

8.323 Problem Set 5 Solutions

March 14, 2023

Question 1: A Useful Formula, and the Path Integral in Phase Space (20 points)

(a) Derive the following equations:

$$\begin{aligned} \left\langle x_{i+1} \left| e^{-i\frac{\hat{p}^2}{2m}\Delta t} e^{-i\Delta t V(\hat{x})} \right| x_i \right\rangle &= \int \tilde{d}p_i \exp \left[-i\Delta t \frac{p_i^2}{2m} - i\Delta t V(x_i) + ip_i(x_{i+1} - x_i) \right] \\ &= \sqrt{\frac{m}{2\pi i\Delta t}} \exp \left[\frac{im\Delta t}{2} \left(\frac{x_{i+1} - x_i}{\Delta t} \right)^2 - i\Delta t V(x_i) \right] \end{aligned}$$

We start by deriving the first equation:

$$\begin{aligned} \left\langle x_{i+1} \left| e^{-i\frac{\hat{p}^2}{2m}\Delta t} e^{-i\Delta t V(\hat{x})} \right| x_i \right\rangle &= \int dp_i \langle x_{i+1} | e^{-i\frac{\hat{p}^2}{2m}\Delta t} | p_i \rangle \langle p_i | e^{-i\Delta t V(\hat{x})} | x_i \rangle \\ &= \int dp_i e^{-i\frac{p_i^2}{2m}\Delta t} e^{-i\Delta t V(x_i)} \langle x_{i+1} | p_i \rangle \langle p_i | x_i \rangle \\ &= \int \tilde{d}p_i e^{-i\frac{p_i^2}{2m}\Delta t} e^{-i\Delta t V(x_i)} e^{ip_i x_{i+1}} e^{-ip_i x_i} \\ &= \int \tilde{d}p_i \exp \left[-i\Delta t \frac{p_i^2}{2m} - i\Delta t V(x_i) + ip_i(x_{i+1} - x_i) \right] \end{aligned}$$

To get the second equation from this, we complete the square and compute the Gaussian integral, or equivalently use the identity $\int dx e^{-ax^2+bx} = \sqrt{\frac{\pi}{a}} e^{b^2/4a}$. Hence,

$$\begin{aligned} \left\langle x_{i+1} \left| e^{-i\frac{\hat{p}^2}{2m}\Delta t} e^{-i\Delta t V(\hat{x})} \right| x_i \right\rangle &= \frac{1}{2\pi} \sqrt{\frac{2\pi m}{i\Delta t}} \exp \left[-\frac{(x_{i+1} - x_i)^2}{2i\Delta t/m} \right] e^{-i\Delta t V(x_i)} \\ &= \sqrt{\frac{m}{2\pi i\Delta t}} \exp \left[\frac{im\Delta t}{2} \left(\frac{x_{i+1} - x_i}{\Delta t} \right)^2 - i\Delta t V(x_i) \right] \end{aligned}$$

(b) Use the first equation in (a) to derive the following:

$$\langle x_a, t_a | x_b, t_b \rangle = \int_{x(t_b)=x_b}^{x(t_a)=x_a} Dx(t) Dp(t) \exp \left[i \int_{t'}^t dt (p\dot{x} - H) \right]$$

The integration in this expression should be understood as

$$\int_{x(t_b)=x_b}^{x(t_a)=x_a} Dx(t) Dp(t) = \lim_{N \rightarrow \infty} \int \frac{dp_0}{2\pi} \int \frac{dx_1 dp_1}{2\pi} \dots \int \frac{dx_{N-1} dp_{N-1}}{2\pi}$$

where we again divide the interval $[t_b, t_a]$ into N segments, with $t_0 = t_b$, $t_N = t_a$.

