

7 Path integrals

7.1 Lagrangian

The Lagrangian $L(\dot{q}, q)$ and the Hamiltonian $H(p, q)$ are related by $H = \dot{q}p - L$, with $p = \partial L / \partial \dot{q}$ the momentum.

a) Verify that $L = \frac{1}{2}m\dot{q}^2 - V$ gives $H = p^2/2m + V$.

b) Check, still for $H = p^2/2m + V$, that Hamilton's equations of motion, $\dot{p} = -\partial H / \partial q$ and $\dot{q} = \partial H / \partial p$ are equivalent to the Euler-Lagrange equation

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0.$$

The action $S[q(t)]$ is a *functional* (function of a function) of the path $q(t)$ that starts at point q_0 at time t_0 and ends at point q_1 at time t_1 :

$$S[q(t)] = \int_{t_0}^{t_1} L(\dot{q}, q, t) dt.$$

The Euler-Lagrange equation says that the action is minimal (more precisely, extremal) for a path $q_{cl}(t)$ that satisfies the classical equations of motion (principle of least action).

c) Demonstrate this explicitly for $L = \frac{1}{2}m\dot{q}^2 - V(q)$, by considering a small perturbation δq of a path q and following these steps (explain every step):

$$\delta S = S[q + \delta q] - S[q] = \int_{t_0}^{t_1} \left[\frac{1}{2}m \frac{d}{dt} (q + \delta q)^2 - V(q + \delta q) \right] dt - S[q] \quad (1)$$

$$= \int_{t_0}^{t_1} \left[\frac{1}{2}m\dot{q}^2 + m\dot{q}\delta\dot{q} - V(q) - V'(q)\delta q \right] dt - S[q] \quad (2)$$

$$= \int_{t_0}^{t_1} \left[m\dot{q}\delta\dot{q} - V'(q)\delta q \right] dt \quad (3)$$

$$= \int_{t_0}^{t_1} \left[-m\ddot{q}\delta q - V'(q)\delta q \right] dt + m\dot{q}\delta q \Big|_{t_0}^{t_1} = 0. \quad (4)$$

7.2 Quantum propagator

The transition amplitude

$$G(q, q'; t) = \langle q | e^{-iHt/\hbar} | q' \rangle$$

is called the “propagator” or the “Green function”.

a) Show that the wave function ψ propagates in time according to

$$\psi(q, t) = \int dq' G(q, q'; t) \psi(q', 0).$$

b) Also show that, in terms of a complete set of energy eigenstates $\psi_n(q)$, one has

$$G(q, q'; t) = \sum_n e^{-iE_n t/\hbar} \psi_n(q) \psi_n^*(q').$$

Hint: Insert the resolution of the identity $\hat{1} = \sum_n |\psi_n\rangle \langle \psi_n|$.

c) Obtain the propagator

$$G(q, q'; t) = \sqrt{\frac{m}{2\pi i \hbar t}} \exp\left(\frac{im(q - q')^2}{2\hbar t}\right).$$

for a free particle by substituting $E_n = p^2/2m$, $\psi_n(q) = (2\pi\hbar)^{-1/2} e^{ipq/\hbar}$, $\sum_n \rightarrow \int_{-\infty}^{\infty} dp$. You may use the formula $\int_{-\infty}^{\infty} e^{-iax^2+ibx} dx = \sqrt{\frac{\pi}{ia}} e^{ib^2/4a}$ (for $a > 0$).

7.3 Feynman's formula

The Feynman path integral expresses the propagator $\langle q_1 | e^{-iHt/\hbar} | q_0 \rangle$ as a sum, or “path integral” $\int \mathcal{D}[q(t)]$, of $e^{iS[q(t)]/\hbar}$ over *all* paths $q(t)$ that go from q_0 to q_1 in a time $T = t_1 - t_0$,

$$G(q_1, q_0; T) = \langle q_1 | e^{-iHT/\hbar} | q_0 \rangle = \sqrt{\frac{m}{2\pi i \hbar T}} \int \mathcal{D}[q(t)] e^{iS[q(t)]/\hbar}.$$

To prove Feynman's path integral formula, we first consider an infinitesimally small time step δt , starting at q and ending at $q + \delta q$.

