Schrodinger's Equation

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1 Schrodinger's Equation

Schrodinger's equation governs the time evolution of quantum states. It says that the time dependence of a state $|\psi\rangle$ is given by

$$\hat{H}\,|\psi\rangle = i\hbar\frac{\partial}{\partial t}\,|\psi\rangle$$

where $\hat{H}$ is the Hamiltonian of the system. We can prove this equation by constructing a time evolution operator.
Let's say that $\hat{U}(dt)$ represents an operator that evolves states by an infinitesimal time dt.[1] That is

$$|\psi(t+dt)\rangle = \hat{U}(dt)\,|\psi(t)\rangle$$

by definition of $\hat{U}(dt)$. We can perform a power series expansion of $\hat{U}(dt)$ in the parameter dt

$$\hat{U}(dt) = \hat{c}_0 + \hat{c}_1 dt + \hat{c}_2(dt)^2 + \cdots = \hat{c}_0 + \hat{c}_1 dt$$

where we have dropped terms of order $(dt)^2$ and higher because the square of an infinitesimal is infinitely negligible. We also know that $U(0)$ is the identity operator, so we must have $\hat{c}_0 = \hat{I}$.
Now by conservation of probability we must have

$$\langle\psi(t+dt)|\,\psi(t+dt)\rangle = \langle\psi(t)|\,\psi(t)\rangle$$

Therefore

$$\langle\psi(t+dt)|\,\psi(t+dt)\rangle = \left\langle\psi(t)\right|(\hat{I}+\hat{c}_1^\dagger dt)(\hat{I}+\hat{c}_1 dt)\left|\psi(t)\right\rangle$$

$$= \left\langle\psi(t)\right|\hat{I}+(\hat{c}_1^\dagger+\hat{c}_1)dt\left|\psi(t)\right\rangle = \langle\psi(t)|\,\psi(t)\rangle + dt\left\langle\psi(t)\right|\hat{c}_1^\dagger+\hat{c}_1\left|\psi(t)\right\rangle$$

Therefore

$$\left\langle\psi(t)\right|\hat{c}_1^\dagger+\hat{c}_1\left|\psi(t)\right\rangle = 0$$

and since $|\psi\rangle$ is arbitrary, this means that $\hat{c}_1^\dagger + \hat{c}_1 = 0$, or in other words $\hat{c}_1$ is anti-Hermitian. We will rewrite $\hat{c}_1 = -i\hat{h}$, where $\hat{h}$ is a Hermitian operator. So we have found

$$\hat{U}(dt) = \hat{I} - i\hat{h}dt$$

for some Hermitian operator $\hat{h}$.
Now we can write down an expression for the time derivative of states.

$$\frac{\partial}{\partial t}\,|\psi(t)\rangle = \lim_{dt\to 0}\frac{|\psi(t+dt)\rangle - |\psi(t)\rangle}{dt}$$

$$= \lim_{dt\to 0}\frac{\hat{U}(dt)\,|\psi(t)\rangle - |\psi(t)\rangle}{dt}$$

$$= \lim_{dt\to 0}\frac{(\hat{I}-i\hat{h}dt)\,|\psi(t)\rangle - |\psi(t)\rangle}{dt}$$

$$= \lim_{dt\to 0}\frac{-i\hat{h}dt\,|\psi(t)\rangle}{dt}$$

[1] We are assuming the existence of such an operator here. Perhaps that could be one of our axioms of quantum mechanics.

$$= -i\hat{h}\left|\psi(t)\right\rangle$$

This already looks quite a bit like Schrodinger's equation, but we don't know what $\hat{h}$ is. Let's specialize to the case where $\hat{h}$ is not explicitly time dependent and check to see if it is a conserved quantity. If it is, then it must be proportional to one of the conserved dynamical quantities: energy, momentum, or angular momentum. Since it is a scalar quantity because it is invariant under rotations, the two momentum cases are automatically ruled out, leaving only the possibility of energy, which is what we want. A quantity corresponding to an operator $\hat{O}$ is conserved if and only if

$$0 = \frac{\partial}{\partial t}\left\langle\psi(t)\middle|\hat{O}\middle|\psi(t)\right\rangle$$

So we let $\hat{O} = \hat{h}$ and compute

$$\frac{\partial}{\partial t}\left\langle\psi(t)\middle|\hat{h}\middle|\psi(t)\right\rangle = \left(\frac{\partial}{\partial t}\left\langle\psi(t)\right|\right)\hat{h}\left|\psi(t)\right\rangle + \left\langle\psi(t)\right|\hat{h}\left(\frac{\partial}{\partial t}\left|\psi(t)\right\rangle\right)$$

$$\left\langle\psi(t)\middle|(i\hat{h})\hat{h}\middle|\left|\psi(t)\right\rangle\right\rangle + \left\langle\psi(t)\middle|\hat{h}(-i\hat{h})\middle|\left|\psi(t)\right\rangle\right\rangle = 0$$

So we have found that $\hat{h}$ corresponds to a conserved scalar dynamical quantity, which means it must be proportional to energy because this is the definition of energy. We write the operator that corresponds directly to energy (without any proportionality constant) as $\hat{H}$, where the H stands for Hamiltonian. The proportionality constant in $\hat{h}$ is found by requiring that $\hat{U}(dt)$ be dimensionless, which means that $\hat{h}dt = (a\hat{H})dt$ is dimensionless, so the proportionality constant a must have dimensions of inverse energy and time. The only fundamental constant that works is $1/\hbar$. If we now insert $\hat{h} = \hat{H}/\hbar$ into our previous result we obtain

$$\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = -i\hat{h}\left|\psi(t)\right\rangle = -\frac{i}{\hbar}\hat{H}\left|\psi(t)\right\rangle$$

Rearranging gives Schrodinger's equation

$$\hat{H}\left|\psi(t)\right\rangle = i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle$$