

Lecture 3: Classical correspondence, superposition, and free particles as wave packets

Planck, Einstein, and de Broglie thus came to point where they had to replace their physics intuition, built up from every-day life, with something new and less intuitive, but in better agreement with what could then be measured at the atomic and subatomic level.

Planck and Einstein found, in very different applications, that light previously thought of as a wave phenomena, can behave on a subatomic scale like a collection of particles, each with an energy $h\nu$ associated with the frequency of the light.

de Broglie argued that a (nonrelativistic) electron, which we “know” is a particle, acts as a wave with a characteristic wavelength of $\lambda_e = h/m_e v$. In the “old quantum mechanics” of Bohr – which we noted raised several conceptual difficulties – his “stationary orbits” in the H atom were obtained by requiring the angular momentum of an orbiting electron to be quantized in units of $n\hbar$ ($\hbar = h/2\pi$). Bohr’s condition for a motion around a circular path can be written

$$\oint p \, dq = nh \quad \text{as this yields for a circular orbit} \quad (m_e v)(2\pi r) = nh \Rightarrow m_e v r = n\hbar$$

where here q is the generalized coordinate that traces out the circular path. de Broglie then gives us another way of thinking about Bohr’s circular orbits

$$\oint dq = n\lambda_e \Rightarrow 2\pi r = n(h/m_e v) \Rightarrow m_e v r = n\hbar$$

The stationary orbits corresponds to an integer number of electron de Broglie wave lengths. We can “*account*” for Bohr’s condition by taking an important intellectual step – stipulating that an electron does behave like a wave with a characteristic wave length that depends of the electron mass and velocity, when the electron is examined on the atomic or subatomic scale.

Correspondence principle - Two limits: The first lecture stressed that conceptional progress in physics is usually a process where an existing theory is not replaced by, but is instead subsumed into, a more general theory that extends the scope and range of validity of the original theory. That is, QM should not replace classical mechanics, but instead should include it within its wider scope.

This concept is incorporated in quantum mechanics through the *correspondence principle*. It states that classical mechanics emerges as a limit of quantum mechanics for large quantum numbers.

For example, we have discussed that the bound states of the hydrogen atom have energies of $-13.6 \text{ eV}/n^2$. Thus n can be increased without limit, and this process ultimately produces bound orbits with binding energies that approach zero, and with radii that steadily increase, scaling as n^2 . Hydrogen (or other atoms) in such highly excited bound states are called Rydberg atoms. Their electron orbits approach the classical limit – the electron moves in a Keplerian orbit. This can be shown explicitly.

The above discussion is in the context of the quantum mechanics of deBroglie and Schroedinger, governed by the h identified by Planck. Another aspect of the correspondence principle is that the classical limit can also be obtained by altering quantum mechanics by taking the limit $h \rightarrow 0$. In classical mechanics when one throws a ball from point x at time t_x that is caught by a receiver at point y at time t_y , the ball follows a precise path that we can calculate from Newton's laws. The path minimizes the action – the difference between the kinetic energy and potential energy, integrate along the time coordinate of the classical path,

$$S = \oint_{t_x}^{t_y} [KE - V] dt.$$

If you sample any path other than the one given by Newton, the action along that path will be higher. (There is a marvelous Feynman lecture on this topic.) Note that the action carries the same units as Planck's constant h – energy \times time.

There is formulation of quantum mechanics, equivalent to the one we will use in this class, in terms of paths. It provides a very intuitive picture of the relationship of quantum mechanics and classical mechanics. In quantum mechanics you are allowed to propagate from x to y by many paths – but the further a path deviates from the classical path, the less probable it is. One pays a “penalty” for increasing the action via a path other than the classical path – the bigger the increase in the action, the stiffer the penalty. Now to convert action to a number – something that could possibly lead to a probability – one needs a unit. h is that unit. The classical path remains the best path, but there are many many others that, though each may be somewhat less probable than the classical path, will contribute. The larger the deviation of the action from its classical path, the bigger the penalty one pays in units of h , and thus the less probable the path. So the difference between classical mechanics and quantum mechanics is that the former has a single defined path, while in the latter many many many paths are allowed, fuzzying (that's probably not a word!) out the classical path – but not too much because of the heavy penalty one pays for taking a distant

path. Classical mechanics is recovered by taking $\hbar \rightarrow 0$ – all penalties become infinite, so only the classical path is allowed.

