Unitary Operators. A unitary operator U, by literal meaning of the word, preserves the normalization of a wavefunction it acts on: $\langle U\Psi, U\Psi\rangle = \langle \Psi, \Psi\rangle$. An even stronger statement is that it preserves the inner product between two wavefunctions: $\langle U\Psi_1, U\Psi_2\rangle = \langle \Psi_1, \Psi_2\rangle$. This is like preserving the "angle" between them, it is a geometrical conservation. Equivalently, $UU^\dagger = U^\dagger U = 1$.

Examples of Unitary Operators. *Translation operator* $D_{\vec{a}} = e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{a}}$, which shifts a wavefunction according to $D_{\vec{a}}\Psi(\vec{r}) = \Psi(\vec{r}-\vec{a})$. *Time evolution operator* $U(t,t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}$ (for a time-independent Hamiltonian), which translates a state forward in time according to $|\Psi(t)\rangle = U(t,t_0)|\Psi(t_0)\rangle$. *Rotation operator* $R_{\hat{n}}(\alpha) = e^{-\frac{i}{\hbar}\alpha\hat{n}\cdot\vec{l}}$, where $\vec{l}$ is angular momentum operator, which rotates a state around axis $\hat{n}$ through angle α according to $|\Psi'\rangle = R_{\hat{n}}(\alpha)|\Psi\rangle$. *Gauge symmetry operator* $U(f) = e^{\frac{ie}{\hbar c}f(\vec{r},t)}$, which effects the change in a wavefunction by $|\Psi'\rangle = U(f)|\Psi\rangle$ when an arbitrary change in electromagnetic gauge is applied according to $\vec{A}' = \vec{A} + \nabla f$, $\varphi' = \varphi - \frac{1}{c}\frac{\partial f}{\partial t}$.

Eigenvalues and Symmetry of Unitary Operators. Unitary operators have (complex) eigenvalues of unit magnitude, like $\lambda = e^{i\alpha}$, where α is a phase angle. Usually a unitary operation is a geometrical symmetry of the system, an operation that may commute with the Hamiltonian and leave expectation values unchanged. (Because it only changes states by an unobservable phase.) An obvious pattern appears in the examples above: the operator within each exponential is a *generator* of the related symmetry process.

Dirac Bra-Ket Notation. Abstract "ket" state vectors written as $|\Psi\rangle$, are not in any particular basis or representation. Dual "bra" vectors written as $\langle\Psi|$ are hermitian conjugate of ket vectors. (Scalar) Inner products of two states written as $\langle\Psi_1|\Psi_2\rangle$, again, no basis expressed.

Projection Operators. Basic projector onto one state $|a\rangle$ is $P_a = |a\rangle\langle a|$. Applied to an arbitrary ket or bra, gives the component of that arbitrary state vector along state $|a\rangle$, specifically $P_a|\Psi\rangle = |a\rangle\langle a|\Psi\rangle$, similarly for application onto a bra vector.

Projection into a Basis. Use a sum over a complete set of eigenstates $|a\rangle$ of some operator A to express a projection operator which is an identity operator, $P_A = 1 = \sum_n |a_n\rangle\langle a_n|$. This type of projector allows easy expansion of an arbitrary state in any basis (any choice of operator A) according to $|\Psi\rangle = P_A|\Psi\rangle = \sum_n |a_n\rangle\langle a_n|\Psi\rangle$. The quantity $\langle a_n|\Psi\rangle$ is the "wavefunction" for Ψ in the "A" representation, as in $\Psi(\vec{r}) = \langle\vec{r}|\Psi\rangle$.

Use of Projectors. Put quantities into desired basis by liberal insertion of $P_A = 1$ operators. Example, $\langle\Psi_1|\Psi_2\rangle = \langle\Psi_1 P_A|\Psi_2\rangle = \sum_n \langle\Psi_1|a_n\rangle\langle a_n|\Psi_2\rangle = \sum_n \Psi_1^*(a_n)\Psi_2(a_n)$ is the usual type of summation expression for an inner product. (For A with a continuous spectrum use an integral in place of the sum.)

