221A Lecture Notes
Path Integral

1 Feynman's Path Integral Formulation

Feynman's formulation of quantum mechanics using the so-called path integral is arguably the most elegant. It can be stated in a single line:

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}x(t) e^{iS[x(t)]/\hbar}. \quad (1)$$

The meaning of this equation is the following. If you want to know the quantum mechanical amplitude for a point particle at a position x_i at time t_i to reach a position x_f at time t_f, you integrate over all possible paths connecting the points with a weight factor given by the classical action for each path. Hence the name path integral. This is it. Note that the position kets form a complete set of basis, and knowing this amplitude for all x is enough information to tell you everything about the system. The expression is generalized for more dimensions and more particles in a straightforward manner.

As we will see, this formulation is completely equivalent to the usual formulation of quantum mechanics. On the other hand, there are many reasons why this expression is just beautiful.

First, the classical equation of motion comes out in a very simple way. If you take the limit $\hbar \to 0$, the weight factor $e^{iS/\hbar}$ oscillates very rapidly. Therefore, we expect that the main contribution to the path integral comes from paths that make the action stationary. This is nothing but the derivation of Euler–Lagrange equation from the classical action. Therefore, the classical trajectory *dominates* the path integral in the small $\hbar$ limit.

Second, we *don't know* what path the particle has chosen, even when we know what the initial and final positions are. This is a natural generalization of the two-slit experiment. Even if we know where the particle originates from and where it hit on the screen, we don't know which slit the particle came through. The path integral is an infinite-slit experiment. Because you can't specficy where the particle goes through, you sum them up.

Third, we gain intuition on what quantum fluctuation does. Around the classical trajectory, a quantum particle "explores" the vicinity. The trajectory can deviate from the classical trajectory if the difference in the action is roughly within $\hbar$. When a classical particle is confined in a potential well, a quantum particle can go on an excursion and see that there is a world outside the potential barrier. Then it can decide to tunnel through. If a classical particle is sitting at the top of a hill, it doesn't fall; but a quantum particle realizes that the potential energy can go down with a little excursion, and decides to fall.

Fourth, whenever we have an integral expression for a quantity, it is often easier to come up with an approximation method to work it out, compared to staring at a differential equation. Good examples are the perturbative expansion and the steepest descent method. One can also think of useful change of variables to simplify the problem. In fact, some techniques in quantum physics couldn't be thought of without the intuition from the path integral.

Fifth, the path integral can also be used to calculate partition functions in statistical mechanics.

Sixth, the connection between the conservation laws and unitarity transformations become much clearer with the path integral. We will talk about it when we discuss symmetries.

There are many more but I stop here.

Unfortunately, there is also a downside with the path integral. The actual calculation of a path integral is somewhat technical and awkward. One might even wonder if an "integral over paths" is mathematically well-defined. Mathematicians figured that it can actually be, but nonetheless it makes some people nervous. Reading off energy eigenvalues is also less transparent than with the Schrödinger equation.

Below, we first derive the path integral from the conventional quantum mechanics. Then we show that the path integral can derive the conventional Schrödinger equation back. After that we look at some examples and actual calculations.

By the way, the original paper by Feynman on the path integral *Rev. Mod. Phys.* **20**, 367-387 (1948) is quite readable for you, and I recommend it. Another highly recommended read is Feynman's Nobel Lecture. You will see that Feynman invented the path integral with the hope of replacing quantum field theory with particle quantum mechanics; he failed. But the path integral survived and did mighty good in the way he didn't imagine.

2 Physical Intuition

Take the two-slit experiment. Each time an electron hits the screen, there is no way to tell which slit the electron has gone through. After repeating the same experiment many many times, a fringe pattern gradually appears on the screen, proving that there is an interference between two waves, one from one slit, the other from the other. We conclude that we need to *sum* amplitudes of these two waves that correspond to different *paths* of the electron. Now imagine that you make more slits. There are now more paths, each of which contributing an amplitude. As you increase the number of slits, eventually the entire obstruction disappears. Yet it is clear that there are many paths that contribute to the final amplitude of the electron propagating to the screen.

