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Alternative "Derivations" of the Schrödinger Equation

As mentioned in Section 3.1 of *A Student's Guide to the Schrödinger Equation*, it's not possible to rigorously derive the Schrödinger Equation from first principles, but it is possible to "justify" an equation by showing that it's consistent with other equations and principles. That's the approach taken in *A Student's Guide to the Schrödinger Equation* by showing that the Schrödinger Equation is consistent with the principle of conservation of energy.

If you're interested in other approaches to justifying the Schrödinger Equation, this document provides a summary of two of those: the path-integral approach and the probability-flow approach. After a short description of each of those approaches, you'll find a list of several helpful references that provide additional details.

Path-integral approach

The path-integral approach to quantum mechanics grew out of the work of P.A.M. Dirac in the early 1930's; Dirac was attempting to apply the Lagrangian function (the difference between kinetic and potential energy) to quantum mechanics. In classical physics, the integral of the Lagrangian over time (which is now called the "action") determines the change in phase of a wave propagating along a specified path, and Dirac speculated that this might be "analogous" to a function that determines the time evolution of a quantum wavefunction (such functions are called "propagators"). Dirac's work didn't lead to the Schrödinger Equation, but almost a decade later Richard Feynman was exploring the consequences of connecting the action to the wavefunction propagator and, in his words, "out came the Schrödinger Equation."

The details of Feynman's path-integral approach are provided in the references listed below, but you can get a sense of how it works by considering a one-dimensional wavefunction $\Psi(x,t)$ given by

$$\Psi(x,t) = Ae^{i(kx-\omega t)}$$

in which ω represents the angular frequency of the wave and k represents the wavenumber of the wave, given by

$$k = \frac{2\pi}{\lambda}.$$

With that definition of the wavenumber, the quantity kx is equivalent to

$$kx = \frac{2\pi}{\lambda}x = 2\pi\frac{x}{\lambda}.$$

In this expression, the factor x/λ is the distance in units of wavelengths (that is, the number of wavelengths the wave has travelled), and multiplying by the factor of 2π converts the number of wavelengths into units of angle (since the phase advances by 2π radians for each wavelength travelled). So kx tells you how much the phase of the wave changes as the wave propagates over distance x.

But what if the wavenumber k varies with distance? Consider, for example, the situation in which the wave travels a distance x_1 through a region with wavenumber k_1, and then distance x_2 through a region with wavenumber k_2. In that case, the phase change over the total path through both regions is

$$\text{Phase change (spatial)} = k_1x_1 + k_2x_2$$

Likewise, if the wave travels along a path that passes through N regions, the phase change over the total path is

$$\text{Phase change (spatial)} = \sum_{i=1}^{N} k_i x_i$$

In the case of continuous variation of wavenumber with distance over path P, the wave's phase change with distance is

$$\text{Phase change (spatial)} = \int_P k\,dx = \int_P \frac{p}{\hbar}\,dx$$

in which the wavenumber has been related to the momentum using the de Broglie relation $k = \frac{p}{\hbar}$.

Now consider the phase change produced by the passage of time (ωt). If the angular frequency (ω) varies continuously with time, a similar analysis gives that phase change as

$$\text{Phase change (temporal)} = \int_T \omega dt = \int_T \frac{E}{\hbar} dt$$

in which T represents the time it takes the wave to travel over path P and the angular frequency has been related to energy using the Planck-Einstein relation $\omega = \frac{E}{\hbar}$.

The next step toward the Schrödinger Equation can be made by using these expressions for phase change to form a propagator that takes a wavefunction $\Psi(x_1, t_1)$ at one point in space (x_1) and time (t_1) and produces the wavefunction $\Psi(x_2, t_2)$ at another point in space (x_2) and later time (t_2). If there is only a single path P to get from (x_1, t_1) to (x_2, t_2), the propagator equation looks like this:

$$\Psi(x_2, t_2) = Ae^{\frac{i}{\hbar}\int_P p dx} e^{-\frac{i}{\hbar}\int_T E dt} \Psi(x_1, t_1)$$

in which A represents a normalization constant. It's helpful to have both these integrals over time, so to convert the position integral $\int_P p dx$ into an integral over time, note that the time that passes as the wave travels can be related to the distance travelled by the wave's velocity. So use the relation $dx = \frac{dx}{dt} dt = v dt$ to write the propagator as

$$\Psi(x_2, t_2) = Ae^{\frac{i}{\hbar}\int_T pv dt} e^{-\frac{i}{\hbar}\int_T E d} \Psi(x_1, t_1)$$

$$= Ae^{\frac{i}{\hbar}\int_T (pv - E) dt} \Psi(x_1, t_1)$$

The next step is to relate the terms inside the integral to the kinetic energy (KE) and the potential energy (PE), which you can do using