Matrix Representation of QM. (Written for discrete spectrum for some operator X here.) State $|\Psi\rangle = \sum_n |x_n\rangle\langle x_n|\Psi\rangle$ in X representation. Probability amplitude $\Psi_n \equiv \langle x_n|\Psi\rangle$. The set of values Ψ_n forms a column vector that represents state $|\Psi\rangle$ in the X representation. Some operator A can be expressed in this X representation by a matrix with elements $A_{m,n} \equiv \langle x_m|A|x_n\rangle$. Action of operator A acting on $|\Psi\rangle$ in X representation produces a state $A|\Psi\rangle$ expressed in matrix form in X representation as $(A\Psi)_m = \sum_n A_{m,n}\Psi_n$, very simple! Use projectors to transform to other representations. Schrodinger equation $H|\Psi\rangle = E|\Psi\rangle$ in matrix notation becomes $\sum_n H_{m,n}\Psi_n = E\Psi_m$.

Change of Basis or Representation Start in Q rep: $\Psi_{q_n} = \langle q_n|\Psi\rangle$. Change to X rep: $\Psi_{x_n} = \langle x_n|\Psi\rangle$. Transformation is via $\langle x_n|P_Q\Psi\rangle = \sum_m \langle x_n|q_m\rangle\langle q_m|\Psi\rangle$ so $\Psi_{x_n} = \sum_m S_{n,m}\Psi_{q_m}$, where the transformation matrix has elements $S_{n,m} = \langle x_n|q_m\rangle$. An arbitrary operator A expressed starting in the new X rep has matrix elements: $A_{x_n,x_m} = \langle x_n|A|x_m\rangle = \langle x_n|P_Q A P_Q|x_m\rangle = \sum_k \sum_l \langle x_n|q_k\rangle\langle q_k|A|q_l\rangle\langle q_l|x_m\rangle$. Then this means $A_{x_n,x_m} = \sum_k \sum_l S_{n,k} A_{q_k,q_l} S^\dagger_{l,m}$. Simply, summarize these as matrix equations like $(\Psi)_X = S \cdot (\Psi)_Q$ and $(A)_X = S \cdot (A)_Q \cdot S^\dagger$, with $(S) = \langle X|Q\rangle$ in fairly obvious notations.

Measurement in QM. We already know, if observable A is measured in an experiment on a system in quantum state $|\Psi\rangle$, the results can only be one of its eigenvalues. We stress two points: 1) The probability that a particular eigenvalue a_i is obtained is given by $w(a_i) = \langle\Psi|P_i|\Psi\rangle/\langle\Psi|\Psi\rangle$, where $P_i \equiv |a_i\rangle\langle a_i|$ is a projection operator onto the desired eigenstate. 2) After the measurement is made, if the value a_i was obtained in a single event, then the final quantum state is $|\Psi\rangle = |a_i\rangle$. This is the so-called "collapse of the wavefunction." The state of the system in modified by the measurement, in an uncontrolled way!

Time Evolution Operator. Advances state vectors forward in time as $|\Psi(t)\rangle = U(t,t_0)|\Psi(t_0)\rangle$. Postulated to solve the operator differential equation $i\hbar\frac{d}{dt}U(t,t_0) = H(t)U(t,t_0)$ with initial condition $U(t_0,t_0) = 1$.

Different Pictures of Dynamics. *Schrodinger Picture:* State vectors $|\Psi(t)\rangle$ depend on time while usual operators do not. This is the usual way we have viewed QM. *Heisenberg Picture:* State vectors $|\Psi\rangle$ are fixed in time while operators have time dependence determined from H, according to $\frac{d}{dt}A_H = \frac{1}{i\hbar}[A_H, H] + \frac{\partial}{\partial t}A_H$. Looks like classical mechanics if we equate $\frac{1}{i\hbar}[A, H]$ with the classical Poisson bracket $\{A, H\}$. Solution is also written as $A_H = U^\dagger(t, t_0)AU(t, t_0)$, where $A = A(t_0)$ is the operator of the Schrodinger picture.

