda)}{d\lambda}$ leading to $\lambda_{min} = -\frac{\langle\psi|\hat{F}|\psi\rangle}{2(\Delta B)^2}$ | $I(\lambda_{min}) \geq 0$ leads to $(\Delta A)^2(\Delta B)^2 \geq \frac{\langle\psi|\hat{F}|\psi\rangle^2}{4}$ or $\Delta A\Delta B \geq \frac{1}{2}\left|\langle\psi|\hat{F}|\psi\rangle\right|$ | $\Delta A\Delta B \geq \frac{1}{2}\left|i\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right|$ | There's a fundamental limit, imposed by quantum mechanics, on two observables whose corresponding Hermitian operators do not commute. | What is the minimum uncertainty principle waveform $\hat{A} = \hat{p}$ and $\hat{B} = x$ so $[\hat{p},x] = -\hbar$, so that $\Delta x\Delta p \geq \frac{\hbar}{2}$ | The minimum is saturated by $0 = |\zeta\rangle \equiv (\hat{p} - \langle\hat{p}\rangle)|\psi\rangle + i\lambda(\hat{x} - \langle\hat{x}\rangle)|\psi\rangle$ | In position space $0 = \zeta(x) \equiv (-i\hbar\frac{d}{dx} - p_0)\psi(x) + i\lambda_{min}(x - x_0)\psi(x)$ where $\lambda_{min} = -\frac{\hbar}{2(\Delta x)^2}$ | Or $\frac{d\psi(x)}{dx} = (\frac{ip_0}{\hbar} - \frac{x-x_0}{2(\Delta x)^2})\psi(x)$ which has a simple solution | $\psi(x)\alpha e^{-(x-x_0)^2/(2\Delta x)^2}e^{ip_0x/\hbar}$ a Gaussian waveform at postion x_0 and with momentum p_0 It is saturated by the ground state of the harmonic oscillator **Time dependence in quantum physics** For stationary states: $\psi(x,t) = \psi_n(x)e^{-iE_nt/\hbar}$ | the expectation value of operators is independent of time $\left\langle\hat{O}\right\rangle = \int_{-\infty}^{\infty}\psi^*(x,t)\hat{O}\psi(x,t)dx = \int_{-\infty}^{\infty}\psi^*(x)e^{+E_nt/\hbar}\hat{O}\psi_n(x)e^{-E_nt/\hbar}dx$ | For a general state, $\psi(x,t) = \sum_n^{\infty}a_n\psi_n(x)e^{-iE_nt/\hbar}$ | the expectation value of operators is generally dependent on time | $\left\langle\hat{O}\right\rangle_t = \int_{-\infty}^{\infty}\psi^*(x,t)\hat{O}\psi(x,t)dx$ | **Conservation laws in quantum physics** $\frac{d(hatO_1)}{dt} = \frac{d}{dt}[\int_{-\infty}^{\infty}\psi^*(x,t)\hat{O}\psi(x,t)dx] = \int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial\hat{O}}{\partial t}\psi(x,t)dx + [\int_{-\infty}^{\infty}[\frac{\partial\psi^*}{\partial t}\hat{O}\psi + \psi^*\hat{O}\frac{\partial\psi}{\partial t}]dx]$ | $i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$ and $-i\hbar\frac{\partial\psi^*}{\partial t} = \hat{H}\psi^*$ | $\frac{d\langle\hat{O}\rangle_t}{dt} = \langle\psi|\frac{\partial\hat{O}}{\partial t}|\psi\rangle + \frac{i}{\hbar}\left\langle\hat{H}\psi\middle|\hat{O}\middle|\psi\right\rangle - \frac{i}{\hbar}\left\langle\psi\middle|\hat{O}\middle|\hat{H}\psi\right\rangle = \langle\psi|\frac{\partial\hat{O}}{\partial t}|\psi\rangle + \frac{i}{\hbar}(\langle\psi|\hat{H}\hat{O}|\psi\rangle - \langle\psi|\hat{O}\hat{H}|\psi\rangle) = \langle\psi|\frac{\partial\hat{O}}{\partial t}|\psi\rangle + \frac{i}{\hbar}\langle\psi|\left[\hat{H},\hat{O}\right]|\psi\rangle$ | If the quantum operator $\hat{O}$ is not an explicit function of time, and it commutes with the Hamiltonian operator of the system, then the corresponding classical observable O is conserved in the average sense **Does it commute with the Hamiltonian** example 1: between Hamiltonian and momentum $\left[\hat{H},\hat{p}\right] = \left[\frac{\hat{p}^2}{2m} + V(x),\hat{p}\right] = \left[\frac{\hat{p}^2}{2m},\hat{p}\right] + [V(x),\hat{p}] = -\frac{\hbar}{i}\frac{dV(x)}{dx}$ | $\frac{d\langle\hat{p}_i\rangle}{dt} = 0 + \frac{i}{\hbar}\left\langle\left[\hat{H},\hat{p}\right]\right\rangle$ | $\frac{d\langle\hat{p}\rangle_i}{dt} = -\left\langle\frac{dV(x)}{dx}\right\rangle = \langle F\rangle$ (Ehrenfest's theorem) | **Classical period and quantum revival time** What time scales are involved in the time evolution of a general state $\psi(x,t) = \sum_n^{\infty}a_n\psi_n(x)e^{-iE_nt/\hbar}$

Chap13 Harmonic Oscillator by algebra 30 points **Factoring differential equation** $\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)$ | $0 = (\frac{d^2}{dx^2} + k^2)\psi(x) = (\frac{d}{dx} + ik)(\frac{d}{dx} - ik)\psi(x) = (\frac{d}{dx} - ik)(\frac{d}{dx} + ik)\psi(x)$ | $(\frac{d}{dx} + ik)\psi(x) = 0$ gives $\psi(x) = e^{-ikx}$ | $(\frac{d}{dx} - ik)\psi(x) = 0$ gives $\psi(x) = e^{+ikx}$ | $\frac{d^2\psi(x)}{dx^2} = +k^2\psi(x)$ | $0 = (\frac{d^2}{dx^2} - k^2)\psi(x) = (\frac{d}{dx} + k)(\frac{d}{dx} - k)\psi(x) = (\frac{d}{dx} - k)(\frac{d}{dx} + k)\psi(x)$ | $(\frac{d}{dx} + k)\psi(x) = 0$ gives $\psi(x) = e^{-kx}$ | $(\frac{d}{dx} - k)\psi(x) = 0$ gives $\psi(x) = e^{+kx}$ **Factoring the harmonic oscillator** The quantum Hamiltonian operator $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2x^2$ can be written as $\hat{H} = \hbar\omega(\frac{m\omega}{2\hbar}x^2 + \frac{\hat{p}^2}{2m\hbar\omega})$ however x and $\hat{p}$ do not commute | Force the issue by introducing operators | $\hat{A}_\pm \equiv x\sqrt{\frac{m\omega}{2\hbar}} \mp i\frac{\hat{p}}{\sqrt{2m\hbar\omega}}$ | It has the inverse $x = \sqrt{\frac{\hbar}{2m\omega}}(\hat{A}_+ + \hat{A}_-)$ and $\hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(\hat{A}_+ - \hat{A}_-)$ | $\left[\hat{A}_-,\hat{A}_+\right] = \hat{A}_-\hat{A}_+ - \hat{A}_+\hat{A}_- = 1$ | $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2x^2 = \frac{1}{2m}(-\frac{m\omega\hbar}{2})(\hat{A}_+ - \hat{A}_-)^2 + \frac{m\omega^2}{2}(\frac{\hbar}{2m\omega})(\hat{A}_+ + \hat{A}_-)^2 = \frac{\hbar\omega}{2}(\hat{A}_+\hat{A}_- + \hat{A}_-\hat{A}_+) = \hbar\omega(\hat{A}_+\hat{A}_- + \frac{1}{2})$ | $\hat{N} \equiv \hat{A}_+\hat{A}_-$ is called the number operator | Or solving the eigenvalue problem for the number operator: $\hat{N}|n\rangle = n|n\rangle$ Solving $\hat{H}\psi(x) = E\psi(x)$ becomes solving $\hbar\omega(\hat{N} + \frac{1}{2})|n\rangle = E|n\rangle$ **Factoring the harmonic oscillator: eigenvalues** $\hat{N}|n_m in\rangle = \hat{A}_+\hat{A}_-|n_m in\rangle = 0 = n_m in|n_m in\rangle$ | We can obtain the energy spectrum purely by algebra $\hat{N}|n\rangle = n|n\rangle$ with $n = 0, 1, 2, \ldots$ and $E_n = (n + \frac{1}{2})\hbar\omega$ | We just need to fin one eigenstate, because all other eigenstates can be produced by raising or lowering operators. The natural choice is the ground state $|0\rangle$ | $\hat{A}_-|0\rangle = 0$ in position space is $(x\sqrt{\frac{m\omega}{2\hbar}} + i\frac{\hat{p}}{\sqrt{2m\hbar\omega}})\psi_0(x) = 0$ | Or $\frac{d\psi_0(x)}{dx} = -\frac{x}{\rho^2}\psi_0(x)$ where $\rho = \sqrt{\frac{\hbar}{m\omega}}$ | So the normalized ground state is $\psi_0(x) = \frac{1}{\sqrt{\rho}\sqrt{\pi}}e^{-x^2/(2\rho^2)}$ | Excited states can be obtained by repeated applying the raising operator on the ground state $\hat{A}_+|n\rangle = c_n|n+1\rangle$ or $\psi_{n+1}(x) = \frac{1}{c_n}(x\sqrt{\frac{m\omega}{2\hbar}} + i\frac{\hat{p}}{\sqrt{2m\hbar\omega}})\psi_n(x)$ But still don't know coefficients c_n **Factoring the harmonic oscillator: coefficients of raising and lowering operations** $\hat{A}_+|n\rangle = c_n|n+1\rangle$ | $\hat{A}_-|n\rangle = b_n|n-1\rangle$ | $\langle n|\hat{A}_- = \langle n+1|c_n$ | $\langle n|\hat{A}_+ = \langle n-1|b_n$ | $\langle n|\hat{A}_-\hat{A}_+|n\rangle = \langle n+1|c_n^2|n+1\rangle$ | $\langle n|\hat{N}+1|n\rangle = c_n^2\langle n+1|n+1\rangle$ | $(n+1)\langle n|n\rangle = c_n^2\langle n=1|n=1\rangle$ | also $\langle n|\hat{A}_+\hat{A}_-|n\rangle = \langle n-1|b_n^2|n-1\rangle$ | $n\langle n|n\rangle = b_n^2\langle n-1|n-1\rangle$ | For normalized states $\langle n|n\rangle = 1$ and $\langle n+1|n+1\rangle = 1$ so $n+1 = c_n^2$ | $\hat{A}_+|n\rangle = \sqrt{n+1}|n+1\rangle$ | $\hat{A}_-|n\rangle = \sqrt{n}|n-1\rangle$ | **Factoring the harmonic oscillator: eigenstates continued** $|n\rangle = \frac{1}{\sqrt{n!}}(\hat{A}_+)^n|0\rangle$ **Factoring the harmonic oscillator: expectation values** $x = \sqrt{\frac{\hbar}{2m\omega}}(\hat{A}_+ + \hat{A}_-)$ | $\hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(\hat{A}_+ - \hat{A}_-)$ **Chap 15 and16 Schrodinger equation in 2D and 3D 30 points** **Transition from 1D to 3D (Cartesian coordinates, position space)** Position $\vec{r} = (x,y,z)$ | Momentum operator $\hat{\vec{p}} = (\hat{p}_x,\hat{p}_y,\hat{p}_z) = \frac{\hbar}{i}\vec{\nabla}$ | Kinetic energy operator $\hat{T} = \frac{\hat{p}_x^2+\hat{p}_y^2+\hat{p}_z^2}{2m} = -\frac{\hbar^2}{2m}nabla^2$ | Potential energy $V(x,y,z,t)$ or $V(\vec{r},t)$ | Hamiltonian operator $\hat{H} = \hat{T} + V$ vs. Energy operator$\hat{E} = ihfracd\partial\partial t$ | Time Dependent Schrodinger Equation $\hat{H}\psi(x,y,z,t) = \hat{E}\psi(x,y,z,t)$ or $(-\frac{\hbar^2}{2m})\nabla^2 + V(\vec{r})\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$ | Time independent Schrodinger Equation $\hat{H}\psi(x,y,z) = \hat{E}\psi(x,y,z)$ or $(-\frac{\hbar^2}{2m})\nabla^2 + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$ | Normalization $\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_{-\infty}^{\infty}dz|\psi(x,y,z,t)|^2 = 1$ or $\int|\psi(\vec{r},t)|^2d\tau^3 = 1$ | Expectation $\left\langle\hat{O}(x,y,z,\hat{p}_x,\hat{p}_y,\hat{p}_z,t)\right\rangle = \int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_{-\infty}^{\infty}dz\psi^*(x,y,z,t)\hat{O}(x,y,z,\hat{p}_x,\hat{p}_y,\hat{p}_z,t)\psi(x,y,z,t)$ or | $\left\langle\hat{O}(\vec{r},\hat{\vec{p}},t)\right\rangle = \int\psi^*(\vec{r},t)\hat{O}(\vec{r},\hat{\vec{p}},t)\psi(\vec{r},t)d\tau^3$ | Gradient operator $\vec{\nabla} = (\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial z})$ | Laplace operator $\nabla^2 = (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})$ **Separation of variables (Cartesian coordinates)** $[-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}) + V(x,y,z)]\psi(x,y,z) = E\psi(x,y,z)$ | if the potential is separable, $V(x,y,z) = V_1(x) + V_2(y) + V_3(z)$ | Try solution $\psi(x,y,z) = \psi_1(x)\psi_2(y)\psi_3(z)$ | $(-\frac{\hbar^2}{2m}\frac{1}{\psi_1(x)}\frac{\partial^2\psi_1(x)}{\partial x^2} + V_1(x)) + (-\frac{\hbar^2}{2m}\frac{1}{\psi_2(y)}\frac{\partial^2\psi_2(y)}{\partial y^2} + V_2(y)) + (-\frac{\hbar^2}{2m}\frac{1}{\psi_3(z)}\frac{\partial^2\psi_3(z)}{\partial z^2} + V_3(z)) = E$ | to be true $E_1 + E_2 + E_3 = E$ | **Example: particle in a rigid 3D box** Infinite potential well $V(x,y,z) = 0$ for$0 < x,y.z < L$ and ∞ everywhere else | $(-\frac{\hbar^2}{2m}\frac{\partial^2\psi_1(x)}{\partial x^2} = E_1\psi_1(x)$ and $\psi_{n_x}(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n_x\pi x}{L}\right)$ and $E_1 = n_x^2\frac{\pi^2\hbar^2}{2mL^2}$ and $n_x = 1, 2, 3, \ldots$ | replace x and 1 with y and 2 and z and 3 | Quantized eigenenergies: $E_{n_xn_yn_z} = E_1 + E_2 + E_3 = (n_x^2 + n_y^2 + n_z^2)\frac{\pi^2\hbar^2}{2mL^2}$ where $n_x, n_y, n_z = 1, 2, 3\ldots$ | Orthonormal eigenfunctions: $\psi_{n_xn_yn_z}(x,y,z) = \sqrt{\frac{8}{L^3}}\sin\left(\frac{n_x\pi x}{L}\right)\sin\left(\frac{n_x\pi y}{L}\right)\sin\left(\frac{n_x\pi z}{L}\right)$ | A new features arises where one wavefunction can have the same energy. For example $(n_x,n_y,n_z) = (1,1,2),(1,2,1),(2,1,1)$ this is called degeneracy **Exchange symmetry** Take 2D square box as example: $E_{n_xn_y} = (n_x^2 + n_y^2)\frac{\pi^2\hbar^2}{2mL^2}$ where $n_x, n_y = 1, 2, 3\ldots$ | $\psi_{n_xn_y}(x,y) = \frac{2}{L}\sin\left(\frac{n_x\pi x}{L}\right)\sin\left(\frac{n_x\pi y}{L}\right)$ Observation: nothing changes if we switch x and y in the wavefunction. This is called exchange

