REVIEW OF QUANTUM MECHANICS

Let us start from classical physics. Imagine a particle of mass m, constrained to move along the x-axis, subject to some force F, which could in general depend on both x and t.
The particle will follow a precise trajectory $x(t)$, and finding $x(t)$ is the program of classical mechanics.
How do we find $x(t)$? We know that $\dot{x}(t) = v(t)$, $\ddot{x}(t) = a(t)$ and $m \cdot a(t) = F(x,t)$
In the case of conservative forces (the <u>only</u> kind that occur at microscopic level in quantum mechanics), I have:

$$F(x,t) = -\frac{\partial V(x,t)}{\partial x} \qquad \text{where } V(x,t) \text{ is some potential}$$

At any instant, particle has specific position, velocity, and acceleration which I can find by solving:

$$m \frac{d^2 x}{dt^2} = -\frac{\partial V}{\partial x} \qquad \underline{\text{Newton's law}}$$

In QM, kinematics plays no rôle: concept of trajectory not compatible with uncertainty principle. Dynamics survives in Schrödinger's equation:

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = \mathcal{H} \psi(x,t) \qquad \underline{\text{Schrödinger's equation}}$$

where $\psi(x,t)$ is the particle's wave function, and $\mathcal{H}$ is the Hamiltonian operator.
The Hamiltonian operator is the QM equivalent of the classical energy; the classical Hamiltonian is: $H = \frac{p^2}{2m} + V = E$

and it is equal to the energy E

Let me apply a substitution of the classical p and E with the corresponding QM operators:

$$p \rightarrow \frac{\hbar}{i}\nabla \qquad E \rightarrow i\hbar\frac{\partial}{\partial t}$$

Then:

$$H = \frac{p^2}{2m} + V \implies \mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 + V$$

Schrödinger's equation becomes:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

Let us take a 1D free particle: $\psi(x,t) = e^{i(kx-\omega t)}$

momentum p: $\frac{\hbar}{i}\nabla\psi = \hbar k\,\psi$: De Broglie $p = \hbar k$

energy E: $i\hbar\frac{\partial\psi}{\partial t} = \hbar\omega\,\psi$: Einstein $E = \hbar\omega$

<u>Fundamental concept</u>:

experimentally measurable observables appear as Hermitian operators acting on a complex-valued wavefunction $\psi(x,t)$ which remains <u>unobservable</u> by direct means

What can we observe, how do we "use" $\psi(x,t)$?

While $\psi(x,t)$ by itself has no physical meaning, it is useful:

- $|\psi(x,t)|^2$ is interpreted (Born) as a probability density
  $\overset{\shortparallel}{\psi^*(x,t)\psi(x,t)}$

  $$\int_a^b |\psi(x,t)|^2 dx = \text{probability of finding the particle between } x=a \text{ and } x=b \text{ at time } t.$$

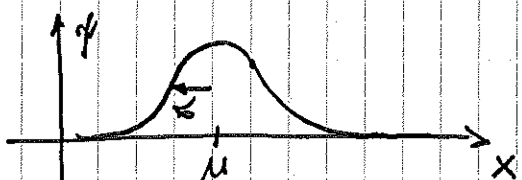
Since the probability of finding the particle anywhere is 1, the wavefunction corresponding to a <u>physical state</u> must be normalized:

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

- observables (position, momentum, energy, angular momentum) are replaced by operators. E.g.: position $\to x$; momentum $\to \frac{\hbar}{i}\frac{\partial}{\partial x}$; energy $\to i\hbar \frac{\partial}{\partial t}$). I can use $\psi(x,t)$ to find their <u>expectation value</u>:

$$\underbrace{\langle x \rangle}_{\text{expectation value of position operator } x} = \int_{-\infty}^{\infty} \psi^*(x,t)\, x\, \psi(x,t)\, dx$$

E.g. Let us take a wavefunction with Gaussian shape:



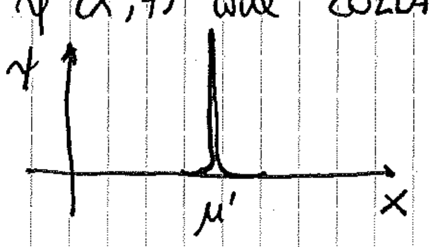
$$\psi(x,t) = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-\frac{(x-\mu)^2}{4\sigma^2}}$$

$$\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1$$

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \psi \, dx = \mu$$

This does NOT tell me that if I measure the position of the particle described by $\psi(x,t)$ I will obtain μ. It does NOT even tell me that if I keep repeating my measurement of position, the average of my measurements will be μ. After the first measurement (let us say I measure $\mu' \neq \mu$) $\psi(x,t)$ will COLLAPSE to:

before $\psi(x,t)$ $\perp$ disperses as time passes



and if I make another measurement quickly enough, I'll still measure μ'.

large...

