A Partial Review of Phys 401

Modern Physics: Important ideas include first quantization – the fact that matter is not continuous but comes in discrete 'chunks'; energy states in atoms are discrete and quantized;

Light carries energy $E = hf$, where h is Planck's constant and f is the frequency of oscillation of the electromagnetic fields;

Light sometimes acts like a particle (photon) in it's interactions;

Particles can sometimes act like waves with a wavelength given by $\lambda = h/p$, where p is the linear momentum of the particle;

The semi-classical Bohr model of the hydrogen atom assumes that electron angular momentum around the proton is quantized in multiples of $\hbar = h/2\pi$ and successfully predicts the main features of the light emission spectrum of the atom;

Quantum Mechanics: the Schrodinger equation makes predictions for the evolution of the complex wavefunction as a function of space and time;

The wavefunction squared $|\Psi(\vec{x}, t)|^2$ can be interpreted probabilistically;

You should be familiar with solutions to these 1D QM problems (eigen-values and eigen-functions): infinite square well, finite square well, harmonic oscillator, delta-function well, step potential, tunneling through a finite-width and finite-height barrier.

Classical Mechanics: Kinematics is the *description of motion*. Classically, a particle is a point-like object that follows a well-defined trajectory given by $\vec{x}(t)$. 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.)

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.

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. The dimensionality of the wavefunction is $[\Psi(\vec{x}, t)] = length^{-dN/2}$, where d is the dimensionality of the system 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.

For time-independent potentials, 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 $\widehat{K} = \frac{\hat{p}_x^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$. An operator is an instruction to do something to the function that follows.

Expectation values for dynamical quantities are defined as $\langle D \rangle \equiv \int \psi^* D\left(x, -i\hbar\frac{\partial}{\partial x}\right)\psi\,dx$. For instance the expectation value of kinetic energy is $\langle T \rangle = -\frac{\hbar^2}{2m}\int \psi^* \frac{\partial^2}{\partial x^2}\psi\,dx$.

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.

There are a concise set of <u>Postulates of Quantum Mechanics</u>. 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.

Two observables A and B which can be simultaneously determined are said to be **compatible observables**. In the Hydrogen atom, the Hamiltonian $\widehat{\mathcal{H}}$ (total energy), angular momentum squared $\widehat{L^2}$, and the z-component of angular momentum $\widehat{L_z}$ are compatible observables, as an example. The hydrogen atom waveunction $\psi_{n,\ell,m}(r,\theta,\varphi)$ 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: $\sigma_A^2\,\sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A}, \hat{B}]\rangle\right)^2$. Here the 'variance' of the operator is defined as $\sigma_A^2 = \langle\left(\hat{A} - \langle\hat{A}\rangle\right)^2\rangle$. In the case of position and momentum this starts with the commutator $[\hat{x}, \hat{p}_x] = i\hbar$, which results in $\sigma_x\,\sigma_{p_x} \geq \hbar/2$.