Path Integrals in Quantum Mechanics: A Review *

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1 Classical Lagrangian mechanics

You may remember from high-school physics the importance of the total energy of a system, and that the total energy can be expressed as the sum of *kinetic* energy, which is inherent in motion, and *potential* energy, which in general depends on the configuration of the physical system (forces, etc.). This sum is called the *Hamiltonian*, and in the absence of external forces, is conserved in the evolution of the system. From the law of conservation of energy, one can thus determine how the system will evolve.

The fundamental quantity in Lagrangian mechanics is not the sum but the difference between the kinetic and potential energies, called the *Lagrangian*:

$$L = K - V.$$

The physical meaning of the Lagrangian is less clear; it is in general not conserved. In many cases, though, the Lagrangian formalism is more useful than the Hamiltonian: for one thing, the Lagrangian is Lorentz-invariant (and therefore appropriate for applications in relativistic field theory), and for another, it gives rise to a quantity known as the *action*, which generalizes nicely to field theory and quantum mechanics. In the following, I will focus on this latter application.

The *action* is defined as the integral over time of the Lagrangian:

$$S = \int L \, dt$$

Once again, the physical meaning of the action is not intuitively obvious. In fact, in the classical theory, its use is limited to the formulation of the *principle of least action*, which states that the space-time path a particle (or field, or system) will follow is that for which the action is extremized. (In this regard, the principle is slightly misnamed; many texts will speak of minimizing

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the action, when all one is really doing is setting the derivative equal to zero. However, in most applications one does indeed find a minimizing path. Cases in which a local maximum can be found are rare, and solutions are called instantons or solitons, depending on their stability. In any case, the extremizing path will often be called the path of least action.) To extremize the action, one follows the usual procedure from calculus: take the derivative, and solve for the path that makes the derivative zero.

What exactly does it mean to take a derivative in this context, though? We appeal to some basic methods in variational calculus. Specifically, we want to find a path for which the infinitesimal variation of the action, δS, is zero, and we assume that the path begins and ends at some fixed points. For clarity, from now on we'll consider the case of a particle moving in one dimension along a path parametrized by $x(t)$. The Lagrangian may depend on x and its time derivative, $\dot{x}$. We have

$$S = \int L(x, \dot{x})\, dt, \tag{1}$$

and

$$\delta S = \int dt \left\{ \frac{\partial L}{\partial x}\delta x + \frac{\partial L}{\partial \dot{x}}\delta \dot{x} \right\} \tag{2}$$

The second term has a factor of $\delta \dot{x} = \delta\left(\frac{d}{dt}x\right)$. We can integrate by parts to write this in terms of δx:

$$\delta S = \int dt \left\{ \frac{\partial L}{\partial x}\delta x - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}}\delta x \right\} + \frac{\partial L}{\partial \dot{x}}\delta x\bigg|_{endpoints}. \tag{3}$$

The boundary term vanishes, since we assumed $\delta x = 0$ at the endpoints. Dividing through by δx (note the wonderful abuse of notation!), we are left with

$$\frac{\delta S}{\delta x} = \int dt \left\{ \frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} \right\} = 0, \tag{4}$$

which means that in general, the integrand must be zero. This requirement produces the *Euler-Lagrange equations of motion*,

$$\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = 0. \tag{5}$$

2 The quantum story

As far as classical mechanics is concerned, the Euler-Lagrange equations are the end of the story. For quantum mechanics, though, it is only the beginning. For systems whose action is much larger than $\hbar$ (Planck's constant), the classical solution can be taken as an approximate or zero-order solution, to which quantum mechanics provides small corrections. However, when dealing with energies large enough (or lengths small enough) to make the action comparable with $\hbar$, the quantum "corrections" generally yield results substantially different from the classical predictions.

The fundamental difference between classical and quantum mechanics is the role of probability in the evolution of a physical system. In classical mechanics, we don't speak of probability amplitudes; the path a particle follows is assumed to be the least action path, with one hundred percent probability. [1] Quantum mechanics, on the other hand, assigns a probability amplitude to every possible path the system may take, and in general these amplitudes are nonzero. In fact, Feynman's formulation gives equal weight to each path, distinguishing their contributions only by a phase factor.

Now suppose we ask what the amplitude is for a particle to propagate from a space-time point a to another point b. Classically, this is not a very interesting question; if the particle starts at a, then either it will go to b (by the path of least action) or it will not – there is no probabilistic ambiguity. Feynman gives us a different approach: amplitude for propagation from x_a to x_b in time T, we sum over all paths beginning at x_a and ending at x_b. If we denote this amplitude as $U(x_a, x_b; T)$, we can write

$$U(x_a, x_b; T) = \sum_{\text{paths}} e^{iS[x(t)]/\hbar}. \tag{6}$$

Note that in the classical limit $\hbar \to 0$ (or $S \gg \hbar$), the exponent blows up, producing rapid oscillation. In this case, a small change δS in the action gives a large change in phase, so those paths for which $\delta S \neq 0$ will tend to cancel in the sum. Thus we recover the least action principle for classical mechanics.