a) Explain the steps in the following calculation of the infinitesimal-time propagator:

$$G(q + \delta q, q; \delta t) = \langle q + \delta q | e^{-iH\delta t/\hbar} | q \rangle \quad (5)$$

$$= \langle q + \delta q | e^{-ip^2\delta t/2m\hbar} e^{-iV(q)\delta t/\hbar} | q \rangle \quad (6)$$

$$= \int dp \int dp' \int dq \langle q + \delta q | p \rangle \langle p | e^{-ip^2\delta t/2m\hbar} | p' \rangle \langle p' | q \rangle \langle q | e^{-iV(q)\delta t/\hbar} | q \rangle \quad (7)$$

$$= \frac{1}{2\pi\hbar} \int dp e^{ip(q+\delta q)/\hbar} e^{-ip^2\delta t/2m\hbar} e^{ipq/\hbar} e^{-iV(q)\delta t/\hbar} \quad (8)$$

$$= \frac{1}{2\pi\hbar} e^{-iV(q)\delta t/\hbar} \int dp e^{-ip^2\delta t/2m\hbar} e^{ip\delta q/\hbar} \quad (9)$$

$$= \sqrt{\frac{m}{2\pi i\hbar\delta t}} e^{-iV(q)\delta t/\hbar} \exp\left(\frac{im\delta q^2}{2\hbar\delta t}\right) \quad (10)$$

$$\rightarrow \sqrt{\frac{m}{2\pi i\hbar\delta t}} \exp([im\dot{q}^2/2\hbar - iV(q)/\hbar]\delta t) \quad (11)$$

$$= \sqrt{\frac{m}{2\pi i\hbar\delta t}} e^{iL(q,\dot{q})\delta t/\hbar}. \quad (12)$$

As a check, show that this result agrees for a *free particle* with what we found in the previous exercise.

b) Explain how you can arrive at the full path integral expression, by combining the contributions from a sequence of infinitesimal time steps. (The $\sqrt{1/T}$ prefactor cannot be explained in a simple way, so you may restrict your discussion to the exponential factor.) Make use of the identity

$$\begin{aligned} \langle q' | e^{-iHt/\hbar} | q \rangle &= \int dq_1 \int dq_2 \cdots \int dq_N \langle q' | e^{-iH\delta t/\hbar} | q_1 \rangle \langle q_1 | e^{-iH\delta t/\hbar} | q_2 \rangle \\ &\quad \times \langle q_2 | e^{-iH\delta t/\hbar} | q_3 \rangle \cdots \langle q_N | e^{-iH\delta t/\hbar} | q \rangle, \end{aligned} \quad (13)$$

with $\delta t = t/(N+1)$. (Why does this identity hold?)

7.4 Stationary phase approximation

a) As a simple application of the stationary phase approximation, we consider the large- x limit of the Bessel function

$$J_n(x) = \int_0^1 \cos[n\pi t - x \sin \pi t] dt = \text{Re} \int_0^1 e^{in\pi t - ix \sin \pi t} dt.$$

Expand the exponent to second order around the extremum $t = 1/2 + \mathcal{O}(1/x)$ (the so-called “point of stationary phase”) and evaluate the Gaussian integral (see exercise 2c) to arrive at the approximation

$$J_n(x) = \sqrt{\frac{2}{\pi x}} \cos(x - n\pi/2 - \pi/4), \text{ for } x \rightarrow \infty.$$

You might want to check the accuracy of this approximation with Mathematica.

We recall the WKB approximation for the wave function,

$$\psi_{\text{WKB}}(q, T) = \frac{1}{\sqrt{v(q)}} \exp\left(\frac{i}{\hbar} \int_{q_0}^q p(q') dq' - iET/\hbar\right),$$

where the integral is along the classical path q_{clas} of a particle with energy E that moves from q_0 to q in a time T . (For simplicity we assume there are no turning points.) We wish to show that the WKB approximation is the stationary phase approximation of the Feynman path integral in the limit $\hbar \rightarrow 0$.

b) Show that ψ_{WKB} is related to the action $S[q_{\text{clas}}(t)]$ of the classical path,

$$\psi_{\text{WKB}}(q, T) = \frac{1}{\sqrt{v(q)}} e^{iS[q_{\text{clas}}(t)]/\hbar}.$$

Hint: recall that $H = \dot{q}p - L$.

c) Show how the stationary phase approximation of the Feynman path integral for $\hbar \rightarrow 0$ produces the exponential factor $e^{iS[q_{\text{clas}}(t)]/\hbar}$.