symmetry. Can formalize by an operator: $\hat{E}_{(x,y)}\psi(x,y) = \psi(y,x)$ **Eigenstates in 3D box as a basis of expansion** Quantized eigenenergies: $E_{n_x n_y n_z} = E_1 + E_2 + E_3 = (n_x^2 + n_y^2 + n_z^2)\frac{\pi^2\hbar^2}{2mL^2}$ where $n_x, n_y, n_z = 1, 2, 3...$ I Orthonormal eigenfunctions: $\psi_{n_x n_y n_z}(x,y,z) = \sqrt{\frac{8}{L^3}}\sin\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right)\sin\left(\frac{n_z \pi z}{L}\right)$ I Orthonormal: $\left\langle \psi_{n_x n_y n_z} \middle| \psi_{m_x m_y m_z} \right\rangle = \delta_{n_x,m_x}\delta_{n_y,m_y}\delta_{n_z,m_z}$ I They form a complete basis I $\psi(x,y,z,0) = \sum_{n_x,n_y,n_z=1}^{\infty} a_{n_x n_y n_z}\psi_{n_x n_y n_z}(x,y,z)$ I $a_{n+x n_y n_z} = \int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_{-\infty}^{\infty}dz\psi(x,y,z,0)\psi_{n_x n_y n_z}(x,y,z)$ I $\psi(x,y,z,t) = \sum_{n_x,n_y,n_z=1}^{\infty} a_{n_x n_y n_z}\psi_{n_x n_y n_z}(x,y,z)e^{-iE_{n_x n - y n_z}t/\hbar}$ I $\langle E\rangle = \langle\psi(x,y,z,t)|\hat{E}|\psi(x,y,z,t)\rangle = \sum_{n_x,n_y,n_z=1}^{\infty}\left|a_{n_x n_y n_z}\right|^2 E_{n_x n_y n_z}$ I The coefficient squared $\left|a_{n_x n_y n_z}\right|^2$ is the probability for getting $E_{n_x n_y n_z}$ if a measurement of the energy is made. **Transition from 1D to 3D (spherical coordinates, position space)** Position $\vec{r} = (r,\theta,\phi)$ I Momentum operator $\hat{\vec{p}} = \frac{\hbar}{i}\vec{\nabla}$ I Kinetic energy operator $\hat{T} = -\frac{\hbar^2}{2m}\nabla^2$ I Potential energy $V(r,\theta,\phi,t)$ or $V(\vec{R},t)$ I Hamiltonian operator $\hat{H} = \hat{T} + V$ vs. Energy operator$\hat{E} = i\hbar frac\partial\partial t$ I Time Dependent Schrodinger Equation $\hat{H}\psi(r,\theta,\phi,t) = \hat{E}\psi(r,\theta,\phi,t)$ or $(-\frac{\hbar^2}{2m})\nabla^2 + V(\vec{r})\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$ I Time independent Schrodinger Equation $\hat{H}\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$ or $(-\frac{\hbar^2}{2m})\nabla^2 + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$ I Normalization $\int_0^{\infty}r^2dr\int_0^{\pi}\sin d\theta\int_0^{2\pi}d\phi|\psi(r,\theta,\phi,t)|^2 = 1$ I Expectation $\left\langle\hat{O}\right\rangle = \int_0^{\infty}r^2dr\int_0^{\pi}\sin d\theta\int_0^{2\pi}d\phi\psi^*(r,\theta,\phi,t)\hat{O}\psi(r,\theta,\phi,t)$ **Angular momentum operator** $\hat{\vec{L}} = \vec{r}\times\hat{\vec{p}} = \begin{vmatrix}\hat{i} & \hat{j} & \hat{k}\\ x & y & z\\ \hat{p}_x & \hat{p}_y & \hat{p}_z\end{vmatrix}$ I $\hat{\vec{L}} = \vec{r}\times\hat{\vec{p}}$ I $\hat{L}_x = y\hat{p}_z - z\hat{p}_y = \frac{\hbar}{i}(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi})$ I $\hat{L}_y = z\hat{p}_x - x\hat{p}_z = \frac{\hbar}{i}(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi})$ I $\hat{L}_z = x\hat{p}_y - y\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial\theta}$ I $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = -\hbar^2(\frac{\partial^2}{\partial\theta^2} + \cot\frac{\partial}{\partial\phi} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\theta^2})$ I Angular momentum operators only depend on angular variables in spherical coordinates **Eigenstates of angular momentum** $\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$ I $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{z}_z^2 = -\hbar^2(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2})$ I $\left[\hat{L}^2, \hat{L}_z\right] = 0$ So they can have simultaneous eigenfunctions. I $\hat{L}^2 Y_{lm}(\theta,\phi) = l(l+1)\hbar^2 Y_{lm}(\theta,\phi)$ and $\hat{L}_Z Y_{lm}(\theta,\phi) = m\hbar Y_{lm}(\theta,\phi)$ and where$l = 0,1,2,\ldots$ and $m = 0,\pm1,\pm2,\ldots$ I Spherical harmonics $Y_{l,m}(\theta,\phi) = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(1+m)!}}P_l^m(\cos\theta)e^{im\phi}$ for $m \geq 0$ I For negative orders of m, $Y_{l,-m}(\theta,\phi) = (-1)^m Y_{l,m}^*(\theta,\phi)$ I Associated Legendre polynomials $P_l^m(x) = (-1)^m(1-x^2)^{m/2}(\frac{d}{dx})^m P_l(x)$ for $m \geq 0$ I $P_l^{-m}(x) = (-1)^m\frac{(l-m)!}{(l+m)!}P_l^m(x)$ I Legendre polynomials $P_l(x) = \frac{1}{2^l l!}(\frac{d}{dx})^2(x^2-1)^l$ I Quantization of angular momentum: 1) $Y_{lm}(\theta,\phi)$ must be well-behaved at $\theta = 0$ and π:l quantization 2) Periodic in ϕ angle: m quantization. 3) l is call the azimuthal quantum number, m is called the magnetic quantum number **The first few spherical harmonics $Y_l^m(\theta,\phi)$** $Y_0^0 = (\frac{1}{4\pi})^{1/2}$ I $Y_1^0 = (\frac{3}{4\pi})^{1/2}\cos\theta$ I $Y_1^{\pm1} = \mp(\frac{3}{8\pi})^{1/2}\sin\theta e^{\pm i\phi}$ I $Y_2^0 = (\frac{5}{16\pi})^{1/2}(3\cos^2\theta - 1)$ I $Y_2^{\pm1} = \mp(\frac{15}{16\pi})^{1/2}\sin\theta\cos\theta e^{\pm i\phi}$ I Spherical harmonics $Y_{l,m}(\theta,\phi)$ form an orthonormal and compete basis: $\left\langle Y_{l',m'}\middle|Y_{l,m}\right\rangle = \int_0^{\pi}\sin\theta d\theta\int_0^{2\pi}d\phi Y_{l',m'}^*(\theta\phi)Y_{l,m}(\theta\phi) = \delta_{l,l'}\delta_{m,m'} = \langle l'm'|lm\rangle$ **Parity of spherical harmonics** $\hat{P}Y_{l,m}(\theta,\phi) = Y_{l,m}(\pi-\theta,\pi_\phi) = (-1)^l Y_{l,m}(\theta,\phi)$ This can be seen as follows: The associated Legendre polynomials gives $(-1)^{l+m}$ and from the exponential function we have $(-1)^m$, giving together for the spherical harmonics a parity of $(-1)^l$ I Spherical harmonics $Y_{l,m}(\theta,\phi) = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\phi}$ for $m \geq 0$ I For negative orders of m $Y_{l,-m}(\theta,\phi) = (-1)^m Y_{l,m}^*(\theta,\phi)$ Associated Legendre polynomials $P_l^m(x) = (-1)^m(1-x^2)^{m/2}(\frac{d}{dx})^m P_l(x)$ for $m \geq 0$, $P_l^{-m}(x) = (-1)^m\frac{(l-m)!}{(l+m)!}P_l^m(x)$ I Legendre polynomials $P_l(x) = \frac{1}{2^l l!}(\frac{d}{dx})^l(x^2-1)^l$ I This means that the Y_{lm} is also an eigenstate of parity (+1 or -1) I Spherical harmonics $Y_{l,m}(\theta,\phi)$ are simultaneous eigenfunctions of $\hat{L}^2$,$\hat{L}_z$, and $\hat{P}$ operators (They are a commuting set) **Eigenstates of angular momentum by algebra method** Simultaneous eigenvalue problem: $\hat{L}^2|Y\rangle = \lambda|Y\rangle$ I $\hat{L}_Z|Y\rangle = \mu|Y\rangle$ Given $\hat{L}^2$ and $\hat{L}_z$, we want to find eigenvalues λ, μ, and eigenstates $|Y\rangle$ I We want to obtain the same result by operator algebra, similar to what we did with the harmonic oscillator. We will work in Cartesian coordinate space, which means x,y, and z components. **Angular momentum by operator algebra** $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$ I Inverse $\hat{L}_x = \frac{1}{2}(\hat{L}_+ + \hat{L}_-)$ and $\hat{L}_y = \frac{1}{2i}(\hat{L}_+ - \hat{L}_-)$ I Following relations should hold (proved in hw) I $\left[\hat{L}_\pm, \hat{L}^2\right] = 0$ I $\left[\hat{L}_z, \hat{L}_\pm\right] = \pm\hbar\hat{L}_\pm$ I $\left[\hat{L}_+, \hat{L}_-\right] = 2\hbar\hat{L}_z$ I $\hat{L}_+\hat{L}_- = \hat{L}^2 - \hat{L}_z^2 + \hbar\hat{L}_z$ I $\hat{L}_-\hat{L}_+ = \hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z$

Eigenstates of angular momentum by operator algebra Simultaneous eigenvalue problem $\hat{L}^2|Y\rangle = \lambda|Y\rangle$ and $\hat{L}_z|Y\rangle = \mu|Y\rangle$ I and Given $\hat{L}^2$ and $\hat{L}_z$ we want to find the eigenvalues λ, μ, and eigenstate $|Y\rangle$ I **Step 1)** If $|Y\rangle$ is and eigenfunction of $\hat{L}^2$ so is $\hat{L}_\pm|Y\rangle$ with the same eigenvalue: $\hat{L}^2(\hat{L}_\pm|Y\rangle) = \hat{L}_\pm\hat{L}^2|L\rangle = \lambda(\hat{L}_\pm|Y\rangle)$ I **step 2)** $\hat{L}_z(\hat{L}_\pm|Y\rangle) = (\hat{L}_\pm\hat{L}_z \pm \hbar\hat{L}_\pm)|Y\rangle = \hat{L}_\pm\mu|Y\rangle \pm \hbar\hat{L}_\pm|Y\rangle = (\mu\pm\hbar)(\hat{L}_\pm|Y\rangle)$ so $\hat{L}_\pm|Y\rangle$ is eigenfunction of $\hat{L}_z$ with eigenvalues raised an lowered by one unit of $\hbar$ I **Step 3)** There must be a a top rung on the ladder $|Y_{max}\rangle$ because the z-component $\hat{L}_z$ cannot exceed the total. Let's call the corresponding eigenvalue $\mu_{max} = \hbar l$ It canot be raised anymore: $\hat{L}_+|Y_{max}\rangle = 0$. $\hat{L}^2|Y_{max}\rangle = (\hat{L_-}\hat{L_+} + \hat{L}_z^2 + \hbar\hat{L}_z)|Y_{max}\rangle = (0 + \hbar^2 l^2 + \hbar^2 l)|Y_{max}\rangle = \hbar^2 l(l+1)|Y_{max}\rangle$ I So the eigenvalue of $\hat{L}^2$ at the top rung is $\lambda = \hbar^2 l(l+1)$ I **Step 4)** By the same, reason, there must be a bottom rung on the latter $|Y_{min}\rangle$. Lets call the corresponding eigenvalue $\mu_{min} = \hbar\bar{l}$. It cannot be lowered anymore: $\hat{L}_-|Y_{min}\rangle = 0$ I $\hat{L}^2|Y_{min}\rangle = (\hat{L}_x\hat{L}_- + \hat{L}_z^2 - \hbar\hat{L}_z)|Y_{min}\rangle = (0 + \hbar^2\bar{l}^2 - \hbar^2\bar{l})|Y_{min}\rangle = \hbar^2\bar{l}(\bar{l}+1)|Y_{min}\rangle$ So the eigenvalues of $\hat{L}^2$ at the bottom run is $\lambda = \hbar^2\bar{l}(\bar{L}+1)$ I **Step 5)** Eigenvalue of $\hat{L}^2$ is the same everywhere on the ladder(It's a ladder for $\hat{L}_z$ at each l) From $l(l+1) = \bar{l}(\bar{l}+1)$, we get $\bar{l} = -l$ (The other root $\hat{l} = l+1$ is unphysical) If we call $m\hbar$ the eigenvalue of $\hat{L}_z$, then m goes from $-l$ to $+l$ in N integer steps, or $l = -l + N$, hence $l = N/2$. So l must be an integer or half integer. This is how we arrive at the quantization of angular momentum I **Therefor** $\hat{L}^2|Y_{lm}\rangle = l(l+1)\hbar^2|Y_{lm}\rangle$ I $\hat{L}_z|Y_{lm}\rangle = m\hbar|Y_{lm}\rangle$ I where $l = 0, \frac{1}{2}, 