

Physics 401 Spring 2021 Prof. Anlage Course Review

Early Quantum Mechanics

JJ Thomson charge-to-mass measurement in E, B fields: $q/m = \frac{v}{RB}$. Millikan oil droplet experiment: revealed the quantization of electric charge.

Blackbody radiation, Stefan-Boltzmann law: $R_{Total} = \sigma T^4$, $\sigma = 5.6703 \times 10^{-8} \frac{W}{m^2 K^4}$.

Wien displacement law says that $\lambda_{max} T = 2.898 \times 10^{-3} m - K$.

Radiation power per unit area related to the energy density of a blackbody: $R(\lambda) = \frac{c}{4} \rho(\lambda)$.

Rayleigh-Jeans (classical equipartition argument) law $\rho(\lambda) = 8\pi k_B T / \lambda^4$ leads to the ‘ultraviolet catastrophe’.

Planck blackbody radiation (treat the atoms as having discrete energy states, and the light as having energy $E = hf$): $\rho(\lambda) = \frac{8\pi hc / \lambda^5}{e^{hc / \lambda k_B T} - 1}$, $h = 6.626 \times 10^{-34} J - s$.

Photoelectric effect: Photoelectric effect and the concept of light as a particle (photon with $E = hf$): $hf = eV_0 + \phi$. Photon collides with one electron and transfers all of its energy, $-V_0$ is the stopping potential.

X-ray production by Bremsstrahlung with cutoff $\lambda_{min} = \frac{1240}{V} nm$ (Duane-Hunt Rule), explained by Einstein as inverse photoemission with $\lambda_{min} = \frac{hc}{eV}$. Sharp emission lines arise from quantized energy levels in the ‘core shells’ of atoms.

Bragg reflection of x-rays from layers of atoms in crystals: $n\lambda = 2d \sin \theta$, where $n = 1, 2, 3, \dots$, d is the spacing between the parallel layers.

Rutherford scattering (Phys 410) suggested that positive charge is concentrated in a very small volume – the nuclear model of the atom.

Empirical rule for wavelengths of light emission from hydrogen $\frac{1}{\lambda_{mn}} = R \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$,

Rydberg constant $R = R_H = 1.096776 \times 10^7 \frac{1}{m}$ for Hydrogen.

Bohr model of the hydrogen atom (assumes stationary states, light comes from transitions between stationary states, electron angular momentum in circular orbits is quantized): $|\vec{L}| = |\vec{r} \times m\vec{v}| = mvr = n\hbar$, with $n = 1, 2, 3, \dots$, Radius of circular orbits:

$r_n = \frac{n^2 a_0}{Z}$ with $a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2} = 0.529 \text{ \AA}$, Total energy of Hydrogen atom: $E_n = -E_0 \frac{Z^2}{n^2}$,

with $E_0 = \frac{mc^2 (e^2 / 4\pi\epsilon_0)^2}{2(\hbar c)^2} = \frac{mc^2}{2} \alpha^2 = 13.6 \text{ eV}$, $\alpha = \frac{e^2 / 4\pi\epsilon_0}{\hbar c} \cong \frac{1}{137}$ is called the ‘fine structure constant’. Explains the Hydrogen atom emission spectrum but not multi-electron atoms.

Davisson-Germer experiment shows that matter (electrons) diffract from periodic structures (Ni atoms on a surface) like waves. It is clear that matter has a strong wave-like character when measured under appropriate conditions.

deBroglie relations: $f = \frac{E}{h}$ and $\lambda_{dB} = \frac{h}{p}$. deBroglie proposed the wavelength of matter waves as $\lambda_{dB} = h/p$, where p is the linear momentum. Classical physics should be recovered in the short- λ_{dB} limit – the Correspondence Principle.

Dispersion relation for a particle: $\hbar\omega = \frac{\hbar^2 k^2}{2m} + V(x, t)$.

The time-dependent Schrodinger equation: $-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V(x, t) \Psi(x, t) = i\hbar \frac{\partial \Psi(x, t)}{\partial t}$;

Separation of variables (assuming $V(x, t) = V(x)$ only) leads to $\Psi(x, t) = \psi(x) e^{-iEt/\hbar}$ (a property of stationary states);

Time-independent Schrodinger equation: $-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x)$;

The wavefunction $\Psi(x, t)$ is complex in general and cannot be measured. Born interpretation of the wave function in terms of a probability density $P(x, t) = \Psi^*(x, t) \Psi(x, t)$;

Probability current: $J(x, t) = \frac{i\hbar}{2m} \left(\Psi \frac{\partial \Psi^*}{\partial x} - \Psi^* \frac{\partial \Psi}{\partial x} \right)$; Normalization

condition: $\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx = 1$ and $\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$.