$$KE = \frac{1}{2} m v^2 = \frac{pv}{2}$$

for kinetic energy and

$$E = KE + PE$$

for total energy. This makes the propagator

$$\Psi(x_2,t_2) = Ae^{\frac{i}{\hbar}\int_T[2KE-(KE+PE)]dt}\Psi(x_1,t_1)$$

$$= Ae^{\frac{i}{\hbar}\int_T(KE-PE)dt}\Psi(x_1,t_1)$$

As you may recall from classical mechanics, the Lagrangian ($\mathcal{L}$) is defined as $\mathcal{L}$ = KE-PE, so this becomes

$$\Psi(x_2,t_2) = Ae^{\frac{i}{\hbar}\int_T \mathcal{L}\,dt}\,\Psi(x_1,t_1)$$

The integral of the Lagrangian over time is the "action" mentioned above, and it's the action that determines the phase change of the propagating wavefunction. But this is the contribution to the wavefunction's evolution for a single path, and Feynman realized that it's necessary to integrate over all possible paths to get the probability for the wavefunction to evolve from (x_1,t_1) to (x_2,t_2). Thus the correct expression

$$\Psi(x_2,t_2) = \sum_{All\ paths} Ae^{\frac{i}{\hbar}\int_T \mathcal{L}\,dt}\,\Psi(x_1,t_1).$$

Now consider an incremental time change ϵ, so write t_2=t and t_1=t-ϵ, over an incremental distance ξ, so write x_2=x and x_1=x-ξ. Then

$$\Psi(x,t) = \sum_{All\ paths} Ae^{\frac{i}{\hbar}\int_T \mathcal{L}\,dt}\,\Psi(x-\xi,t-\epsilon).$$

Feynman's next trick was to expand wavefunction $\Psi(x-\xi,t-\epsilon)$ using a Taylor series (you can see the details in the references listed below), giving

$$\Psi(x,t) = A\sqrt{\frac{2\pi i\hbar\epsilon}{m}}\left[\Psi(x,t) + \left(-\frac{\partial\Psi(x,t)}{\partial t} - \frac{i}{\hbar}V\Psi(x,t) + \frac{i\hbar}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}\right)\epsilon\right] + O(\epsilon^2)$$

in which $O(\epsilon^2)$ represents terms of order ϵ^2 and higher. For this equation to be true, the constant *A* must be

$$A = \sqrt{\frac{m}{2\pi i\hbar\epsilon}}$$

and the three terms inside the parentheses must sum to zero. That means that

$$-\frac{\partial\Psi(x,t)}{\partial t} - \frac{i}{\hbar}V\Psi(x,t) + \frac{i\hbar}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} = 0$$

Now rearrange the terms and multiply through by $i\hbar$ to get

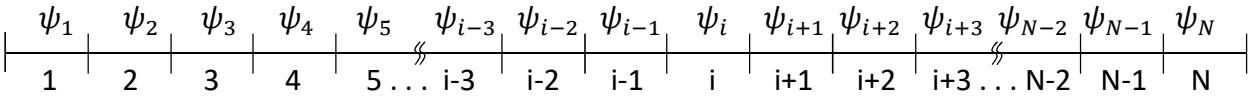
$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V\Psi(x,t)$$

which is the time-dependent Schrödinger Equation.

Probability-flow approach

In discussing the change of probability over space and time, most quantum textbooks begin with the Schrödinger equation and manipulate that equation to arrive at a definition of probability flow (also called "probability current"), but it's also possible to go the other way. That approach begins by writing an expression for the change of probability in a given spatial interval and then manipulates that expression to arrive at a version of the Schrödinger equation. This section will give you an idea of how that approach works, and if you'd like more detail, take a look at the references listed below.

To understand probability flow, start by considering a quantum particle in some spatial region of interest and dividing that region into N discrete intervals. Assigning an index to each interval (from 1 to N) makes the x-axis look like this (this section uses the notation in Baym's *Lectures on Quantum Mechanics*):



Within each interval, there exists a one-dimensional quantum wavefunction ψ, the square magnitude of which ($|\psi|^2$) gives the probability that the quantum particle will be found within that interval. As you can see above the sketch of the intervals, over each interval in position (x), the wavefunction for that interval has a subscript with the interval's index number. So the probability of finding the particle in interval 1 is $|\psi_1|^2$ and the probability in interval i is $|\psi_i|^2$.

Now consider how the probability amplitude in interval i (ψ_i) might change over time – some probability amplitude from the neighboring intervals (i-1 on the left and i+1 on the right) might "flow in" to interval i, and some probability amplitude from interval

i might flow out into those regions. What about the other intervals? By considering the probability amplitude change over very short time periods, the flow of probability amlitude from those regions will be negligible.