1, \ldots$ and $m = -l, -l+1, \ldots, l-1, l$ for each l I Also $\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z$ I $\left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x$ I $\left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y$ We obtained the eigenvalues purely by operator algebra, integer, values are allowed and so are half integer values, which can be used to describe particle spin. The only assumption used is the commutation relation on the three components **What about eigenfunctions of angular momentum** For angular momentum must know $\hat{L}_x = \frac{\hbar}{i}(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi})$ I $\hat{L}_y = \frac{\hbar}{i}(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi})$ I $\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$ I $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y = \pm\frac{\hbar}{i}e^{\pm i\phi}(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi})$ I **Step 1)** The condition at the top rung $\hat{L}_+|Yll\rangle = 0$ can be cast into the following differential equation in spherical coordinates: $\hat{L}_+Y_{ll}(\theta,\phi) = 0$, where $Y_{ll}(\theta,\phi) = \Theta_{ll}(\theta)e^{il\phi}$ is separable in θ and ϕ I **Step 2)** Using $\hat{L}_+$ in spherical coordinates, we obtain $0 = \frac{\hbar}{i}e^{i\phi}(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi})(\Theta_{ll}(\theta)e^{il\phi})$ Or $0 = (\frac{\partial}{\partial\theta} - l\cot\theta)\Theta_{ll}(\theta)$, which can be integrated to give $\Theta_{ll}(\theta) = sin^l\theta$ I **Step 3)** Starting form $Y_{ll}(\theta,\phi) = (\sin^l\theta)e^{il\phi}$, all other $Y_{lm}(\theta,\phi)$ can be obtained by repeatedly applying the lowering operator $\hat{L}_-$ The only thing to watch for is normalization I $Y_{l,m}(\theta,\phi) = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\phi}$ I $Y_{l,-m}(\theta,\phi) = (-1)^m Y_{l,m}^*(\theta,\phi)$ I Associated Legendre polynomials $P_l^m(x) = (-1)^m(1-x^2)^{m/2}(\frac{d}{dx})^m P_l(x)$ for $m > 0$ I and $P_l^{-m}(x) = (-1)^m\frac{(l-m)!}{(l-m)!}P_l^m(x)$ I Legendre polynomials $P_l(x) = \frac{1}{2^l l!}(\frac{d}{dx})^l(x^2-1)^l$

Semi-classical representations of angular momentum $L = \sqrt{l(l+1)\hbar}$ for $l = 0,1,2,\ldots$ and $L_z = h\hbar$ for $m = 0,\pm1,\pm2,\ldots,\pm1$ The smallest angle with the z axis corresponds to the maximum projection $L_z = l\hbar$ I $\cos\theta = \frac{|L_z|}{L} = \frac{l}{\sqrt{l(l+1)}} = \frac{l}{\sqrt{(l+1/1}} < 1$ for $l \neq 0$ So it can never point to the z-axis **Spin** Starting from the trio of fundamental commutation relations: $\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z$, $\left[\hat{S}_y, \hat{S}_z\right] = i\hbar\hat{S}_x$, $\left[\hat{S}_z, \hat{S}_x\right] = i\hbar\hat{S}_y$ a carbon copy of the theorem was derived for $\hat{L}$ can be used to describe an important property every particle processes: its spin angular momentum (denoted by $\hat{S}$) $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$ $\hat{S}_\pm|sm\rangle = \hbar\sqrt{s(s+1) - m(m\pm1)|sm\pm1\rangle}$ I **Therefor** $\hat{S}^2|sm\rangle = s(s+1)\hbar^2|sm\rangle$ I $\hat{S}_z|sm\rangle = m\hbar|sm\rangle$ I where $s = 0, \frac{1}{2}, 1, \ldots$ and $m = -s, -s+1, \ldots, s-1, s$ for each s I On quantum mechanics, S is fundamentally differs from L -L is called the orbital angualr momentum, such as the motion of the elctron around the nucealus; can be described by spherical harmonics $Y_{lm}(r,\theta,\phi)$ I S is the insrinsic propert of a particle, which has nothing to do with motion in space; therefore cannot be described by functions of position like $Y_{lm}(r,\theta,\phi)$ I A particle can have both intrinsic S and extrinsic L angular momentum I In classical mechanics, we also have the concepts of orbital angular momentum, like the earth orbiting around the sun, and spin angular momentum, like the earth spinning around its own axis. But the distinction is superficial: the spin angular momentum is nothing but the sum all orbital angular momentum of individual rocks making up the earth I In quantum mechanics, most particles are point-like, with no spatial structure. I Elementary particle in nature can be divided into two categories according to their spin angular momentum: I Those with integer spin are called Bosons, like the photon, pion, graviton, Higgs boson I Those with half-integer spin are called Fermions, like the electron, proton, and neutron **Spin 1/2** Spin-1/2 has fixed eigenvalues $s(s+1)\hbar^2 = \frac{1}{2}(1+\frac{1}{2})\hbar^2 = \frac{3}{4}\hbar^2$ and $m\hbar = -\frac{\hbar}{2}, \frac{\hbar}{2}$ I We need to find a representation for the eigenstate of spin 1/2, the simplest non-trivial spin I Since s = 1/2, we only have two eigenstates, $m = -1/2$ and $+1/2$ I We call $\left|\frac{1}{2}\frac{1}{2}\right\rangle$ spin-up (or ↑) and $|sm\rangle = \left|\frac{1}{2} - \frac{1}{2}\right\rangle$ spin-down or(↓) I We can use a two-component column matrix (called a spinor) to represent the two eigenstates: $\chi_x\begin{pmatrix}1\\0\end{pmatrix}$ and $\chi_-\begin{pmatrix}0\\1\end{pmatrix}$ They are normalized and orthogonal I **Normalization:** $\left\langle\chi_+\middle|\chi_+\right\rangle = (\chi_+)^\dagger\chi_+ = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 1$ I $\left\langle\chi_-\middle|\chi_-\right\rangle = (\chi_-)^\dagger\chi_+ = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 1$ I **Orthogonality:** $\left\langle\chi_+\middle|\chi_+\right\rangle = (\chi_+)^\dagger\chi_+ = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 0$ I $\left\langle\chi_-\middle|\chi_-\right\rangle = (\chi_-)^\dagger\chi_+ = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 0$ I Since the eigenstates are represented by two-component column , the spin operators $\hat{S}^2$ and $\hat{S}_x$,$\hat{S}_y$,$\hat{S}_z$ must be represented by 2×2 matrices I Assume $\hat{S}^2 = \begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}$ with a_{ij} to be determined I From $\hat{S}^2\chi_+ = \frac{3}{4}\hbar^2\chi_+$ or $\begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix}1\\0\end{pmatrix}$, we get $\begin{pmatrix}a_{11}\\ a_{21}\end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix}1\\0\end{pmatrix}$, or $a_{11} = \frac{3}{4}\hbar^2$, $a_{21} = 0$ I From $\hat{S}^2\chi_- = \frac{3}{4}\hbar^2\chi_-$ or $\begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix}0\\1\end{pmatrix}$, we get $\begin{pmatrix}a_{12}\\ a_{22}\end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix}0\\1\end{pmatrix}$, or $a_{12} = 0$, $a_{22} = \frac{3}{4}\hbar^2$ I **Therefore** $\hat{S}^2 = \frac{3}{4}\hbar^2\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \frac{3}{4}\hbar^2 I$ I Similarly, assume $\hat{S}_z = \begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}$ with a_{ij} to be determined I From $\hat{S}_z\chi_+ = \frac{\hbar}{2}\chi_+$ or $\begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}1\\0\end{pmatrix}$, we get $\begin{pmatrix}a_{11}\\ a_{21}\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}1\\0\end{pmatrix}$, or $a_{11} = \frac{\hbar}{w}$, $a_{21} = 0$ I From $\hat{S}_z\chi_- = -\frac{\hbar}{2}\chi_-$ or $\begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix}0\\1\end{pmatrix}$, we get $\begin{pmatrix}a_{12}\\ a_{22}\end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix}0\\1\end{pmatrix}$, or $a_{12} = 0$, $a_{22} = -\frac{\hbar}{2}$ I **Therefore** $\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ I $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$ I $\hat{S}_\pm|sm\rangle = \hbar\sqrt{s(s+1) - m(m\pm1)|sm\pm1\rangle}$ I **More spin 1/2** I Similarly, assume $\hat{S}_+ = \begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}$ with a_{ij} to be determined I From $\hat{S}_+\chi_- = \hbar\chi_+$ or $\begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \hbar\begin{pmatrix}1\\0\end{pmatrix}$, we get $\begin{pmatrix}a_{12}\\ a_{22}\end{pmatrix} = \hbar\begin{pmatrix}1\\0\end{pmatrix}$, or $a_{12} = \hbar$, $a_{22} = 0$ I From $\hat{S}_+\chi_+ = 0$ or $\begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \hbar\begin{pmatrix}0\\0\end{pmatrix}$, we get $\begin{pmatrix}a_{11}\\ a_{21}\end{pmatrix} = \hbar\begin{pmatrix}0\\0\end{pmatrix}$, or $a_{11} = 0$, $a_{21} = 0$ So $\hat{S}_+ = \hbar\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}$ I Similarly, assume $\hat{S}_0- = \begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}$ with a_{ij} to be determined I From $\hat{S}_-\chi_+ = \hbar\chi_+$ or $\begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \hbar\begin{pmatrix}0\\1\end{pmatrix}$, we get $\begin{pmatrix}a_{11}\\ a_{21}\end{pmatrix} = \hbar\begin{pmatrix}0\\1\end{pmatrix}$, or $a_{11} = 0$, $a_{21} = \hbar$ I From $\hat{S}_-\chi_- = 0$ or $\begin{pmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \hbar\begin{pmatrix}0\\0\end{pmatrix}$, we get $\begin{pmatrix}a_{12}\\ a_{22}\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix}$, or $a_{12} = 0$, $a_{22} = 0$ So $\hat{S}_- = \hbar\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}$ I **In conclusion** $\hat{S}_x = \frac{1}{2}(\hat{S}_x + \hat{S}_-) = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$ I $\hat{S}_y = \frac{1}{2i}(\hat{S}_+ - \hat{S}_-) = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$ I Sometimes they are written in terms of Pauli matrices $\hat{S} = \frac{\hbar}{2}\vec{\sigma}$ I $\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$ I $\sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$ I $\sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ I A general spin -1/2 state $\chi = \begin{pmatrix}a\\b\end{pmatrix}$ can be expanded as a linear combination of the two eigenstates: $\chi = a\begin{pmatrix}1\\0\end{pmatrix} + b\begin{pmatrix}0\\1\end{pmatrix} = a\chi_= + b\chi_-$ I The normalization condition $\langle\chi|\chi\rangle = 1$ means $|a|^2 + |b|^2 = 1$ I Then $|a|^2$ is interpreted as the probability of getting spin-up $|b|^2$ spin-down, if the spin of the particle is measured I Since χ_x and χ_- are eigenstates of $\hat{S}_z$, $|a|^2$ and $|b|^2$ are also the probabilities of getting $\frac{+\hbar}{2}$ and $\frac{-\hbar}{2}$ respectively, if $\hat{S}_z$ is measured I Expectation values are calculated by $\left\langle\hat{O}\right\rangle = \langle\chi|\hat{O}|\chi\rangle = \chi^\dagger\hat{O}\chi$ as matrix linear algebra operations.