One-Dimensional Piecewise Constant Potentials. Match logarithmic derivatives at interfaces: $\frac{d}{dx}ln(\psi_I(x)) = \frac{d}{dx}ln(\Psi_{II}(x))$ at a boundary point $x = a$. Probability current in $\psi = e^{ikx}$ is $J = \hbar k/m$. Define reflection or transmission coefficients using ratios of probability currents. Define time-delay of a wave by $t_{delay} = \hbar\frac{d(2\phi)}{dE}$ where (2ϕ) is a phase shift between two waves. Review solution methods for finite depth square wells. Understand condition for oscillatory $(E > V)$ vs. decaying or growing exponential $(E < V)$ wavefunctions, tunneling, etc.

One-Dimensional Harmonic Oscillators. Energy eigenvalues $E_n = \hbar\omega(n + 1/2)$. Energy eigenfunctions $\psi_n(x) = (\frac{m\omega}{\hbar})^{1/4}(\sqrt{\pi}2^n n!)^{-1/2}e^{-\xi^2/2}H_n(\xi)$, in terms of $\xi = \sqrt{\frac{m\omega}{\hbar}}x$ and Hermite polynomials. Similar expression in momentum space. Parity of solutions is $(-1)^n$. Have simultaneous eigenfunctions of energy and parity because parity operation commutes with H, as H is invariant under inversion.

Operator Method for Harmonic Oscillator. Creation/annihilation (or raising/lowering) operators defined via $x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$, $ip = \sqrt{\frac{\hbar}{2m\omega}}(a - a^\dagger)$. Basic commutation relation $[a, a^\dagger] = 1$. Hamiltonian $H = \hbar\omega(aa^\dagger + 1/2)$. Number operator that counts quanta of excitation is $N = a^\dagger a$. Creation/annihilation commutations $[N, a^\dagger] = a^\dagger$, $[N, a] = -a$. Action of creation/annihilation on energy eigenstates is $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$, $a|n\rangle = \sqrt{n}|n-1\rangle$, which can be used to find arbitrary matrix elements. Normalized eigenstates obtained from ground state by $|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$.

Multi-dimensional Harmonic Oscillators. For dynamics of a sum of d degrees of freedom following identical harmonic oscillator hamiltonians, normalized eigenstates $|n_1, n_2, ...n_d\rangle = \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1!}}\frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2!}}...\frac{(a_d^\dagger)^{n_d}}{\sqrt{n_d!}}|0\rangle$. Energies of states are $E_n = \hbar\omega(n + d/2)$, with large degeneracy increasing with n. Principle quantum number $n = n_1 + n_2 + ... + n_d$.

Two-dimensional Harmonic Oscillator. Degeneracy related to a conserved angular momentum, $L_z = i\hbar(a_1a_2^\dagger - a_1^\dagger a_2)$. Creation operators $A_\pm^\dagger = \frac{1}{\sqrt{2}}(a_1^\dagger \pm a_2^\dagger)$ produce quanta with energy $\hbar\omega$ and angular momentum $\pm\hbar$. Number operators $N_+ = A_+^\dagger A_+$, and $N_- = A_-^\dagger A_-$. Total quanta number operator $N = N_1 + N_2 = N_+ + N_-$. Net angular momentum operator $L_z = \hbar(N_+ - N_-)$. Normalized simultaneous eigenstates of H and L_z with energy $\hbar\omega(n + 1)$ and angular momentum $l\hbar$ produced by $|n, l\rangle = \frac{(A_+^\dagger)^{n_+}}{\sqrt{n_+!}}\frac{(A_-^\dagger)^{n_-}}{\sqrt{n_-!}}|0\rangle$, where $n_+ = (n + l)/2$, and $n_- = (n - l)/2$.

