III. PROBABILITY DENSITY AND CONSERVATION

A. Where is the particle?

Okay, I avoided the hard question with some painful mathematical interlude. I learned this from a mathematician friend of mine - everytime I asked him about his dating life, he changed the subject to algebraic topology.

So - where is the particle? Last class we talked about wave interference, and I asked you a similar question - where is the light beam? The answer was where the energy flux is, and the energy flux is determined by the square of the wave function. We guessed:

$$\rho \propto |\psi|^2. \tag{47}$$

But now we are not considering a barrage of photons - we are considering a single electron. Still there is this itch to use this expression for something. What is ρ then? You guess (or know!) *probability density.* This is true, but we must give an excuse - intuition is no longer enough for a Nobel Prize!

B. Probability conservation

If it is probability, what does it have to obey? A conservation law. For starters, the total probability must remain constant:

$$\frac{d}{dt}\int\limits_{-\infty}^{\infty} dx|\psi|^2 = 0 \tag{48}$$

Let's verify this:

$$\frac{d}{dt}\int\limits_{-\infty}^{\infty} dx|\psi|^2 = \frac{d}{dt}\int\limits_{-\infty}^{\infty} dx\left(\psi^*\frac{\partial\psi}{\partial t} - \frac{\partial\psi^*}{\partial t}\psi\right) \tag{49}$$

but for this we can use the Schrödinger equation. For $\frac{\partial\psi}{\partial t}$ it is obvious, for $\frac{\partial\psi^*}{\partial t}$ it is also obvious, but I'll write it here just the same:

$$\frac{\partial\psi^*}{\partial t} = -\frac{1}{(i\hbar)^*}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi^* = -i\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi^* \tag{50}$$

and we see easily that:

$$\psi^*\frac{\partial\psi}{\partial t} + \frac{\partial\psi^*}{\partial t}\psi = i\frac{\hbar}{2m}(\psi^*\frac{\partial^2\psi}{\partial x^2} - \frac{\partial^2\psi^*}{\partial x^2}\psi) \tag{51}$$

And at this point we must begin to worry! We know that $|\psi|^2$ is the probability density - we read it in the modern physics books back in highschool! But this doesn't seem to be zero. No worries; everything becomes clearer when we realize that:

$$\psi^*\frac{\partial^2\psi}{\partial x^2} - \frac{\partial^2\psi^*}{\partial x^2}\psi = \frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right) \tag{52}$$

Once we put this in the integral, we get:

$$\begin{aligned}\frac{d}{dt}\int\limits_{-\infty}^{\infty} dx|\psi|^2 &= i\frac{\hbar}{2m}\int\limits_{-\infty}^{\infty} dx\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)\\ &= i\frac{\hbar}{2m}\left[\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right]_{-\infty}^{\infty} = 0\end{aligned} \tag{53}$$

assuming that $\psi \to 0$ when $x \to \pm\infty$.

What we just showed is a global conservation. There is another condition, however, which has to do with our expectation that the underlying particle motion is still local: the probability needs to be locally conserved. If you think about an imaginary 1d box, and a denisty of something (e.g., probability), this density can change if there are currents of the same something going in and out of it. We take them to be positive in the $+x$ direction. Now:

$$-\frac{\partial dx \cdot \rho}{\partial t} = j(x+dx) - j(x) \tag{54}$$

or:

$$-\frac{\partial \rho}{\partial t} = \frac{\partial j}{\partial x} \tag{55}$$

In a 3d world, $\vec{j}$ is a vector, and this relationship is easily seen to become:

$$-\frac{\partial \rho}{\partial t} = \nabla \cdot \vec{j}. \tag{56}$$

Does the Schrödinger equation define a j? Let's see:

$$\frac{\partial \psi^* \psi}{\partial t} = \psi^* \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi = \frac{\partial}{\partial x}\left[i\frac{\hbar}{2m}(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi)\right] \tag{57}$$

as we saw before. And we recognize:

$$j = \frac{\hbar}{2mi}(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi). \tag{58}$$

Nice! We now have an expression for the probability current.

Let's check it. If we are thinking of a wave solution, $\psi = e^{ikx - i\omega t}$ then we end up with:

$$j = \frac{1}{m}\hbar k |\psi|^2 \tag{59}$$

This we can interpret as velocity times density: $j \sim v\rho$, which we recall from E&M to be correct.