Spin 1 The methodology is exactly the same, except we are dealing with 3×3 linear albebra I Spin 1 has fixed eigenvalues $s(s+1)\hbar^2 = 2\hbar^2$ for $\hat{S}^2$ and $m\hbar = -\hbar, 0, \hbar$ for $\vec{S_z}$ I $\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z$ I $\left[\hat{S}_y, \hat{S}_z\right] = i\hbar\hat{S}_x$ I $\left[\hat{S}_z, \hat{S}_x\right] = i\hbar\hat{S}_y$ are found to be: I $\hat{S}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}$ I $\hat{S}_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0\end{pmatrix}$ I $\hat{S}_y = \hbar\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}$ I Eigenstates $\hat{S}_z$ (orthonormal): $\chi_1 = \begin{pmatrix}1\\0\\0\end{pmatrix}$ for $\hbar$ I $\chi_0 = \begin{pmatrix}0\\1\\0\end{pmatrix}$ for 0 I $\chi_{-1} = \begin{pmatrix}0\\0\\1\end{pmatrix}$ for $-\hbar$ I A general spin 1 state: $\chi = \begin{pmatrix}a\\b\\c\end{pmatrix} = a\chi_1 + b\chi_0 + c\chi_{-1}$ I Normalization: $|a|^2 + |b|^2 + |c|^2 = 1$ **Addition of angular momenta** In classical physics, the addition of angular momenta is like any addition of two vector $\vec{J} = \vec{J_1} + \vec{J_2}$ I The maxmum magnitude of the sum is when the two are parallel, the minimum when anti-parallel. All values in between are allowed depending on the relative orientation of $\vec{J_1}$ and $\vec{J_2}$ In quantum mechanics, we often need to add two angular momenta. For example, when two electrons are put together, how do their spins add up? Or how does electron's orbital angular momentum couple to its spin? I Generically, the total angular momentum is the sum of two vector operators $\hat{\vec{J}} = \hat{\vec{J_1}} + \hat{\vec{J_2}}$ Two complications arise in quantum mechanics **1)** Angular momentum is quantized **2)** The components of an angular momentum do not commute with each other The operators $\hat{J}_1^2$, $\hat{J}_{1Z}$, $\hat{J}_2^2$, $\hat{J}_{2Z}$ form a commuting set so they have simultaneous eigenstates that are simply the product of the individual states $|j_1m_1\rangle|j_2m_2\rangle$ or $|j_1m_1j_2m_2\rangle$ I They are called the composite basis of "uncoupled basis" satisfying I $\hat{J}_1^2 = |j_1m_1\rangle|j_2m_2\rangle = j_1(j_1+1)\hbar^2|j_1m_1\rangle|j_2m_2\rangle$ I $\hat{J}_{1Z}|j_1m_1\rangle|j_2m_2\rangle = m_1\hbar|j_1m_1\rangle|j_2m_2\rangle$ I $\hat{J}_2^2|j_1m_1\rangle|j_2m_2\rangle = j_2(j_2+1)\hbar^2|j_1m_1\rangle|j_2m_2\rangle$ I $\hat{J}_{2Z}|j_1m_1\rangle|j_2m_2\rangle = m_2\hbar|j_1m_1\rangle|j_2m_2\rangle$ I For the total angular momentum, the operators $\hat{J}_1^2$, $\hat{J}_{1Z}$, $\hat{J}_2^2$, $\hat{J}_{2Z}$ form a commuting set so they have simultaneous eigenstates. They from the so-called "coupled basis" denoted by $|JMj_1j_2\rangle$ or simply $|JM\rangle$ satisfying I $\hat{J}^2|JM\rangle = J(J+1)\hbar^2|JM\rangle$ and $\hat{J}_z|JM\rangle = M\hbar|JM\rangle$ I The problem of angular momentum addition boils down to: Given the uncoupled basis $|j_1m_1\rangle|j_2m_2\rangle$ how to find the coupled basis $|JM\rangle$ (both eigenvalues and eigenstate) **Rules for eigenvalues addition:** J can take values from $|j_1 - j_2|$ to $j_1 + j_2$n in steps of 1. For each J value, M can take values from $-J$ to J in steps of 1. **Rules for eigenvalues addition:** The coupled state is a linear combination of the uncoupled states: $|JM\rangle = \sum_{m1=-j_1}^{j_1}\sum_{m2=-j_2}^{j_2}C_{m_1m_2M}^{j_1j_2J}|j_1m_1\rangle|j_2m_2\rangle$ (non-zero only for $m_1 + m_2 = M$) I Where $C_{m_1m_2M}^{j_1j_2J}$ are called Clebsch- Gordan coefficients **Coupling of angular momenta** How to compute the coupling between $\hat{J}_1$ and $\hat{J}_2$ defined $\hat{J}_1\cdot\hat{J}_2$ in the coupled basis $|JMj_1j_2\rangle$ (or simply $|JM\rangle$) $\hat{J}^2 = (\hat{J}_1 + \hat{J}_2)^2 = \hat{J}_1^2 + 2\hat{J}_1\cdot\hat{J}_2^2$ So $\hat{J}_1\cdot\hat{J}_2 = \frac{1}{2}(\hat{J}^2 - \hat{J}_1^2 - \hat{J}_2^2) = \frac{\hbar^2}{2}[J(J+1) - j_1(j_1+1) - j_2(j_2+1)]$ I Example: what is the coupling between two spin 1/2's I For $j_1 = 1/2$ and $j_2 = 1/2$ the total spin $J = 0, 1$ I $\hat{J}_1\cdot\hat{J}_2 = \frac{\hbar^2}{2}[J(J+1) - j_1(j_1+1) - j_2(j_2+1)] = \frac{\hbar^2}{2}[J(J+1) - \frac{3}{4} - \frac{3}{4}] = \frac{\hbar^2}{2}[J(J+1) - \frac{3}{4} - \frac{3}{4}] = \hbar^2/4$ for $J = 1$, $-3\hbar^2/4$ for $J = 0$ **Example: adding the spins of two electrons** In general, the total number of states from adding j_1 and j_2 is $(2j_1+1)(2j_2+1)$ I We have $j_1 = 1/2$ and $j_2 = 1/2$ So $J = 0, 1$ From $J = 0, M = 0$ for $J = 1, M = -1, 0, 1$ So there are $4\,|JM\rangle$ states in total. The $|JM\rangle$ states can be found from tables of Clebsch-Gordan coefficients I $|JM\rangle = \sum_{m_1=-j_1}^{j_1}\sum_{m_2=-j_2}^{j_2}C_{m_1m_2M}^{j_1j_2J}|j_1m_1\rangle|j_2m_2\rangle$ (non-zero only for $m_1 + m_2 = M$) I (handwritten)

Final **Chap 17 The Hydrogen atom** Proton carries 1 unit of positive charge, has sping 1/2 and mass1.67×10^{-27} kg or 938 MeV Electron carries 1 unit of negative charge, has spin 1/2 and mass of 9.11×10^{-31} kg **Two-body probem** $\hat{H} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} = V(\hat{r}_1 - \hat{r}_2)$ I changing to center of mass and relative coordinates $\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1+m_2}$ and $\vec{r} = \vec{r}_1 - \vec{r}_2$ I $\hat{\vec{p}}_1 = frac m_1 M\hat{\vec{P}} + \hat{\vec{p}}$ and $\hat{\vec{p}}_2 = frac m_2 M\hat{\vec{P}} + \hat{\vec{p}}$ where $M = m_1 + m_2$ I leads to transformed $\hat{H} = \frac{\hat{P}^2}{2M} + \frac{\hat{p}^2}{2\mu} + V(\vec{r})$ I where $\mu = \frac{m_1+m_2}{m_1+m_2}$ is called the reduced mass two-body problem is separable into center-of-mass motion plus one-body relative motion. **Schrodiner equation** the coulomb potential between the

proton $V(r) = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$ Since the potential is spherically symmetric $V(r)$, the Time Independent Schrodinger Equation $(-\frac{\hbar^2}{2\mu}\Delta^2 + V(\vec{r}))\psi(\vec{r}) = E\psi(\vec{r})$ I spherical coordinates $\psi(r,\theta,\psi) = R(r)Y_{lm}(\theta,\phi)$ I kinetic energy term separable into radial and rotational parts $\hat{T} = -\frac{\hbar^2}{2\mu}\Delta^2 = \hat{T}_r + \frac{\hat{L}^2}{s\mu r^2}$ where $\hat{T}_r = -\frac{\hbar^2}{2\mu}(\frac{\partial}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r})$ I Using the eigenfunction of angular momentum $\hat{L}t^2Y_{lm}(\theta,\phi) = l(l+1)\hbar^2Y_{lm}(\theta,\phi)$ I obtain the radial equation $[\hat{T}_r + \frac{\hat{L}^2}{2\mu r^2} + V(r)]R(r)Y_{lm}(\theta,\phi) = ER(r)Y_{lm}(\theta,\phi)$ I or $[-\frac{\hbar^2}{2\mu}(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr}) + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)]R(r) = ER(r)$ **solving radial equation** $[-\frac{\hbar^2}{2\mu}(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr}) + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)]R(r) = ER(r)$ for $V(r) = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$ I **step 1)**Change to dimensionless variables $\rho = r\sqrt{\frac{8\mu|E|}{\hbar^2}}$ and $\sigma = \alpha\sqrt{\frac{\mu c^2}{2|E|}}$ where $\alpha = \frac{1}{4\pi\epsilon_0}\frac{e^2}{\hbar c} \approx \frac{1}{137}$ is the fine structure constant I $\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + (\frac{\sigma}{\rho} - \frac{l(l+1)}{\rho^2} - \frac{1}{4})R = 0$ I **step 2)**For large ρ: $\frac{d^2R}{d\rho^2} - \frac{R}{4} = 0$ which leads to $R \to e^{-\rho/2}$ For small ρ: $\frac{d^2R}{d\rho^2} - \frac{l(l+1)}{\rho^2}R = 0$ which leads to $R \to \rho^l$ I It suggests a solution of the form $R(\rho) = G(\rho)\rho^l e^{-\rho/2}$ leading to differential equation for G: $\frac{d^2G}{d\rho^2} + (\frac{2l+2}{\rho} - 1)\frac{dG}{d\rho} + (\frac{\sigma}{\rho} - \frac{l(l+1)}{\rho^2} - \frac{1}{4})G = 0$ **step 3)** A standard power series solution $G = \sum_{s=0}^{\infty} a_s\rho^s$ yields the recursion relation on the coefficients: $\frac{a_{s+1}}{a_s} = \frac{s-(\sigma-l-1)}{(s+1)(s+2l+1)} \to \frac{1}{s}$ for large s. I It means that $G(\rho) \to e^\rho$ which leads to $R \to e^\rho\rho^l e^{-\rho/2} \to \infty$ for the large ρ I **Step 4)** The series must terminate (to become a polynomial) in order for R to be well-behaved($R \to 0$) at large ρ It happens at some maximum power $s_{max} = \sigma - l - 1$ which counts the number of radial nodes in $G(\rho)$, often denoted by n_r (called radial quantum number) I **Step 5)** The condition $n_r = \sigma - l - 1$ yields the quantization of energy $\sigma = n$ where $n = n_r + l + 1$ is called principal quantum number ($n \geq l+1$) Converting back to physical units from $\sigma = \alpha\sqrt{\mu c^2/(2|E|)}$ $E_n = -\frac{\mu c^2\alpha^2}{2n^2}$ therefore $n = 1, 2, 3, \ldots$ If we approximate $\mu \approx m_e$ then $E_n = -\frac{13.6}{n^2}$ eV $n = 1, 2, 3, \ldots$ **radial wavefunction** We can rewrite ρ as $\rho = \frac{2r}{na_0}$ where $a_0 = \frac{\hbar}{\mu c\alpha} \approx 0.529\mathring{A}$ is the Bohr radius I The normalized radial wavefunction in terms of r is $R_{nl}(r) = \sqrt{(\frac{2}{na_0})^3\frac{(n-l-1)!}{2n[(n+l)!]^3}}(\frac{2r}{na_0})^l L^{2l+1}_{n-l-1}(\frac{2r}{na_0})e^{\frac{-r}{na_0}}$ I where $L^{2l+1}_{n-l-1}(\rho)$ is the associated Laguerre polynomial They form a orthonormal basis: $\langle R_{nl}|R_{n'l'}\rangle = \int_0^\infty r^2R^*_{nl}(r)R_{n'l'}(r)dr = \delta_{nn'}\delta_{ll'}$ **notations** wave function depends on 3 quantum numbers n: principal l: angular momentum m: magnetic Restriction on quantum numbers $n = 1, 2, 3, \ldots$ (quantized energy levels) $l = 0, 1, 2, \ldots, n-1$(angular momentum constrained by total energy) $m = 0, \pm1, \ldots, \pm l$ **energy levels** Degeneracy for fixed n: $\sum_{l=0}^{n-1}(2l+1) = n^2$ Double if electron spin is included **transitions** Jumping between two energy levels emits or absorbs photons: $|E - f - E_i| = h\nu = \hbar\omega$ I $R\left|\frac{1}{n_f^2} - \frac{1}{n_i^2}\right| = \frac{1}{\lambda}$ I $R = 1.097 \times 10^7\,\mathrm{m}^{-1}$ is Rydberg constant I Selection rules: Angular momentum conservation dictates that only certain transitions are allowed leading to conditions for Δn = anything, $\Delta l = \pm1$, and $\Delta m = 0, \pm1$, angular momentum of photon = $\pm\hbar$ **where is the electron** the total probability of finding the electron within a small colume dV of position (r,θ,ϕ) is given by $P = |\psi_{nlm}(r,\theta,\phi)|^2dV = P_rP^\theta$ I Volume element: $dV = r^2drd\theta$ Angular element: $d\theta = \sin\theta d\theta d\phi$ I Radial Probability $P_r = |R_{nl}(r)|^2r^2dr$ I Angular Probability $P_\omega = |Y_{lm}(\theta,\phi)|^2d\theta$ I $\langle\psi_{nlm}|\psi_{nlm}\rangle = 1 = (\int_0^\infty|R_{nl}(r)|^2r^2dr)(\int_0^\pi\sin\theta d\theta\int_0^{2\pi}d\phi|Y_{lm}(\theta,\phi)|^2)$ **ground state** $n = 1, l = 0, m = 0$ wavefunction spherically symmetric $E_1 = -13.6$ eV I $\psi_{100}(\vec{r}) = R_{10}(r)Y_{00}(\theta,\phi)$ I $R_{10}(r) = \frac{2}{(a_0)^{3/2}}e^{-r/a_0}$ I $Y_{00}(\theta,\phi) = \frac{1}{\sqrt{4\pi}}$ **combined wavefunction of space and spin** when electron spin is included, a general wavefunction could be written as an expansion in spatial eigenstates and spin eigenstates: $\psi(\vec{r},\chi) = \sum_{nlm}(a^+_n\psi_{nlm}(r,\theta,\phi)\chi_+ + a^-_n\psi_{nlm}(r,\theta,\phi)\chi_-)$ I Then $\left|a^+_n\right|^2$ is the probability of getting spin-up and other eigenvalues ($\hat{H}$, $\hat{L}^2$, $\hat{L}_z$, $\hat{P}$), and $\left|a^-_n\right|^2$ spin-up and others **Hydrogen-like systems** All the result