As we generalize this thought experiment further, we are led to conclude that the amplitude of a particle moving from a point x_i to another point x_f consists of many components each of which corresponds to a particular path that connects these two points. One such path is a classical trajectory. However, there are infinitely many other paths that are not possible classically, yet contribute to the quantum mechanical amplitude. This argument leads to the notion of a *path integral*, where you sum over all possible paths connecting the initial and final points to obtain the amplitude.

The question then is how you weight individual paths. One point is clear: the weight factor must be chosen such that the classical path is singled out in the limit $\hbar \to 0$. The correct choice turns out to be $e^{iS[x(t)]/\hbar}$, where $S[x(t)] = \int_{t_i}^{t_f} dt L(x(t), \dot{x}(t))$ is the classical action for the path $x(t)$ that satisfies the boundary condition $x(t_i) = x_i$, $x(t_f) = x_f$. In the limit $\hbar \to 0$, the phase factor oscillates so rapidly that nearly all the paths would cancel each other out in the final amplitude. However, there is a path that makes the action stationary, whose contribution is not canceled. This particular path is nothing but the classical trajectory. This way, we see that the classical trajectory *dominates* the path integral in the $\hbar \to 0$ limit.

As we increase $\hbar$, the path becomes "fuzzy." The classical trajectory still dominates, but there are other paths close to it whose action is within $\Delta S \simeq \hbar$ and contribute significantly to the amplitude. The particle does an excursion around the classical trajectory.

3 Propagator

The quantity*

$$K(x_f, t_f; x_i, t_i) = \langle x_f, t_f | x_i, t_i \rangle \tag{2}$$

is called a *propagator*. It knows everything about how a wave function "propagates" in time, because

$$\begin{aligned} \psi(x_f, t_f) &= \langle x_f, t_f | \psi \rangle = \int \langle x_f, t_f | x_i, t_i \rangle dx_i \langle x_i, t_i | \psi \rangle \\ &= \int K(x_f, t_f; x_i, t_i) \psi(x_i, t_i) dx_i. \end{aligned} \tag{3}$$

In other words, it is the Green's function for the Schrödinger equation.

The propagator can also be written using energy eigenvalues and eigenstates (if the Hamiltonian does not depend on time),

$$\begin{aligned} K(x_f, t_f; x_i, t_i) &= \langle x_f | e^{-iH(t_f - t_i)/\hbar} | x_i \rangle = \sum_n \langle x_f | n \rangle e^{-iE_n(t_f - t_i)/\hbar} \langle n | x_i \rangle \\ &= \sum_n e^{-iE_n(t_f - t_i)/\hbar} \psi_n^*(x_f) \psi_n(x_i). \end{aligned} \tag{4}$$

In particular, Fourier analyzing the propagator tells you all energy eigenvalues, and each Fourier coefficients the wave functions of each energy eigenstates.

The propagator is a nice package that contains all dynamical information about a quantum system.

4 Derivation of the Path Integral

The basic point is that the propagator for a short interval is given by the classical Lagrangian

$$\langle x_1, t + \Delta t | x_0, t \rangle = c e^{i(L(t)\Delta t + O(\Delta t)^2)/\hbar}, \tag{5}$$

where c is a normalization constant. This can be shown easily for a simple Hamiltonian

$$H = \frac{p^2}{2m} + V(x). \tag{6}$$

*Note that the expression here is in the Heisenberg picture. The base kets $|x\rangle$ and the operator x depend on time, while the state ket $|\psi\rangle$ doesn't.

