Advanced Quantum Theory
Homework 2

Tim Lawson

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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:

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

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

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

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:

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

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:

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

First, evaluate the action for the deviation:

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

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

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

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}:

$$\sum_{i=0}^{N-1} (\delta x_{i+1} - \delta x_i)^2 = \sum_{i=1}^{N-1}\sum_{j=1}^{N-1} \left(2\delta_{ij} - (\delta_{i+1,j} + \delta_{i,j+1})\right)(\vec{\delta x})_i(\vec{\delta x})_j$$

$$S[\delta x] = \lim_{N\to\infty} \frac{mN}{2t} \vec{\delta x} \cdot B_{N-1}\vec{\delta x}\,, \quad B_{N-1} = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ 0 & -1 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

The functional integral in equation 2.3.4 becomes:

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

We have that:

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

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

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

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

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

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

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

The action for the classical solution is:

$$S\left[x_{\text{cl}}\right] = \int_0^t \frac{1}{2}m\dot{x_{\text{cl}}}(t')^2 \mathrm{d}t' = \frac{1}{2}m\frac{\left(x_f - x_0\right)^2}{t} \tag{2.3.8}$$

Substitute equations 2.3.7 and 2.3.8 into equation 2.3.4:

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

2.7 Elastic chain

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

The Lagrangian is:

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

As previously, the propagator is:

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

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

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

Define $\vec{\Phi}_i(t') = \begin{bmatrix}\Phi_{i1}(t') & \Phi_{i2}(t')\end{bmatrix}^\top$. Hence:

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

Replace $\vec{\Phi}_i(t')$ with $\vec{\Phi}(ia, t') = \begin{bmatrix}\Phi_1(ia, t') & \Phi_2(ia, t')\end{bmatrix}^\top$ in the summand:

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

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

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

Combine the summands:

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

The propagator is given by equation 2.7.2.

I think there is also more to do where 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:

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

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