Why Angular Momentum is Fun. Total momentum squared $\vec{p}^{\,2} = p_r^2 + \vec{l}^{\,2}/r^2$, radial momentum $p_r = -i\hbar \frac{1}{r}\frac{\partial}{\partial r}(r\cdot\ )$, orbital angular momentum $\vec{l} = \vec{r}\times\vec{p} = -i\hbar\vec{r}\times\vec{\nabla}$. Angular momentum is a good quantum number if Hamiltonian is spherically symmetric, which implies $[\vec{l}^{\,2}, H] = \vec{l}, H] = 0$. Kinetic energy has a radial and an angular part.

General Angular Momentum Properties. Any set of three quantities (J_x, J_y, J_z) with commutation relations like $[J_x, J_y] = i\hbar J_z$ and its cyclic permutations is an angular momentum. The possible (eigen-)values of squared angular momentum $\vec{J}^{\,2}$ in Nature are $j(j+1)\hbar^2$, where $j = 0, 1/2, 1, 3/2, ...$ etc. The possible (eigen-)values of any component of an angular momentum, for a given j, are from $-j\hbar$ to $+j\hbar$, in increments of $\hbar$. For a given j, there are $2j+1$ substates with different projection of angular momentum on a chosen axis. Usually that chosen axis is the z-axis.

Raising and Lowering of Angular Momentum Eigenstates. Eigenstates $|j, m\rangle$ have $\vec{J}^{\,2}$ and J_z eigenvalues of $j(j+1)\hbar^2$ and $m\hbar$, respectively. j can be integer or half-integer. m ranges from $-j$ to $+j$ in unit increments. Raising operator $J_+ = J_x + iJ_y$ increases m by one: $J_+|j, m\rangle = \hbar\sqrt{j(j+1) - m(m+1)}|j, m+1\rangle$. Lowering operator $J_- = J_x - iJ_y$ decreases m by one: $J_-|j, m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}|j, m-1\rangle$. These new states will be unit normalized if the original ones were.

Commutation and other Operator Relations. The J_z operator acts something like a number operator with respect to the raising/lowering operators: $[J_z, J_+] = \hbar J_+$, and $[J_z, J_-] = -\hbar J_-$ (compare relations between N and $a^\dagger$ and a for a harmonic oscillator). Also have relations like $[J_+, J_-] = 2\hbar J_z$ and $\vec{J}^{\,2} = \frac{1}{2}(J_+J_- + J_-J_+) + J_z^2$, from which $J_-J_+ = \vec{J}^{\,2} - J_z(J_z + \hbar)$, and $J_+J_- = \vec{J}^{\,2} - J_z(J_z - \hbar)$.

Orbital Angular Momentum, Spherical Coordinates. Orbital angular momentum, l must be integer. From basic definitions and algebra: $l_x = i\hbar(\sin\phi\frac{\partial}{\partial\theta} + \cos\phi\cot\theta\frac{\partial}{\partial\phi})$, $l_y = i\hbar(-\cos\phi\frac{\partial}{\partial\theta} + \sin\phi\cot\theta\frac{\partial}{\partial\phi})$, $l_z = -i\hbar\frac{\partial}{\partial\phi}$. Raising and lowering are $l_+ = l_x + il_y = \hbar e^{i\phi}(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi})$. $l_- = l_x - il_y = -\hbar e^{-i\phi}(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\phi})$.

Why Care about Spherical Harmonics. The coordinate space representation of the orbital angular momentum states $|l, m\rangle$ are the spherical harmonics: $\langle\hat{r}|l, m\rangle = Y_l^m(\theta, \phi)$, where $\hat{r} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is the unit vector to position $\vec{r}$. Then they have obvious orthogonality relations $\langle l, m|l', m'\rangle = \int d\Omega\ Y_l^m(\Omega)Y_{l'}^{m'}(\Omega) = \delta_{l,l'}\delta_{m,m'}$, where $d\Omega = d\phi\ d(\cos\theta)$. Under inversion (parity operation), $PY_l^m(\theta, \phi) = Y_l^m(\pi - \theta, \phi + \pi) = (-l)^l Y_l^m(\theta, \phi)$. The Y_l^m form a complete set (basis) in which arbitrary functions of θ and ϕ can be expanded (for chosen l). This makes for easy evaluation of $\langle\vec{l}^{\,2}\rangle$ and $\langle l_z\rangle$.