The quantity we want is

$$\langle x_1, t+\Delta t|x_0, t\rangle = \langle x_1|e^{-iH\Delta t/\hbar}|x_0\rangle = \int dp \langle x_1|p\rangle\langle p|e^{-iH\Delta t/\hbar}|x_0\rangle. \quad (7)$$

Because we are interested in the phase factor only at $O(\Delta t)$, the last factor can be estimated as

$$\begin{aligned}
&\langle p|e^{-iH\Delta t/\hbar}|x_0\rangle \\
&\quad = \langle p|1 - iH\Delta t/\hbar + (\Delta t)^2|x_0\rangle \\
&\quad = \left(1 - \frac{i}{\hbar}\frac{p^2}{2m}\Delta t - \frac{i}{\hbar}V(x_0)\Delta t + O(\Delta t)^2\right)\frac{e^{-ipx_0/\hbar}}{\sqrt{2\pi\hbar}} \\
&\quad = \frac{1}{\sqrt{2\pi\hbar}} \exp\frac{-i}{\hbar}\left(px_0 + \frac{p^2}{2m}\Delta t + V(x_0)\Delta t + O(\Delta t)^2\right). \qquad (8)
\end{aligned}$$

Then the p-integral is a Fresnel integral

$$\begin{aligned}
&\langle x_1, t+\Delta t|x_0, t\rangle \\
&\quad = \int \frac{dp}{2\pi\hbar} e^{ipx_1/\hbar} e^{-i(px_0 + \frac{p^2}{2m}\Delta t + V(x_0)\Delta t + O(\Delta t)^2)/\hbar} \\
&\quad = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \exp\frac{i}{\hbar}\left(\frac{m}{2}\frac{(x_1-x_0)^2}{\Delta t} - V(x_0)\Delta t + O(\Delta t)^2\right). \qquad (9)
\end{aligned}$$

The quantity in the parentheses is nothing but the classical Lagrangian[†] times Δt by identifying $\dot{x}^2 = (x_1 - x_0)^2/(\Delta t)^2$.

Once Eq. (5) is shown, we use many time slices to obtain the propagator for a finite time interval. Using the completeness relation many many times,

$$\begin{aligned}
\langle x_f, t_f|x_i, t_i\rangle &= \int \langle x_f, t_f|x_{N-1}, t_{N-1}\rangle dx_{N-1}\langle x_{N-1}, t_{N-1}|x_{N-2}, t_{N-2}\rangle dx_{N-2} \\
&\quad \cdots dx_2\langle x_2, t_2|x_1, t_1\rangle dx_1\langle x_1, t_1|x_i, t_i\rangle. \qquad (10)
\end{aligned}$$

The time interval for each factor is $\Delta t = (t_f - t_i)/N$. By taking the limit $N \to \infty$, Δt is small enough that we can use the formula Eq. (5), and we find

$$\langle x_f, t_f|x_i, t_i\rangle = \int \prod_{i=1}^{N-1} dx_i e^{i\sum_{i=0}^{N-1} L(t_i)\Delta t/\hbar}, \qquad (11)$$

[†]The expression is asymmetrical between x_1 and x_0, but the difference between $V(x_0)\Delta t$ and $V(x_1)\Delta t$ is approximately $V'\Delta t(x_0 - x_1) \simeq V'\dot{x}(\Delta t)^2$ and hence of higher oder.

up to a normalization. (Here, $t_0 = t_i$.) In the limit $N \to \infty$, the integral over positions at each time slice can be said to be an integral over all possible paths. The exponent becomes a time-integral of the Lagrangian, namely the action for each path.

This completes the derivation of the path integral in quantum mechanics. As clear from the derivation, the overall normalization of the path integral is a tricky business.

