PHY 115A
Lecture Notes 3:
Formalism
(Griffith's Chapter 3)

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Chapter 3

Formalism

3.1 Matter Waves

Early in the development of quantum mechanics it became clear that light was quantized as photons with discrete energy:

$$E = h\nu$$

but for a massless particle, we know that:

$$E = pc$$

and:

$$pc = h\nu$$

so that:

$$\frac{h}{p} = \frac{\nu}{c} = \lambda$$

where λ is the wavelength of the light. De Broglie made the hypothesis that matter was also described by a wave with frequency:

$$\nu = \frac{E}{h}$$

and wavelength:

$$\lambda = \frac{h}{p}$$

We are using the reduced Planck's constant:

$$\hbar = \frac{h}{2\pi}$$

so we write these relations equivalently as:

$$E = h\nu = \hbar(2\pi\nu) = \hbar\omega$$

and:

$$p = \frac{h}{\lambda} = \hbar\frac{2\pi}{\lambda} = \hbar k$$

Recall that in general a right traveling wave has the format:

$$f(k\,x - \omega\,t)$$

for $k > 0$ and $\omega > 0$. So we can imagine several different functional forms for de Broglie's "matter waves" traveling left:

$$\Psi_1(x,t) = \cos(kx - \omega t)$$

or:

$$\Psi_2(x,t) = \sin(kx - \omega t)$$

or

$$\Psi_3(x,t) = \exp(ikx - i\omega t)$$

where we don't care about the amplitude of the function yet. But take care to note that:

$$g(-k\,x + \omega\,t) = g(-(k\,x - \omega\,t))$$

is also a right traveling wave, because it can be written as:

$$f(k\,x - \omega\,t) \equiv g(-(k\,x - \omega\,t))$$

But since:

$$\cos(-k\,x + \omega\,t) = \cos(k\,x - \omega\,t)$$

we don't need to consider that case. And since:

$$\sin(-k\,x + \omega\,t) = -\sin(k\,x - \omega\,t)$$

and we don't care about the amplitude of the function yet, we can ignore that as well. That only leaves one additional possibility to consider:

$$\Psi_4(x,t) = \exp(-ikx + i\omega t)$$

It seems like we could use any of these four options, but let's see what happens when we try to construct a standing wave by adding am equal mixture of right traveling and left traveling waves. To switch to a left traveling wave, we just put:

$$k \to -k$$

Our standing wave using Ψ_1 is:

$$\Psi(x) = \cos(k\,x - \omega\,t) + \cos(-k\,x - \omega\,t)$$

but using:

$$\cos(\alpha + \beta) = \cos(\alpha)\cos(\beta) - \sin(\alpha)\sin(\beta)$$

we conclude:

$$\Psi(x) = 2\cos(k\,x)\cos(\omega\,t)$$

which is an utter catastrophe, since the wave function vanishes everywhere whenever:

$$\omega t = \frac{n\pi}{2} \qquad\qquad n = 1, 3, 5$$

This would describe a particle that disappears and reappears from existence... not the theory we are trying to build! So we discard option Ψ_1. Likewise for Ψ_2:

$$\Psi(x) = \sin(k\,x - \omega\,t) + \sin(-k\,x - \omega\,t)$$

but using:

$$\sin(\alpha+\beta) = \sin(\alpha)\cos(\beta) + \cos(\alpha)\sin(\beta)$$

we conclude:

$$\Psi(x) = -2\cos(k\,x)\sin(\omega\,t)$$

which is another catastrophe, since the wave function vanishes everywhere whenever:

$$\omega t = n\pi \qquad\qquad n = 1, 2, 3, 4, 5$$

But there is no such problem with Ψ_3 where:

$$\Psi(x) = \exp(ik\,x - i\omega\,t) + \exp(-ik\,x - i\omega\,t) = 2\cos(kx)e^{-i\omega t}$$

this vanishes at specific locations in space, where the particle will never be found, but this is exactly what we would expect for a standing wave. The only time-dependent factor

$$e^{-i\omega t}$$

is never zero at any point in time. Similarly, for Ψ_4:

$$\Psi(x) = \exp(-ik\,x + i\omega\,t) + \exp(ik\,x + i\omega\,t) = 2\cos(kx)e^{i\omega t}$$

