Quantum Mechanics
Day 6

Today

I. Last Time

- We generalized Fermat's principle to the case of a spatially varying index of refraction: the physical path of a light ray extremizes the travel time
$$T = \frac{1}{c}\int_S^D n(s)ds.$$
- By analogy we introduced the action
$$S = \int_{x_i}^{x_f} p dx,$$
where $p = \sqrt{2m[E - V(x)]}$ and Hamilton's principle: the physical trajectories connecting x_i and x_f are extremals of the action.
- We saw that Huygens' principle helped to explain Fermat's principle; rays and their behavior arise naturally as a short wavelength limit of the wave theory. We wondered whether a 'wave theory of mechanics' might also shed light on Hamilton's principle.

II. Refresher on Taylor series

Recall that given a function $f(x)$ it is often quite useful to expand it in a power series about some specific point x_0. Taylor series are a systematic way to do this and give

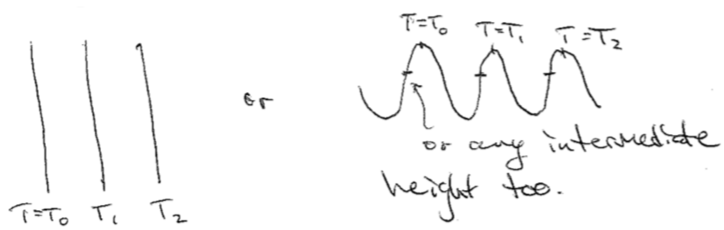
$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2!}f''(x_0)(x - x_0)^2 + \frac{1}{3!}f'''(x_0)(x - x_0)^3 + \cdots .$$

One of the reasons this series is so useful is that it gives us a controlled way to approximate the function $f(x)$ near the point x_0. If we are very close to x_0, then $f(x_0)$ is a good approximation to the value of $f(x)$. But, if we start to deviate more we can approximate the adjustment by the slope of the function f at the point x_0 times the amount that we have moved away. This gives a linear approximation to f in the neighborhood of x_0. Next the series takes into account how the function is quadratically curved and so on. The Taylor series systematically builds up these approximations and takes into account more and more features of how f varies near the point x_0.

III. Schrödinger's Insight

In 1925-1926 E. Schrödinger was challenged to develop and had the insight to find a wave theory for particle mechanics.

Starting from a wavefront $T_0 = \text{const.}$ we reach the next wave front by following wavelets for a fixed period of time. Hence, all the *level sets* of the wave field are given by surfaces of constant T, graphically



So, let's require the same thing for $S = S(x, t)$, that is,

$$\frac{1}{\hbar} S(x + \lambda, t) = \frac{1}{\hbar} S(x, t) + 2\pi.$$

Notice that $\hbar$ is required in this formula for dimensional consistency, and again we have no physical interpretation for it yet.

Now, let's suppose that λ is small, that is, that we are close to the ray limit of the theory, then we can Taylor expand and find

$$\frac{1}{\hbar}\left(S(x,t) + \lambda \frac{\partial S}{\partial x} + \cdots \right) = \frac{1}{\hbar} S(x,t) + 2\pi.$$

Simplifying between the two sides, this is

$$\frac{\partial S}{\partial x} = \frac{2\pi\hbar}{\lambda}.$$

Recalling the definition of the action

$$S = \int p dx$$

we have,

$$\boxed{\frac{\partial S}{\partial x} = p = \frac{h}{\lambda};}$$

de Broglie's hypothesis comes right out of the idea to treat mechanics as a wave theory analogous to the relationship between waves and rays in optics! Next we will start to build this wave theory towards Schrödinger's equation.

IV. The Schrödinger Equation

So far we have developed the particle mechanics in close analogy with optics. In optics we only considered an index of refraction that varied spatially $n = n(x)$ and similarly in mechanics we only considered momenta that varied spatially $p = p(x)$, explicitly we found

$$p(x) = \sqrt{2m[E - V(x)]}.$$

In both the optical and the mechanical contexts we will want to consider more general, time-varying quantities.

To hint at how to construct these quantities, let me leverage another analogy. You have studied electric plane waves, which have the form

$$\vec{E}_{\text{plane}} = \vec{E}_0 e^{i(kx-\omega t)},$$

where $\vec{E}_0$ is an constant vector determining the amplitude and direction of the electric field. The 'wave number' k is directly related to the momentum of the wave and ω is related to the energy that it carries.

