Derivation of Quantum Probability Continuity Equation for EM Schrödinger

Drew Silcock

Here's the equation we want to derive, called the probability continuity equation for Quantum Mechanics:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0 \tag{1}$$

Given the definitions of ρ and $\mathbf{J}$ as follows:

$$\rho \stackrel{\text{def}}{=} |\Psi|^2 \tag{2}$$

$$\mathbf{J} \stackrel{\text{def}}{=} \frac{1}{2m}\Psi^*(-\imath\hbar\nabla - \frac{e}{c}\mathbf{A})\Psi + \frac{1}{2m}\Psi(\imath\hbar\nabla - \frac{e}{c}\mathbf{A})\Psi^* \tag{3}$$

Where Ψ is our quantum wavefunction and $\mathbf{A}$ is our vector potential.
First, let's note that

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial t}\left(\Psi^*\Psi\right) \tag{4}$$

$$= \Psi\frac{\partial \Psi^*}{\partial t} + \Psi^*\frac{\partial \Psi}{\partial t} \tag{5}$$

Before taking the div of $\mathbf{J}$, we first note that

$$\mathbf{J} = \frac{1}{2m}\left[\Psi^*\left(-\imath\hbar\nabla\right)\Psi + \Psi\left(\imath\hbar\nabla\right)\Psi^*\right] - \frac{e}{mc}\mathbf{A}|\Psi|^2 \tag{6}$$

$$= \frac{1}{2m}\left[\left\{\Psi^*\left(-\imath\hbar\nabla\right)\Psi\right\} + \left\{\Psi^*\left(-\imath\hbar\nabla\right)\Psi\right\}^*\right] - \frac{e}{mc}\rho\mathbf{A} \tag{7}$$

Next we use the fact that $\Re(z) = \frac{z+z^*}{2}$, we see that

$$\mathbf{J} = -\frac{\hbar}{m}\Re(\Psi^*\imath\nabla\Psi) - \frac{e}{mc}\rho\mathbf{A} \tag{8}$$

Using the equation

$$\Re(\imath z) = \frac{(\imath z) + (\imath z)^*}{2} \tag{9}$$

$$= \imath\frac{z - z^*}{2} \tag{10}$$

$$= -\frac{z - z^*}{2\imath} \tag{11}$$

$$= -\Im(z) \tag{12}$$

We can simplify the above to

$$\mathbf{J} = \frac{\hbar}{m}\Im(\Psi^*\nabla\Psi) - \frac{e}{mc}\rho\mathbf{A} \tag{13}$$

Now we're ready to take its divergence, and try and show that it's equal to $\frac{\partial\rho}{\partial t}$:

$$\nabla\cdot\mathbf{J} = \frac{\hbar}{m}\nabla\cdot\Im(\Psi^*\nabla\Psi) - \nabla\left(\frac{e}{mc}\rho\mathbf{A}\right) \tag{14}$$

$$= \frac{\hbar}{m}\Im(\nabla\cdot[\Psi^*\nabla\Psi]) - \frac{e}{mc}\left(\nabla\rho\cdot\mathbf{A} + \rho\nabla\cdot\mathbf{A}\right) \tag{15}$$

$$= \frac{\hbar}{m}\Im\left(\nabla\Psi^*\cdot\nabla\Psi + \Psi^*\nabla^2\Psi\right) - \frac{e}{mc}\left(\nabla\rho\cdot\mathbf{A} + \rho\nabla\cdot\mathbf{A}\right) \tag{16}$$

We can simply this by realising that

$$\nabla\Psi^*\cdot\nabla\Psi = (\nabla\Psi)^*\cdot\nabla\Psi \tag{17}$$

$$= |\nabla\Psi|^2 \in \mathbb{R} \tag{18}$$

$$\Rightarrow \Im\left(\nabla\Psi^*\cdot\nabla\Psi\right) = 0 \tag{19}$$

Thus we have

$$\nabla\cdot\mathbf{J} = \frac{\hbar}{m}\Im\left(\Psi^*\nabla^2\Psi\right) - \frac{e}{mc}\left(\nabla\rho\cdot\mathbf{A} + \rho\nabla\cdot\mathbf{A}\right) \tag{20}$$