for the hydrogen atom can be transmuted to describe a system with an "electron" of charge $-Z_1e$ and mass m_1 bound to a proton of charge Z_2e and mass m_2 Specifically **1** Replace e^2 by $Z_1Z_2e^2$ everywhere. Recall potential $V(r) = -\frac{1}{4\pi\epsilon_0}\frac{Z_1Z_2e^2}{r}$ **2** New reduced mass: $\mu = \frac{m_1m_2}{m_1+m_2}$ I Energy $E_n = -\frac{\mu c^2(Z_1Z_2)^2\alpha^2}{2n^2}$, $n = 1, 2, 3, \ldots$ I where $\alpha = \frac{1}{4\pi\epsilon_0}\frac{e^2}{\hbar c} \approx \frac{1}{137}$ I Bohr radius $a_0 = \frac{\hbar}{\mu cZ_1Z_2\alpha}$ **in a magnetic field** electron has two kinds of magnetic moment Orbital $\vec{\mu}_L = -g_l\frac{e}{2m}\vec{L}$ where $g_L = 1$ I Spin $\vec{\mu}_s = -g_s\frac{e}{2m}\vec{S}$ where $g_s \approx 2$ **Identical particles** **Two-particle system** The hamiltonian operator for the whole system $\hat{H} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + V(x_1,x_2,t) = -\frac{\hbar^2}{2m_1}\frac{\partial^2}{dx_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{dx_2^2} + V(x_1,x_2,t)$ I The time-dependent schrodinger equation (TDSE) $\hat{H}\psi(x_1,x_2,t) = i\hbar\frac{\partial\psi(x_1,x_2,t)}{\partial t}$ is a hard problem to solve I If the potential is independnet of time $V(x_1,x_2)$ then we have the usual soultion states $\psi(x_1,x_2,t) = \psi(x_1,x_2)e^{iEt/\hbar}$ I where we only need to solve the Time Independent Schrodinger equation (an eigenvalue problem): $\hat{H}\psi(x_1,x_2) = E\psi(x_1,x_2)$ This is progress but still hard to solve. If the potential is separable $V(x_1,x_2) = V_a(x_1) + V_b(x_2)$ meaning there is no interaction between the two particles $V(x_1-x_2)$, just interaction with outside potentials, the the total wavefunction of the system is simply the product of individual ones: $psi(x_1,x_2) = \psi_a(x_1)\psi_b(x_2)$ then the total energy is simply the sum: $E = E_1 + E_2$ **Example: two non-interacting particles in the standard infinite well** $(-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2})\psi(x_1,x_2) = E\psi(x_1,x_2)$ I $-\frac{\hbar^2}{2m}\frac{d^2\psi_a(x_1)}{dx_1^2} = E_1\psi_a(x_1)$ and $\psi_{n_1}(x_1) = \sqrt{\frac{2}{L}}\sin\left(\frac{n_1\pi x_1}{L}\right)$ and $E_1 = n_1^2\frac{\pi^2\hbar^2}{2m_1L^2}$ where $n_1 = 1, 2, 3, \ldots$ I $-\frac{\hbar^2}{2m}\frac{d^2\psi_a(x_2)}{dx_1^2} = E_1\psi_a(x_1)$ and $\psi_{n_2}(y) = \sqrt{\frac{2}{L}}\sin\left(\frac{n_2\pi x_2}{L}\right)$ and $E_2 = n_2^2\frac{\pi^2\hbar^2}{2m_2L^2}$ where $n_2 = 1, 2, 3, \ldots$ I Quantized eigen energies: $E_{n_1n_2} = E_1 + E_2 = \frac{n_1^2\pi^2\hbar^2}{2m_1L^2} + \frac{n_2^2\pi^2\hbar^2}{2m_2L^2}$ where $n_1, n_2 = 1, 2, 3, \ldots$ I Orthonormal eigenfunctions: $\psi_{n_1n_2}(x_1,x_2) = \frac{2}{L}\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right)$ I If the two particles have the same mass, than degeneracy emerges. **Identical particles** IN classical physics, not two particles can be truly identical, in the sense that you can always tell them apart in some way, by observing their trajectories, by painting them with colors, and so on. The quantum physics, the situation is fundamentally different: Identical particles are truly identical in the sense you can never tell them apart. Example: there are two electrons in the Helium atom, but you can't tell which one is which. The same is true for the electrons in other atoms. In fact, you can push it to the extreme: all electrons in the universe are identical. The same is true for all photons, and all protons, and so on. This is a fundamental principle of quantum mechanics: called the indistinguishability of identical particles, which has profound consequences. **Identical particles exchange operator** The indistinguishability of identical particles in quantum mechanics can be formalized by the exchange operator, which simply switches two particles in the wavefuncion $\hat{E}_{12}\psi(x_1,x_2) \equiv \psi(x_2,x_1)$ I It can be shown that the exchange operator is Hermitian, commutes with the Hamiltonian of the system, and has eigenvalues +1 or -1 Hermitian proof $\left\langle\hat{E}_{12}\right\rangle^* = [\int_{-\infty}^\infty dx_1\int_{-\infty}^\infty dx_2\psi^*(x_1,x_2)\hat{E_{12}}\psi(x_1,x_2)]^* = \int_{-\infty}^\infty dx_1\int_{-\infty}^\infty dx_2\psi(x_1,x_2)\psi^*(x_2,x_1) = \int_{-\infty}^\infty dx_1\int_{-\infty}^\infty dx_2\psi(x_2,x_1)\psi^*(x_1,x_2)$ (relabeling dummy integration variable) $\int_{-\infty}^\infty dx_1\int_{-\infty}^\infty dx_2\psi^*(x_1,x_2)\hat{E_{12}}\psi^*(x_1,x_2) = \left\langle\hat{E}_{12}\right\rangle^*$ I The Hamiltonian $\hat{H} = -\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} + V(x_1,x_2)$ is invariant under exchange of x_1 and x_2 because $m_1 = m_2$ and $V(x_1,x_2) = V(x_2,x_1)$. So $\left[\hat{E}_{12},\hat{H}\right] = 0$ I Applying the exchange operator twice $\hat{E}^2_{12}\psi(x_1,x_2) = \hat{E}_{12}\psi(x_2,x_1) = \psi(x_1,x_2)$ So $E^2_{12} = 1$ or $E_{12} = \pm1$ **Identical particles: symmetrization requirement** Therefor, the indistinguishability of identical particles in quantum mechanics implies that the total wave function of the system must satisfy the requirement: $\psi(x_1,x_2) = \pm\psi(x_2,x_1)$ Nature accommodates this requirement through two kinds of identical particles: 1) Bosons which take the plus sign, example include photons, pions, muons, Higgs boson, and so on 2) Ferminons which take the minus sign. Examples include electrons, neutrinos, protons and neutrons, and so on. I In other words, the total wavefunction of identical bosons must be symmetric under exchange of any two of them; the total wavefunction of identical fermions must be anti-symmetric under exchange of any two of them. I 1)The symmetrization requirement applies to all identical particles of the same species in nature. 2) The total wavefunction includes both position-space wavefunction and spin-space wavefunction: $\psi_{total}(1,2) = \psi_{position}(x_1,x_2)\chi_{spin}(1,2)$ **Example: two non-interacting particles in the standard 1D infinite well** Quantized eigenenergies: $E_{n_1n_2} = E_1 + E_2 = (n_1^2 + n_2^2)\frac{\pi^2\hbar^2}{2mL^2}$ and $n_1, n_2 = 1, 2, 3, \ldots$ I Orthonormal eigenfunctions: $\psi_{n_1n_2}(x_1,x_2) = u_{n_1}(x_1)u_{n_2}(x_2) = \frac{2}{L}\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right)$ If the two identical particles are distinguishable, The first energy level is non-degenerate: $E_{11} = 2E_0$ and $\psi_{11}(x_1,x_2) = u_1(x_1)u_1(x_2)$ I The 2nd level is double-degenerate: $E_{12} = E_{21} = 5E_0$ I $\psi_{12}(x_1,x_2) = u_1(x_1)u_2(x_2)$ and $\psi_{21}(x_1,x_2) = u_2(x_1)u_1(x_2)$ I If the two identical particles are indistinguishable bosons, the first level is unchanged because it's already symmetric I $\psi^{(boson)}_{2nd}(x_1,x_2) = \frac{1}{\sqrt{2}}[u_1(x_1)u_2(x_2) + u_2(x_1)u_1(x_2)]$ (symmetric) I We see that the symmetrization requirement removed the degeneracy. I If the two identical particles are indistinguishable fermions, the first energy level has quantum numbers (1,2) or (2,1) because (1,1) is symmetric (we need anti-symmetric for fermions) I So the first level has energy $5E_0$ and $\psi^{fermions}_{1st}(x_1,x_2) = \frac{1}{\sqrt{2}}[u_1(x_1)u_2(x_2) - u_2(x_1)u_1(x_2)]$ (anti-symmetric) I The 2nd energy level comes in at (1,3) or (3,1), not (2,2) since it's symmetric, has energy $10E_0$ and $\psi^{fermion}_{2nd}(x_1,x_2) = \frac{1}{\sqrt{2}}[u_1(x_1)u_3(x_2) - u_3(x_1)u_1(x_2)]$(anti-symmetric) I We see that if two fermions occupy the same state ($x_1 = x_2$) in this example, than the total wavefunction vanishes. This is the origin of the Pauli exclusion principle (no two fermions can occupy the same quantum state). There's no such restriction for identical bosons. You can have as many bosons as you want to occupy the same quantum state. Example: Bose-Einstein condensate. **Example: what if 3 non-interacting particles in the standard 1D infinite well** Quantized eigenenergies $E_{n_1n_2n_3} = E_1 + E_2 + E_3 = (n_1^2 + n_2^2 + n_3^2)\frac{\pi^2\hbar^2}{2mL^2}$ and $n_1, n_2, n_3 = 1, 2, 3, \ldots$ I Orthonormal eigenfunctions: $\psi_{n_1n_2n_3}(x_1,x_2,x_3) = u_{n_1}(x_1)u_{n_2}(x_2)u_{n_3}(x_3) = \frac{8}{L^3}\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right)\sin\left(\frac{n_3\pi x_3}{L}\right)$ I Let's consider an energy level for which each particle can have one of three different quantum numbers a,b or c. This level is 6-fold degenerate, with energy $(a^2 + b^2 + c^2)E_0$ I If the 3 identical particles are distinguishable, The 6 degenerate states are (a,b,c),(b,c,a),(c,a,b),(a,c,b),(b,a,c),(c,b,a) I If the 3 identical particles have indistinguishable bosons, the total wavefunction must be symmetric under exchange of an two particles. I The normalized and symmetrized total wavefunction can be expressed in **slater determinant** $\psi^{(boson)}(x_1,x_2,x_3) = \frac{1}{\sqrt{3!}}det\begin{vmatrix}u_a(x_1) & u_b(x_1) & u_c(x_1)\\ u_a(x_2) & u_b(x_2) & u_c(x_2)\\ u_a(x_3) & u_b(x_2) & u_c(x_3)\end{vmatrix}_+$ (symmetric) The + sign means taking all plus signs in the determinant I If the three identical particles are indistinguishable fermions, the total wavefunction be anti-symmetric under exchange of any two particles I The normalized and symmetrized total wavefunction can be expressed in **slater determinant** $\psi^{(fermion)}(x_1,x_2,x_3) = \frac{1}{\sqrt{3!}}det\begin{vmatrix}u_a(x_1) & u_b(x_1) & u_c(x_1)\\ u_a(x_2) & u_b(x_2) & u_c(x_2)\\ u_a(x_3) & u_b(x_2) & u_c(x_3)\end{vmatrix}_+$ (anti-symmetric) I $= \frac{1}{\sqrt{6}}[+u_a(x_1)u_b(x_2)u_c(x_3) + u_b(x_1)u_c(x_2)u_a(x_3) + +u_c(x_1)u_a(x_2)u_b(x_3) - u_a(x_1)u_c(x_2)u_b(x_3) - u_b(x_1)u_a(x_2)u_c(x_3) - u_c(x_1)u_b(x_2)u_a(x_3)]$ I The exclusion principle in this case lies in the fact that the determinant is zero when any two rows are the same. The Slater determined can be easily generalized to N identical fermions. **what happens if we include spin** $\psi_{total} = \psi_{position}\chi spin$ Lets consider the simplest scenario: two non-interacting electrons in a 1D box. We know the electon spins can couple to from the singlet or triplet: The ground state is symmetric in position, so it must be paired with the anti-symmetric spin singlet to make the total anti-symmetric, as required for fermions. So the normalized total wavefunction $\psi_{gs}(1,2) = \frac{1}{\sqrt{2}}det\begin{vmatrix}u_1(x_1)|\uparrow\rangle & u_1(x_1)|\downarrow\rangle\\ u_1(x_2)|\uparrow\rangle & u_1(x_2)|\downarrow\rangle\end{vmatrix} = u_1(x_1)u_1(x_2)\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ I The next state is doubly-degenerate in position space, (1,2) or (2,1) so we have four possibilites when paired with spin: $\psi_a(1,2) = \frac{1}{\sqrt{2}}det\begin{vmatrix}u_1(x_1)|\uparrow\rangle & u_2(x_1)|\downarrow\rangle\\ u_1(x_2)|\uparrow\rangle & u_2(x_2)|\downarrow\rangle\end{vmatrix} = \frac{1}{\sqrt{2}}[u_1(x_1)u_2(x_2)|\uparrow\downarrow\rangle - u_2(x_1)u_2(x_2)|\downarrow\uparrow\rangle]$ I $\psi_b(1,2) = \frac{1}{\sqrt{2}}det\begin{vmatrix}u_1(x_1)|\downarrow\rangle & u_2(x_1)|\uparrow\rangle\\ u_1(x_2)|\downarrow\rangle & u_2(x_2)|\uparrow\rangle\end{vmatrix} = \frac{1}{\sqrt{2}}[u_1(x_1)u_2(x_2)|\downarrow\uparrow\rangle - u_2(x_1)u_2(x_2)|\uparrow\downarrow\rangle]$ I $\psi_c(1,2) = \frac{1}{\sqrt{2}}det\begin{vmatrix}u_1(x_1)|\uparrow\rangle & u_2(x_1)|\uparrow\rangle\\ u_1(x_2)|\uparrow\rangle & u_2(x_2)|\uparrow\rangle\end{vmatrix} = \frac{1}{\sqrt{2}}[u_1(x_1)u_2(x_2) - u_2(x_1)u_2(x_2)]|\uparrow\uparrow\rangle$ I $\psi_d(1,2) = \frac{1}{\sqrt{2}}det\begin{vmatrix}u_1(x_1)|\downarrow\rangle & u_2(x_1)|\downarrow\rangle\\ u_1(x_2)|\downarrow\rangle & u_2(x_2)|\downarrow\rangle\end{vmatrix} = \frac{1}{\sqrt{2}}[u_1(x_1)u_2(x_2) - u_2(x_1)u_2(x_2)]|\downarrow\downarrow\rangle$ I The energy of this level is $E_2 = 5E_0$, more possibilities arise when spin is included **identical particles: exchange forces** Consider two non-interacting identical particles, Suppose one particle is in state ψ_a the other in state ψ_b The two states are normalized and orthogonal. We know the total wave function is: If distinguishable: $\psi(x_1,x_2) = \psi_a(x_1)\psi_b(x_2)$ I If identical bosons: $\psi(x_1,x_2) = \frac{1}{\sqrt{2}}[\psi_a(x_1)\psi_b(x_2) + \psi_b(x_1)\psi_a(x_2)]$ (symmetric) I If identical fermions: $\psi(x_1,x_2) = \frac{1}{\sqrt{2}}[\psi_a(x_1)\psi_b(x_2) - \psi_b(x_1)\psi_a(x_2)]$ (anti-symmetric) I Lets calculate the expectation value of the square of the separation distance between the two particles $\left\langle(x_1-x_2)^2\right\rangle = \left\langle x_1^2\right\rangle + \left\langle x_2^2\right\rangle - 2\langle x_1x_2\rangle$ I If distinguishable: $\left\langle x_1^2\right\rangle = \int x_1^2|\psi_a(x_1)|^2dx_1\int|\psi_b(x_2)|^2dx_2 = \left\langle x^2\right\rangle_a$ I $\left\langle x_2^2\right\rangle = \int|\psi_a(x_1)|^2dx_1\int intx_2^2|\psi_b(x_2)|^2dx_2 = \left\langle x^2\right\rangle_b$ I $\langle x_1x_2\rangle = \int x_1|\psi_a(x_1)|^2dx_1\int intx_2|\psi_b(x_2)|^2dx_2 = \langle x\rangle_a\langle x\rangle_b$ I So $\left\langle(x_1-x_2)^2\right\rangle = \left\langle x^2\right\rangle_a + \left\langle x^2\right\rangle_b - 2\langle x\rangle_a\langle x\rangle_b$ I If identical bosons: $\left\langle(x_1-x_2)^2\right\rangle = \left\langle x^2\right\rangle_a + \left\langle x^2\right\rangle_b - 2\langle x\rangle_a\langle x\rangle_b + 2\left|\langle x\rangle_{ab}\right|^2$ I If identical fermions: $\left\langle(x_1-x_2)^2\right\rangle = \left\langle x^2\right\rangle_a + \left\langle x^2\right\rangle_b - 2\langle x\rangle_a\langle x\rangle_b - 2\left|\langle x\rangle_{ab}\right|^2$ I where $\langle x\rangle_{ab} = \int\psi_a^*(x)x\psi_b(x)dx$ is called the overlap integral. The the effect of symmetrization requirement is that identical bosons tend to be closer together, and identical fermions farther apart, than distinguishable particles in the same two states. In other words, when tow identical bosons are brought together, there is a a force of attraction; when two identical fermions are brought together, there's a force of repulsion. We call them **exchange forces**. In fact, they are not forces in the classical sense because there is no interaction potential between them. They are purely quantum effects due to the indistinguishability of identical particles **Perturbation theory** **Perturbation theory** The hamiltonian can be written as a main part plus a small 'perturbation' $\hat{H} = H_0 + \lambda\hat{H}'$ I where for $\hat{H}_0$ we know the exact solutions: $\hat{H}_0\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)}$ then we can try to solve the real problem by expanding $E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2E_n^{(2)} + \ldots$ and $\psi_n = \psi_n^0 + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \ldots$ I and try to find the energy and wavefunction order by order in λ, λ is a real parameter between 0 and 1 introduced for book keeping. Once the solution is found, it will be set to 1, so we are solving the true Hamiltonian: $\hat{H} = \hat{H}_0 + \hat{H}'$ I By substituting the expansion into the schrodinger equation $\hat{H}\psi_n = E_n\psi_n$ I $(\hat{H}_0 + \lambda\hat{H}')(\psi_n^0 + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \ldots) = (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2E_n^{(2)} + \ldots)(\psi_n^0 + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \ldots)$ and comparing order by order in powers of λ we can find I $E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \ldots$. I First order $E_n^{(1)} = \left\langle\psi_n^{(0)}\left|\hat{H}'\right|\psi_n^{(0)}\right\rangle = H'_{nn}$ and $\psi_n^1 = \sum_{k\neq n}a_{nk}^{(1)}\psi_k^{(0)}$ I Second order $E_n^{(2)} = \sum_{k\neq n}\frac{\left|\left\langle\psi_n^{(0)}\left|\hat{H}'\right|\psi_n^{(0)}\right\rangle\right|^2}{E_n^{(0)}-E_k^{(0)}} = \sum_{k\neq n}\frac{\left|\left\langle H'_{nk}\right\rangle\right|}{E_n^{(0)}-E_k^{(0)}}$ and $\psi_n^{(2)} = \sum_{k\neq n}a_{nk}^2\psi_k^{(1)}$ I Matrix elements $H'_{nk} \equiv \left\langle\psi_n^{(0)}\left|\hat{H}'\right|\psi_n^{(0)}\right\rangle$ I Comments: 1) need matrix element of the perturbation in un-perturbed eigenfunctions: H'_{nk}. 2) Fails if there is degeneracy. A different solution is needed to deal with degeneracy, 3) 2nd-order correction to energy is positive for states below n, negative above n. 4)K-th order correction can be built from (k-1)th order **10.9 Harmonic oscillator in applied electric field** $V(x) = \frac{1}{2}m\omega^2x^2 - Fx$ where $F = qE$ I $\hat{H} = \hat{H}_0 + \hat{H}'$ and $\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2x^2$ and $\hat{H}' = -Fx$ I problem can be solved by completing square $E_n = (n+\frac{1}{2})\hbar\omega - \frac{F^2}{2m\omega^2}$ (where $n = 0, 1, 2, \ldots$) I and First order energy correction $E_n^{(1)} = H'_{nn} \approx \langle n|H'|n\rangle = -F\langle n|x|n\rangle = 0$ I and Second-order energy correction $E_n^{(2)} = \sum_{k\neq n}\frac{\left|H'_{nk}\right|^2}{E_n^{(0)}-E_k^{(0)}} = F^2\sum_{k\neq n}\frac{|\langle n|x|k\rangle|^2}{(n-k)\hbar\omega} = \frac{F^2}{2m\omega^2}(\frac{n}{1} + \frac{n+1}{-1}) = -\frac{F^2}{2m\omega^2}$ I which happens to be the exact answer. This means all higher-order corrections vanish. **Useful integrals (matrix elements):** $\langle\psi_n|x|\psi_k\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\delta_{n,k-1}\sqrt{k} + \delta_{n,k+1}\sqrt{k+1})$ I $\langle\psi_n|\hat{p}|\psi_k\rangle = -i\sqrt{\frac{\hbar}{2m\omega}}(\delta_{n,k-1}\sqrt{k} + \delta_{n,k+1}\sqrt{k+1})$ **10.10 symmetric infinite well plus δ function** I $\hat{H} = \hat{H}_0 + \hat{H}'$ and $\hat{H}_0 = \frac{\hat{p}^2}{2m} + V(x)$ and $\hat{H}' = g\delta(x)$ I no corrections to odd-parity energies, because $H'_{nk} \equiv \langle n|H'|k\rangle = \left\langle u_n^{(-)}\left|g\delta(x)\right|u_k^{(-)}\right\rangle = 0$ to all orders in perturbation theory I First-order energy correction for even-parity(for all levels): $(E_n^{(+)})^{(1)} = \langle n|H'|n\rangle = \left\langle u_n^{(+)}\left|\delta(x)\right|u_n^{(+)}\right\rangle = \frac{g}{a} = \lambda(\frac{\hbar^2}{2ma^2})$, where$\lambda \equiv \frac{2ma^2g}{\hbar^2}$ I Second-order energy correction to ground-state(n=1): $H'_{nk} = \left\langle u_n^{(+)}\left|g\delta(x)\right|u_k^{(x)}\right\rangle = \int_{-a}^a dx\frac{1}{\sqrt{a}}\cos\left(\frac{(n-1/2)\pi x}{a}\right)g\delta(x)\frac{1}{\sqrt{a}}\cos\left(\frac{(k-1/2)\pi x}{a}\right) = \frac{g}{a}$ and $(E_1^{(+)})^{(2)} = \frac{8m_ea^2}{\pi^2\hbar^2}(\frac{g}{a})^2\sum_{k=2}^\infty\frac{1}{1-(2k-1)^2} = \frac{8m_ea^2}{\pi^2\hbar^2}(\frac{g}{a})^2(-\frac{1}{4}) = -\lambda^2(\frac{\hbar^2}{2\pi^2ma^2})$ From this Even-parity solutions:$E_n^{(+)} = \frac{(2n-1)^2\pi^2\hbar^2}{8ma^2}$ and $u_n^{(+)}(x) = \frac{1}{\sqrt{a}}\cos\left(\frac{(n-1/2)\pi x}{a}\right)$ with $n = 1, 2, 3, \ldots$ and Odd-parity soltuions: $E_n^{--} = \frac{n^2\pi^2\hbar^2}{2ma^2}$ and

$u_n^-(x) = \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi x}{a}\right)$ **Degenerate perturbation theory** Lets consider the simple case of two-fold degeneracy: two orthonormal states $\psi_a^{(0)}$ and $\psi_b^{(0)}$ correspond to the smae energy $E^{(0)}$. the key idea is to use a linear combination of the degenerate states $\psi^{(0)} = a\psi_a^{(0)} + b\psi_b^{(0)}$ with to-be-determined coefficients a and b. To first-order in λ the Schrodinger equation $\hat{H}\psi_n = E_n\psi_n$ yields a 2 × 2 eigenvalue problem $\begin{pmatrix} H'_{aa} & H'_{ab} \\ H'_{ba} & H'_{bb} \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = E^{(1)}\begin{pmatrix} a \\ b \end{pmatrix}$ I The eigenvalue is determined from the characteristic equation $det\begin{vmatrix} H'_{aa} - E^{(1)} & H'_{ab} \\ H'_{ba} & H'_{bb} - E^{(1)} \end{vmatrix} = 0$ which gives $E^{(1)}_{\pm} = \frac{1}{2}(H'_{aa} + H'_{bb} \pm \sqrt{(H'_{aa} - H'_{bb})^2 + 4\left|H'_{ab}\right|^2})$ **Key: lifting of degeneracy by perturbation**

Perturbation in 3D cubic box $\hat{H} = \hat{H}_0 + \hat{H}'$ where $\hat{H}' = V_0$ for $0 < x < a/2$ and $0 < y < a/2$ and $= 0$ otherwise The perturbation raises the potential by V_0 in 1/4 of the box. The unperturbed states for $\hat{H}_0$ are: $E_{n_x n_y n_z} = (n_x^2 + n_y^2 + n_z^2)\frac{\pi^2\hbar^2}{2ma^2}$ where $n_x, n_y, n_z = 1, 2, 3, \ldots$ and $\psi_{n_x n_y n_z}(x, y, z) = \sqrt{\frac{8}{a^3}}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{a}\right)\sin\left(\frac{n_z\pi z}{a}\right)$ I The ground state is (1,1,1), which is non-degenerate, with unperturbed energy $E_1 = 3E_0$ Standard non-degenerate perturbation theory gives the 1st correction: **should this be a/2** $E_1^{(1)} = \langle 111|\hat{H}'|111\rangle = \frac{8V_0}{a^3}\int_0^{a/2}\sin^2(\frac{\pi x}{a})dx\int_0^{a/2}\sin^2(\frac{\pi y}{a})dy\int_0^{a}\sin^2(\frac{\pi z}{a})dz = \frac{8V_0}{a^3}\frac{a}{4}\frac{a}{4}\frac{a}{2} = \frac{V_0}{4}$ I The first excited state is 3-fold degenerate, with unperturbed energy $E_2 = 6E_0$ let's call $\psi_{112} = \psi_a, \psi_{121} = \psi_b, \psi_{211} = \psi_c$ For 1st-order energy correction $E = E_2^{(1)}$ we need to solve the matrix equation eigenvalue problem I $\begin{pmatrix} H'_{aa} & H'_{ab} & H'_{ac} \\ H'_{ba} & H'_{bb} & H'_{bc} \\ H'_{ca} & H'_{cb} & H'_{cc} \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = E\begin{pmatrix} a \\ b \\ c \end{pmatrix}$ Where the matrix elements are: $H'_{aa} = H'_{bb} = H'_{cc} = \langle 112|\hat{H}'|112\rangle = \frac{V_0}{4}$ I $H'_{ab} = H'_{ba} = H'_{ac} = H'_{ca} = 0$ I $H'_{bc} = H'_{cb} = \frac{16V_0}{9\pi^2} = k\frac{V_0}{4}$ where $k = \frac{64}{9\pi^2} = 0.7205$ I The eigenvalues are determine from the characteristic equation $det\begin{vmatrix} 1-w & 0 & 0 \\ 0 & 1-w & k \\ 0 & k & 1-w \end{vmatrix} = 0$ where $w = \frac{4}{V_0}E$ where $(1-w)^3 - k^3(1-w) = 0$, $w = 1,\ 1+k,\ 1-k = 1,\ 1.705\ 0.2795$ So to first-order in λ where $E_2(\lambda) = 6E_0 + 0.25V_0\lambda$ and $= 6E_0 + 0.426V_0\lambda$ and $6E_0 + 0.07V_0\lambda$ The degeneracy is lifted by the perturbation. The eigenvectors give the corresponding wave functions in terms of linear combination of the 3 degenerate ones. $\psi_2 = \psi_{112}$ and $(\psi_{121} + \psi_{211})/\sqrt{2}$ and $(\psi_{121} - \psi_{211})/\sqrt{2}$ **Ground state of Helium atom** We need to solve Time Independent Schrodinger Equation $\hat{H}\psi = E\psi$ for $\hat{H} = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{Ze^2}{4\pi\epsilon_0 r_1} - \frac{Ze^2}{4\pi\epsilon_0 r_2} + \frac{e^2}{4\pi\epsilon_0|\vec{r}_1 - \vec{r}_2|}$ I We can treat the electron-electron interaction as a perturbation: $\hat{H} = \hat{H}_0 + \hat{H}'$ I We know the solution for $\hat{H}_0$: $\psi(\vec{r}_1, \vec{r}_2) = \psi_{n_1 l_1 m_1}(\vec{r}_1)\psi_{n_2 l_2 m_2}(\vec{r}_2)$ I $E_{n_1 n_2} = -Z^2\frac{13.6\,eV}{n_1^2} - Z^2\frac{13.6\,eV}{n_2^2}$ where $Z = 2$ for Helium atom I The ground state: $\psi_0(\vec{r}_1, \vec{r}_2) = \psi_{100}(\vec{r}_1)\psi_{100}(\vec{r}_2) = \frac{8}{\pi a^6}e^{-2(r_1+r_2)/a}$ and $E_0 = 8E_1 = 8 \times (-13.6\,eV) = -108.8\,eV$ vs Experiment $E_0 = -78.975\,eV$ I First-order