We denote the left-hand side of the equation in (a) by M_i . Now we do the same trick from class to derive the path-integral:

$$\begin{aligned}
\langle x_a, t_a | x_b, t_b \rangle &= \langle x_a | e^{-i\hat{H}(t_a-t_b)} | x_b \rangle = \langle x_a | (e^{-i\hat{H}\Delta t})^N | x_b \rangle \\
&= \int dx_1 \cdots dx_{N-1} \langle x_a | e^{-i\hat{H}\Delta t} | x_{N-1} \rangle \langle x_{N-1} | \cdots | x_1 \rangle \langle x_1 | e^{-i\hat{H}\Delta t} | x_b \rangle \\
&= \int dx_1 \cdots dx_{N-1} M_{N-1} \cdots M_0 \\
&= \int dx_1 \cdots dx_{N-1} \bar{d}p_0 \cdots \bar{d}p_{N-1} \prod_{i=0}^{N-1} \exp \left[-i\Delta t \frac{p_i^2}{2m} - i\Delta t V(x_i) + ip_i(x_{i+1} - x_i) \right] \\
&= \int_{x(t_b)=x_b}^{x(t_a)=x_a} Dx(t) Dp(t) \exp \left[i \sum_{i=0}^{N-1} \Delta t \left(p_i \frac{x_{i+1} - x_i}{\Delta t} - \frac{p_i^2}{2m} - V(x_i) \right) \right] \\
&= \int_{x(t_b)=x_b}^{x(t_a)=x_a} Dx(t) Dp(t) \exp \left[i \int_{t_b}^{t_a} dt (p\dot{x} - H) \right]
\end{aligned}$$

In the second line we insert the identity $N - 1$ times, so that we can use the formula from (a) for each matrix element in the 4th line. In the 5th line the product of exponentials becomes a sum of exponents, which in the continuum case reduces to the integral in the last line.

Question 2: The Schrödinger Equation, Rederived (20 points)

The wavefunction $\psi(t, x)$ for a system at time t can be obtained from that at time t' by

$$\psi(t, x) = \int dx' K(x, t; x', t') \psi(x', t')$$

for the propagator given by

$$K(x, t; x', t') = \langle x, t | x', t' \rangle = \int_{x(t_b)=x_b}^{x(t_a)=x_a} Dx(t) \exp \left[i \int_{t'}^t dt L(\dot{x}, x) \right]$$

Show that $\psi(t, x)$ satisfies the Schrödinger equation,

$$i\partial_t \psi(t, x) = -\frac{1}{2m} \partial_x^2 \psi(t, x) + V(x) \psi(t, x)$$

We therefore consider the wavefunction after an infinitesimal time step δt :

$$\psi(t + \delta t, x) = \int dy K(t + \delta t, x; t, y) \psi(t, y)$$

Equating both sides of this equation to order δ will lead to the Schrödinger equation. The left hand side is simple:

$$\text{LHS} = \psi(t + \delta t, x) = \psi(t, x) + \delta t \partial_t \psi(t, x) + \mathcal{O}(\delta t^2)$$

To expand the right hand side, note for an infinitesimal δt that the propagator $K(t + \delta t, x; t, y)$ can be written as a single infinitesimal time step:

$$K(t + \delta t, x; t, y) = \left(\frac{m}{2\pi i \delta t} \right)^{1/2} \exp \left[i \delta t \left(\frac{m}{2} \left(\frac{x - y}{\delta t} \right)^2 - V(y) \right) \right]$$

Therefore we expand:

$$\begin{aligned} \text{RHS} &= \int dy K(t + \delta t, x; t, y) \psi(t, y) \\ &= \left(\frac{m}{2\pi i \delta t} \right)^{1/2} \int dy e^{i \delta t \left(\frac{m}{2} \left(\frac{x-y}{\delta t} \right)^2 - V(y) \right)} \psi(t, y) \\ &= \left(\frac{m}{2\pi i} \right)^{1/2} \int du e^{i \left(\frac{m}{2} u^2 - \delta t V(x + u\sqrt{\delta t}) \right)} \psi(t, x + u\sqrt{\delta t}) \\ &= \left(\frac{m}{2\pi i} \right)^{1/2} \int du e^{i \frac{m}{2} u^2} (1 - \delta t V(x)) \left(\psi(t, x) + \sqrt{\delta t} \partial_x \psi(t, x) u + \frac{\delta t}{2} \partial_x^2 \psi(t, x) u^2 \right) + \mathcal{O}(\delta t^2) \\ &= \psi(t, x) + \delta t \left(-iV(x) \psi(t, x) + \frac{i}{2m} \partial_x^2 \psi(t, x) \right) + \mathcal{O}(\delta t^2) \end{aligned}$$

