Connecting Path Integral Formalism with Schrodinger Formalism

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The full time dependent Schrodinger equation is

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

(As a brief aside, the shortest notation for the Hamiltonian in x-space is $\langle x| H = \langle x| \frac{\mathbf{P}^2}{2m} + V(x)\langle x|$)

In order to evaluate the LHS we should compare the wavefunction at t to that at a (shortly) later time, $t+\delta t$. So what is $\Psi(x, t+\delta t)$ according to Path Integral Formalism (PIF)? This can be evaluated by applying the PIF propagator

$$\Psi(x,t+\delta t) = A\int d(\delta x)\int d[x_{path}]e^{i/\hbar\int_t^{t+\delta t}\mathcal{L}(x,\dot{x},t')dt'}\Psi(x-\delta x,t)$$

where all paths connect the two endpoints, $x-\delta x$ and x. Only a small range of δx contribute, even though the integral goes from $-\infty \to \infty$.

As long as we don't go too far from x, we can approximate $V(x)$ like a constant, then

$$\lim_{\Delta t\to 0} \to \int d(\delta x)\sqrt{\frac{m}{2\pi i\hbar\delta t}}e^{\frac{i(\delta x)^2 m}{\hbar\delta t 2}}e^{-\frac{iV(x)\delta t}{\hbar}}\Psi(x-\delta x,t)$$

The trick is knowing which terms to drop and which to keep. Doing a Taylor expansion around small quantities

$$e^{-\frac{iV(x)\delta t}{\hbar}} \to (1-\frac{i}{\hbar}V(x)\delta t)$$

if δt is small, therefore we can ignore the higher terms
if δx is small, then

$$\Psi(x-\delta x,t) \to \big(\Psi(x,t) - \frac{\partial\Psi}{\partial x}\delta x + \frac{1}{2}\frac{\partial^2\Psi}{\partial x^2}(\delta x)^2\big)$$

we can reduce this further by kicking out products of small quantities when we multiply these simplifications together

$$\left(1-\frac{i}{\hbar}V(x)\delta t\right)\left(\Psi(x,t) - \frac{\partial\Psi}{\partial x}\delta x\right) + \frac{1}{2}\frac{\partial^2\Psi}{\partial x^2}(\delta x)^2$$

now looking at the first part of the integral

$$\int d(\delta x)\sqrt{\frac{m}{2\pi i\hbar\delta t}}e^{\frac{i(\delta x)^2 m}{\hbar\delta t 2}}$$

we can rewrite the term in the exponent as

$$\frac{-(\delta x)^2}{2(\sqrt{i\hbar\delta t/m})^2}$$

This gives us our familiar gaussian integral form. Recalling that

$$\int_{-\infty}^{\infty} ye^{-y^2/2\sigma^2}dy = 0$$

and

$$\int_{-\infty}^{\infty} y^2 e^{-y^2/2\sigma^2} dy = \sigma^2$$

our expression becomes

$$\Psi(x,t+\delta t) = (1 - \frac{i}{\hbar}V(x)\delta t)\Psi(x,t) + 0 + \frac{1}{2}\frac{\partial^2\Psi}{\partial x^2}\frac{i\hbar\delta t}{m}$$

doing a little rearranging

$$\Psi(x,t+\delta t) - \Psi(x,t) = \frac{\partial\Psi}{\partial t}\delta t = \frac{1}{i\hbar}V(x)\delta t\Psi(x,t) - \frac{\hbar}{2im}\delta t\frac{\partial^2\Psi}{\partial x^2}$$

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

and we see that our Path Integral Formalism recovers our Time Dependent Schrodinger Equation

Variational Method

How can we find an approximate solution to the Schrodinger equation making quantum mechanical approximations vice classical approximations?

Let's say we had some complicated Hamiltonian and we are trying to find the solution to

$$H|\Psi_E\rangle = E|\Psi_E\rangle$$

We first ask, "can we find the ground state solution?"

