Lecture 1 Highlights
Phys 402

We started with a brief review of classical physics. Kinematics is the description of motion. Classically, a particle is a point-like object that follows a well-defined trajectory given by $\vec{x}(t)$. In principle, the trajectory of a particle can be determined with arbitrary precision, and the act of measuring the trajectory does not disturb the particle. At any instant it has a velocity vector $\vec{v}(t)$ and acceleration vector $\vec{a}(t)$. Dynamics is the study of why motion occurs. It is summarized by Newton's second law of motion, relating a kinematic quantity to the net unbalanced force acting on the particle of mass m: $\vec{a} = \vec{F}_{net} / m$. Conservative forces can be derived from a scalar potential V as $\vec{F} = -\vec{\nabla} V$, and manipulation of the scalar potential is often easier than solving problems directly with the vector force. (In quantum mechanics all microscopic forces are conservative.)

We also briefly reviewed Lagrangian and Hamiltonian mechanics, the idea of generalized coordinates and their conjugate momenta. Generalized coordinates are the minimal set of coordinates required to describe the most general motion of the system. It is important to recognize that these coordinates do not have to be spatial variables (i.e. x, y, z), but can represent any degree of freedom of the system, such as charge on a capacitor, magnetic flux in a loop, etc. The *conjugate momenta* are derived from the Lagrangian. The Hamiltonian is a description of the system in terms of only the generalized coordinates and their conjugate momenta.

In quantum mechanics, kinematics plays essentially no role, since the concept of trajectory is not compatible with the uncertainty principle for position and momentum. Dynamics survives in the form of the time-dependent Schrödinger equation.

Quantum mechanics is a wave theory of matter. The theory revolves around determination and use of the wavefunction Ψ. The statistical interpretation of quantum mechanics means that we calculate probabilities of finding the particle in a given location, rather than calculating a precisely defined trajectory. For example, $|\Psi(\vec{x},t)|^2\, d^3x$ is the probability of finding a particle within a differential volume d^3x of location $\vec{x}$ at time t. The wavefunction is normalized so that $\iiint |\Psi(\vec{x},t)|^2\, d^3x = 1$ for all time t. Among other things, this constraint means that we only consider physically relevant solutions to the Schrodinger equation. The dimensionality of the wavefunction is $[\Psi(\vec{x},t)] = length^{-dN/2}$, where d is the dimensionality of the system (1, 2, or 3) and N is the number of particles described by the wavefunction.

Quantum dynamics are described by the time-dependent Schrodinger equation: $-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$, where $V(x,t)$ is the total potential associated with all conservative forces acting on the particle, in one dimension. Separation of variables leads to $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$ (a property of stationary states). This leads to the time-independent Schrodinger equation: $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\,\psi(x) = E\psi(x)$, where E is the energy eigenvalue.

Dynamical variables are replaced by operators: position x becomes the position operator $\hat{x}$, momentum p becomes the momentum operator $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$. The kinetic energy operator is $\hat{K} = \frac{\hat{p}_x{}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$. An operator is an instruction to do something to the function that follows. Expectation values for dynamical quantities are defined as $\langle\hat{Q}\rangle \equiv \int \psi^* \, \hat{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right) \psi \, dx$. For instance, the expectation value of kinetic energy is $\langle\hat{T}\rangle = -\frac{\hbar^2}{2m}\int \psi^* \, \frac{\partial^2}{\partial x^2} \, \psi \, dx$. The expectation value is the average of repeated measurements on an *ensemble* of identically prepared systems. It is NOT the average of repeated measurements on one single system.

We next reviewed the Postulates of Quantum Mechanics. These are assumptions that we make, and we then explore the logical consequences of these assumptions in the description of the physical world. So far, they have allowed us to calculate many properties of the microscopic world, in excellent agreement with experimental results.