General solution to TDSE: $\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$; $\sum_{n=1}^{\infty} |c_n|^2 = 1$; $\langle \hat{\mathcal{H}} \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$;

Expectation values: $\langle x \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) x \Psi(x, t) dx$, and for any function of position: $\langle f(x) \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) f(x) \Psi(x, t) dx$

Linear momentum operator: $\hat{p} = -i\hbar \frac{\partial}{\partial x}$, Hamiltonian operator: $\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(x)$, the time independent Schrodinger equation written as an operator equation: $\hat{\mathcal{H}} \psi(x) = E \psi(x)$.

Definition of uncertainty: $\sigma = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$; The Uncertainty Principle: $\sigma_x \sigma_{p_x} \geq \hbar/2$;

One example of Ehrenfest's theorem: $\frac{d\langle x \rangle}{dt} = \frac{1}{m} \langle p \rangle$; Expectation values obey classical laws of motion!

Infinite square well of width a for a particle of mass m : Energy eigenvalues $E_n = \frac{\hbar^2 k_n^2}{2m} = n^2 \frac{\pi^2 \hbar^2}{2ma^2}$ with $n = 1, 2, 3, \dots$, and eigenfunctions $\psi_n(x) = \sqrt{2/a} \sin k_n x$, with $k_n = n\pi/a$; These eigenfunctions form a complete ortho-normal set on the interval $[0, a]$: $\int_{-\infty}^{+\infty} \psi_m^*(x) \psi_n(x) dx = \delta_{n,m}$; Use this to find the above expansion coefficients: $c_m = \int_{-\infty}^{+\infty} \psi_m^*(x) \Psi(x, 0) dx$, for $m = 1, 2, 3, \dots$

Harmonic oscillator: $V(x) = \frac{1}{2} m \omega^2 x^2$, leading to the TISE: $-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + \frac{1}{2} m \omega^2 x^2 \psi(x) = E \psi(x)$; Raising and Lowering operators: $\hat{a}_+ = \frac{1}{\sqrt{2m\hbar\omega}} (-i\hat{p} + m\omega\hat{x})$; $\hat{a}_- = \frac{1}{\sqrt{2m\hbar\omega}} (+i\hat{p} + m\omega\hat{x})$; Commutator: $[\hat{x}, \hat{p}] = i\hbar$; $\hat{a}_- \hat{a}_+ = \frac{1}{\hbar\omega} \hat{\mathcal{H}} + \frac{1}{2}$;

Moving up and down the ladder of states: $\hat{a}_+ \psi_n(x) = \sqrt{n+1} \psi_{n+1}(x)$; $\hat{a}_- \psi_n(x) = \sqrt{n} \psi_{n-1}(x)$;

Harmonic oscillator wavefunctions: $\psi_n(x) = \frac{1}{\sqrt{n!}} (\hat{a}_+)^n \psi_0(x)$; $\psi_n(x) =$

$\left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{m\omega x^2}{2\hbar}}$ $E_n = \left(n + \frac{1}{2} \right) \hbar\omega$, where $n = 0, 1, 2, 3, \dots$, and $H_n(x)$

are the Hermite polynomials. The number operator: $\hat{N} \psi_n = \hat{a}_+ \hat{a}_- \psi_n = n \psi_n$;

Expressing x and \hat{p} in terms of the raising and lowering operators: $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_+ + \hat{a}_-)$;

$\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}_+ - \hat{a}_-)$. This is a good shortcut for finding $\langle x \rangle$, $\langle \hat{p} \rangle$, etc.

The classical turning points are inflection points in $\psi(x)$.

Parity operator: $\hat{\Pi}\psi(x) = \psi(-x)$. Problems with symmetric potential have only even and odd parity wavefunction solutions. Parity alternates going up the energy ladder of states.

