PATH INTEGRAL TO SCHRÖDINGER EQUATION FOR A VECTOR POTENTIAL

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 8. Section 8.6, Exercise 8.6.4.

When we showed that the path integral approach is equivalent to the Schrödinger equation, we did so for a scalar potential V, so that the Lagrangian is the usual $L = T - V$, and we can use that to calculate the action over an infinitestimal time interval ε, during which time the particle moves from x' to x. In the calculation, we chose the value of V at the midpoint of this interval, that is $V\left(\frac{x+x'}{2}\right)$. In fact, in this derivation it didn't matter where in the interval $[x', x]$ we chose to evaluate V, since we took only terms up to first order in ε, and moving the point at which we evaluate V introduced terms only of order ε^2 or higher.

Things get a bit more complicated if we consider a system such as the electromagnetic force, where the Lagrangian is no longer just $T - V$, but becomes

$$L = \frac{1}{2}m\mathbf{v}\cdot\mathbf{v} - q\phi + \frac{q}{c}\mathbf{v}\cdot\mathbf{A} \tag{1}$$

To examine the effect this has on the demonstration that the path integral approach is equivalent to the Schrödinger equation, we'll consider only one dimension, and leave out the electrostatic potential ϕ since it's just a scalar potential and we already know that such potentials do indeed convert to the Schrödinger equation. Thus the Lagrangian we'll consider is

$$L = \frac{1}{2}mv^2 + \frac{q}{c}vA \tag{2}$$

Over the infinitesimal time interval ε we have

$$v = \frac{x - x'}{\varepsilon} \tag{3}$$

The propagator over this time interval is

(4)
$$U\left(x,\varepsilon;x',0\right)=\sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\frac{(x-x')^{2}}{\varepsilon}+\varepsilon\frac{q}{c}\frac{x-x'}{\varepsilon}A\left(x+\alpha\left(x-x'\right)\right)\right)\right]$$

(5)
$$=\sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\frac{\eta^{2}}{\varepsilon}-\frac{q}{c}\eta A\left(x+\alpha\eta\right)\right)\right]$$

(6)
$$=\sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\exp\left(\frac{im\eta^{2}}{2\hbar\varepsilon}\right)\exp\left[-\frac{iq}{\hbar c}\eta A\left(x+\alpha\eta\right)\right]$$

where α is a parameter that we can vary between 0 and 1 in order to vary the point along the path from x' to x at which we evaluate the vector potential A. Also,

(7)
$$\eta\equiv x'-x$$

Using the same argument as before, we require

(8)
$$|\eta|\lesssim\sqrt{\frac{2\hbar\varepsilon\pi}{m}}$$

so calculations to first order in ε must include terms up to second order in η.

Once we have $U\left(x,\varepsilon;x',0\right)$, we can find $\psi\left(x,\varepsilon\right)$ from

(9)
$$\psi\left(x,\varepsilon\right)=\int_{-\infty}^{\infty}U\left(x,\varepsilon;x',0\right)\psi\left(x',0\right)dx'$$

To find U to first order in ε, we need to expand the second exponential in 6 out to terms in η^{2}, so we first look at the argument of the exponential:

(10)
$$-\frac{iq}{\hbar c}\eta A\left(x+\alpha\eta\right)=-\frac{iq}{\hbar c}\left(\eta A\left(x\right)+\alpha\eta^{2}\frac{\partial A}{\partial x}+\ldots\right)$$

where the derivative is evaluated at the endpoint x and is constant in the integral. The second exponential in 6 now becomes, to second order in η:

(11)
$$\exp\left[-\frac{iq}{\hbar c}\eta A\left(x+\alpha\eta\right)\right]=1-\frac{iq}{\hbar c}\left(\eta A\left(x\right)+\alpha\eta^{2}\frac{\partial A}{\partial x}\right)-\left(\frac{q}{\hbar c}\right)^{2}\frac{\eta^{2}A^{2}\left(x\right)}{2}$$

We also need the expansion of the wave function in 9 up to second order in η:

$$\psi(x+\eta,0)=\psi(x,0)+\eta\frac{\partial\psi}{\partial x}+\frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2} \tag{12}$$

Again, both derivatives are evaluated at the endpoint x and are constants in the integral.