A useful point to notice is that even matrix elements of operators can be written in terms of path integrals. For example,

$$\begin{aligned} \langle x_f, t_f | x(t_0) | x_i, t_i \rangle &= \int dx(t_0) \langle x_f, t_f | x(t_0), t_0 \rangle x(t_0) \langle x(t_0), t_0 | x_i, t_i \rangle \\ &= \int dx(t_0) \int_{t_f > t > t_0} \mathcal{D}x(t) e^{iS[x(t)]/\hbar} x(t_0) \int_{t_0 > t > t_i} \mathcal{D}x(t) e^{iS[x(t)]/\hbar} \\ &= \int_{t_f > t > t_i} \mathcal{D}x(t) e^{iS[x(t)]/\hbar} x(t_0), \end{aligned} \tag{12}$$

At the last step, we used the fact that an integral over all paths from x_i to $x(t_0)$, all paths from $x(t_0)$ to x_f, further integrated over the intermediate position $x(t_0)$ is the same as the integral over all paths from x_i to x_f. The last expression is literally an expectation value of the position in the form of an integral. If we have multiple insertions, by following the same steps,

$$\langle x_f, t_f | x(t_2) x(t_1) | x_i, t_i \rangle = \int_{t_f > t > t_i} \mathcal{D}x(t) e^{iS[x(t)]/\hbar} x(t_2) x(t_1). \tag{13}$$

Here we assumed that $t_2 > t_1$ to be consistent with successive insertion of positions in the correct order. Therefore, expectation values in the path integral corresponds to matrix elements of operators with correct ordering in time. Such a product of operators is called “timed-ordered” $Tx(t_2)x(t_1)$ defined by $x(t_2)x(t_1)$ as long as $t_2 > t_1$, while by $x(t_1)x(t_2)$ if $t_1 > t_2$.

Another useful point is that Euler–Lagrange equation is obtained by the change of variable $x(t) \to x(t) + \delta x(t)$ with $x_i = x(t_i)$ and $x_f = x(t_f)$ held fixed. A change of variable of course does not change the result of the integral, and we find

$$\int \mathcal{D}x(t) e^{iS[x(t)+\delta x(t)]/\hbar} = \int \mathcal{D}x(t) e^{iS[x(t)]/\hbar}, \tag{14}$$

and hence

$$\int \mathcal{D}x(t) e^{iS[x(t)+\delta x(t)]/\hbar} - \int \mathcal{D}x(t) e^{iS[x(t)]/\hbar} = \int \mathcal{D}x(t) e^{iS[x(t)]/\hbar} \frac{i}{\hbar} \delta S = 0. \tag{15}$$

Recall (see Note on Classical Mechanics I)

$$\delta S = S[x(t) + \delta(t)] - S[x(t)] = \int \left(\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} \right) \delta x(t) dt. \tag{16}$$

Therefore,

$$\int \mathcal{D}x(t) e^{iS[x(t)]/\hbar} \frac{i}{\hbar} \int \left(\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} \right) \delta x(t) dt = 0. \tag{17}$$

Because $\delta x(t)$ is an arbitrary change of variable, the expression must be zero at all t independently,

$$\int \mathcal{D}x(t) e^{iS[x(t)]/\hbar} \frac{i}{\hbar} \left(\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} \right) = 0. \tag{18}$$

Therefore, the Euler–Lagrange equation must hold as an expectation value, nothing but the Ehrenfest's theorem.

5 Schrödinger Equation from Path Integral

Here we would like to see that the path integral contains all information we need. In particular, we rederive Schrödinger equation from the path integral.

Let us first see that the momentum is given by a derivative. Starting from the path integral

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}x(t) e^{iS[x(t)]/\hbar}, \tag{19}$$

we shift the trajectory $x(t)$ by a small amount $x(t) + \delta x(t)$ with the boundary condition that x_i is held fixed ($\delta x(t_i) = 0$) while x_f is varied ($\delta x(t_f) \neq 0$). Under this variation, the propagator changes by

$$\langle x_f + \delta x(t_f), t_f | x_i, t_i \rangle - \langle x_f, t_f | x_i, t_i \rangle = \frac{\partial}{\partial x_f} \langle x_f, t_f | x_i, t_i \rangle \delta x(t_f). \tag{20}$$