Free particle: $\Psi(x, t) = Ae^{i(kx - \hbar k^2 t/2m)}$, with $k = \pm\sqrt{\frac{2mE}{\hbar^2}}$; $\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \varphi(k) e^{i(kx - \hbar k^2 t/2m)} dk$; $\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \varphi(k) e^{ikx} dk$; $\varphi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x, 0) e^{-ikx} dk$; $v_{\text{phase}} = \frac{\omega}{k} = \frac{\hbar k}{2m} = \frac{p}{2m} = v_{\text{classical}}/2$; $v_{\text{group}} = \frac{d\omega}{dk} = \frac{\hbar k}{m} = v_{\text{classical}}$.

Delta function potential well: $V(x) = -\alpha \delta(x)$, with $\alpha > 0$; $\left. \frac{d\psi}{dx} \right|_{x=0^+} - \left. \frac{d\psi}{dx} \right|_{x=0^-} = -\frac{2m\alpha}{\hbar^2} \psi(0)$; single bound state ($E < 0$): $\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2}$ with $E = -\frac{m\alpha^2}{2\hbar^2} < 0$. Scattering states ($E > 0$): $\psi_I(x) = Ae^{ikx} + Be^{-ikx}$ for region I ($x < 0$), and $\psi_{II}(x) = Fe^{ikx} + Ge^{-ikx}$ for region II ($x > 0$), where $k^2 = +\frac{2mE}{\hbar^2} > 0$. $R = |B/A|^2 = \frac{\beta^2}{1+\beta^2} =$

$$\frac{1}{1+\frac{2\hbar^2}{m\alpha^2 E}}, T = |F/A|^2 = \frac{1/\beta^2}{1+1/\beta^2} = \frac{\frac{2\hbar^2}{m\alpha^2 E}}{1+\frac{2\hbar^2}{m\alpha^2 E}},$$

Scattering matrix treatment: express outgoing wave amplitudes in terms of incoming wave amplitudes: $\begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ G \end{pmatrix} = \bar{S} \begin{pmatrix} A \\ G \end{pmatrix}$.

Finite square well: $V(x) = \begin{cases} -V_0 & \text{for } -a < x < a \\ 0 & \text{for } x < -a \text{ and } x > a \end{cases}$. Finite square well of width $2a$

bound states given by solutions to the transcendental equation: $\tan(z) = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$ with $z = \frac{a}{\hbar} \sqrt{2m(E + V_0)}$ and $z_0 = \frac{a}{\hbar} \sqrt{2mV_0}$ (even parity solutions). There is always at least one solution!

Step potential $V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x > 0 \end{cases}$ has reflection probability $R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$, and transmission probability $T = \frac{4k_1 k_2}{(k_1 + k_2)^2}$, where $k_1 = \sqrt{2mE}/\hbar$ and $k_2 = \sqrt{2m(E - V_0)}/\hbar$.

Tunneling probability through a barrier $T = \left[1 + \frac{\sinh^2(\alpha a)}{4 \frac{E}{V_0} \left(1 - \frac{E}{V_0}\right)}\right]^{-1} \approx 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0}\right) e^{-2\alpha a}$, where a is the barrier width, and $\alpha = \sqrt{2m(V_0 - E)}/\hbar$.

Hilbert Space:

Originally defined as a function space: inner product or “projection” $\langle f|g \rangle = \int_{-\infty}^{\infty} f^*(x)g(x)dx$ $\langle f|g \rangle^* = \langle g|f \rangle$

A set of functions $\{f_n\}$ is orthonormal if they satisfy $\langle f_m | f_n \rangle = \int_{-\infty}^{\infty} f_m^*(x) f_n(x) dx = \delta_{m,n}$ with this one can express any function in Hilbert space: $f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$.

Hermitian conjugate of an operator: $\langle f | \hat{Q} g \rangle = \langle \hat{Q}^+ f | g \rangle$. For a Hermitian operator \hat{Q} : $\langle \psi | \hat{Q} \psi \rangle = \langle \hat{Q} \psi | \psi \rangle$. Operators can operate on kets or bras.

The momentum operator eigenfunction as expressed in real space. $\hat{p} f_p(x) = p f_p(x)$ yields $f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$ and Dirac orthogonality $\langle f_{p'} | f_p \rangle = \delta(p - p')$.

The position operator eigenfunction in position space: $g_y(x) = \delta(x - y)$

Generalized Statistical Interpretation:

Operator with a discrete spectrum: $\hat{Q} f_n = q_n f_n$, in state $|\Psi\rangle$ the probability of measuring q_n is $|\langle f_n | \Psi \rangle|^2$ and $\langle Q \rangle = \sum_n |\langle f_n | \Psi \rangle|^2 q_n$. Collapse of the wavefunction: measurement “projects out” an eigenstate of the \hat{Q} operator, and $|\Psi\rangle$ collapses to eigenfunction f_n .