So it seems at this point that both Ψ_3 and Ψ_4 are valid options for a right-traveling matter waves, but if they are both valid, then we should be able to superimpose them:

$$\Psi_3(x,t) + \Psi_4(x,t) = \exp(ik\,x - i\omega\,t) + \exp(-ik\,x + i\omega\,t) = 2\cos(k\,x - \omega\,t)$$

which we already saw was a problematic right traveling wave. So we conclude that we can have Ψ_3 or Ψ_4, but **not both**. We choose the one that has $k > 0$ for a right traveling wave, so that our right traveling matter wave is finally uniquely identified as:

$$\Psi_{\rm k}(x,t) \equiv \exp(ik\,x - i\omega\,t) \tag{3.1}$$

with where:

$$p = \hbar k, \qquad \text{and} \qquad E = \hbar\omega.$$

For the free particle, we also have:

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \tag{3.2}$$

and so:

$$\omega(k) = \frac{\hbar k^2}{2m} \tag{3.3}$$

The free particles have phase velocity:

$$v_{\rm phase} = \frac{\omega}{k} = \frac{\hbar k}{2m}$$

and group velocity:

$$v_{\rm group} = \frac{d\omega}{dk} = \frac{\hbar k}{m}$$

which is the classical velocity of the particle. In chapter 2, we showed that this phase velocity is the velocity of a wave packet consisting of waves with wave numbers close to k.

3.2 From Matter Waves to the Schrödinger Equation

With the matter waves in hand, we now will try to identify the wave equation that predicts matter waves for a free particle ($V(x) = 0$), in the hope that we can generalize that equation in other contexts ($V(x) \neq 0$).

The first thing we will try to do is determine the momentum of the matter wave. Now, knowing that:

$$\Psi_k(x,t) = \exp(ik\,x - i\omega\,t)$$

we can of course simply read off the wave number k and determine the momentum $p = \hbar k$. But we cannot *generalize* that approach to other wave functions $\Psi(x,t)$. In the general case, we will only know $\Psi(x,t)$, so we can only do things involving x and t. Here's something:

$$-i\hbar\frac{\partial}{\partial x}\Psi_k(x,t) = (-i\hbar)(ik)\Psi_k(x,t) = \hbar k\Psi_k(x,t) = p\Psi_k(x,t)$$

so we define the momentum operator:

$$\hat{p} \equiv -i\hbar\frac{\partial}{\partial x} \tag{3.4}$$

and note that for our matter wave for free particles:

$$\hat{p}\,\Psi_k(x,t) = p\,\Psi_k(x,t) \tag{3.5}$$

We say that the free particle solutions $\Psi_k(x,t)$ is an eigenstate of the momentum operator $\hat{p}$. Note that this is true only for eigenstates. For a general state with wave function $\Psi(x,t)$ generally:

$$\hat{p}\,\Psi(x,t) \neq p\,\Psi(x,t)$$

Note also that $\hat{p}$ and p are two very different things. Whereas p is just a number, $\hat{p}$ is a complicated beast: an operator that when given a wave function returns a (possibly different) wave function.

What about the position operator $\hat{x}$? Since we have access to x and t, for any wave function $\Psi(x,t)$, we need only write:

$$\hat{x} = x \tag{3.6}$$

and so for *any wave function* $\Psi(x,t)$

$$\hat{x}\,\Psi(x,t) = x\,\Psi(x,t)$$

which looks like any $\Psi(x,t)$ is also an eigenstate of $\hat{x}$, but that is not so, because x is not just a number here, and

$$x\,\Psi(x,t)$$

is a new wave function that is distinct from $\Psi(x,t)$.

Next we will try to find a recipe for determining the energy $E = \hbar\omega$ only through $\Psi(x,t)$. We can try something similar:

$$i\hbar\frac{\partial}{\partial t}\,\Psi_k(x,t) = (i\hbar)(-i\omega)\,\Psi_k(x,t) = \hbar\omega\,\Psi_k(x,t) = E\,\Psi_k(x,t)$$

We also know that for the free particle:

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

So let's find an operator $\hat{H}$ such that:

