

## PATH INTEGRAL TO SCHRÖDINGER EQUATION FOR A VECTOR POTENTIAL

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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 infinitesimal time interval  $\epsilon$ , 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  $\epsilon$ , and moving the point at which we evaluate  $V$  introduced terms only of order  $\epsilon^2$  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

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

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  $\phi$  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

$$L = \frac{1}{2}mv^2 + \frac{q}{c}vA \quad (2)$$

Over the infinitesimal time interval  $\epsilon$  we have

$$v = \frac{x - x'}{\epsilon} \quad (3)$$

The propagator over this time interval is

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

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

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

where  $\alpha$  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,

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

Using the same argument as before, we require

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

so calculations to first order in  $\varepsilon$  must include terms up to second order in  $\eta$ .

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

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

To find  $U$  to first order in  $\varepsilon$ , we need to expand the second exponential in 6 out to terms in  $\eta^2$ , so we first look at the argument of the exponential:

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

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  $\eta$ :

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

We also need the expansion of the wave function in 9 up to second order in  $\eta$ :

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

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

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

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

$$\sqrt{\frac{m}{2\pi\hbar\varepsilon i}} \left( \frac{1}{2} \frac{\partial^2\psi}{\partial x^2} - \frac{iq}{\hbar c} A(x) \frac{\partial\psi}{\partial x} + \psi(x, 0) \left( -\frac{iq\alpha}{\hbar c} \frac{\partial A}{\partial x} - \frac{1}{2} \left( \frac{qA(x)}{\hbar c} \right)^2 \right) \right) \int_{-\infty}^{\infty} \exp\left(\frac{im\eta^2}{2\hbar\varepsilon}\right) \eta^2 d\eta \quad (15)$$

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

We can now do the integrals:

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

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

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

Plugging these in we get

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \quad (29)$$

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.