Choosing the Coulumb gauge, $\nabla\cdot\mathbf{A} = 0$, allows us to simply this further to

$$\nabla\cdot\mathbf{J} = \frac{\hbar}{m}\Im\left(\Psi^*\nabla^2\Psi\right) - \frac{e}{mc}\left(\nabla\rho\cdot\mathbf{A}\right) \tag{21}$$

Now Schrödinger's equation gives us an expression for $\nabla^2\Psi$ which we might be able to substitute back in

$$\imath\hbar\frac{\partial\Psi}{\partial t} = \left[\frac{1}{2m}\left(-\imath\hbar\nabla - \frac{e}{c}\mathbf{A}\right)^2 + eV\right]\Psi \tag{22}$$

But first, let's expand it and rearrange it into a more useful form:

$$\imath\hbar\frac{\partial\Psi}{\partial t} = \frac{1}{2m}\left(-\hbar^2\nabla^2 + \frac{e^2}{c^2}A^2 + \frac{\imath\hbar e}{c}\nabla\cdot\mathbf{A} + \frac{\imath\hbar e}{c}\mathbf{A}\cdot\nabla\right)\Psi + eV\Psi \tag{23}$$

$$= \frac{1}{2m}\left(-\hbar^2\nabla^2\Psi + \frac{e^2}{c^2}A^2 + \frac{\imath\hbar e}{c}\nabla\cdot[\mathbf{A}\Psi] + \frac{\imath\hbar e}{c}\mathbf{A}\cdot[\nabla\Psi]\right) + eV\Psi \tag{24}$$

By the product rule:

$$\nabla\cdot(\mathbf{A}\Psi) = \Psi\nabla\cdot\mathbf{A} + \mathbf{A}\cdot\nabla\Psi \tag{25}$$

Thus, we can write this as:

$$\imath\hbar\frac{\partial\Psi}{\partial t} = \frac{1}{2m}\left(-\hbar^2\nabla^2\Psi + \frac{e^2}{c^2}A^2 + \frac{\imath\hbar e}{c}\Psi\nabla\cdot\mathbf{A} + \frac{2\imath\hbar e}{c}\mathbf{A}\cdot\nabla\Psi\right) + eV\Psi \tag{26}$$

Remembering that $\nabla\cdot\mathbf{A} = 0$, due to our choice of gauge:

$$\imath\hbar\frac{\partial\Psi}{\partial t} = \frac{1}{2m}\left(-\hbar^2\nabla^2 + \frac{e^2}{c^2}A^2 + \frac{2\imath\hbar e}{c}\mathbf{A}\cdot\nabla\right)\Psi + eV\Psi \tag{27}$$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi = \imath\hbar\frac{\partial\Psi}{\partial t} - \frac{e^2}{c^2}A^2\Psi - \frac{\imath\hbar e}{mc}\mathbf{A}\cdot\nabla\Psi + eV\Psi \tag{28}$$

$$\nabla^2\Psi = -\frac{2m\imath}{\hbar}\frac{\partial\Psi}{\partial t} + \frac{2me^2}{\hbar^2c^2}A^2\Psi + \frac{2\imath e}{\hbar c}\mathbf{A}\cdot\nabla\Psi + eV\Psi \tag{29}$$