Rotations of Quantum States. Operation $\mathcal{R}$ rotates a statevector, or wavefunction, to give a rotated wavefunction according to $\Psi'(\vec{r}) \equiv \mathcal{R}[\Psi(\vec{r}\ )] = \Psi(\mathcal{R}^{-1}[\vec{r}\ ])$. The rotation only moves the probability density around in space.

Unitary Operators for Rotations. State vector of rotated state is related to unrotated by $|\Psi'\rangle = R|\Psi\rangle$, where unitary operator R produces the effect of some rotation operation $\mathcal{R}$. An observable is changed by rotation into the rotated observable according to $Q' = RQR^\dagger$. For an infinitesimal rotation thru angle ε around axis $\hat{n}$, the unitary operator is $R_{\hat{n}}(\varepsilon) = 1 - \frac{i}{\hbar}\varepsilon\hat{n}\cdot\vec{J}$. For a finite rotation thru angle α around axis $\hat{n}$, the unitary operator is $R_{\hat{n}}(\alpha) = e^{-\frac{i}{\hbar}\alpha\hat{n}\cdot\vec{J}}$. Can be used to modify states or operators as desired, by given rotations.

QM States of Spherically Symmetric Potentials. If Hamiltonian H has spherical symmetry, i.e., $V(\vec{r}) = V(r)$, then $\vec{l}^{\,2}$ and l_z commute with H and are (conserved) good quantum numbers. Wavefunctions must have form $\Psi(\vec{r}) = R(r)Y_l^m(\theta,\phi)$. Scaled radial wavefunction $u(r) \equiv rR(r)$ satisfies a 1D Schrodinger equation, with an added centrifugal potential: $\frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[\frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]u = Eu$. Particular solutions depend on the potential form.

Region of Constant Spherically Symmetric Potential V_0. $R(r)$ satisfies Bessel equation of half-integer order, $\nu = l + 1/2$. Solutions are spherical Bessel functions $R(r) = j_l(kr), n_l(kr)$, where $k = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$. $j_l(kr)$ is finite at $r \to 0$, $n_l(kr)$ diverges at $r \to 0$. Related are spherical Hankel functions $h_l^{(\alpha)}(kr) = j_l(kr) + i\alpha n_l(kr)$, $\alpha = \pm 1$ usually denoted as "first type" ($\alpha = +1$) or "second type" ($\alpha = -1$). $h_l^{(1)}$ represents outgoing spherical waves, $h_l^{(2)}$ represents incoming spherical waves; application is in scattering problems.

Spherically Symmetric Coulomb Potential $V(r) = -\frac{Ze^2}{r}$. Asymptotic behaviors lead to bound state scaled radial wavefunction $u(\rho) = \rho^{\,l+1}e^{-\rho}w(\rho)$. Scaled radial coordinate is $\rho = kr = \sqrt{\frac{2m|E|}{\hbar^2}}r$. Power series solution leads to associated Laguerre polynomials. Energies given by Balmer formula $E_n = \frac{E_1}{n^2}$, ground state energy $E_1 = -\frac{Z^2e^2}{2a_B}$ using Bohr radius $a_B = \frac{\hbar^2}{me^2}$. Radial length scale is $a_n = \frac{na_B}{Z}$, depends on principal quantum number n and on atomic number Z. Principal quantum number n must be greater than l, that is, $l = 0, 1, 2...(n-1)$. Degeneracy of each of the infinite number of bound energy levels is determined by the angular momentum (e.g., $2l + 1$ due to orbital angular momentum symmetry). Wavefunctions $\psi_{l,m,n}$ and associated probability densities have both radial and angular dependencies, determined by quantum numbers n, l, m.