energy correction: $E_0^1 = \left\langle \hat{H}\middle|\psi_0\middle|\hat{H}\right\rangle = \frac{e^2}{4\pi\epsilon_0}\int dr_1^3\int dr_2^3\frac{|\psi_0(\vec{r}_1,\vec{r}_2)|^2}{|\vec{r}_1 - \vec{r}_2|} = \frac{e^2}{4\pi\epsilon_0}(\frac{5}{4a}) = -\frac{5}{2}E_1 = 34\,eV$ I So 1st-order perturbation theory gives $E_0 = -108.8 + 34 = -74.8\,eV$ close **Variational principle** **Variational principle** In quantum mechanics, we often need to solve the eigenvalue problem: $\hat{H}\psi_n = E_n\psi_n$ How do we make progress if we are faced with problems with no exact solutions $E[\psi] = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}$ If $\psi = \psi_n$, then it returns the eigenenergy $E[\psi_n] = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = E_n$ I In general wavefunction, then the expansion $\psi = \sum_n a_n\psi_n$ leads to the following condition $E[\psi_n] = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_n |a_n|^2 E_n}{\sum_n |a_n|^2} \le \frac{\sum_n |a_n|^2 E_0}{\sum_n |a_n|^2} = E_0$ (assume ordered energies) $E_0 \le E_1 \le E_2 \ldots$ I It provides the basis for the variational principle: devise trial wavefunctions ψ with adjustable parameters, and minimize the energy functional. It guarantees an upper bound on the ground-state energy $E[\psi] \ge E_0$ I General property: First-order deviations in trial wave functions from the true ground-state solution give rise to second-order changes in energies. $E[\psi_0 + \lambda\phi] = \frac{\langle\psi_0+\lambda\phi|\hat{H}|\psi_0+\lambda\phi\rangle}{\langle\psi_0+\lambda\phi|\psi_0+\lambda\phi\rangle} = \frac{E_0\langle\psi_0|\psi_0\rangle + \lambda\langle\psi_0|\hat{H}|\phi\rangle + \lambda\langle\phi|\hat{H}|\psi_0\rangle + \lambda^2\langle\phi|\hat{H}|\phi\rangle}{\langle\psi_0|\psi_0\rangle + \lambda\langle\psi_0|\phi\rangle + \lambda\langle\phi|\psi_0\rangle + \lambda^2\langle\phi|\phi\rangle} = E_0\frac{1+\lambda(\langle\psi_0|\phi\rangle + \langle\phi|\psi_0\rangle) + \lambda^2\langle\phi|\hat{H}|\phi\rangle/E_0}{1+\lambda(\langle\psi_0|\phi\rangle + \langle\phi|\psi_0\rangle) + \lambda^2\langle\phi|\phi\rangle} = E_0[1 + O(\lambda^2)]$ I This means that the key in getting good estimates of the energy is to find good trial wavefunctions. Theres great freedom for exploring trial wavefunctions, because "lower is always better" **example: ground state of standard infinite well 1** $\hat{H} = \hat{T} + V = \frac{\hat{p}^2}{2m} + V(x)$ using this I Note, for $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$ I $\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ with $n = 1, 2, 3, \ldots$ I The trial wavefunction $\psi = x(L-x)$ seems reasonable because it satisfies the boundary conditions. I $\langle\psi|\psi\rangle = \int_0^L x^2(L-x)^2dx = \frac{L^5}{30}$ I $\langle\psi|\hat{T}|\psi\rangle = \int_{-\infty}^{\infty}x(L-x)(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2})x(L-x)dx = -\frac{\hbar^2}{2m}(-\frac{L^3}{3})$ I $E(L) = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{5\hbar^2}{mL^2} = \frac{10}{\pi^2}E_1 = 1.013E_1$ Not bad, even with no adjustable parameter. The normalized wavefunction $\psi(x) = \sqrt{\frac{30}{L^5}}x(L-x)$ is compared to the exact solution **example: ground state of standard infinite well 2** The trial wavefunction $\psi = x^2(L-x)^2$ also satisfies the boundary conditions. I note that Note, for $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$ I $\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ with $n = 1, 2, 3, \ldots$ I $\langle\psi|\psi\rangle = \int_0^L x^4(L-x)^4dx = \frac{L^9}{630}$ I $\langle\psi|\hat{T}|\psi\rangle = \int_{-\infty}^{\infty}x^2(L-x)^2(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2})x^2(L-x)^2dx = -\frac{\hbar^2}{2m}(-\frac{2L^7}{105})$ I $E(L) = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{6\hbar^2}{mL^2} = \frac{12}{\pi^2}E_1 = 1.216E_1$ I Not as good. The normalized wavefunction $\psi(x) = \sqrt{\frac{630}{L^9}}x^2(L-x)^2$ is compared to the exact solution **example: ground state of standard infinite well 3** What about $\psi = x(L-x)^2$ Note, for $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$ I $\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ with $n = 1, 2, 3, \ldots$ I $\langle\psi|\psi\rangle = \int_0^L x^2(L-x)^4dx = \frac{L^7}{105}$ I $\langle\psi|\hat{T}|\psi\rangle = \int_{-\infty}^{\infty}x(L-x)^2(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2})(L-x)^2dx = -\frac{\hbar^2}{2m}(-\frac{2L^7}{105})$ I $E(L) = \frac{\langle\psi|\hat{T}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{7\hbar^2}{mL^2} = \frac{14}{\pi^2}E_1 = 1.4185E_1$ I Even worse. The normalized wavefunction $\psi(x) = \sqrt{\frac{105}{L^7}}x(L-x)^2$ is compared to the exact solution **example: ground state of harmonic oscillator 1** $\hat{H} = \hat{T} + V = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2x^2$ I use trial wavefunction $\psi(x) = e^{-ax^2}$ with a as variational parameter I $\langle\psi|\psi\rangle = \int_{-\infty}^{\infty}e^{-2ax^2}dx = \sqrt{\frac{\pi}{2a}}$ I $\langle\psi|V(x)|\psi\rangle = \frac{1}{2}m\omega^2\int_{-\infty}^{\infty}x^2e^{-2ax^2}dx = \frac{1}{2}m\omega^2(\frac{1}{4a^2}\sqrt{\frac{\pi}{2a}})$ I $\langle\psi|\hat{T}|\psi\rangle = \int_{-\infty}^{\infty}e^{-ax^2}(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2})e^{-ax^2}dx = -\frac{\hbar^2}{2m}(-\sqrt{\frac{\pi a}{2}})$ I $E(a) = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{a\hbar^2}{2m} + \frac{m\omega^2}{8a}$ I $\frac{dE(a)}{da} = 0$ gives $a = \frac{m\omega}{2\hbar} = \frac{1}{2\rho^2}$ I So $E_{min} = \frac{1}{2}\hbar\omega$ I which happens to be the exact answer. Reason: the trial wavefunction happens to have the correct functional form. I The normalized wavefunction $\psi(x) = (\frac{2a}{\pi})^{1/4}$ with $a = \frac{m\omega}{2\hbar} = \frac{1}{2\rho^2}$ is the exact wavefunction for the ground state. **example: ground state of harmonic oscillator 2** $\hat{H} = \hat{T} + V = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2x^2$ I Trial wave $\psi(x) = 0$ for $|x| > a$ and $(a^2 - x^2)^2$ for $|x| < a$ with a as variational parameter I $\langle\psi|\psi\rangle = \int_{-a}^{a}(a^2 - x^2)^4dx = \frac{256a^9}{315}$ I $\langle\psi|V(x)|\psi\rangle = \frac{1}{2}m\omega^2\int_{-a}^{+a}x^2(a^2 - x^2)^4dx = \frac{1}{2}m\omega^2(\frac{256a^{11}}{3465})$ I $\langle\psi|\hat{T}|\psi\rangle = \int_{-a}^{+a}(a^2 - x^2)^2(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2})(a^2 - x^2)^2dx = -\frac{\hbar^2}{2m}(-\frac{256a^9}{105})$ I $E(a) = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{3\hbar^2}{2ma^2} + \frac{a^2m\omega^2}{22}$ I $\frac{dE(a)}{da} = 0$ gives $a = 33^{(1/4)}\sqrt{\frac{\hbar}{m\omega}} = 2.3968\sqrt{\frac{\hbar}{m\omega}}$ I So $E_{min} = \sqrt{\frac{3}{11}}\hbar\omega = 0.522\hbar\omega$ compare to exact value of $0.5\hbar\omega$ I Normalized wavefcuntion$\psi(x) = 0$ for $|x| > a$ and $\sqrt{\frac{315}{256a^9}}(a^2 - x^2)^2$ for $|x| < a$ I 1st-order changes in wavefunction give 2nd order changes in energy **example: ground state of harmonic oscillator 3 two-parameter minimization** $\hat{H} = \hat{T} + V = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2x^2$ I Trial wavefunction $\psi(x) = 0$ for $|x| > a$ and $= (a^2 - x^2)^2(1 + bx^2)$ for $|x| < a$ with a and b as variational parameters I $E(a,b) = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{39(11+a^4b^2)\hbar^2+(13+6a^2b+a^4b^2)m^2\omega^2}{2ma^2(143+26a^2b+3a^4b^2)}$ I $\frac{\partial E(a,b)}{\partial a} = 0$ and $\frac{\partial E(a,b)}{\partial b} = 0$ give I $a = 2.7656\sqrt{\frac{\hbar}{m\omega}}$ and $b = -0.1307\frac{m\omega}{\hbar}$ I So $E_{min} = 0.5099\hbar\omega$ compared to exact value of $0.5\hbar\omega$ I Variational principle: Lower is always better **variational principle: excited states** If the trial wavefunction ψ is such that it is orthogonal to the ground state, then $a_0 = \langle\psi_0|\psi\rangle = 0$ so the expansion $psi = \sum_n a_n\psi_n$ leas to an upper bound on the next state(excited state): $E[\psi] = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_{n=0}|a_n|^2E_n}{\sum_{n=0}|a_n|^2} = \frac{\sum_{n=1}|a_n|^2E_n}{\sum_{n=1}|a_n|^2} \ge \frac{\sum_{n=1}|a_n|^2E_1}{\sum_{n=1}|a_n|^2} = E_1$ (assume ordered energies $E_0 \le E_1 \le E_2 \ldots$) I To get an upper bound on E_2, the trial wavefunction ψ must be othogonal to both ψ_0 and ψ_1 (so $a_0 = 0$ and $a_1 = 0$) And so on for higher excited states I The key is orthogonality, which is not guaranteed, in special cases: we can rely on parity to guarantee orthogonality **example: First excited state of harmonic oscillator** $\hat{H} = \hat{T} + V = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2x^2$ I Because the potential is symmetric, the states alternative in parity, with the ground state even-parity. So the odd-parity trial wavefunction $\psi(x) = xe^{-ax^2}$ with a as variational parameter seems a reasonable choice for the first excited state. $\langle\psi|\psi\rangle = \int_{-\infty}^{\infty}x^2theee^{-2ax^2}dx = \frac{1}{4a}\sqrt{\frac{\pi}{2a}}$ I $E(a) = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{3a\hbar^2}{2m} + \frac{3m\omega^2}{8a}$ I $\langle\psi|V(x)|\psi\rangle = \frac{1}{2}m\omega^2\int_{-\infty}^{\infty}x^4e^{-2ax^2}dx = \frac{1}{2}m\omega^2(\frac{3}{16a^2}\sqrt{\frac{\pi}{2a}})$ I $\langle\psi|\hat{T}|\psi\rangle = \int_{-\infty}^{\infty}e^{-ax^2}(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2})e^{-ax^2}dx = -\frac{\hbar^2}{2m}(-\frac{3}{4}\sqrt{\frac{\pi a}{2}})$ I $E(a) = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{3a\hbar^2}{2m} + \frac{3m\omega^2}{8a}$ I $fracdE(a)da = 0$ gives $a = \frac{m\omega}{2\hbar} = \frac{1}{2\rho^2}$ I $E_{min} = \frac{3}{2}\hbar\omega$ I which happens to be the exact answer. Reason: the trial wavefunction happens to have the correct functional form. I Normalized wavefunction $\psi(x) = (4a)^{1/2}(\frac{2a}{\pi})^{1/4}xe^{-ax^2}$ with $a = \frac{m\omega}{2\hbar} = \frac{1}{2\rho^2}$ I is the exact wavefunction for the first excited state. **ground state of Helium atom (perturbation theory)** We need to solve Time Independent Schrodinger Equation $\hat{H}\psi = E\psi$ for $\hat{H} = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{Ze^2}{4\pi\epsilon_0 r_1} - \frac{Ze^2}{4\pi\epsilon_0 r_2} + \frac{e^2}{4\pi\epsilon_0|\vec{r}_1 - \vec{r}_2|}$ I We can treat the electron-electron interaction as a perturbation: $\hat{H} = \hat{H}_0 + \hat{H}'$ I We know the solution for $\hat{H}_0$: $\psi(\vec{r}_1, \vec{r}_2) = \psi_{n_1 l_1 m_1}(\vec{r}_1)\psi_{n_2 l_2 m_2}(\vec{r}_2)$ I $E_{n_1 n_2} = -Z^2\frac{13.6\,eV}{n_1^2} - Z^2\frac{13.6\,eV}{n_2^2}$ where $Z = 2$ for Helium atom I The ground state: $\psi_0(\vec{r}_1, \vec{r}_2) = \psi_{100}(\vec{r}_1)\psi_{100}(\vec{r}_2) = \frac{8}{\pi a^6}e^{-2(r_1+r_2)/a}$ and $E_0 = 8E_1 = 8 \times (-13.6\,eV) = -108.8\,eV$ vs Experiment $E_0 = -78.975\,eV$ I First-order energy correction: $E_0^1 = \left\langle \hat{H}\middle|\psi_0\middle|\hat{H}\right\rangle = \frac{e^2}{4\pi\epsilon_0}\int dr_1^3\int dr_2^3\frac{|\psi_0(\vec{r}_1,\vec{r}_2)|^2}{|\vec{r}_1 - \vec{r}_2|} = \frac{e^2}{4\pi\epsilon_0}(\frac{5}{4a}) = -\frac{5}{2}E_1 = 34\,eV$ I So 1st-order perturbation theory gives $E_0 = -108.8 + 34 = -74.8\,eV$ close **ground state of Helium atom (variational principle)** $\hat{H}\psi = E\psi$ for $\hat{H} = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{Ze^2}{4\pi\epsilon_0 r_1} - \frac{Ze^2}{4\pi\epsilon_0 r_2} + \frac{e^2}{4\pi\epsilon_0|\vec{r}_1 - \vec{r}_2|}$ I Trial