When S and $\hbar$ are of comparable size, though, we have to worry about evaluating this sum. Since the set of all paths is in general a continuous infinity, and we assume that a path can go anywhere in the universe, this sum becomes an infinite product of integrals, each one taken over all space. As an example of the methods used to define this integral, let us once again consider the one particle, one dimension case. A general path is given by $x(t)$, and the object we want to define is the *path integral* (or *functional integral*),

$$\int \mathcal{D}x(t).$$

In analogy with the definition of the Riemann integral, we break up the time parameter into n discrete slices of duration ϵ. We then fix $x(0) = x(t_0) = x_a$ and $x(T) = x(t_n) = x_b$, and let $x(t_j)$

[1] An *amplitude* is just a complex number assigned to a given state; the probability of measuring that state is given by the squared magnitude of this number, i.e. the number times its complex conjugate.

vary for each t_j in the partition $0 = t_0 < t_1 < \ldots < t_n = T$. Our integral thus becomes

$$\int \mathcal{D}x(t) = \frac{1}{C(\epsilon)} \int \frac{dx_{n-1}}{C(\epsilon)} \int \frac{dx_{n-2}}{C(\epsilon)} \cdots \int \frac{dx_1}{C(\epsilon)}, \tag{7}$$

where I have abbreviated $x(t_j) = x_j$. The numbers $C(\epsilon)$ are convergence factors and, as suggested, dependent on ϵ; for some simple cases they can be found explicitly, but the general problem of defining the integration measure is unsolved. Fortunately for physicists (and to the continuing horror of mathematicians), these simple cases suffice for most known physical situations, so nobody worries too much about the fact that the path integral is not generally well-defined.

3 A path integral calculation

To see the use of the path integral formalism, let us consider the Lagrangian

$$L = \frac{1}{2} m \dot{x}^2 - V(x).$$

Then the propagation amplitude is

$$\begin{aligned} U(x_a, x_b; T) &= \int \mathcal{D}x(t) e^{\frac{i}{\hbar} \int dt \left[\frac{1}{2} m \dot{x}^2 - V(x)\right]} \qquad (8) \\ &= \frac{1}{C(\epsilon)} \left(\prod \int \frac{dx_j}{C(\epsilon)} \right) \exp \left\{ \frac{i}{\hbar} \sum_{j=0}^{n} \left[\frac{m}{2} \frac{(x_{j+1} - x_j)^2}{\epsilon} - \epsilon V \left(\frac{x_{j+1} + x_j}{2} \right) \right] \right\} \end{aligned}$$

We can derive the equation of motion for this amplitude by examining the integral over the last time slice. For convenience, we'll call the variable of integration x' instead of x_{n-1}. We have

$$\begin{aligned} U(x_a, x_b; T) &= \frac{1}{C(\epsilon)} \int dx' \exp \left\{ \frac{i}{\hbar} \left[\frac{m}{2} \frac{(x_b - x')^2}{\epsilon} - \epsilon V \left(\frac{x_b + x'}{2} \right) \right] \right\} \\ &\quad \times U(x_a, x'; T - \epsilon). \end{aligned} \tag{9}$$

Assuming x' is close to x_b, we expand about x_b. The integrand is now

$$\begin{aligned} &\exp \left\{ \frac{i}{\hbar} \frac{m}{2\epsilon} (x_b - x')^2 \right\} \times \left[1 - \frac{i}{\hbar} \epsilon V(x_b) + \mathcal{O}(\epsilon^2) \right] \\ &\times \left[1 + (x' - x_b) \frac{\partial}{\partial x_b} + \frac{1}{2} (x' - x_b)^2 \frac{\partial^2}{\partial x_b^2} + \mathcal{O}((x' - x_b)^3) \right] U(x_a, x_b; T - \epsilon), \end{aligned} \tag{10}$$

where the derivatives may be understood as taken with respect to x' and evaluated at x_b. In doing the dx' integral, we can take out the second factor and use the Gaussian integration formulae for the rest. Recall that

$$\begin{aligned}
\int_{-\infty}^{\infty} e^{-\alpha\zeta^2} d\zeta &= \sqrt{\frac{\pi}{\alpha}} \\
\int_{-\infty}^{\infty} \zeta e^{-\alpha\zeta^2} d\zeta &= 0 \\
\int_{-\infty}^{\infty} \zeta^2 e^{-\alpha\zeta^2} d\zeta &= \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}.
\end{aligned}$$

Integrating (10), we get

$$\left(1 - \frac{i}{\hbar}\epsilon V(x_b)\right)\left(\sqrt{\frac{2\pi\hbar\epsilon}{-im}} - \frac{\hbar\epsilon}{2im}\sqrt{\frac{2\pi\hbar\epsilon}{-im}}\frac{\partial^2}{\partial x^2}\right) U(x_a, x_b; T - \epsilon). \tag{11}$$

Rewriting the above and returning to (8),

$$U(x_a, x_b; T) = \frac{1}{C(\epsilon)}\sqrt{\frac{2\pi\hbar\epsilon}{-im}}\left[1 - \frac{\hbar\epsilon}{2im}\frac{\partial^2}{\partial x^2} - \frac{i\epsilon}{\hbar}V(x_b) + \mathcal{O}(\epsilon^2)\right] U(x_a, x_b; T - \epsilon), \tag{12}$$

so for the limit $\epsilon \to 0$ to make sense, we must have

$$C(\epsilon) = \sqrt{\frac{2\pi\hbar\epsilon}{-im}}.$$

Using this value of C, we can factor out ϵ in (12) and form a difference quotient, obtaining

$$\frac{1}{\epsilon}\left[U(x_a, x_b; T) - U(x_a, x_b; T - \epsilon)\right] = \left(-\frac{\hbar}{im}\frac{\partial^2}{\partial x^2} - \frac{i}{\hbar}V(x)\right) U(x_a, x_b; T - \epsilon),$$

or

$$i\hbar\frac{\partial}{\partial T}U = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}U + V(x)U. \tag{13}$$

This is the *Schrödinger equation*, the equation of motion governing non-relativistic wave functions in quantum mechanics.

References

[1] M. E. Peskin and D. V. Schroeder. *An Introduction to Quantum Field Theory*, chapter 9. Perseus, 1995.

[2] R.P. Feynman. *Quantum Mechanics and Path Integrals.* McGraw-Hill, 1965.