C. Consequences

It the wave function is indeed a probability density then the first thing we have to do is make sure it is normalized. Let's go back to our old initial wave function:

$$\psi(x,0) = Ne^{-\frac{x^2}{4\Delta x^2}}. \tag{60}$$

This is an unnormalized wave function until we have chosen N properly. The total probabilty is then:

$$1 = p = \int\limits_{-\infty}^{\infty} dx|\psi(x)|^2 = \int\limits_{-\infty}^{\infty} dx N^2 e^{-\frac{x^2}{2\Delta x^2}} = N^2\sqrt{2\pi}\Delta x. \tag{61}$$

This yields:

$$N = \frac{1}{\sqrt{\sqrt{2\pi}\Delta x}}. \tag{62}$$

At this point w can start calculating things like averages, and standard deviation. The first, is easily defined as:

$$\langle y \rangle = \sum_y p_y y \tag{63}$$

Note that the notation $\langle \ldots \rangle$ indicates an *expectation value* of whatever is inside, with respect to the quantum-mechanical wave function.

The latter, is an old favorite in quantum mechanics. The standard deviation of a variable y, σ_y, is given by:

$$\sigma_y^2 = \sum_y p_y (y - \langle y \rangle)^2 \tag{64}$$

which we can expand:

$$= \sum_y p_y(y^2 + \langle y\rangle^2 - 2y\langle y\rangle) = \langle y^2\rangle - \langle y\rangle^2 \tag{65}$$

Let's calculate this for the location of our particle at the initial time. Instead of the discrete sum above, we can write an integral. One can definitely visualize the integral as a discrete sum over bins of size dx in the parameter space at hand. The average is thus:

$$\langle x\rangle = \int_{-\infty}^{\infty} dx|\psi(x)|^2 x = 0 \tag{66}$$

and the standard deviation is:

$$\sigma_x^2 = \langle x^2\rangle = \int_{-\infty}^{\infty} dx|\psi(x)|^2 x^2 = \frac{1}{\sqrt{2\pi}\Delta x}\int_{-\infty}^{\infty} dx e^{-\alpha x^2} \tag{67}$$

with $\alpha = \frac{1}{2\Delta x^2}$. I'm writing this deliberatly so, because I wanted to show you a trick. We already know how to calculate the gaussian integral. Now we have a variation of it with an extra x^2. Check this out:

$$N^2\int_{-\infty}^{\infty} dx x^2 e^{-\alpha x^2} = -N^2\frac{\partial}{\partial\alpha}\int_{-\infty}^{\infty} dx e^{-\alpha x^2} \tag{68}$$

This trick is called differentiating inside the integral, and it is deeply rooted in the Feynman heritage. In fact, he dedicated a whole chapter to this trick in his masterpiece "surely you're joking" book. That's where I learned it from. Let's see how it works:

$$= -N^2\frac{\partial}{\partial\alpha}\sqrt{\frac{\pi}{\alpha}} = N^2\frac{1}{2}\frac{\sqrt{\pi}}{\alpha^{3/2}} \tag{69}$$

substituting back α and N we get:

$$\frac{1}{\sqrt{2\pi}\Delta x}\frac{1}{2}\sqrt{\pi}(2\Delta x^2)^{3/2} = \Delta x^2 \tag{70}$$

Now you see why I had the 4 there in the first place. Δx gives us the spread of the probability distribution of the particle.

D. Probability density in momentum space

The interpretation of the wave function as a probability density in real space is neat. But it turns out that the probability density picture could be extended to other spaces, for example, momentum space. Before we can deal with this, for my own peace of mind, I'd like to recount the equations of Fourier transform. Given a function $f(x)$, we can define the Fourier transform, f_k as follows:

$$f_k = \int_{-\infty}^{\infty} dx e^{-ikx} f(x) \tag{71}$$

This is useful because we can then recover hte function $f(x)$ by simply:

$$f(x) = \int \frac{dk}{2\pi} f_k e^{ikx} \tag{72}$$

An interesting special case, and a number one favorite in quantum mechanics classes, is the δ-function:

$$f(x) = \delta(x - x_0) \tag{73}$$

Where $\int \delta(x) = 1$, but $\delta(x) = 0$ for all $x \neq 0$.
Plugging $f(x)$ in gives immediately:

$$f_k = e^{-ikx_0} \tag{74}$$

Every mathematical formula requires some checking. Substituting back:

$$f(x) = \int \frac{dk}{2\pi} e^{ik(x-x_0)} \tag{75}$$

wow. This is not a trivial formula. Okay - if $x \neq x_0$, then clearly this should be zero. When $x = x_0$, we get infinity. But there are many kinds of infinity, here we see that the δ-function infinity is exactly an integral withteh 2π below:

$$\int dk e^{ik(x-x_0)} = 2\pi\delta(x - x_0) \tag{76}$$

This also has a dual form:

$$\int dx e^{ix(k-k_0)} = 2\pi\delta(k - k_0). \tag{77}$$