

Advanced Quantum Theory

Homework 2

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2.3 Propagator for a free particle

Evaluate the path integral for the propagator of a particle moving freely in one dimension without potential, i.e., a particle with the Lagrangian $L = \frac{1}{2}m\dot{x}^2$.

The action is:

$$S[x] = \int_0^t \frac{1}{2}m\dot{x}(t')^2 dt' \quad (2.3.1)$$

Split $x(t')$ into the classical solution $x_{\text{cl}}(t')$ and deviation $\delta x(t')$:

$$x(t') = x_{\text{cl}}(t') + \delta x(t'), \quad x(0) = x_0, \quad x(t) = x_f, \quad \delta x(0) = \delta x(t) = 0 \quad (2.3.2)$$

Substitute equation 2.3.2 into equation 2.3.1. The Taylor expansion is around a stationary point of the action, so the linear term vanishes:

$$\begin{aligned} S[x] &= \int_0^t \frac{1}{2}m\dot{x}_{\text{cl}}(t')^2 dt' + \int_0^t m\dot{x}_{\text{cl}}(t')\dot{\delta x}(t') dt' + \int_0^t \frac{1}{2}m\dot{\delta x}(t')^2 dt' \\ &= \int_0^t \frac{1}{2}m\dot{x}_{\text{cl}}(t')^2 dt' + \int_0^t \frac{1}{2}m\dot{\delta x}(t')^2 dt' \\ &= S[x_{\text{cl}}] + S[\delta x] \end{aligned} \quad (2.3.3)$$

Substitute equation 2.3.3 into the path integral for the propagator and replace the functional integral over x by a functional integral over δx :

$$\begin{aligned} K(x_f, x_0, t) &= \int D[x] e^{\frac{i}{\hbar}S[x]} \\ &= \int D[x] e^{\frac{i}{\hbar}(S[x_{\text{cl}}] + S[\delta x])} \\ &= e^{\frac{i}{\hbar}S[x_{\text{cl}}]} \int D[\delta x] e^{\frac{i}{\hbar}S[\delta x]} \end{aligned} \quad (2.3.4)$$

First, evaluate the action for the deviation:

$$S[\delta x] = \int_0^t \frac{1}{2}m\dot{\delta x}(t')^2 dt'$$

Discretise the integral and define $\tau = \frac{t}{N}$, $\delta x_i = \delta x(t'_i) = \delta x(i\tau)$:

$$S[\delta x] = \lim_{N \rightarrow \infty} \sum_{i=0}^{N-1} \frac{1}{2}m \left(\frac{\delta x_{i+1} - \delta x_i}{\tau} \right)^2 \tau = \lim_{N \rightarrow \infty} \frac{m}{2\tau} \sum_{i=0}^{N-1} (\delta x_{i+1} - \delta x_i)^2$$

The boundary conditions $\delta x(0) = \delta x(t) = 0$ imply $\delta x_0 = \delta x_N = 0$. Rearrange the sum:

$$\begin{aligned} \sum_{i=0}^{N-1} (\delta x_{i+1} - \delta x_i)^2 &= \sum_{i=0}^{N-1} \delta x_{i+1}^2 - 2 \sum_{i=0}^{N-1} \delta x_{i+1} \delta x_i + \sum_{i=0}^{N-1} \delta x_i^2 \\ &= \sum_{i=0}^{N-2} \delta x_{i+1}^2 - 2 \sum_{i=1}^{N-2} \delta x_{i+1} \delta x_i + \sum_{i=0}^{N-2} \delta x_i^2 \\ &= 2 \sum_{i=1}^{N-1} \delta x_i^2 - 2 \sum_{i=1}^{N-2} \delta x_{i+1} \delta x_i \end{aligned}$$

In terms of the vector $\vec{\delta x} = [\delta x_1 \ \delta x_2 \ \dots \ \delta x_{N-1}]^\top$ and Kronecker delta δ_{ij} :

$$\begin{aligned} \sum_{i=0}^{N-1} (\delta x_{i+1} - \delta x_i)^2 &= \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} (2\delta_{ij} - (\delta_{i+1,j} + \delta_{i,j+1})) (\vec{\delta x})_i (\vec{\delta x})_j \\ S[\delta x] &= \lim_{N \rightarrow \infty} \frac{mN}{2t} \vec{\delta x} \cdot B_{N-1} \vec{\delta x}, \quad B_{N-1} = \begin{bmatrix} 2 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & \dots & 0 \\ 0 & -1 & 2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix} \end{aligned}$$

The functional integral in equation 2.3.4 becomes:

$$\begin{aligned} \int D[\delta x] e^{\frac{i}{\hbar} S[\delta x]} &= \lim_{N \rightarrow \infty} \left(\frac{mN}{2\pi i \hbar t} \right)^{N/2} \int d\delta x_1 \int d\delta x_2 \dots \\ &\dots \int d\delta x_{N-1} \exp \left(i \frac{mN}{2\hbar t} \vec{\delta x} \cdot B_{N-1} \vec{\delta x} \right) \end{aligned} \quad (2.3.5)$$

We have that:

$$\int d\delta x_1 \int d\delta x_2 \dots \int d\delta x_{\nu-1} \exp \left(i \vec{\delta x} \cdot A \vec{\delta x} \right) = \left(\frac{(i\pi)^\nu}{\det A} \right)^{1/2} \quad (2.3.6)$$

With $\nu = N - 1$, $A = \frac{mN}{2\hbar t} B_{N-1}$:

$$\int D[\delta x] e^{\frac{i}{\hbar} S[\delta x]} = \lim_{N \rightarrow \infty} \left(\frac{mN}{2\pi i \hbar t} \right)^{N/2} \left(\frac{(i\pi)^{N-1}}{\det \left(\frac{mN}{2\hbar t} B_{N-1} \right)} \right)^{1/2}$$