As V is a real scalar, $\Psi^* eV\Psi = eV|\Psi^2| \in \mathbb{R}$, thus this term goes to zero when we take the imaginary part. Our expression thus becomes:

$$\nabla\cdot\mathbf{J} = \frac{\hbar}{m}\Im\left(\Psi^*\left[-\frac{2m\imath}{\hbar}\frac{\partial\Psi}{\partial t} + \frac{2me^2}{\hbar^2c^2}A^2\Psi + \frac{2\imath e}{\hbar c}\mathbf{A}\cdot\nabla\Psi\right]\right) - \frac{e}{mc}\left(\nabla\rho\cdot\mathbf{A}\right) \tag{30}$$

$$\tag{31}$$

Assuming $\mathbf{A} \in \mathbb{R}$, the term $\Im\left(\Psi^*\frac{2me^2}{\hbar^2c^2}A^2\Psi\right) = 0$, meaning we have the following:

$$\nabla\cdot\mathbf{J} = \frac{\hbar}{m}\Im\left(-\frac{2m\imath}{\hbar}\Psi^*\frac{\partial\Psi}{\partial t} + \frac{2\imath e}{\hbar c}\Psi^*\mathbf{A}\cdot\nabla\Psi\right) - \frac{e}{mc}\left(\nabla\rho\cdot\mathbf{A}\right) \tag{32}$$

Let's look at that second term in the $\Im$:

$$\frac{\hbar}{m}\Im\left(\frac{2\imath e}{\hbar c}\Psi^*\mathbf{A}\cdot\nabla\Psi\right) = \frac{2e}{mc}\Im\left(\imath\mathbf{A}\cdot[\Psi^*\nabla\Psi]\right) \tag{33}$$

$$\frac{2e}{mc}\Re\left(\mathbf{A}\cdot[\Psi^*\nabla\Psi]\right) \tag{34}$$

$$\frac{e}{mc}\left(\{\mathbf{A}\cdot[\Psi^*\nabla\Psi]\} + \{\mathbf{A}\cdot[\Psi^*\nabla\Psi]\}^*\right) \tag{35}$$

$$\frac{e}{mc}\left(\mathbf{A}\cdot[\Psi^*\nabla\Psi + \Psi\nabla\Psi^*]\right) \tag{36}$$

Remembering that $\nabla\rho = \nabla(\Psi^*\Psi) = \Psi^*\nabla\Psi + \Psi\nabla\Psi^*$, this can be simplified to:

$$\frac{e}{mc}(\mathbf{A}\cdot[\Psi^*\nabla\Psi + \Psi\nabla\Psi^*]) = \frac{e}{mc}(\mathbf{A}\cdot\nabla\rho) \tag{37}$$

$$= \frac{e}{mc}(\nabla\rho\cdot\mathbf{A}) \tag{38}$$

Inputting this back into Equation 32 gives:

$$\nabla\cdot\mathbf{J} = \frac{\hbar}{m}\Im\left(-\frac{2m\imath}{\hbar}\Psi^*\frac{\partial\Psi}{\partial t}\right) + \frac{e}{mc}(\nabla\rho\cdot\mathbf{A}) - \frac{e}{mc}(\nabla\rho\cdot\mathbf{A}) \tag{39}$$

$$= \frac{\hbar}{m}\Im\left(-\frac{2m\imath}{\hbar}\Psi^*\frac{\partial\Psi}{\partial t}\right) \tag{40}$$

$$= -\Re\left(2\Psi^*\frac{\partial\Psi}{\partial t}\right) \tag{41}$$

$$= -\left(\left\{\Psi^*\frac{\partial\Psi}{\partial t}\right\} + \left\{\Psi^*\frac{\partial\Psi}{\partial t}\right\}^*\right) \tag{42}$$

$$= -\left(\Psi^*\frac{\partial\Psi}{\partial t} + \Psi\frac{\Psi^*}{\partial t}\right) \tag{43}$$

We showed at the beginning in Equation that this is simply:

$$\nabla\cdot\mathbf{J} = -\frac{\partial\rho}{\partial t} \tag{44}$$

$$\Rightarrow \frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{J} = 0 \tag{45}$$

We have thus proven the continuity equation demonstrating conservation of probability in quantum mechanics, from the definitions of ρ and $\mathbf{J}$.

□