In the third line we have made the substitution $u\sqrt{\delta t} = y - x$, and in the 4th line we expand each term to order δt , neglecting higher order terms. In the subsequent line we perform the Gaussian integrals over u , noting that the order $(\delta t)^{1/2}$ term because the integral is odd.

Setting the 2 sides equal, we have the Schrödinger equation as desired:

$$i\partial_t \psi(t, x) = \left(-\frac{1}{2m} \partial_x^2 + V(x) \right) \psi(t, x)$$

Question 3: The Free Particle (20 points)

For a free particle, i.e. $V(x) = 0$, perform explicitly the integrals over x_i , $i = 1, \dots, N - 1$ to show that

$$K(x_a, t_a; x_b, t_b) = \left(\frac{m}{2\pi i(t_a - t_b)} \right)^{1/2} \exp \left[\frac{im(x_a - x_b)^2}{2(t_a - t_b)} \right]$$

We evaluate the integrals in order, starting with the one over x_1 . We denote $x_0 = x_b$ and $x_N = x_a$.

$$\begin{aligned} K(x_a, t_a; x_b, t_b) &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \Delta t} \right)^{N/2} \int dx_1 \cdots dx_{N-1} e^{i \frac{m}{2\Delta t} ((x_N - x_{N-1})^2 + \cdots + (x_2 - x_1)^2 + (x_1 - x_0)^2)} \\ &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \Delta t} \right)^{N/2} \left(\frac{i\pi \Delta t}{m} \right)^{1/2} \int dx_2 \cdots dx_{N-1} e^{i \frac{m}{2\Delta t} ((x_N - x_{N-1})^2 + \cdots + (x_3 - x_2)^2 + \frac{1}{2}(x_2 - x_0)^2)} \\ &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \Delta t} \right)^{\frac{N-1}{2}} \frac{1}{\sqrt{2}} \int dx_2 \cdots dx_{N-1} e^{i \frac{m}{2\Delta t} ((x_N - x_{N-1})^2 + \cdots + (x_3 - x_2)^2 + \frac{1}{2}(x_2 - x_0)^2)} \\ &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \Delta t} \right)^{\frac{N-1}{2}} \frac{2}{\sqrt{2}} \left(\frac{i\pi \Delta t}{3m} \right)^{1/2} \int dx_3 \cdots dx_{N-1} e^{i \frac{m}{2\Delta t} ((x_N - x_{N-1})^2 + \cdots + \frac{1}{3}(x_3 - x_0)^2)} \\ &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \Delta t} \right)^{\frac{N-2}{2}} \frac{1}{\sqrt{3}} \int dx_3 \cdots dx_{N-1} e^{i \frac{m}{2\Delta t} ((x_N - x_{N-1})^2 + \cdots + (x_4 - x_3)^2 + \frac{1}{3}(x_3 - x_0)^2)} \\ &= \cdots = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i N \Delta t} \right)^{1/2} e^{i \frac{m}{2N\Delta t} (x_a - x_b)^2} \\ &= \sqrt{\frac{m}{2\pi i N(t_a - t_b)}} e^{i \frac{m}{2} \frac{(x_a - x_b)^2}{t_a - t_b}} \end{aligned}$$

Question 4: The Path Integral for a Free Particle, Revisited (20 points)

In this problem we evaluate the path integral for a free particle using a different method than Problem 3. For simplicity, take $x_a = x_b = 0, t_b = 0, t_a = T$. As discussed in class, K is a Gaussian path-integral of form:

$$K(0, T; 0, 0) = \int_{x(0)=0}^{x(T)=0} Dx(t) \exp \left[\frac{i}{2} \int dt dt' x(t) A(t, t') x(t') \right]$$

for some differential operator A .