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

for our free particles. Working with our definition of the momentum operator:

$$\hat{H}\,\Psi_k(x,t) = \frac{p^2}{2m}\Psi_k(x,t) = \frac{p}{2m}(p\,\Psi_k(x,t)) = \frac{p}{2m}\,\left(-i\hbar\frac{\partial}{\partial x}\,\Psi_k(x,t)\right)$$

but p here is just a number (unlike $\hat{p}$ or $\partial/\partial x$) so we are free to move it right up against $\Psi_k(x,t)$ and continue on:

$$\hat{H}\,\Psi_k(x,t) = \frac{-i\hbar}{2m}\,\frac{\partial}{\partial x}\,(p\,\Psi_k(x,t)) = \frac{-i\hbar}{2m}\,\frac{\partial}{\partial x}\,\left(-i\hbar\frac{\partial}{\partial x}\,\Psi_k(x,t)\right) = -\frac{\hbar^2}{2m}\,\frac{\partial^2}{\partial x^2}\,\Psi_k(x,t)$$

from which we read off the operator $\hat{H}$ for the free particle:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} = \frac{\hat{p}^2}{2m}$$

this is the Hamiltonian operator (for the free particle) which does not have any potential energy. For a general potential, we need to find an operator $\hat{V}$ and the total energy will be obtained by:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}$$

But the potentials we will encounter will depend only on x and t, so the operator $\hat{V}$ is trivial:

$$\hat{V} = V(\hat{x},t) = V(x,t)$$

So for the free particle with $V(x,t) = 0$ we have shown that:

$$i\hbar\frac{\partial}{\partial t}\Psi_k(x,t) = \hat{H}\,\Psi_k(x,t)$$

but our assumption is that when $V(x,t) \neq 0$ we can determine the possible states as solutions to the equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\,\Psi(x,t) \tag{3.7}$$

or equivalently

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\,\Psi(x,t) + V(x,t)\Psi(x,t) \tag{3.8}$$

So we have plausibly deduced the Schrödinger Equation from the deBroglie hypothesis via the Matter Waves.

3.3 The Fourier Transform Revisited

Our inner product now extends between positive and negative infinity:

$$\langle\Psi,\phi\rangle \equiv \int_{-\infty}^{\infty}\Psi^*(x)\phi(x)\,dx \tag{3.9}$$

Our basis functions, which are now defined for any value of k,

$$e_k = \frac{1}{\sqrt{2\pi}} \exp(ikx) \tag{3.10}$$

are still orthonormal, but the condition looks a bit different in the continuum case:

$$\langle e_k, e_{k'} \rangle \quad = \quad \delta(k - k')$$

See the appendix for more details on the Dirac delta function $\delta(x)$, which is zero everywhere but at $x = 0$, where it is infinite. It is the continuous version of δ_{nm}.

Our basis functions are also still complete. In the discrete case we have a complex Fourier coefficient for every integer n. Now we have a complex Fourier coefficient for any real value of k. In place of Fourier coefficients, we have instead a function of k which we call the Fourier transform: $\widetilde{\Psi}(k)$. Instead of a sum over discrete terms, we now have to integrate over all values of k:

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{\Psi}(k) \exp(ikx)\, dk. \tag{3.11}$$

Just as in the discrete case, we determine the Fourier transform from the inner product:

$$\widetilde{\Psi}(k) = \langle e_k, \Psi \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ikx)\, dx \tag{3.12}$$

Equation 3.12 is generally referred to as the *Fourier Transform*, while Equation 3.11 is referred to as the *Inverse Fourier Transform*.

3.4 The Fourier Transform in Quantum Mechanics

So far we have been considering the Fourier transform with respect to position x and wave-number k. A much more useful pair of variables for Quantum Mechanics turns out to be momentum p and position x. To relate p to k we need only apply the DeBroglie relation to the wavelength in the definition of the wavenumber:

$$k \equiv \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{\hbar}$$

We could therefore make the substitution $k \to p/\hbar$ (and $dk \to dp/\hbar$)) in Equations 3.11 and 3.12. It turns out that a marginally more useful equation results if we make the normalization factors symmetric, by splitting the normalization factor of $1/\hbar$ across both equations with $1/\sqrt{\hbar}$ applied to each:

$$\Psi(x) \quad = \quad \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widetilde{\Psi}(p) \exp(ipx/\hbar)\, dp \tag{3.13}$$

$$\widetilde{\Psi}(p) \quad = \quad \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ipx/\hbar)\, dx \tag{3.14}$$

The major benefit of this symmetric form is that the normalization of $\Psi(x)$ and $\widetilde{\Psi}(p)$ in this case turns out to be the same:

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = \int_{-\infty}^{\infty} |\widetilde{\Psi}(p)|^2 dp = 1$$

Because we can always calculate $\Psi(x)$ from $\widetilde{\Psi}(p)$ either one completely describes the quantum mechanical state. We call $\widetilde{\Psi}(p)$ the momentum wave function. Whereas $|\Psi(x)|^2$ gives us the probability density for the quanton to be at position x, $|\Psi(p)|^2$ gives us the probability density for the quanton to have momentum p.