On the other hand, the path integral changes by

$$\int \mathcal{D}x(t) e^{iS[x(t)+\delta x(t)]/\hbar} - \int \mathcal{D}x(t) e^{iS[x(t)]/\hbar} = \int \mathcal{D}x(t) e^{iS[x(t)]/\hbar} \frac{i\delta S}{\hbar}. \tag{21}$$

Recall that the action changes by (see Note on Classical Mechanics II)

$$\begin{aligned}
\delta S &= S[x(t)+\delta x(t)] - S[x(t)] \\
&= \int_{t_i}^{t_f} dt \left(\frac{\partial L}{\partial x}\delta x + \frac{\partial L}{\partial \dot{x}}\delta \dot{x} \right) \\
&= \frac{\partial L}{\partial \dot{x}}\delta x \bigg|_{x_i}^{x_f} + \int_{t_i}^{t_f} dt \left(\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} \right) \delta x. \qquad (22)
\end{aligned}$$

The last terms vanishes because of the equation of motion (which holds as an expectation value, as we saw in the previous section), and we are left with

$$\delta S = \frac{\partial L}{\partial \dot{x}}\delta x(t_f) = p(t_f)\delta x(t_f). \qquad (23)$$

By putting them together, and dropping $\delta x(t_f)$, we find

$$\frac{\partial}{\partial x_f}\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}x(t) e^{iS[x(t)]/\hbar} \frac{i}{\hbar} p(t_f). \qquad (24)$$

This is precisely how the momentum operator is represented in the position space.

Now the Schrödinger equation can be derived by taking a variation with respect to t_f. Again recall (see Note on Classical Mechanics II)

$$\frac{\partial S}{\partial t_f} = -H(t_f) \qquad (25)$$

after using the equation of motion. Therefore,

$$\frac{\partial}{\partial t_f}\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}x(t) e^{iS[x(t)]/\hbar} \frac{-i}{\hbar} H(t_f). \qquad (26)$$

If

$$H = \frac{p^2}{2m} + V(x), \qquad (27)$$

the momentum can be rewritten using Eq. (24), and we recover the Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t}\langle x_f, t_f | x_i, t_i \rangle = \left(\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x_f} \right)^2 + V(x_f) \right) \langle x_f, t_f | x_i, t_i \rangle. \qquad (28)$$

In other words, the path integral contains the same information as the conventional formulation of the quantum mechanics.

6 Examples

6.1 Free Particle and Normalization

Here we calculate the path integral for a free particle in one-dimension. We need to calculate

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}x(t) e^{i \int \frac{m}{2} \dot{x}^2 dt/\hbar}, \tag{29}$$

over all paths with the boundary condition $x(t_i) = x_i$, $x(t_f) = x_f$.

First, we do it somewhat sloppily, but we can obtain dependences on important parameters nonetheless. We will come back to much more careful calculation with close attention to the overall normalization later on.

The classical path is

$$x_c(t) = x_i + \frac{x_f - x_i}{t_f - t_i}(t - t_i). \tag{30}$$

We can write $x(t) = x_c(t) + \delta x(t)$, where the left-over piece (a.k.a. quantum fluctuation) must vanish at the initial and the final time. Therefore, we can expand $\delta x(t)$ in Fourier series

$$\delta x(t) = \sum_{n=1}^{\infty} a_n \sin \frac{n\pi}{t_f - t_i}(t - t_i). \tag{31}$$

The integral over all paths can then be viewed as integrals over all a_n,

$$\int \mathcal{D}x(t) = c \int \prod_{n=1}^{\infty} da_n. \tag{32}$$

The overall normalization factor c that depends on m and $t_f - t_i$ will be fixed later. The action, on the other hand, can be calculated. The starting point is

$$\dot{x} = \dot{x}_c + \delta\dot{x} = \frac{x_f - x_i}{t_f - t_i} + \sum_{n=1}^{\infty} \frac{n\pi}{t_f - t_i} a_n \cos \frac{\pi n}{t_f - t_i}(t - t_i). \tag{33}$$