For a scalar k and $n \times n$ matrix A , $\det kA = k^n \det A$. Hence:

$$\begin{aligned} \int D[\delta x] e^{\frac{i}{\hbar} S[\delta x]} &= \lim_{N \rightarrow \infty} \left(\frac{mN}{2\pi i \hbar t} \right)^{N/2} \left(\frac{(i\pi)^{N-1}}{\left(\frac{mN}{2\hbar t} \right)^{N-1} \det B_{N-1}} \right)^{1/2} \\ &= \lim_{N \rightarrow \infty} \left(\frac{mN}{2\pi i \hbar t} \right)^{N/2} \left(\frac{2\pi i \hbar t}{mN} \right)^{(N-1)/2} \\ &= \sqrt{\frac{m}{2\pi i \hbar t}} \end{aligned} \quad (2.3.7)$$

Next, evaluate the action for the classical solution. The classical solution $x_{\text{cl}}(t')$ is the solution of Lagrange's equation:

$$\frac{\partial L}{\partial x} = \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \implies \ddot{x}_{\text{cl}}(t') = 0, \quad \dot{x}_{\text{cl}}(t') = \frac{x_f - x_0}{t}$$

The action for the classical solution is:

$$S[x_{\text{cl}}] = \int_0^t \frac{1}{2} m \dot{x}_{\text{cl}}(t')^2 dt' = \frac{1}{2} m \frac{(x_f - x_0)^2}{t} \quad (2.3.8)$$

Substitute equations 2.3.7 and 2.3.8 into equation 2.3.4:

$$K(x_f, x_0, t) = \sqrt{\frac{m}{2\pi i \hbar t}} \exp\left(\frac{i}{\hbar} \frac{m}{2t} (x_f - x_0)^2\right) \quad (2.3.9)$$

2.7 Elastic chain

(a) Write the propagator of the system as a path integral.

The Lagrangian is:

$$L(\Phi, \dot{\Phi}) = \sum_{i=1}^{N-1} \sum_{j=1}^2 \frac{1}{2} m \dot{\Phi}_{ij}^2 - \sum_{i=0}^{N-1} \sum_{j=1}^2 \frac{1}{2} k (\Phi_{i+1,j} - \Phi_{ij})^2 - \sum_{i=1}^{N-1} m g \Phi_{i2} \quad (2.7.1)$$

As previously, the propagator is:

$$K(\Phi_f, \Phi_0, t) = \int_{\Phi(0)=\Phi_0, \Phi(t)=\Phi_f} D[\Phi] e^{\frac{i}{\hbar} S[\Phi]}, \quad S[\Phi] = \int_0^t dt' L(\Phi(t'), \dot{\Phi}(t')) \quad (2.7.2)$$

I think there is more to do here but I don't know what.

(b) Take the limit $N \rightarrow \infty$ and replace the index i in Φ_{i1} by a continuous parameter x .

Define $\vec{\Phi}_i(t') = [\Phi_{i1}(t') \quad \Phi_{i2}(t')]^\top$. Hence:

$$L(\Phi, \dot{\Phi}) = \sum_{i=1}^{N-1} \frac{1}{2} m \left\| \frac{d}{dt} \vec{\Phi}_i(t') \right\|^2 - \sum_{i=0}^{N-1} \frac{1}{2} k \left\| \vec{\Phi}_{i+1}(t') - \vec{\Phi}_i(t') \right\|^2 - \sum_{i=1}^{N-1} m g \Phi_{i2}$$

Replace $\vec{\Phi}_i(t')$ with $\vec{\Phi}(ia, t') = [\Phi_1(ia, t') \quad \Phi_2(ia, t')]^\top$ in the summand:

$$\frac{1}{2} m \left\| \frac{d}{dt} \vec{\Phi}(ia, t') \right\|^2 - \frac{1}{2} k \left\| \vec{\Phi}((i+1)a, t') - \vec{\Phi}(ia, t') \right\|^2 - m g \Phi_2(x, t')$$

By a Taylor expansion, the second term $\approx \frac{1}{2} k a^2 \left\| \frac{d}{dx} \vec{\Phi}(a, t') \right\|^2$ and the summand is:

$$\approx \int_{ia}^{(i+1)a} dx \left(\frac{1}{2} \frac{m}{a} \left\| \frac{d}{dt} \vec{\Phi}(x, t') \right\|^2 - \frac{1}{2} k a \left\| \frac{d}{dx} \vec{\Phi}(x, t') \right\|^2 - m g \Phi_2(x, t') \right)$$

Combine the summands:

$$L(\Phi, \dot{\Phi}) \approx \int_0^C dx \left(\frac{1}{2} \frac{m}{a} \left\| \frac{d}{dt} \vec{\Phi}(x, t') \right\|^2 - \frac{1}{2} k a \left\| \frac{d}{dx} \vec{\Phi}(x, t') \right\|^2 - m g \Phi_2(x, t') \right)$$

The propagator is given by equation 2.7.2.

I think there is more to do here also but I don't know what.

(c) Write down a path integral analogous to (b) for the matrix elements of $e^{-\beta\hat{H}}$.

The path integral for $\langle \vec{r}_f | e^{-\beta\hat{H}} | \vec{r}_0 \rangle$ is:

$$\langle \vec{r}_f | e^{-\beta\hat{H}} | \vec{r}_0 \rangle = \int D[\vec{r}] \exp \left(- \int_0^\beta d\beta' \left(\frac{1}{2} m \left(\frac{1}{\hbar} \frac{d\vec{r}}{d\beta'} \right)^2 + U(\vec{r}(\beta')) \right) \right)$$

This is from p. 17 of the notes. There must be more to do here!