$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = \begin{cases} 0 & \text{Compatible} \\ \neq 0 & \text{Incompatible} \end{cases} \quad \sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2 \quad \text{with } \sigma_A^2 = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$.

Generalized Ehrenfest theorem: $\frac{d}{dt} \langle \hat{Q} \rangle = \frac{i}{\hbar} \langle [\hat{\mathcal{H}}, \hat{Q}] \rangle + \langle \frac{\partial \hat{Q}}{\partial t} \rangle$

$\Psi(x, t) = \langle x | S(t) \rangle$, $\Phi(p, t) = \langle p | S(t) \rangle$

$\Phi(p, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \Psi(x, t) dx$ and $\Psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{+ipx/\hbar} \Phi(p, t) dp$

Orthonormal basis $|e_n\rangle$, $\langle e_m | e_n \rangle = \delta_{n,m}$ Operator as a set of matrix elements: $Q_{mn} \equiv \langle e_m | \hat{Q} | e_n \rangle$.

Example of 2-level system: $i\hbar \frac{d}{dt} |S(t)\rangle = \hat{\mathcal{H}} |S(t)\rangle$, $|S(t)\rangle = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$, $i\hbar \frac{d}{dt} \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \begin{pmatrix} \epsilon & -\Delta \\ -\Delta & \epsilon \end{pmatrix} \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$. TISE: $\hat{\mathcal{H}} |s\rangle = E |s\rangle$, with $E = \epsilon + \Delta$ with $|s_-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$; and $E = \epsilon - \Delta$ with $|s_+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$. $\langle s_+ | s_+ \rangle = \langle s_- | s_- \rangle = 1$ and $\langle s_+ | s_- \rangle = \langle s_- | s_+ \rangle = 0$.

Definition of bra: $\langle f | \cdots = \int f^*(x) \cdots dx$ $|\beta\rangle = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix}$ and $\langle \beta | = (b_1^* \quad b_2^* \quad b_3^* \quad \cdots)$ so

$\langle \alpha | \beta \rangle = a_1^* b_1 + a_2^* b_2 + a_3^* b_3 + \cdots$

Projection operator: $\hat{P}_\alpha = |\alpha\rangle \langle \alpha|$

Completeness: $\hat{1} = \sum_{n=1}^{\infty} |e_n\rangle \langle e_n|$ (discrete basis), $\hat{1} = \int |e_z\rangle \langle e_z| dz$ (continuous basis).

General state $|S(t)\rangle = \int \langle x | S(t) \rangle |x\rangle dx = \int \Psi(x, t) |x\rangle dx$, $|S(t)\rangle = \int \langle p | S(t) \rangle |p\rangle dp = \int \Phi(p, t) |p\rangle dp$, $|S(t)\rangle = \sum_{n=1}^{\infty} \langle n | S(t) \rangle |n\rangle = \sum_{n=1}^{\infty} c_n(t) |n\rangle$

$\hat{x} \rightarrow x$ in position space and $\hat{x} \rightarrow i\hbar \frac{\partial}{\partial p}$ in momentum space; $\hat{p} \rightarrow -i\hbar \frac{\partial}{\partial x}$ in position space and $\hat{p} \rightarrow p$ in momentum space.

3D QM Schrodinger equation $i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = \hat{\mathcal{H}} \Psi(\vec{r}, t)$ Probability density: $|\Psi(\vec{r}, t)|^2 d^3r$ is the probability of finding the particle within differential volume d^3r of the location \vec{r} in 3D space. Normalization $\iiint |\Psi(\vec{r}, t)|^2 d^3r = 1$.

3D momentum operator: $\hat{\vec{p}} = -i\hbar \left(\hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \right) = -i\hbar \vec{\nabla}$.

Separation of variables: $\Psi(\vec{r}, t) = \psi(\vec{r}) e^{-iEt/\hbar}$ if $V = V(\vec{r})$ only, independent of time.