$\langle x \rangle = \mu$ means that if I start from a <u>set</u> of particles all prepared in the wavefunction $\psi(x,t)$ and I measure each of them once, the distribution of those measurements (made on <u>different</u> particles) will have average μ.

Back to Hamiltonian and Schrödinger, some parallel with classical cases. Let us look at the potential V:

- $V(x,t) =$ constant, boundary at $\pm\infty$

  this is a <u>free</u> particle. Solutions are plane waves $\psi(x,t) = e^{i(kx-\omega t)}$

  Classical wave: $\omega(k) = k \cdot v$: no dispersion

  We saw before: $i\hbar \dfrac{\partial \psi}{\partial t} = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2 \psi}{\partial x^2} \Longrightarrow \omega(k) = \dfrac{\hbar k^2}{2m}$

  dispersion relation non trivial, but still expect familiar wave phenomena (interference, diffraction...)

- $V(x,t) = V(x)$ [i.e., no dependency on time]

  Schrödinger equation can now be separated:

  $$\psi(x,t) = \psi(x) \cdot e^{-i\frac{E}{\hbar}t}$$

  where $\psi(x)$ solves the equation $-\dfrac{\hbar^2}{2m}\dfrac{\partial^2 \psi}{\partial x^2} + V\psi = E$

  <u>constraints</u>: boundary conditions (possibly) and normalization
  ↳ for both cases above

Solutions of $-\dfrac{\hbar^2}{2m}\dfrac{\partial^2 \psi}{\partial x^2} + V\psi = E$ are "stationary" states: while the complete wavefunction does depend on time ($\psi(x,t) = \psi(x) e^{-i\frac{E}{\hbar}t}$), the expectation value of <u>any</u> operator is <u>constant</u> on a stationary state easy to prove: $e^{-i\frac{E}{\hbar}t}$ is a number, not an operator:

$$\langle Q \rangle = \int \psi(x,t)^* Q \psi(x,t) dx = \int \psi^*(x) e^{i\frac{E}{\hbar}t} Q \psi(x) e^{-i\frac{E}{\hbar}t} dx =$$

$$= \cancel{e^{+iE/\hbar t}} \cancel{e^{-i\frac{E}{\hbar}t}} \int \psi^*(x) Q \psi(x) dx = \int \psi^*(x) Q \psi(x) dx$$

What happens if I have confined stationary state? Similarly to what happens in classical closed system such as strings, the energy values become quantized:

	$\psi(x)$	E
particle in a box (V= const and finite in finite x interval)	sinusoidal waves	$E \propto n^2$
harmonic oscillator $V \propto x^2$	Gaussian × Hermite	$E \propto n$
Dirac delta $V \propto -\alpha\delta$	exponential decay	$E \propto -\alpha^2$ (only one bound state)

Now all boils down to finding Hamiltonian, and identifying the conjugate variables, the ones that, in QM, give rise to non-commuting (incompatible) observables.

One of the "surprising" aspects of QM is that there are quantities that cannot be measured at the same time (Heisenberg uncertainty principle). The first example is the pair position and momentum. Since now x and p are OPERATORS, not numbers, $xp \neq px$: applying the x operator to a wavefunction and then the p operator yields a result that is different had I swapped the two.

We express this by saying:

$$[x, p] = xp - px \neq 0$$

commutator

If I use the definition of p, $\frac{\hbar}{i}\frac{\partial}{\partial x}$, I can calculate the commutator:

$$[x, p]\psi = \frac{\hbar}{i} x \frac{\partial \psi}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x}(x\psi) =$$

$$= \cancel{\frac{\hbar}{i} x \frac{\partial \psi}{\partial x}} - \frac{\hbar}{i}\psi - \cancel{\frac{\hbar}{i} x \frac{\partial \psi}{\partial x}} = i\hbar\psi \quad \forall \psi$$

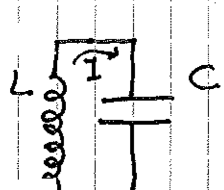
$$\Longrightarrow [x, p] = i\hbar$$

Heinsenberg uncertainty principle states that, given that $\sigma_A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$:

$$\sigma_A \cdot \sigma_B \geq \left| \frac{1}{2i}\langle [A, B]\rangle \right| \qquad \text{(all expectation values)}$$

How do I identify conjugate variables? The answer is in classical physics, with the concept of generalized coordinates q, the minimum number of quantities required to describe a system. "Generalized" is used to underline the fact that spatial coordinates are not always the best choice.

