The Schrödinger Equation - Corrections

Originally appeared at:
http://behindtheguesses.blogspot.com/2009/06/schrodinger-equation-corrections.html

Eli Lansey — elansey@gmail.com
June 4, 2009

CC BY-NC-SA

In my last post,[1] I claimed

> Additionally, we can extend from here that any quantum operator $\mathcal{G}$ is written in terms of its classical counterpart G by
> $$\mathcal{G} = -iG/\hbar.$$

Peeter Joot correctly pointed out[2] that this result does not follow from the argument involving the Hamiltonian. While it is true that

> any arbitrary unitary transformation, $\mathcal{U}$, can be written as
> $$\mathcal{U} = e^{-i\frac{\alpha}{\hbar}G},$$
> where G is an Hermitian operator,

the relationship between a classical G and its quantum counterpart is not as straightforward as I claimed. In reality, we can only relate the classical Poisson brackets to the quantum mechanical commutators, and we must work from there. Perhaps I will discuss this further in a later post.

In any case, though, the derivation of the Schrödinger equation only makes use of the relationship between the classical and quantum mechanical Hamiltonians, so the remainder of the derivation still holds. I am leaving the original post up as reference, but the corrected, restructured version (with some additional, although slight, notation changes) is below.

A brief walk through classical mechanics

Say we have a function of $f(x)$ and we want to translate it in space to a point $(x + \Delta x)$, where Δx need not be small. To do this, we'll find a "space translation" operator $S_{\Delta x}$ which, when applied to $f(x)$, gives $f(x + \Delta x)$. That is,

$$f(x + \Delta x) = S_{\Delta x} f(x) \tag{1}$$

We'll expand $f(x + \Delta x)$ in a Taylor series:

$$\begin{aligned} f(x + \Delta x) &= f(x) + \Delta x \frac{df(x)}{dx} + \frac{(\Delta x)^2}{2!}\frac{d^2 f(x)}{dx^2} + \dots \\ &= \left[1 + \Delta x \frac{d}{dx} + \frac{(\Delta x)^2}{2!}\frac{d^2}{dx^2} + \dots\right] f(x) \end{aligned} \tag{2}$$

[1] http://behindtheguesses.blogspot.com/2009/05/schrodinger-equation.html

[2] http://behindtheguesses.blogspot.com/...
2009/05/schrodinger-equation.html?showComment=1243377144823#c3781014951742869278

which can be simplified using the series expansion of the exponential[3] to

$$e^{\left[\Delta x \frac{d}{dx}\right]} f(x) \tag{3}$$

from which we can conclude that

$$S_{\Delta x} = e^{\left[\Delta x \frac{d}{dx}\right]} \tag{4}$$

If you do a similar thing with rotations around the z-axis, you'll find that the rotation operator is

$$R_{\Delta\theta} = e^{\Delta\theta\, L_z}, \tag{5}$$

where L_z is the z-component of the angular momentum.

Comparing (4) and (5), we see that both have an exponential with a parameter (distance or angle) multiplied by something ($\frac{d}{dx}$ or L). We'll call the something the "generator of the transformation." So, the generator of space translation is $\frac{d}{dx}$ and the generator of rotation is L. So, we'll write an arbitrary transformation operator O through a parameter $\Delta\alpha$ as

$$O_{\Delta\alpha} = e^{\Delta\alpha\, G} \tag{6}$$

where G is the generator of this particular transformation.[4] See [1] for an example with Lorentz transformations.

From classical to quantum

Generalizing (6), we'll postulate that any arbitrary quantum mechanical (unitary) transformation operator $\mathcal{O}$ through a parameter $\Delta\alpha$ can be written as

$$\mathcal{O}_{\Delta\alpha} = e^{\Delta\alpha\, \mathcal{G}}, \tag{7}$$

where $\mathcal{G}$ is the quantum mechanical version of the classical operator G. We'll call this the "quantum mechanical generator of the transformation." If we have a way of relating a classical generator to a quantum mechanical one, then we have a way of finding a quantum mechanical transformation operator.