wavefunction $\psi(\vec{r}_a, \vec{r}_2, Z) = \frac{Z^3}{\pi a^3}e^{-Z(r_1+r_2)/a}$ and treat Z as a variational parameter $\hat{H} = (-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{Ze^2}{4\pi\epsilon_0 r_1}) + (-\frac{\hbar^2}{2m}\nabla_2^2 - \frac{Ze^2}{4\pi\epsilon_0 r_2}) + \frac{(Z-2)e^2}{4\pi\epsilon_0 r_1} + \frac{(Z-2)e^2}{4\pi\epsilon_0 r_2} + \frac{e^2}{4\pi\epsilon_0|\vec{r}_1 - \vec{r}_2|}$ I To perform calculation one must use $\langle\psi|\frac{1}{r_1}|\psi\rangle = \langle\psi|\frac{1}{r_2}|\psi\rangle = \frac{Z}{a}$ I $\langle\psi|\frac{1}{|\vec{r}_1 - \vec{r}_2|}|\psi\rangle = \frac{5Z}{8a}$ I $E_1 = -\frac{e^2}{4\pi\epsilon_0}(\frac{1}{2a}) = -13.6\,eV$ I use this to solve Energy function $E(Z) = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = -\frac{even^2}{4\pi\epsilon_0}(\frac{Z^2}{2a}) - \frac{e^2}{4\pi\epsilon_0}(\frac{Z^2}{2a}) + \frac{(Z-2)e^2}{4\pi\epsilon_0}\langle\psi|\frac{1}{r_1}|\psi\rangle + \frac{(Z-2)e^2}{4\pi\epsilon_0}\langle\psi|\frac{1}{r_2}|\psi\rangle + \frac{e^2}{4\pi\epsilon_0}\langle\psi|\frac{1}{|\vec{r}_1 - \vec{r}_2|}|\psi\rangle = (2Z^2 + 4(Z-2)Z - 5Z/4)E_1 = (-2Z^2 + 27Z/4)E_1$ I $\frac{dE(Z)}{dZ} = 0$ gives $Z = 27/16 = 1.69$ I So $E_{min} = 5.6953E_1 = -77.45\,eV$ Close to experiment value $-79\,eV$ than perturbation of $-74.8\,eV$ I Physics reasons: one electron screen the nuclear charge form the other electron, effectively from $Z = 2$ down to $Z = 1.69$ **Variational principle in electrodynamics** Theorem: Among all the potentials which take constant values on a set of conductor surfaces, the electrostatic energy $U_E[\psi] = \frac{\epsilon_0}{2}\int\left|\vec{E}^2\right|dr^3 = \frac{\epsilon_0}{2}\int\Delta\psi\cdot\Delta\psi dr^3)$ (recall $\vec{E} = -\nabla\psi$) is the lowest for the particular potential function which satisfies the Laplace equation $\Delta^2\psi = 0$ in the volume bounded by the surfaces. When this theorem is applied to trial potentials with adjustable parameters, we have a variational principle that can be used to find approximate solutions to the Laplace equation. We can trust that lower U_E is always better. Example: Find the potential in a conducting slot shown in the figure: The trial potential $\psi(x, y) = \psi_0 x(a-x)e^{-py}$, which p treated as variational parameter, seems reasonable. (based on boundary conditions in x, and y-dependence) $U_E(p) = \frac{\epsilon_0}{12}\psi_0^2a^3(\frac{1}{p} + \frac{pa^2}{10})$ which has minimum at $p = \sqrt{10}/a$ I So the optimal potential is $\psi(x, y) = \psi_0 x(a-x)e^{-\sqrt{10}y/L}$ I It compares well with the exact solution that can be found by separation of variables **Fine structure in the hydrogen atom** **Relativistic kinetic energy correction** How fast is the electron in the hydrogen atom? Electron kinetic energy is $\langle T\rangle = \frac{-}{+}2\langle V\rangle = -E_n$ where $E_n = -\frac{13.6\,eV}{n^2}$, $n = 1, 2, 3, ..$ So $\left\langle\frac{mv^2}{2}\right\rangle = \frac{13.6\,eV}{n^2}$, or $\left\langle\frac{v}{c}\right\rangle \approx 7.3 \times 10^{-3} \approx \frac{1}{137}$ in the ground state. Relativistic effects may be important I $T = E - mc^2 = \sqrt{p^2c^2 + m^2c^4} - mc^2$ I $(1+x)^a = 1 + ax + \frac{a(a-1)}{2!}x^2 + \ldots$ I $= mc^2[\sqrt{a + (\frac{p}{mc})^2} - 1] = mc^2[1 + \frac{1}{2}(\frac{p}{mc})^2 + \frac{1/2(1/2-1)}{2!}(\frac{p}{mc})^4 + \ldots - 1]$ I $= \frac{p^2}{2m} - \frac{pa\dot{i}d^4}{8m^3c^2} + \ldots$ I The relativistic correction is $H' = -\frac{\hat{p}^4}{8m^3c^2}$, now use perturbation theory to estimate its contribution to energy levels **needed for Relativistic correction** $(\frac{\hat{p}^2}{2m} + V(r))\psi_{nlm} = E_n\psi_{nlm}$ I $V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$ I $E_n = -(\frac{e^2}{4\pi\epsilon_0})\frac{1}{2n^2a_0} = -\frac{mc^2\alpha^2}{2n^2}$ I $\alpha = \frac{1}{4\pi\epsilon_0}\frac{e^2}{\hbar c} \approx \frac{1}{137}$ I $a_0 = \frac{\hbar}{\mu c\alpha} \approx 0.529\,\text{Å}$ **Virial theorem** $\langle V\rangle = -2\langle T\rangle = 2E_n$ I $\left\langle\frac{1}{r}\right\rangle = \frac{1}{n^2a_0}$ **Feynman-Hellman theorem** (treat l as a parameter) $n = n_r + l + 1$ I $\left\langle\frac{1}{r^2}\right\rangle = \frac{1}{(l+1/2)n^3a_0^2}$ I We can use this to keep solving $E^{(1)} = \langle\psi_{nlm}|\hat{H}'|\psi_{nlm}\rangle = -\frac{1}{8m^3c^2}\langle\psi_{nlm}|\hat{p}^4|\psi_{nlm}\rangle = -\frac{1}{2mc^2}\langle\psi_{nlm}|(E_n - V)^2|\psi_{nlm}\rangle = -\frac{1}{2mc^2}[E_n^2 - 2E_n\langle\psi_{nlm}|V(r)|\psi_{nlm}\rangle + (\frac{e^2}{4\pi\epsilon_0})^2\langle\psi_{nlm}|\frac{1}{r^2}|\psi_{nlm}\rangle] = -\frac{E_n^2}{2mc^2}[\frac{4n}{l+1/2} - 3]$ I So the relativistic correction is a small negative shift about 9×10^{-4} eV on the ground state energy energy of 13.6 eV Or $|\frac{E_n^{(1)}}{E_n}| = \frac{\alpha^2}{2n^2} \sim 3 \times 10^{-5}$ in relative magnitude I Every energy level experiences a shift; but the higher the energy, the smaller the shift **Spin-orbit coupling** interaction between electron orbital motion and its spin, from the vantage point of the electron, the proton produces an internal magnetic field on the electron. This internal magnetic field can then interact with the spin of the electron $H' = -\vec{\mu}\cdot\vec{B}$ I proton $\vec{B} = \frac{\mu_0 I}{2r} = \frac{e}{4\pi\epsilon_0}\frac{1}{mc^2r^3}\vec{L} \sim 12\,T$ I electron $\vec{\mu_s} = \frac{g_s q}{2m}\vec{S} = \frac{-e}{m}\vec{S}$ I The final spin-orbit correction is $H' = (\frac{1}{2})\frac{e^2}{4\pi\epsilon_0}\frac{1}{morc^2r^3}\vec{S}\cdot\vec{L}$ I The extra factor of 1/2 comes from Thomas precession, a relativistic effect to correct for the dact that electron is not in inertial frame. It takes into account the relativistic dilation between between the electron and the proton. **In the coupled basis** $(\vec{J} = \vec{L} + \vec{S})$ I $\left\langle\vec{S}\cdot\vec{L}\right\rangle = \left\langle\frac{1}{2}(\hat{J}^2 - \hat{L}^2 - \hat{S}^2)\right\rangle$ I $= \frac{\hbar^2}{2}[j(j+1) - l(l+1) - s(s+1)]$ I $= \frac{\hbar^2}{2} = l$ for $l + 1/2$ and $-(l+1)$ for $j = l - 1/2$ I Because of spin-orbit coupling, the good quantum numbers are (n, l, s, j, M), not (n, l, m_l, s, m_s) I With this in mind we can continue to solve $\hat{H}' = \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2r^3}\vec{S}\cdot\vec{L}$ I $E^{(1)} = \langle\psi_{nlm}|\hat{H}'|\psi_{nlm}\rangle$ I $= \frac{E_n^2}{mc^2}\frac{n[j(j+1)-l(l+1)-s(s+1)]}{l(l+1/2)(l+1)}$ for $(l \ne 0)$ So the spin-orbit interaction has not effect on the ground state, but splits each $l > 0$ into 2 levels. The gap between the two is on the order of 10^{-4} eV I From recursion relation $\left\langle\frac{1}{r^3}\right\rangle = \frac{1}{l(l+1/2)(l+1)n^3a_0^3}$ I The relative magnitude is $|\frac{E_3^{(1)}}{E_n}| \approx = \frac{\alpha^2}{2n^2} \sim 3 \times 10^{-5}$ on the order as the relativistic kinetic-energy correction. **Darwin term** The electron is in a frantic back and forth motion The position of the electron is "smeared out" by a distance characterized by its Compton wavelength $\lambda = \frac{\hbar}{mc} \sim 4 \times 10^{-11}$ m I This argument leads to a correction very close to the final form $\hat{H}' = \frac{e^2}{4\pi\epsilon_0}\frac{\pi\hbar^2}{2m^2c^2}\delta(\vec{r})$ I We know the exact form because it can be derived from the Dirac equation. It acts only at the origin I $E^{(1)} = \left\langle\psi_{ylm}\middle|\hat{H}'\middle|\psi_{ylm}\right\rangle = \frac{e^2}{4\pi\epsilon_0}\frac{\pi\hbar^2}{2m^2c^2}|\psi_{n00}(0)|^2 = \frac{E_n^2}{mc^2}(2n)$ (only for $l = 0$) I **wave function at the origin**

$\psi_{nlm}(0) = R_{nl}(0)Y_{lm}(0,\phi)$ is only non-zero for $l = 0$ due to radial wavefunction ▮ $R_{nl}(r) = \sqrt{(\frac{2}{na_0})^3 \frac{(n-l-1)!}{2n[(n+1)!]^3}} (\frac{2r}{na_0})^l L^{2l+1}_{n-l-l}(\frac{2r}{na_0})$ ▮ So $|\psi_{n00}(0)|^2 = \frac{1}{\pi a_0^3 n^3}$ The Darwin shift is positive, affects only the s states (l=0), and is on the same order as the other two shifts **Fine structure: combined** $\hat{H} H_0 + \hat{H'_{rel}} + \hat{H'_{so}} + \hat{H'_{Darwin}}$ ▮ First -order perturbation $E^1 = \langle\psi_{nlm}|\hat{H'}|\psi_{nlm}\rangle$ ▮ $\hat{H'_{rel}} = -\frac{\hat{p}^4}{8m^3c^2}$ and $E^{(1)}_{rel} = -\frac{E_n^2}{2mc^2}[\frac{4n}{l+1/2} - 3]$ ▮ $\hat{H'_{so}} = \frac{1}{2}\frac{e^2}{4\pi\epsilon_0}\frac{1}{m^2c^2r^3}\vec{S}\cdot\vec{L}$ and $E^{(1)}_{so} = \frac{E_n^2}{mc^2}\frac{n[j(j+1/2)-l(l+1)-s(s+1)]}{l(l+1/2)(l+1)}$ only for $l \neq 0$ ▮ $\hat{H'_{Darwin}} = \frac{e^2}{4\pi\epsilon_0}\frac{\pi\hbar^2}{2m^2c^2}\delta\vec{r}$ and $E^{(1)}_{Darwin} = \frac{E_n^2}{mc^2}(2n)$ only for $l = 0$ ▮ $E_{nj} = E_n + E^{(1)}_{rel} + E^{(1)}_{so} + E^{(1)}_{Darwin} = E_n[1 + \frac{\alpha^2}{n^2}(\frac{4n}{j+1/2} - \frac{3}{4})]$ **Dirac equation** $\hat{H}\psi = E\psi$ ▮ $\hat{H} = c\vec{\alpha}\cdot\vec{p} + mc^2\beta + V(\vec{r})$ ▮ $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$ ▮ $\vec{\beta} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$ ▮ Relativity is built in, electron spin is built in, wave function has 4 components, has negative-energy solution (the positron), A non-relativistic reduction of it yields the 3 contributions for the fine structure. Has an exact solution for hydrogen ▮ $E_{nj} = mc^2\{[1 + (\frac{\alpha}{n-(j+1/2)+\sqrt{(j+1/2)^2-\alpha^2}})^2]^{-1/2} - 1\}$

Hyperfine spitting Interaction between electron spin and proton spin **In the coupled basis** $(vecS = \vec{S}_p + \vec{S}_e)\left\langle \vec{S}_p\cdot\vec{S}_e\right\rangle = \left\langle \frac{1}{2}(\vec{S}^2 - S)^2_p - \vec{S}^2_p\right\rangle = \frac{\hbar^2}{2} = [s(s+1) - \frac{1}{2}(\frac{1}{2}+1) - \frac{1}{2}(\frac{1}{2}+1)]$ ▮ $= \frac{\hbar^2}{2} = 1/2$ for $s = 1$ (triplet) and $= -3/2$ for $s = 0$(singlet) ▮ proton $\vec{\mu}_p = \frac{g_p e}{2m_p}\vec{S}_p$ (where $g_p \approx 5.59$) ▮ electron $\vec{\mu}_e = \frac{g_e(-e)}{2m_e}\vec{S}_e$ where $g_e \approx 2.0$ ▮ Magnetic field of a dipole (including the origin): $\vec{B}(\vec{r}) = \frac{\mu_0}{4\pi}\frac{3(\vec{m}\cdot\hat{r})\hat{r} - \vec{\mu}}{r^3} + \frac{2\mu_0}{3}\vec{\mu}\delta(\vec{r})$ ▮ $H' = -\vec{\mu}\cdot\vec{B} = \frac{\mu_0 g_p g_e e^2}{16\pi m_p m_e}\frac{3(\vec{S}_p\cdot\hat{r})(\vec{S}_e\cdot\hat{r}) - \vec{S}_p\cdot\vec{S}_e}{r^3} + \frac{\mu_0 g_p g_e e^2}{6m_p m_e}\vec{S}_p\cdot\vec{S}_e\delta(\vec{r})$ ▮ When evaluated in the ground state, the 1st term vanishes, leaving only the 2nd term: ▮ $|\psi_{100}(0)|^2 = \frac{1}{\pi a_0^3}$ ▮ $E^{(1)} = \langle\psi_{100}|\hat{H'}|\psi_{100}\rangle = \frac{\mu_0 g_p g_e e^2}{6m_p m_e}\left\langle \vec{S}_p\cdot\vec{S}_e\right\rangle|\psi_{100}(0)|^2 = \frac{g_p g_e \hbar^4}{3m_p m_e^2 c^2 a_0^3}$ such that $1/2$ for $s = 1$(triplet) and $-3/2$ for $s = 0$ (singlet) ▮ The transition between the two states has an energy gap $\Delta E^(1) = \frac{2g_p g_e \hbar^4}{3m_p m_e^2 c^2 a_0^4} \approx 5.88 \times 10^{-6}$ eV Or a photon of frequency $f = \Delta E^{(1)}/h \approx 1420$ MHz or a wavelength of $\lambda \approx 21$ cm **Lamb shift** There is a small energy difference between $2s_{1/2}$ and $2p_{1/2}$, equal to 4.372×10^{-6} eV (equivalent to 1057 MHz or 28 cm **hydrogen atom: overview** Relative orders of magnitudes $E_n = -\frac{\mu c^2\alpha^2}{2n^2} = \frac{-13.6eV}{n^2}$ ▮ Fine structure $\frac{\Delta E}{E_n} \sim \alpha^2 \sim 1 \times 10^{-5}$ ▮ Hyperfine splittings: $\frac{\Delta E}{E_n} \sim \frac{m_e}{m_p}\alpha^2$ ▮ Lamb shift: $\frac{\Delta E}{E_n} \sim 0.1\alpha^3$ ▮ $\alpha = \frac{1}{137}$ ▮ $\frac{m_e}{m_p} = \frac{1}{1836}$