3D TISE: $\frac{-\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r})$ and $\Psi(\vec{r}, t) = \sum_n c_n \psi_n(\vec{r}) e^{-iE_n t/\hbar}$

In spherical coordinates: $\frac{-\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi(r, \theta, \phi)}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi(r, \theta, \phi)}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \left(\frac{\partial^2 \psi(r, \theta, \phi)}{\partial \phi^2} \right) \right] + V(r, \theta, \phi) \psi(r, \theta, \phi) = E \psi(r, \theta, \phi)$ Consider central forces only, such that $V = V(r)$ only. Separate variables as $\psi(r, \theta, \phi) = R(r) Y(\theta, \phi)$ to arrive at two new equations: Radial $\frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - \frac{2mr^2}{\hbar^2} [V(r) - E] R = \ell(\ell + 1) R$ and Angular $\left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \left(\frac{\partial^2 Y}{\partial \phi^2} \right) \right] = -\ell(\ell + 1) Y$.

The TISE in sphericals can be regarded as: $\left(\frac{p_r^2}{2m} + \frac{p_\perp^2}{2m} + V(r) \right) \psi = E \psi$, with $\frac{p_r^2}{2m} = \frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right)$ for the radial kinetic energy operator, and $\frac{p_\perp^2}{2m} = \frac{|\vec{L}|^2}{2mr^2} = \frac{-\hbar^2}{2m} \left[\frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \left(\frac{\partial^2}{\partial \phi^2} \right) \right]$ for the “angular momentum squared” operator.

Solution to the angular equation: $Y_\ell^m(\theta, \phi) = \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} P_\ell^m(\cos \theta) e^{im\phi}$. Also note that $\ell \geq 0$, and $|m| \leq \ell$. The spherical harmonics are an orthonormal set of functions “on the sphere”: $\int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta Y_\ell^{m*}(\theta, \phi) Y_{\ell'}^{m'}(\theta, \phi) = \delta_{\ell, \ell'} \delta_{m, m'}$ any express any function of angle $f(\theta, \phi) = \sum_{\ell=0}^\infty \sum_{m=-\ell}^\ell c_{\ell, m} Y_\ell^m(\theta, \phi)$.

For the radial equation, define the effective potential $V_{eff}(r) = V(r) + \frac{\hbar^2 \ell(\ell+1)}{2m r^2}$ that includes the “centrifugal term” that pushes the particle away from the force center.

Infinite spherical well $V(r) = \begin{cases} 0 & r < a \\ \infty & r \geq a \end{cases}$ $\psi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r) Y_\ell^m(\theta, \phi) = A_{n\ell} j_\ell(\beta_{n\ell} r/a) Y_\ell^m(\theta, \phi)$, involving spherical Bessel functions where $n = 1, 2, 3, 4, \dots$ and $\ell = 0, 1, 2, 3, 4, \dots$ and $m \in \{-\ell, -\ell+1, -\ell+2, \dots, 0, \dots, \ell-2, \ell-1, \ell\}$.

Hydrogen atom: $V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$, radial Eq. $-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left[-\frac{e^2}{4\pi\epsilon_0 r} + \frac{\hbar^2 \ell(\ell+1)}{2m r^2} \right] u = E u$,

terminating the infinite series solution leads to $E_n = -\left[\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \right] \frac{1}{n^2}$, where $n =$

$1, 2, 3, \dots$, $E_1 = -13.6 \text{ eV}$. $a = \frac{4\pi\epsilon_0 \hbar^2}{me^2} = 0.529 \times 10^{-10} \text{ m}$, known as the Bohr radius.

Full solution: $\psi_{n\ell m}(r, \theta, \phi) = \sqrt{\left(\frac{2}{na} \right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!} \left(\frac{2r}{na} \right)^\ell} L_{n-\ell-1}^{2\ell+1} \left(\frac{2r}{na} \right) e^{-r/na} Y_\ell^m(\theta, \phi)$

Degeneracy of the n^{th} state of the hydrogen atom is given by $d(n) = \sum_{\ell=0}^{n-1} (2\ell+1) = n^2$. Transitions from higher energy states to lower states can be accomplished with photon emission with energy $E_\gamma = -13.6 \text{ eV} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$, $\frac{1}{\lambda} = R \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$, where R is the Rydberg constant.