This discussion is a bit hand-wavy: the penalty one pays actually arises from the interference among paths. If we represent the action by S , the weighting of a path is

$$e^{iS/\hbar}$$

so that a large excess in the action causes rapid fluctuations with respect to the classical path and its nearest neighbors, leading to destructive interference among paths. In contrast paths near the classical path have slowly varying relative phases, and thus tend to cohere. If one drives $\hbar \rightarrow 0$ constructive interference among paths only occurs for paths increasingly near the classical one. At $\hbar = 0$ one converges to the classical path.

I think this gives one a much deeper feel for the physics of Planck's constant – how it governs the deviations from classical mechanics – and helps one visualize how the classical limit is achieved as $\hbar \rightarrow 0$. In summary,

Correspondence principle: QM becomes classical as $n \rightarrow \infty$ or as $\hbar \rightarrow 0$

The principle of superposition and wave packets: Any theory that would generalize classical mechanics should be required to reproduce classical mechanics in appropriate limits – but surely there are many generalizations possible that would have this property. However, the accumulation of phenomena in the early years of the 20th century indicating that light could behave as particle, and that particles could behave as wave, led us to a path where particles with definite positions and momenta gave way to a description in terms of waves and wave packets. Therefore, before we introduce the wave equation, we should remind ourselves of some of the properties that might be achievable through waves.

Familiar wave equations are those for sound in air or waves on water, which in 1D take the form

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2}$$

We can look for solutions of this equation in the form of an oscillation wave.

$$\psi(x, t) = \phi(x)e^{i\omega t} \Rightarrow \frac{\partial^2 \phi(x)}{\partial x^2} = -\frac{\omega^2}{c^2} \phi(x)$$

and we find

$$\phi(x) = e^{ikx} \quad \text{where} \quad c^2 k^2 = \omega^2 \quad \text{so that} \quad \psi(x, t) = e^{i(kx - \omega t)} \quad \text{with} \quad k(\omega) = \pm \frac{\omega}{c}$$

These plane wave solutions are extended, covering the entire range of x . An important property of this equation is that it is linear in ψ . This leads to the principle of superposition:

If $\psi_1(\vec{x}, t)$ and $\psi_2(\vec{x}, t)$ satisfy the wave equation, so does $\psi_1(\vec{x}, t) + \psi_2(\vec{x}, t)$

This property allows one to build *wave packets*, as you would get by throwing a stone into the middle of a quiet pond. Such a localized wave can be made from superpositions of the extended plane waves derived above. (An example is given just below.)

It would be very difficult to envision a successful theory of quantum mechanics that lacked this property. The correspondence principle requires us to be able to create localized particles in QM, and we know how to build localized wave packets from waves through Fourier analysis

$$\psi(x, t=0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} dk \quad \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x, t=0) e^{-ikx} dx$$

For example,

$$\psi(x, t=0) = e^{-x^2/a^2} \Rightarrow \psi(x, t=0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-a^2 k^2/4} e^{ikx} dk$$

We can easily build the Gaussian wave packet out of plane waves, but this infinite sum of plane waves will not be a solution of our QM wave equation unless the superposition principle holds.

Wave packets and uncertainty relationships: The simple Gaussian example used above illustrates another important property of wave packets. There is a size scale associate with our coordinate-space wave packet, with $\Delta x \sim a$. But we see the smaller a – the more localized in x – the broader the range of contributing momentum-space waves. That is

$$e^{-a^2 k^2/4} = e^{-k^2/(2/a)^2} \Rightarrow \Delta k = \frac{2}{a} \quad \text{consequently} \quad \Delta x \Delta k \sim 1$$