Because different modes are orthogonal upon t-integral, the action is

$$S = \frac{m}{2} \frac{(x_f - x_i)^2}{t_f - t_i} + \frac{m}{2} \sum_{n=1}^{\infty} \frac{1}{2} \frac{(n\pi)^2}{t_f - t_i} a_n^2. \tag{34}$$

The first term is nothing but the classical action. Then the path integral reduces to an infinite collection of Fresnel integrals,

$$c \int \prod_{n=1}^{\infty} da_n \exp\left[\frac{i}{\hbar}\frac{m}{2}\left(\frac{(x_f - x_i)^2}{t_f - t_i} + \sum_{n=1}^{\infty} \frac{1}{2}\frac{(n\pi)^2}{t_f - t_i} a_n^2\right)\right]. \tag{35}$$

We now obtain

$$\langle x_f, t_f | x_i, t_i \rangle = c \prod_{n=1}^{\infty} \left(-\frac{i}{\pi\hbar}\frac{m}{2}\frac{1}{2}\frac{(n\pi)^2}{t_f - t_i}\right)^{-1/2} \exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(x_f - x_i)^2}{t_f - t_i}\right]. \tag{36}$$

Therefore, the result is simply

$$\langle x_f, t_f | x_i, t_i \rangle = c'(t_f - t_i) \exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(x_f - x_i)^2}{t_f - t_i}\right]. \tag{37}$$

The normalization constant c can depend only on the time interval $t_f - t_i$, and is determined by the requirement that

$$\int dx \langle x_f, t_f | x, t \rangle \langle x, t | x_i, t_i \rangle = \langle x_f, t_f | x_i, t_i \rangle. \tag{38}$$

And hence[‡]

$$c'(t_f - t) c'(t - t_i) \sqrt{\frac{2\pi i\hbar (t_f - t)(t - t_i)}{m(t_f - t_i)}} = c'(t_f - t_i). \tag{39}$$

We therefore find

$$c'(t) = \sqrt{\frac{m}{2\pi i\hbar t}}, \tag{40}$$

recovering Eq. (2.5.16) of Sakurai precisely.

In order to obtain this result directly from the path integral, we should have chosen the normalization of the measure to be

$$\mathcal{D}x(t) = \sqrt{\frac{m}{2\pi i\hbar (t_f - t_i)}} \prod_{n=1}^{\infty} \sqrt{\frac{m}{2\pi i\hbar (t_f - t_i)}} \frac{n\pi}{\sqrt{2}} da_n. \tag{41}$$

[‡]This argument does not eliminate the possible factor $e^{-i\omega_0(t_f - t_i)}$, which would correspond to a zero point in the energy $\hbar\omega_0$. Mahiko Suzuki pointed out this problem to me. Here we take the point of view that the normalization is fixed by comparison to the conventional method.

Now we do it much more carefully with close attention to the overall normalization. The path integral for the time interval $t_f - t_i$ is divided up into N time slices each with $\Delta t = (t_f - t_i)/N$,

$$K = \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2} \int \prod_{n=1}^{N-1} dx_n e^{iS/\hbar}, \tag{42}$$

where

$$S = \frac{1}{2} m \sum_{n=1}^{N-1} \frac{(x_{n+1} - x_n)^2}{\Delta t}. \tag{43}$$

The point is that this is nothing but a big Gaussian (to be more precise, Fresnel) integral, because the action is quadratic in the integration variables $x_1, \cdots, x_{N-1}$. To make this point clear, we rewrite the action into the following form:

$$S = \frac{1}{2}\frac{m}{\Delta t}(x_N^2 + x_0^2) - \frac{m}{\Delta t}(x_{N-1}, x_{N-2}, x_{N-3}, \cdots, x_2, x_1) \begin{pmatrix} x_N \\ 0 \\ 0 \\ \vdots \\ 0 \\ x_0 \end{pmatrix} + \frac{1}{2}\frac{m}{\Delta t} \times$$
$$(x_{N-1}, x_{N-2}, x_{N-3}, \cdots, x_2, x_1) \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 \\ 0 & 0 & 0 & \cdots & -1 & 2 \end{pmatrix} \begin{pmatrix} x_{N-1} \\ x_{N-2} \\ x_{N-3} \\ \vdots \\ x_2 \\ x_1 \end{pmatrix} \tag{44}$$