Hamilton was deeply aware of this comparison, and actually introduced a more general action than I discussed last time, it is given by

$$S = \int_{t_i}^{t_f} (p\dot{x} - H)dt. \quad (1)$$

Notice that the first piece, $p\dot{x}dt = pdx$, is precisely our initial definition of the action. In this new action, the function $H = H(x, p, t)$ is known as the 'Hamiltonian' and in very many cases is just given by

$$H(x, p, t) = \frac{p^2}{2m} + V(x, t).$$

You will recognize this as the total energy of the system expressed as a function, in this case a function of x and p (and sometimes t if V happens to depend on t).

In time-dependent problems Hamilton's principle remains the same: the physical trajectories are those that extremize the action. The difference is that the word action now refers to the extended action function defined in Eq. (1).

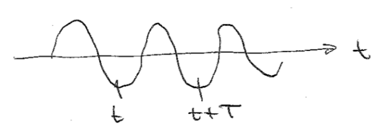


Figure 1: The wavefronts of a point source with rays traced as a guide.

Now that we have the full, time-dependent action, we can try to apply Schrödinger's insight again, this time to the time dependence. In the time domain, a wave repeats after a period T (instead of after a wavelength λ), and so we are looking to require

$$\frac{1}{\hbar} S(x, t + T) = \frac{1}{\hbar} S(x, t) - 2\pi,$$

here the minus sign is motivated by the minus signs in Eq. (1) and in the electric plane wave. Once again Taylor expanding the left hand side gives

$$\frac{1}{\hbar} \frac{\partial S}{\partial t} T = -2\pi \qquad \text{or} \qquad \frac{\partial S}{\partial t} = -\hbar \frac{2\pi}{T} = -\hbar\omega.$$

But, from the action

$$\frac{\partial S}{\partial t} = -E,$$

where E is a level set of H, that is, all points such that $H(x,p,t) = E$. Setting these expressions equal gives

$$E = \hbar\omega,$$

the Einstein relation!

Encouraged by the fact that we are recovering these pieces of the history leading up to quantum theory, we proceed to derive a full wave equation for mechanics, this will be the equation that governs quantum mechanics. Again by way of analogy we note that we can always break an arbitrary electric wave up into a superposition of plane waves of the form

$$\vec{E}_{\text{plane}} = \vec{E}_0 e^{i(kx-\omega t)}.$$

Let's try to do the same with our matter wave

$$\Psi_{\text{plane}}(x,t) = Re^{\frac{i}{\hbar}S},$$

here we think of R as an amplitude for the wave, and we intend for S to be the action. Why the action? Well, the reason is closely related to what we've seen above, with this choice and with the standard form for the energy

$$H(x,p,t) = \frac{p^2}{2m} + V(x,t),$$

we notice that

$$\begin{aligned}\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi_{\text{plane}} &= \frac{\hbar}{i}Re^{\frac{i}{\hbar}S}\cdot\frac{i}{\hbar}\frac{\partial S}{\partial x}\\ &= p\cdot\Psi_{\text{plane}},\end{aligned}$$

and

$$\begin{aligned}\frac{\hbar}{i}\frac{\partial}{\partial t}\Psi_{\text{plane}} &= \frac{\hbar}{i}Re^{\frac{i}{\hbar}S}\cdot\frac{i}{\hbar}\frac{\partial S}{\partial t}\\ &= -E\cdot\Psi_{\text{plane}}.\end{aligned}$$

Then this way of writing things gives us the opportunity to express the conservation of mechanical energy, one of the deepest foundations of mechanics, as a differential condition on our matter wave:

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\Psi_{\text{plane}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi_{\text{plane}} + V(x,t)\cdot\Psi_{\text{plane}}$$

Putting these observations together (Fermat, Huygens, Hamilton, ...) Schrödinger guessed that *any* quantum wave should satisfy

$$\boxed{i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi, \qquad \text{Schrödinger's Eq.}} \tag{2}$$

I think this is a beautiful piece of theoretical physics—he drew together several different strands of ideas and used an inductive leap to arrive at the correct generalization of all of them.

Notice the subtle, but profound shift in the meaning of momentum too. It is both a physical property of the particle and a differential operator that acts on the particle's wave description.