For example, in classical dynamics, the time derivative of a quantity f is given by the Poisson bracket:

$$\frac{df}{dt} = \{f, H\} \tag{8}$$

where H is the classical Hamiltonian of the system and $\{\ ,\ \}$ is shorthand for a messy equation.[2] In quantum mechanics this equation is replaced with

$$\frac{df}{dt} = i\hbar[f, \mathcal{H}] \tag{9}$$

where the square brackets signify a commutation relation and $\mathcal{H}$ is the quantum mechanical Hamiltonian.[3] This holds true for any quantity f, and $i\hbar$ is a number which commutes with everything, so we can argue that the quantum mechanical Hamiltonian operator is related to the classical Hamiltonian by

$$H = i\hbar\mathcal{H} \Rightarrow \mathcal{H} = -iH/\hbar. \tag{10}$$

[3] $e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \ldots$

[4] There are other ways to do this, differing by factors of i in the definition of the generators and in the construction of the exponential, but I'm sticking with this one for now.

Time translation of a quantum state

Consider a quantum state at time t described by the wavefunction $\psi(\vec{r},t)$. To see how the state changes with time, we want to find a "time-translation" operator $\mathcal{T}_{\Delta t}$ which, when applied to the state $\psi(\vec{r},t)$, will give $\psi(\vec{r},t+\Delta t)$. That is,

$$\psi(\vec{r},t+\Delta t) = \mathcal{T}_{\Delta t}\psi(\vec{r},t). \tag{11}$$

From our previous discussion we know that we can write $\mathcal{T}$ using (7). Classically, the generator of time translations is the Hamiltonian![4] So we can write

$$\begin{aligned}\mathcal{T}_{\Delta t} &= e^{\Delta t\,\mathcal{H}} \\ &= e^{-i\frac{\Delta t}{\hbar}H}\end{aligned} \tag{12}$$

where we've made the substitution from (10). Then (11) becomes

$$\psi(\vec{r},t+\Delta t) = e^{-i\frac{\Delta t}{\hbar}H}\,\psi(\vec{r},t). \tag{13}$$

This holds true for any time translation, so we'll consider a small time translation and expand (13) using a Taylor expansion[5] dropping all quadratic and higher terms:

$$\psi(\vec{r},t+\Delta t) \approx \left[1 - i\frac{\Delta t}{\hbar}H + \ldots\right]\psi(\vec{r},t) \tag{14}$$

Moving things around gives

$$H\psi(\vec{r},t) = i\hbar\left[\frac{\psi(\vec{r},t+\Delta t) - \psi(\vec{r},t)}{\Delta t}\right] \tag{15}$$

In the limit $\Delta t \to 0$ the right-hand side becomes a partial derivative giving the Schrödinger equation

$$H\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} \tag{16}$$

For a system with conserved total energy, the classical Hamiltonian is the total energy

$$H = \frac{\vec{p}^2}{2m} + V \tag{17}$$

which, making the substitution for quantum mechanical momentum $\vec{p} = i\hbar\nabla$ and substituting into (16) gives the familiar differential equation form of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} \tag{18}$$

References

[1] J.D. Jackson. *Classical Electrodynamics*. John Wiley & Sons, Inc., 3rd edition, 1998.

[2] L.D. Landau and E.M. Lifshitz. *Mechanics*. Pergamon Press, Oxford, UK.

[3] L.D. Landau and E.M. Lifshitz. *Quantum Mechanics*. Butterworth-Heinemann, Oxford, UK.

[4] H. Goldstein, C. Poole, and J. Safko. *Classical Mechanics*. Cambridge University Press, San Francisco, CA, 3rd edition, 2002.

[5] Kind of the reverse of how we got to this whole exponential notation in the first place...