A property of wave packets is the more they are localized in coordinate space, the more they delocalize in momentum space. Thus as a wave theory, we would expect quantum mechanics to have an uncertainty principle that prevents us from simultaneously having precise particle locations

and momenta. As the de Broglie relation gives us $p = \frac{h}{\lambda} = \frac{h}{2\pi}k$ so that $\Delta k = \Delta p/\hbar$, it is not surprising that QM would have an uncertainty principle relating the product of coordinate and momentum uncertainties to \hbar . Its precise form is

$$\text{Uncertainty principle: } \Delta x \Delta p \geq \frac{\hbar}{2}$$

Schrödinger's equation: These kinds of considerations no doubt helped inspire Schrödinger's ansatz for a wave equation that might account for the apparent dual particle-wave nature of the electron and other elementary particles. While we live in 3D, we here write the equation in 1D

$$\text{Schrödinger equation: } \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t)$$

with the external potential $V(x)$ unspecified, but might be the Coulomb potential generated by the nucleus were we trying to understand the hydrogen atom. This equation is a fairly gentle variation of the sound/water wave equation just discussed, though with a couple of interesting differences.

So what does this equation mean? Staring at the LHS the potential is clear, while the derivative term can be rewritten in a way that clarifies the units

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} = -\frac{\hbar^2 c^2}{2mc^2} \frac{\partial^2}{\partial x^2}$$

As $(\hbar c)^2$ has units of (Energy-distance)², mc^2 is an energy, and $\partial^2/\partial x^2$ has units of (distance)⁻², the first term on the left hand side is an energy, and by the “what else can it be” argument, must be the kinetic energy. Classically this is $p^2/2m$. But $p^2/2m + V = E$, so on the RHS, the differential operator must be generating E. The requirement that the Schrödinger equation with its differential operators corresponds with classical mechanics allows us to identify the equation's differential operators with the physics

$$\text{Schrödinger equation operators: } \hat{p} \leftrightarrow \frac{\hbar}{i} \frac{\partial}{\partial x} \qquad \hat{E} \leftrightarrow i\hbar \frac{\partial}{\partial t}$$

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t) \leftrightarrow \left[\frac{\hat{p}^2}{2m} + V(x) \right] \psi(x, t) = \hat{E} \psi(x, t)$$

We indicate that \hat{p} and \hat{E} are QM operators by giving them “hats:” as expressed above, they are differential operators that act on the wave function.

Consider a free particle, so $V \rightarrow 0$, and write down a candidate solution

$$\psi(x, t) = e^{-i(Et - px)/\hbar}$$

where E and p are numbers. We note

$$\hat{p}\psi(x, t) = p\psi(x, t) \quad \hat{E}\psi(x, t) = E\psi(x, t)$$

while plugging into the Schroedinger equation yields the constraint

$$\frac{p^2}{2m} = E$$

Thus there are infinite set of plane-wave solutions labeled by the real number p , with $E(p) = p^2/2m$. One of the important differences between the wave equation we discussed for sound and the Schrödinger equation is that the former is quadratic in its space and time differential operators, while the Schrödinger equation is quadratic in space *but linear in time*. The latter is a reflection of the nonrelativistic relationship between a particle’s momentum and its energy – a consequence of building a theory beyond classical mechanics that extends our reach to and beyond the atomic scale, but shares with classical mechanics nonrelativistic restrictions. The linear-in-time nature of the Schrödinger equation leads naturally to complex wave functions. As measurements involve real quantities, the connect between wave functions and observables requires discussion – that is a topic for the next lecture.

We also note that our plane-wave solution of the Schrödinger equation has a characteristic wavelength. The length of a wave corresponds to the distance required to change the phase by 2π , at fixed time t . That is

$$2\pi = \frac{p\Delta x}{\hbar} \equiv \frac{p\lambda}{\hbar} \Rightarrow \lambda = \frac{2\pi\hbar}{p} = \frac{h}{p}$$

That’s de Broglie’s wave length! Further, we can anticipate that if solve the Schrödinger equation, obtaining continuous wave functions for problems like the hydrogen atom, the quantization conditions postulated by Bohr will emerge naturally, but in a wave theory where the paradoxes of the “old QM” have disappeared.