(a) Write down the explicit expression for A .

The action for a free particle is given by

$$\begin{aligned} S[x(t)] &= \int dt \frac{m}{2} \partial_t x \partial_t x = -\frac{m}{2} \int dt x \partial_t^2 x = -\frac{m}{2} \int dt dt' x(t) \delta(t-t') \partial_t^2 x(t) \\ &= \frac{1}{2} \int dt dt' x(t') A(t', t) x(t), \quad A(t', t) = -m \delta(t-t') \partial_t^2 \end{aligned}$$

Then, we write the propagator as

$$K(0, T; 0, 0) = \int_{x(0)=0}^{x(T)=0} Dx e^{iS} = \int_{x(0)=0}^{x(T)=0} Dx \exp \left[\frac{i}{2} \int_0^T dt dt' x(t') A(t', t) x(t) \right]$$

for the differential operator $A(t', t) = -m \delta(t-t') \partial_t^2$.

(b) Find all the eigenvalues of A . Show that the determinant of A can be written as

$$\det A = \prod_{n=1}^{\infty} m \frac{n^2 \pi^2}{T^2}$$

The eigenvectors of a second order derivative operator are precisely exponentials, $x(t) = f_\lambda(t) = e^{i\lambda t}$. We further need our eigenvectors to satisfy the boundary conditions $x(0) = x(T) = 0$, since the endpoints of our trajectory are fixed. Hence, a complete set of eigenvectors are given by sine functions, with momenta integer multiples of π/T . Without loss of generality we can restrict to $n > 0$.

$$f_{\lambda_n}(t) = \sqrt{\frac{2}{T}} \sin \left(\frac{n\pi t}{T} \right)$$

Furthermore,

$$\int dt A(t', t) f_{\lambda_n}(t) = -m \int dt \delta(t-t') \sqrt{\frac{2}{T}} \partial_t^2 \sin \left(\frac{n\pi t}{T} \right) = m \frac{n^2 \pi^2}{T^2} \sqrt{\frac{2}{T}} \sin \left(\frac{n\pi t}{T} \right) = \lambda_n f_{\lambda_n}(t)$$

for the eigenvalue $\lambda_n = m \frac{n^2 \pi^2}{T^2}$. In this basis A is diagonal: $A_{mn} = m \frac{n^2 \pi^2}{T^2} \delta_{nm}$. Finally, the determinant of an operator is obtained by multiplying all of its eigenvalues, giving us the desired expression:

$$\det A = \prod_{n=1}^{\infty} m \frac{n^2 \pi^2}{T^2}$$

(c) Since our propagator is Gaussian, it can be evaluated as

$$K(0, T; 0, 0) = \frac{C}{\sqrt{\det A}}$$

where C is some constant. By comparing this equation with the solution to Problem 3, show that the consistency of the 2 approaches requires

$$\frac{C}{\sqrt{\det A}} = \left(\frac{m}{2\pi iT}\right)^{1/2}$$

We substitute $x_a = x_b = 0, t_a = T, t_b = 0$ into the result in Problem 3:

$$K(0, T; 0, 0) = \left(\frac{m}{2\pi iT}\right)^{1/2} \exp\left[\frac{im0^2}{2T}\right] = \left(\frac{m}{2\pi iT}\right)^{1/2}$$

It therefore follows immediately from our work in (b) that

$$K(0, T; 0, 0) = \left(\frac{m}{2\pi iT}\right)^{1/2} = \frac{C}{\sqrt{\det A}} = \frac{CT}{\pi\sqrt{m}} \prod_{n=1}^{\infty} \frac{1}{n}$$

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