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

Our first care is if we can find the energy eigenvalues. We care far less about whether we can find the actual wavefunction itself, so we make a very crude approximation. We pick an arbitrary ϕ where $H|\phi\rangle$ may not be an eigenstate, but we can ask, "what is $\langle E\rangle$?"

$$\langle E\rangle_\phi = \langle\phi| H |\phi\rangle = \left\langle \phi \middle| H \sum_n a_n \middle| \Psi_n \right\rangle$$

where $a_n = \langle\Psi_n|\,\phi\rangle$
the eigenstates of H form a complete basis

$$\left\langle \phi \middle| E_n \sum_n a_n \middle| \Phi_n \right\rangle = |a_n|^2 E_n \geq E_0$$

This becomes an iterative process where by choosing ϕ "cleverly" you get closer and closer to E_0. This process converges much more quickly to the correct ground state energy than to the correct ground state wave function. Assume at some point you have $|\phi\rangle = |\Psi_n\rangle + |\Psi_\perp\rangle$, where

$$\delta|\Psi_\perp\rangle = \sum_{n=1}^{\infty} a_n |\Psi_n\rangle$$

is a (small correction). Then what is $\langle\phi| H |\phi\rangle$?

$$\langle\phi| H |\phi\rangle = \langle\phi_0| H\phi_0\rangle + \langle\phi_0| H |\Psi_\perp\rangle + \langle\Psi_\perp| H |\phi_0\rangle + \delta\langle\Psi_\perp| H |\delta\Psi_\perp\rangle$$

The middle two terms are zero by orthogonality, the first term is E_0 (what we want), and the final term is how far off we are from the actual answer. So if we're close, then our error is $\delta\left|\Psi_\perp\right|^2$, which is even smaller. The trick is in guessing well.
One thing we can do is try several wavefunctions at once by parameterizing $\phi(a,b,c...)$, then we find $\langle E(a,b,c...)\rangle$, and just minimize this function.

$$\langle E\rangle_{min} = \frac{\partial E}{\partial allparameters} = 0$$

Let's test it on a system where we already know the answer, the good ol' harmonic oscillator. We already know that

$$H = \frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{m\omega^2 x^2}{2}\Psi$$

and let's make our assumption that

$$\phi(x) = Ae^{-x^2/4\sigma^2}$$

where $A = (2\pi\sigma^2)^{-1/4}$ and σ is our fit parameter. We can take the derivatives and plug them into the time independent Schrodinger equation

$$\frac{\partial^2\phi/A}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{-2x}{4\sigma^2}e^{-x^2/4\sigma^2}\right) = \frac{-2}{4\sigma^2}e^{-x^2/4\sigma^2} + \frac{x^2}{4\sigma^4}e^{-x^2/4\sigma^2}$$

$$H\phi(x) = Ae^{-x^2/4\sigma^2}\left[\frac{-\hbar^2}{2m}\left(\frac{-2}{4\sigma^2} + \frac{x^2}{4\sigma^4}\right) + \frac{m\omega^2 x^2}{2}\Psi\right]$$

so then

$$\langle E\rangle = A^2\int e^{-x^2/2\sigma^2}\left(\frac{\hbar^2}{4\sigma^2 m} - \frac{\hbar^2 x^2}{8m\sigma^4} + \frac{m\omega^2 x^2}{2}\right)dx$$

$$= \left(\frac{\hbar^2}{4\sigma^2 m} - \frac{\hbar^2\sigma^2}{8m\sigma^4} + \frac{m\omega^2\sigma^2}{2}\right) = \left(\frac{\hbar^2}{8m\sigma^2} + \frac{m\omega^2\sigma^2}{2}\right)$$

now minimizing

$$\frac{\partial\langle E\rangle}{\partial\sigma^2} = \left(\frac{-\hbar^2}{8m\sigma^4} + \frac{m\omega^2}{2}\right) = 0$$

$$\frac{m\omega^2}{2} = \frac{\hbar^2}{8m\sigma^4}$$

$$\therefore\ \sigma^2 = \frac{\hbar}{2m\omega}$$

plugging this back into our assumption for ϕ

$$\phi = Ae^{-m\omega x^2/2\hbar}$$

which is of course the correct answer.