We also reviewed the concepts of compatible and incompatible operators. Two observables A and B which can be simultaneously determined are said to be compatible observables. In the Hydrogen atom, the Hamiltonian $\mathcal{H}$ (total energy), angular momentum squared L^2, and the z-component of angular momentum L_z are compatible observables, as an example. The hydrogen atom wavefunction $\psi_{n,\ell,m}(r,\theta,\varphi)$ is a simultaneous eigenfunction of all three observables: $\widehat{\mathcal{H}}\,\psi_{n,\ell,m}(r,\theta,\varphi) = E_n\psi_{n,\ell,m}(r,\theta,\varphi)$, $\widehat{L^2}\,\psi_{n,\ell,m}(r,\theta,\varphi) = \hbar^2\ell(\ell+1)\psi_{n,\ell,m}(r,\theta,\varphi)$, and $\widehat{L_z}\,\psi_{n,\ell,m}(r,\theta,\varphi) = m\hbar\,\psi_{n,\ell,m}(r,\theta,\varphi)$. These eigenvalues can be simultaneously determined, and it does not matter which order these observables are measured, the outcome will be the same. In other words, $\widehat{\mathcal{H}}\,\widehat{L^2}\,\psi_{n,\ell,m}(r,\theta,\varphi) = \widehat{L^2}\,\widehat{\mathcal{H}}\,\psi_{n,\ell,m}(r,\theta,\varphi)$, or more compactly $\left(\widehat{\mathcal{H}}\,\widehat{L^2} - \widehat{L^2}\,\widehat{\mathcal{H}}\right)\psi_{n,\ell,m}(r,\theta,\varphi) = 0$, or since this is actually just a property of the operators and not the eigenfunction, $\left(\widehat{\mathcal{H}}\,\widehat{L^2} - \widehat{L^2}\,\widehat{\mathcal{H}}\right) = 0$, or $\left[\widehat{\mathcal{H}}, \widehat{L^2}\right] = 0$. Incompatible operators cannot be determined simultaneously. The measurement of the second observable causes the information supplied by the first observable to be lost. One cannot construct simultaneous eigenfunctions of incompatible observables. The outcome of the measurement of the two observables depends on the order in which they are measured: $\hat{A}\,\hat{B}\,\psi \neq \hat{B}\,\hat{A}\,\psi$. This can be expressed in terms of a non-zero commutator: $\left[\hat{A},\hat{B}\right] \neq 0$. This leads to the "generalized uncertainty principle" for any two incompatible observables: $\sigma_A^2\,\sigma_B^2 \geq \left(\frac{1}{2i}\langle[A,B]\rangle\right)^2$ (this is Griffiths Eq. [3.62]). Here the 'variance' of the operator is defined as $\sigma_A^2 = \langle(A - \langle A\rangle)^2\rangle$. In the case of position and momentum this starts with the commutator $[\hat{x},\hat{p}_x] = i\hbar$, which results in $\sigma_x\,\sigma_{p_x} \geq \hbar/2$.

We then began a review of the full 3D solution to the Schrodinger equation for the basic (no spin, non-relativistic) hydrogen atom. The interaction force between the proton and electron is the Coulomb force: $\vec{F} = \frac{q_1 q_1}{4\pi\varepsilon_0 r^2}\hat{r}$, where $q_1 = +e$ for the proton and $q_2 = -e$ for the electron. Here we assume that the proton is infinitely massive and locate the origin there. (In reality we perform a transformation of the original problem to the center of mass and relative coordinates, and this will be reviewed in a homework problem later in the semester.) The unit vector $\hat{r}$ points from the proton to the electron. We also adopt a spherical coordinate system (r,θ,φ) with the z-axis in an arbitrary direction. All forces at the microscopic scale are conservative (work done between two points is independent of the path taken), hence they can be represented in terms of a scalar potential $V(r)$ as $\vec{F} =$

$-\vec{\nabla} V$. For the Coulomb interaction this is $V(r) = \frac{-e^2}{4\pi\varepsilon_0 r}$. We use the scalar potential in the Schrodinger equation as a stand-in for the force interaction.

In Phys 401 we solved the time-dependent Schrodinger equation for the hydrogen atom: $-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{x},t) - \frac{e^2}{4\pi\varepsilon_0 r}\Psi(\vec{x},t) = i\hbar\frac{\partial\Psi(\vec{x},t)}{\partial t}$, where m is the (reduced) mass of the electron. The first step is to separate variables by assuming the hydrogen atom is in a stationary state of well-defined energy E (i.e. it is in an energy eigen-state): $\Psi(x,t) = u(r,\theta,\varphi)e^{-iEt/\hbar}$. This leads to the time-independent Schrodinger equation: $-\frac{\hbar^2}{2m}\nabla^2 \mathrm{u} - \frac{e^2}{4\pi\varepsilon_0 r}\mathrm{u} = E\,u$.

The full solution to the (un-perturbed, and no-spin) Hydrogen atom wavefunction is:

$$u_{n,\ell,m}(r,\theta,\varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}}\; e^{-\frac{r}{na_0}} \left(\frac{2r}{na_0}\right)^\ell L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right) Y_{\ell,m}(\theta,\varphi),$$

where $n = 1, 2, 3, \ldots$, $\ell = 0, 1, 2, \ldots, n-1$ and m runs from $-\ell$ to $+\ell$ in integer steps. As a function of radial coordinate r, this wavefunction has a power-law behavior at small r, it wiggles with $n-\ell-1$ zero-crossings, and then has an exponential decay at large r. The full time-dependent wavefunction is,

$$\Psi_{n,\ell,m}(r,\theta,\varphi,t) = u_{n,\ell,m}(r,\theta,\varphi)e^{-iE_n t/\hbar}.$$

The degeneracy $d(n) = n^2$ in the un-perturbed hydrogen atom. All will be broken by the end of this semester!