Comapring to the identity Eq. (106),

$$\int \prod_{n=1}^{N} dx_n e^{-\frac{1}{2}\mathbf{x}^T A\mathbf{x} - \mathbf{x}^T\mathbf{y}} = (2\pi)^{N/2} (\det A)^{-1/2} e^{+\frac{1}{2}\mathbf{y}^T A^{-1}\mathbf{y}} \tag{45}$$

we identify

$$A = -\frac{i}{\hbar}\frac{2m}{\Delta t}\begin{pmatrix} 1 & -1/2 & 0 & \cdots & 0 & 0 \\ -1/2 & 1 & -1/2 & \cdots & 0 & 0 \\ 0 & -1/2 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1/2 \\ 0 & 0 & 0 & \cdots & -1/2 & 1 \end{pmatrix} \tag{46}$$

This is nothing but the matrix K_{N-1} in Eq. (106) with $a = 1/2$ up to a factor of $-\frac{i}{\hbar}\frac{2m}{\Delta t}$. One problem is that, for $a = 1/2$, $\lambda_+ = \lambda_- = 1/2$ and hence Eq. (111) is singular. Fortunately, it can be rewritten as

$$\det K_{N-1} = \frac{\lambda_+^N - \lambda_-^N}{\lambda_+ - \lambda_-} = \lambda_+^{N-1} + \lambda_+^{N-2}\lambda_- + + \cdots + \lambda_+\lambda_-^{N-2} + \lambda_-^{N-1} = N\left(\frac{1}{2}\right)^{N-1}. \tag{47}$$

Therefore,

$$\det A = \left(\frac{2m}{i\hbar\Delta t}\right)^{N-1} N\frac{1}{2^{N-1}} = N\left(\frac{m}{i\hbar\Delta t}\right)^{N-1}. \tag{48}$$

Therefore, the prefactor of the path integral is

$$\begin{aligned} & \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2} (2\pi)^{(N-1)/2} (\det A)^{-1/2} \\ & = \left(\frac{m}{i\hbar\Delta t}\right)^{N/2} (2\pi)^{-1/2} N^{-1/2} \left(\frac{m}{i\hbar\Delta t}\right)^{-(N-1)/2} \\ & = \left(\frac{m}{2\pi i\hbar N\Delta t}\right)^{1/2} = \left(\frac{m}{2\pi i\hbar(t_f - t_i)}\right)^{1/2}. \end{aligned} \tag{49}$$

The exponent is given by

$$\frac{i}{\hbar}\frac{1}{2}\frac{im}{\hbar\Delta t}(x_N^2 + x_0^2) + \frac{1}{2}\left(\frac{m}{\Delta t}\right)^2 (x_N, 0, 0, \cdots, 0, x_0) A^{-1} \begin{pmatrix} x_N \\ 0 \\ 0 \\ \vdots \\ 0 \\ x_0 \end{pmatrix} \tag{50}$$

We need only $(1,1)$, $(N-1, N-1)$, $(1, N-1)$, and $(N-1, 1)$ components of A^{-1}.

$$(A^{-1})_{1,1} = (A^{-1})_{N-1,N-1} = \frac{i\hbar\Delta t}{2m}\frac{\det K_{N-2}}{\det K_{N-1}} = \frac{i\hbar\Delta t}{m}\frac{N-1}{N}. \tag{51}$$