Orbital Angular Momentum of the electron: $\vec{L} = \vec{r} \times \vec{p}$ classically. Angular momentum operator components: $\hat{L}_x = y \hat{p}_z - z \hat{p}_y$, $\hat{L}_y = z \hat{p}_x - x \hat{p}_z$, $\hat{L}_z = x \hat{p}_y - y \hat{p}_x$. None of the components commute: $[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$; $[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$; $[\hat{L}_z, \hat{L}_x] =$

$i\hbar\hat{L}_y$. This leads to an uncertainty relation for the components: $\sigma_{L_x}\sigma_{L_y} \geq \frac{\hbar}{2}|\langle\hat{L}_z\rangle|$ and cyclic permutations of x, y, z . Angular momentum squared operator $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$. $[\hat{L}^2, \hat{L}_z] = 0$. Ladder operators $\hat{L}_+ = \hat{L}_x + i\hat{L}_y$ and $\hat{L}_- = \hat{L}_x - i\hat{L}_y$.

One can show that $\hat{L}^2 = \hat{L}_\pm\hat{L}_\mp + \hat{L}_z^2 \mp \hbar\hat{L}_z$. The ladder of states associated with orbital angular momentum has these properties:

- 1) The ladder is centered on $m = 0$ (i.e. the ladder includes the value of $0\hbar$).
- 2) The ladder is symmetric about $m = 0$.
- 3) The ladder has steps in units of \hbar .

The corresponding differential operators for angular momentum: $\hat{L}_x = -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right)$, $\hat{L}_y = -i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right)$, $\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$. $\hat{L}_\pm = \pm\hbar e^{\pm i\phi}\left[\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right]$; $\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$

The Hydrogen atom wave functions as simultaneous eigenfunctions of the Hamiltonian and two angular momentum operators: $\hat{\mathcal{H}}\psi_{n\ell m}(r, \theta, \phi) = E_n\psi_{n\ell m}(r, \theta, \phi)$, $\hat{L}^2\psi_{n\ell m}(r, \theta, \phi) = \ell(\ell+1)\hbar^2\psi_{n\ell m}(r, \theta, \phi)$, $\hat{L}_z\psi_{n\ell m}(r, \theta, \phi) = m\hbar\psi_{n\ell m}(r, \theta, \phi)$

Spin Angular Momentum: Spin-1/2: a “two-valuedness not describable classically.” We adopt the same kets and operators as those developed for orbital angular momentum: $\hat{S}^2|s, m_s\rangle = s(s+1)\hbar^2|s, m_s\rangle$, and $\hat{S}_z|s, m_s\rangle = m_s\hbar|s, m_s\rangle$. $[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$, and all cyclic permutations. There is an associated ladder of states with properties:

- 1) The ladder is symmetric about $m_s = 0$.
- 2) The ladder has steps in units of \hbar .

Note that there are total of $2s+1$ steps in the ladder.

Spin raising and lowering operators: $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$, and $\hat{S}_\pm|s, m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s \pm 1)}|s, m_s \pm 1\rangle$.

Spin-1/2: Two-dimensional Hilbert space $|\Psi\rangle = \alpha\left|\frac{1}{2}, +\frac{1}{2}\right\rangle + \beta\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$, or going over to a column vector description, $|\Psi\rangle = \alpha\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. $\hat{S}^2 = \frac{3}{4}\hbar^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\sigma_z$, $\hat{S}_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ and $\hat{S}_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$, $\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_x$, $\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_y$.

The Pauli Spin Matrices square to the unit matrix: $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

Pauli spin matrices obey the commutation relations like the spin components, namely $[\sigma_x, \sigma_y] = i2\sigma_z$, and cyclic permutations. The two eigenvalues are $\lambda_1 = +1$, and $\lambda_2 = -1$ for all of the Pauli spin matrices.

The “up” eigenvector for the \hat{S}_x operator, expressed in the “ \hat{S}_z basis”: $(\chi_+)_x = \frac{1}{\sqrt{2}}\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right)$.

Spin in a magnetic field. The spin of a charged particle has a magnetic moment associated with it: $\vec{\mu} = \gamma\vec{S}$, where γ is called the gyromagnetic ratio. Spin in a magnetic field: $\mathcal{H} = -\vec{\mu} \cdot \vec{B}$. For $\vec{B} = B_0\hat{z}$, $\hat{\mathcal{H}} = -\gamma\hat{S}_zB_0$ and the matrix form of this Hamiltonian

