PROBABILITY CURRENT IN 3-D

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We've seen the concept of the probability current in one dimension. A generalization to 3-d gives the vector

$$\mathbf{J}=\frac{i\hbar}{2m}\left(\Psi\nabla\Psi^{*}-\Psi^{*}\nabla\Psi\right) \tag{1}$$

We can use the product rule from vector calculus to get

$$\begin{aligned}\nabla\cdot\mathbf{J} &= \frac{i\hbar}{2m}\left(\left|\nabla\Psi\right|^{2}+\Psi\nabla^{2}\Psi^{*}-\left|\nabla\Psi\right|^{2}-\Psi^{*}\nabla^{2}\Psi\right) &(2)\\ &= \frac{i\hbar}{2m}\left(\Psi\nabla^{2}\Psi^{*}-\Psi^{*}\nabla^{2}\Psi\right) &(3)\\ &= \Psi\left(-\frac{\partial\Psi^{*}}{\partial t}+\frac{i}{\hbar}\Psi^{*}V\right)-\Psi^{*}\left(\frac{\partial\Psi}{\partial t}+\frac{i}{\hbar}\Psi V\right) &(4)\\ &= -\frac{\partial}{\partial t}\left|\Psi\right|^{2} &(5)\end{aligned}$$

where in the third line we used the Schrodinger equation rearranged to:

$$\frac{i\hbar}{2m}\nabla^{2}\Psi=\frac{\partial\Psi}{\partial t}+\frac{i}{\hbar}\Psi V \tag{6}$$

Again generalizing the 1-d case, if we integrate the outward component of $\mathbf{J}$ over the surface area of a volume, this gives us the net rate at which probability 'flows' across the surface, and should, therefore, be equal to the rate at which probability changes within the volume. From the divergence theorem, we know that

$$\begin{aligned}\int_{A}\mathbf{J}\cdot d\mathbf{a} &= \int_{V}\nabla\cdot\mathbf{J}d^{3}\mathbf{r} &(7)\\ &= -\frac{d}{dt}\int_{V}\left|\Psi\right|^{2}d^{3}\mathbf{r} &(8)\end{aligned}$$

Since $|\Psi|^{2}$ is the probability density, this equation expresses exactly this idea.

As an example, we can look at the ψ_{211} state of the hydrogen atom. We worked out this function earlier, so we quote the result here:

$$\psi_{211} = -\frac{1}{8a^2\sqrt{\pi a}} r e^{-r/2a} \sin\theta e^{i\phi} \tag{9}$$

The gradient in spherical coordinates is

$$\nabla = \hat{\mathbf{r}}\frac{\partial}{\partial r} + \frac{1}{r}\hat{\theta}\frac{\partial}{\partial \theta} + \frac{1}{r\sin\theta}\hat{\phi}\frac{\partial}{\partial \phi} \tag{10}$$

so we can calculate $\nabla\psi_{211}$:

$$\nabla\psi_{211} = \frac{-1}{8a^2\sqrt{\pi a}} e^{-r/2a} e^{i\phi}\left[\left(1-\frac{r}{2a}\right)\sin\theta\hat{\mathbf{r}} + \cos\theta\hat{\theta} + i\hat{\phi}\right] \tag{11}$$

We can now calculate $\mathbf{J}$ from 1. The contributions along the $\hat{\mathbf{r}}$ and $\hat{\theta}$ directions cancel out, so we are left with

$$\mathbf{J} = \frac{i\hbar}{2m}\left[-\frac{1}{8a^2\sqrt{\pi a}} r e^{-r/2a} \sin\theta e^{i\phi} \frac{i}{8a^2\sqrt{\pi a}} e^{-r/2a} e^{-i\phi}\right. \tag{12}$$

$$\left. -\frac{1}{8a^2\sqrt{\pi a}} r e^{-r/2a} \sin\theta e^{-i\phi} \frac{i}{8a^2\sqrt{\pi a}} e^{-r/2a} e^{i\phi}\right]\hat{\phi} \tag{13}$$

$$= \frac{\hbar}{64\pi m a^5} r e^{-r/a} \sin\theta\hat{\phi} \tag{14}$$

From 1, we see that the dimensions of $\mathbf{J}$ are those of velocity, since $\hbar$ has dimensions of energy $\times$ time $=$ mass $\times$ length^2 $\times$ time^{-1} so $\frac{\hbar}{m}\nabla$ has dimensions of length $\times$ time^{-1}. The quantity $m\mathbf{J}$ therefore has dimensions of momentum, and can be interpreted as the flow of mass. This makes sense, since the probability density is the probability density of finding the particle within a given infintesimal volume, and the particle consists of its mass.

From $\mathbf{L} = \mathbf{r}\times\mathbf{p}$, we can therefore write the (orbital, ignoring spin) angular momentum as

$$\mathbf{L} = \int_V \mathbf{r}\times(m\mathbf{J})\, d^3\mathbf{r} \tag{15}$$

Since $\mathbf{J}$ is parallel to $\hat{\phi}$ and $\hat{\mathbf{r}}\times\hat{\phi} = -\hat{\theta}$, we have for the hydrogen atom above:

$$\mathbf{r}\times\mathbf{J} = \frac{-\hbar}{64\pi m a^5} e^{-r/a} r^2 \sin\theta\hat{\theta} \tag{16}$$

If we want to find L_z, we need the component of $\mathbf{r}\times\mathbf{J}$ along the unit vector $\hat{\mathbf{k}}$. The component of $\hat{\theta}$ along $\hat{\mathbf{k}}$ is $-\sin\theta\hat{\mathbf{k}}$ so to find L_z we must do the integral

$$L_z = m\int |\mathbf{r}\times\mathbf{J}|\sin\theta d^3\mathbf{r} \tag{17}$$

$$= \frac{\hbar}{64\pi a^5}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} r^4 e^{-r/a}\sin^3\theta dr d\theta d\phi \tag{18}$$

$$= \hbar \tag{19}$$

where we used Maple to do the integral. This is correct for the state ψ_{211} since for quantum number (not mass) $m=+1$ we would expect $L_z=+\hbar$.