Expressing this "inflow and outflow" concept mathematically looks like this:

$\psi_i(t + \Delta t) = \psi_i(t)$ +Probability amplitude flowing in – Probability amplitude flowing out

The next logical question is how to write an expression for the probability amplitude flowing from an adjacent interval (i-1, for example) into interval i. For short time periods, it seems reasonable to make that flow proportional to the amount of time (Δt) as well as the amount of probability amplitude present in the source interval (i-1 in this case). As for the constant of proportionality, Baym writes it as $-\sqrt{-1}w_{i,i-1}$, in which the first subscript specifies the destination interval (the interval into which the probability amplitude is flowing), and the second subscript specifies the source interval (the interval from which the probability amplitude is flowing). The reason for including the factor $-\sqrt{-1}$ is straightforward: it connects the terms of the probability-flow equation to the terms of the Schrödinger Equation.

Using this notation and writing the complex unit i=$\sqrt{-1}$ (be careful not to confuse the "i" with the "i" interval index), you can write

Probability amplitude flowing in to interval i from interval i-1 = $-i\Delta t w_{i,i-1}\psi_{i-1}(t)$

and

Probability amplitude flowing in to interval i from interval i+1 = $-i\Delta t w_{i,i+1}\psi_{i+1}(t)$.

For the probability amplitude outflow from interval i, Baym uses a slightly different notation. That's because the probability amplitude (the wavefunction) in any interval may change not only by flowing out into adjacent intervals, but it's also possible for the wavefunction phase to change. That phase change doesn't cause a change in the probability within the interval, since it drops out when the wavefunction is squared ($|\psi_i|^2 = \psi_i * \psi_i$), but it's related to the potential energy of the particle. Baym includes the effect of phase change into the coefficient for probability

amplitude outflow (in either direction) and writes that coefficient as w_{ii}. The same factors of $-i\Delta t$ apply to this term, and the "source" interval (i in this case) has initial probability amplitude ψ_i(t), so the final term in the expression for $\psi_i(t+\Delta t)$ is

Probability amplitude flowing out (or changing phase) of interval i = $-i\Delta t w_{ii}\psi_i$(t)

Thus

$$\psi_i(t+\Delta t) = \psi_i(t) - i\Delta t w_{i,i-1}\psi_{i-1}(t) - i\Delta t w_{i,i+1}\psi_{i+1}(t) - i\Delta t w_{ii}\psi_i(\text{t}),$$

and moving $\psi_i(t)$ to the left side and dividing by $-i\Delta t$ makes this

$$\frac{\psi_i(t+\Delta t)-\psi_i(t)}{-i\Delta t} = i\frac{\psi_i(t+\Delta t)-\psi_i(t)}{\Delta t} = w_{i,i-1}\psi_{i-1}(t) + w_{i,i+1}\psi_{i+1}(t) + w_{ii}\psi_i(\text{t})$$

Over a very small time period (so Δt approaches zero), the fraction between the equals signs becomes the partial derivative of $\psi_i(t)$ with respect to time. So this is

$$i\frac{\partial\psi_i(t)}{\partial t} = w_{i,i-1}\psi_{i-1}(t) + w_{i,i+1}\psi_{i+1}(t) + w_{ii}\psi_i(\text{t})$$

which at least has one element in common with the Schrödinger Equation (the leftmost term). To make the next step, write the outflow/phase change coefficient as

$$w_{ii} = -w_{i,i+1} - w_{i,i+1} + \frac{v_i}{\hbar}.$$

At first glance, this may look a bit opaque, but the first two terms are simply the "outflow" coefficients, which are just the negative of the "inflow" coefficients, since the total probability must be conserved (don't confuse these negative signs with the negative signs in the $-i\Delta t$ factors, because you'll need both in the next step). The term involving v_i and Planck's modified constant (ħ) allows for wavefunction phase change within an interval; the form is chosen to connect to the potential-energy term in the Schrödinger Equation.

Inserting this expression for w_{ii} gives

$$i\frac{\partial\psi_i(t)}{\partial t} = w_{i,i-1}\psi_{i-1}(t) + w_{i,i+1}\psi_{i+1}(t) + (-w_{i,i+1} - w_{i,i+1} + \frac{v_i}{\hbar})\psi_i(\mathrm{t})$$

or

$$i\frac{\partial\psi_i(t)}{\partial t} = w_{i,i-1}[\psi_{i-1}(t) - \psi_i(\mathrm{t})] + w_{i,i+1}[\psi_{i+1}(t) - \psi_i(\mathrm{t})] + (\frac{v_i}{\hbar})\psi_i(\mathrm{t})$$

This is beginning to look promising – the left side of this equation already matches a term in the Schrödinger Equation, and the right side contains terms related to the spatial change in the wavefunction and the potential energy.

To take the final steps, shrink the discrete intervals to infinitesimally small extent, so the wavefunction $\psi(x)$ varies continuously across the region of interest. Expanding the wavefunction over an incremental distance using a Taylor introduces first- and second-order spatial derivatives, and the first-order derivatives cancel (you can see the details in the references listed below), leading to

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + v(x,t)\psi(x,t)$$

which is the time-dependent Schrödinger Equation.

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