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 $q_{\mathrm{cl}}(t)$ 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):

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

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

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

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

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 $E_n = p^2/2m$, $\psi_n(q) = (2\pi\hbar)^{-1/2}e^{ipq/\hbar}$, $\sum_n \to \int_{-\infty}^{\infty} dp$. 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” $\int \mathscr{D}[q(t)]$, of $e^{iS[q(t)]/\hbar}$ over *all* paths $q(t)$ that go from q_0 to q_1 in a time $T = t_1 - t_0$,

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

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:

$$\begin{aligned}
G(q+\delta q, q; \delta t) &= \langle q+\delta q| e^{-iH\delta t/\hbar} |q\rangle && (5)\\
&= \langle q+\delta q| e^{-ip^2\delta t/2m\hbar} e^{-iV(q)\delta t/\hbar} |q\rangle && (6)\\
&= \int dp \int dp' \int dq \, \langle q+\delta q|p\rangle\langle p|e^{-ip^2\delta t/2m\hbar}|p'\rangle\langle p'|q\rangle\langle q|e^{-iV(q)\delta t/\hbar}|q\rangle && (7)\\
&= \frac{1}{2\pi\hbar}\int dp \, e^{ip(q+\delta q)/\hbar} e^{-ip^2\delta t/2m\hbar} e^{-ipq/\hbar} e^{-iV(q)\delta t/\hbar} && (8)\\
&= \frac{1}{2\pi\hbar} e^{-iV(q)\delta t/\hbar}\int dp \, e^{-ip^2\delta t/2m\hbar} e^{ip\delta q/\hbar} && (9)\\
&= \sqrt{\frac{m}{2\pi i\hbar\delta t}} e^{-iV(q)\delta t/\hbar} \exp\left(\frac{im\delta q^2}{2\hbar\delta t}\right) && (10)\\
&\to \sqrt{\frac{m}{2\pi i\hbar\delta t}} \exp\left([im\dot{q}^2/2\hbar - iV(q)/\hbar]\delta t\right) && (11)\\
&= \sqrt{\frac{m}{2\pi i\hbar\delta t}} e^{iL(q,\dot{q})\delta t/\hbar}. && (12)
\end{aligned}$$

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

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

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

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

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

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

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

We recall the WKB approximation for the wave function,

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

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 $\hbar \to 0$.

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

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

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

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