is $\hat{\mathcal{H}} = -\gamma B_0 \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. TISE energy eigenvalues $E_{\mp} = \pm \gamma B_0 \frac{\hbar}{2}$. The corresponding eigenvectors are $\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, so we use “+” to refer to the “up” spin which is aligned with \vec{B} and therefore has lower energy $E_+ = -\gamma B_0 \frac{\hbar}{2}$. Time dependent Schrodinger equation for the spinor wavefunction: $i\hbar \frac{\partial \chi}{\partial t} = \hat{\mathcal{H}} \chi$. Time evolution of the spinor wavefunction: $\chi(t) = \begin{pmatrix} \cos(\alpha/2) e^{i\omega_L t/2} \\ \sin(\alpha/2) e^{-i\omega_L t/2} \end{pmatrix}$. An additional perpendicular rf magnetic field acts as a perturbation and can cause a transition of the spin to the higher energy state (ESR, NMR): $\hat{\mathcal{H}}_{pert} = -\gamma \hat{\vec{S}} \cdot \vec{B}_{rf} \cos(\omega_{rf} t)$.

Combining two spins: $\vec{S} = \vec{S}_1 + \vec{S}_2$. $S_z = S_{1z} + S_{2z}$. $S^2 = (\vec{S}_1 + \vec{S}_2)^2 = S_1^2 + S_2^2 + 2\vec{S}_1 \cdot \vec{S}_2$. Two spin-1/2 creates two ladders of states. First the $s = 1$ ladder of 3 states.

TRIPLET $|1 \ 1\rangle = |\uparrow\rangle|\uparrow\rangle$, $|1 \ 0\rangle = \frac{1}{\sqrt{2}}(|\downarrow\rangle|\uparrow\rangle + |\uparrow\rangle|\downarrow\rangle)$, and $|1 \ -1\rangle = |\downarrow\rangle|\downarrow\rangle$. And the $s = 0$ ladder of 1 state. **SINGLET** $|0 \ 0\rangle = \frac{1}{\sqrt{2}}(|\downarrow\rangle|\uparrow\rangle - |\uparrow\rangle|\downarrow\rangle)$. The states $|1 \ 1\rangle$, $|0 \ 0\rangle$, etc. are in the ‘coupled representation’, while the states $|\uparrow\rangle|\downarrow\rangle$, etc. are in the ‘un-coupled’ representation.

Combining general spins: $\vec{J} = \vec{J}_1 + \vec{J}_2$, this sum spin has possible quantum numbers j ranging from $\{j_1 + j_2, j_1 + j_2 - 1, \dots, |j_1 - j_2|\}$. Each of these j values is a ladder of states with $2j + 1$ rungs each.

Observation: For the Hermite, Legendre and Laguerre polynomials: all required that a parameter in the corresponding differential equation take on an integer value in order to terminate an infinite series which would otherwise diverge and give a non-normalizable wavefunction.

So **What is important?**

Understanding the motivation for a wave theory of matter

The Bohr model of the hydrogen atom – a good starting point!

Solving the TISE quickly and efficiently and accurately

Stationary states vs. full time-dependent solutions to the TDSE

Operators and how to form their expectation values {momentum, kinetic energy,

Hamiltonian, raising and lowering, angular momentum, ...}

Properties of the ubiquitous QM problems:

Infinite Square Well, Harmonic Oscillator, Free Particle, Finite square well, Dirac delta function well, scattering problems, radial equation with various choices for $V(r)$

Energy values, wavefunctions, orthonormality, quantum numbers and their possible values and constraints, degeneracies

Being able to sketch wavefunctions for new potentials using intuition about the properties of the wavefunction in one dimension

Copenhagen Interpretation of Quantum mechanics. All that we know about a quantum system is given by its wavefunction. There are no hidden variables or additional degrees of freedom, or trajectories, etc. A measurement collapses the wavefunction into an eigenstate of the operator representing the observable quantity.

Matrix mechanics – heavy use of linear algebra (see Appendix A)

Hilbert space generalization of QM (the natural setting for ang. mom. and spins!)

Bras and Kets representing quantum states and Matrix Elements representing operators

Utilizing orthonormal bases to represent arbitrary states

Evaluating commutators, recognizing incompatible operators, constructing uncertainty relations

Understanding that quantum states exist in Hilbert space, and can be projected into a number of different representations, as needed

Structure and properties of the Hydrogen atom

Angular and Radial equation solutions

This is the basis for atomic physics and understanding the periodic table

Spin Angular Momentum is the paradigm of “simple” quantum systems that live in Hilbert space

It is the basis for quantum bits (qubits)

Phys 401 has presented a series of exactly solvable QM problems

Phys 402 develops approximation methods to do with more realistic QM problems