Let us take as an example a LC resonator circuit:



The energy stored in the system is the sum of U_L and U_C, the energies stored in the inductor and capacitor, respectively.

$$U_L = \frac{1}{2} L I^2 = \frac{1}{2} L \dot{Q}^2$$ (since the current is the time derivative of the charge)

where $L = \Phi / I$ and Φ = magnetic flux in inductor generated by current I $= \oint \vec{B} \cdot d\vec{A}$

Incidentally, Lenz's law states that $V = \dot{\Phi}$ (V - voltage drop across inductor)
(let me remove minus sign and call V a voltage drop) — V: voltage drop

I can also write $U_L = \frac{1}{2} \frac{\Phi^2}{L}$, using definition of L

$$U_C = \frac{1}{2} C V^2 = \frac{1}{2} C \dot{\Phi}^2$$ using Lenz's law

I also have $U_C = \frac{1}{2} \frac{Q^2}{C}$ using definition of $C = \frac{Q}{V}$

Let me now make a parallel with a mechanical oscillator:

<u>mechanical</u>		<u>electrical 1</u>	<u>electrical 2</u>
position	x	charge on capacitor Q	flux in inductor Φ
mass	m	inductance L	capacitance C
spring constant	k	$1/C$	$1/L$
kinetic energy	$\frac{1}{2} m \dot{x}^2$	$\frac{1}{2} L \dot{Q}^2$ (U_L)	$\frac{1}{2} C \dot{\Phi}^2$ (U_C)
potential energy	$\frac{1}{2} k x^2$	$\frac{1}{2} \frac{Q^2}{C}$ (U_C)	$\frac{1}{2} \frac{\Phi^2}{L}$ (U_L)

Let us take the electrical-2 case. ϕ is our generalized coordinate. What is its conjugate momentum? When I will replace the classical ϕ with its equivalent quantum operator $\hat{\phi}$, which will be the observable incompatible with $\hat{\phi}$?

Let us build the system Lagrangian:

$$\mathcal{L} = T - V = \frac{1}{2} C \dot{\phi}^2 - \frac{1}{2} \frac{\phi^2}{L}$$

The conjugate momentum is:

$$\frac{\partial \mathcal{L}}{\partial \dot{\phi}} = C\dot{\phi} \underset{\text{Lenz}}{=} CV \underset{\text{definition of } C}{=} Q$$

Hence, the Hamiltonian becomes:

$$H = p\dot{q} - \mathcal{L}(q, \dot{q}(p,q)) = \frac{Q^2}{2C} + \frac{\phi^2}{2L}$$

Now we convert Q and ϕ into operators $\hat{Q}$ and $\hat{\phi}$, and we write (and solve) Schrödinger's equation.

Interestingly enough, classical physicists predicted that classically conjugate variables will become incompatible observables in Quantum mechanics.

Long ago, Poisson brackets $\{f, g\}$ were defined for any pair of dynamical quantities:

$$\{f, g\} = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right)$$

where Σ is a sum over all generalized coordinates q_i and their corresponding conjugate variable $p_i = \dfrac{\partial \mathcal{L}}{\partial \dot{q}_i}$.

You can verify that canonically conjugate variables have a Poisson bracket equal to 1*. Very easy in our case:

$$\{\phi, Q\} = \frac{\partial \phi}{\partial \phi} \cdot \frac{\partial Q}{\partial Q} - \frac{\partial \phi}{\partial Q} \cdot \frac{\partial Q}{\partial \phi} = 1 \cdot 1 - 0 \cdot 0 = 1$$

Dirac POSTULATES that quantum operators derived from classically conjugate variables will have a quantum Poisson bracket (the commutator) whose value is $i\hbar$:

$$[\hat{\phi}, \hat{Q}] = i\hbar$$

Hence, I can't measure with arbitrary precision both flux and charge at the same time, and will have that:

$$\Delta\phi \, \Delta Q \geq \hbar/2$$

* this is the very definition of canonical conjugate coordinates