We now need to do the integral 9, which consists of several standard Gaussian integrals. From 7, $dx'=d\eta$, so

$$\int_{-\infty}^{\infty}U\left(x,\varepsilon;x',0\right)\psi\left(x',0\right)dx'=\sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\psi(x,0)\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)d\eta+ \tag{13}$$

$$\sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\left(\frac{\partial\psi}{\partial x}-\frac{iq}{\hbar c}A(x)\psi(x,0)\right)\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)\eta\,d\eta+ \tag{14}$$

$$\sqrt{\frac{m}{2\pi\hbar\varepsilon i}}\left(\frac{1}{2}\frac{\partial^2\psi}{\partial x^2}-\frac{iq}{\hbar c}A(x)\frac{\partial\psi}{\partial x}+\psi(x,0)\left(-\frac{iq\alpha}{\hbar c}\frac{\partial A}{\partial x}-\frac{1}{2}\left(\frac{qA(x)}{\hbar c}\right)^2\right)\right. \tag{15}$$

$$\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)\eta^2d\eta \tag{16}$$

We can now do the integrals:

$$\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)d\eta=\sqrt{\frac{2\pi\hbar\varepsilon i}{m}} \tag{17}$$

$$\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)\eta\,d\eta=0 \tag{18}$$

$$\int_{-\infty}^{\infty}\exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right)\eta^2d\eta=-\frac{\hbar\varepsilon}{im}\sqrt{\frac{2\pi\hbar\varepsilon i}{m}} \tag{19}$$

Plugging these in we get

(20)
$$\psi(x,\varepsilon)=\psi(x,0)-\frac{\hbar\varepsilon}{im}\left[\frac{1}{2}\frac{\partial^2\psi}{\partial x^2}-\frac{iq}{\hbar c}A(x)\frac{\partial\psi}{\partial x}+\psi(x,0)\left(-\frac{iq\alpha}{\hbar c}\frac{\partial A}{\partial x}-\frac{1}{2}\left(\frac{qA(x)}{\hbar c}\right)^2\right)\right]$$

(21)
$$=\psi(x,0)+\frac{\varepsilon}{i\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+\frac{i\hbar q}{mc}A(x)\frac{\partial\psi}{\partial x}+\psi(x,0)\left(\frac{i\hbar q\alpha}{mc}\frac{\partial A}{\partial x}+\frac{1}{2m}\left(\frac{qA(x)}{c}\right)^2\right)\right]$$

We can compare this with the quantum version of the Hamiltonian for the vector potential part of the electromagnetic force. The classical Hamiltonian is

$$H=\frac{|\mathbf{p}-q\mathbf{A}/c|^2}{2m} \tag{22}$$

Because $\mathbf{A}$ depends on x, it doesn't commute with $\mathbf{p}$ so to get the quantum version we need to symmetrize when we expand the square. The one dimensional version is

$$H=\frac{P^2}{2m}-\frac{q}{2mc}PA-\frac{q}{2mc}AP+\frac{q^2A^2}{2mc^2} \tag{23}$$

In the coordinate basis, we have, using $P=-i\hbar\partial/\partial x$

$$H\psi=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+\frac{i\hbar q}{2mc}\left(\frac{\partial(A\psi)}{\partial x}+A\frac{\partial\psi}{\partial x}\right)+\frac{q^2A^2}{2mc^2}\psi \tag{24}$$

$$=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+\frac{i\hbar q}{2mc}\left(2A\frac{\partial\psi}{\partial x}+\psi\frac{\partial A}{\partial x}\right)+\frac{q^2A^2}{2mc^2}\psi \tag{25}$$

$$=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+\frac{i\hbar q}{mc}\left(A\frac{\partial\psi}{\partial x}+\frac{1}{2}\psi\frac{\partial A}{\partial x}\right)+\frac{q^2A^2}{2mc^2}\psi \tag{26}$$

Returning to the result we got from the path integral, upon rearranging 21 we get

(27)
$$i\hbar\frac{\psi(x,\varepsilon)-\psi(x,0)}{\varepsilon}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+\frac{i\hbar q}{mc}\left(A(x)\frac{\partial\psi}{\partial x}+\alpha\psi(x,0)\frac{\partial A}{\partial x}\right)+\frac{\psi(x,0)}{2m}\left(\frac{qA(x)}{c}\right)^2$$

(28)
$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+\frac{i\hbar q}{mc}\left(A(x)\frac{\partial\psi}{\partial x}+\alpha\psi\frac{\partial A}{\partial x}\right)+\frac{\psi}{2m}\left(\frac{qA(x)}{c}\right)^2$$

where in the last line we took the limit as $\varepsilon \to 0$ on the LHS to get Schrödinger's equation in the form

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \tag{29}$$

Comparing the RHS of 28 with 26, we see that they are equal provided we take $\alpha = \frac{1}{2}$. Thus in this case, we really do need to evaluate the vector potential A at the midpoint of the path.