On the other hand,

$$
\begin{aligned}
(A^{-1})_{1,N-1} &= (A^{-1})_{N-1,1} \\
&= \frac{i\hbar\Delta t}{2m}\frac{1}{\det K_{N-1}}(-1)^{N-2}\det\begin{pmatrix} -1/2 & 1 & -1/2 & \cdots & 0 \\ 0 & -1/2 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -1/2 \end{pmatrix} \\
&= \frac{i\hbar\Delta t}{2m}\frac{2^{N-1}}{N}\frac{1}{2^{N-2}} \\
&= \frac{i\hbar\Delta t}{Nm}. \qquad (52)
\end{aligned}
$$

We hence find the exponent

$$
\begin{aligned}
&\frac{i}{\hbar}\frac{1}{2}\frac{m}{\Delta t}(x_N^2+x_0^2)+\frac{1}{2}\left(\frac{m}{\Delta t}\right)^2(x_N,0,0,\cdots,0,x_0)A^{-1}\begin{pmatrix} x_N \\ 0 \\ 0 \\ \vdots \\ 0 \\ x_0 \end{pmatrix} \\
= \;& \frac{i}{\hbar}\frac{1}{2}\frac{m}{\Delta t}(x_N^2+x_0^2)+\frac{1}{2}\left(\frac{im}{\hbar\Delta t}\right)^2\left(\frac{i\hbar\Delta t}{m}\frac{N-1}{N}(x_N^2+x_0^2)+2\frac{i\hbar\Delta t}{Nm}x_Nx_0\right) \\
= \;& \frac{i}{\hbar}\frac{1}{2}\frac{m}{\Delta t}\frac{1}{N}(x_N^2+x_0^2)-\frac{1}{2}\frac{im}{\hbar N\Delta t}2x_Nx_0 \\
= \;& \frac{i}{\hbar}\frac{m}{2}\frac{(x_N-x_0)^2}{N\Delta t} \\
= \;& \frac{i}{\hbar}\frac{m}{2}\frac{(x_f-x_i)^2}{t_f-t_i}. \qquad (53)
\end{aligned}
$$

Putting the prefactor Eq. (49) and the exponent Eq. (53) together, we find the propagator

$$
K = \left(\frac{m}{2\pi i\hbar(t_f-t_i)}\right)^{1/2} e^{\frac{i}{\hbar}\frac{m}{2}\frac{(x_f-x_i)^2}{t_f-t_i}}. \qquad (54)
$$

We recovered Eq. (2.5.16) of Sakurai without any handwaving this time!

6.2 Harmonic Oscillator

Now that we have fixed the normalization of the path integral, we calculate the path integral for a harmonic oscillator in one-dimension. We need to calculate

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}x(t) e^{i \int \left(\frac{m}{2}\dot{x}^2 - \frac{1}{2} m\omega^2 x^2 \right) dt/\hbar}, \tag{55}$$

over all paths with the boundary condition $x(t_i) = x_i$, $x(t_f) = x_f$. The classical path is

$$x_c(t) = x_i \frac{\sin \omega(t_f - t)}{\sin \omega(t_f - t_i)} + x_f \frac{\sin \omega(t - t_i)}{\sin \omega(t_f - t_i)}. \tag{56}$$

The action along the classical path is

$$S_c = \int_{t_i}^{t_f} \left(\frac{m}{2}\dot{x}^2 - \frac{1}{2} m\omega^2 x^2 \right) dt = \frac{1}{2} m\omega \frac{(x_i^2 + x_f^2) \cos \omega(t_f - t_i) - 2x_i x_f}{\sin \omega(t_f - t_i)}. \tag{57}$$

The quantum fluctuation around the classical path contributes as the $O(\hbar)$ correction to the amplitude, relative to the leading piece $e^{iS_c/\hbar}$. We expand the quantum fluctuation in Fourier series as in the case of free particle. Noting that the action is stationary with respect to the variation of $x(t)$ around $x_c(t)$, there is no linear piece in a_n. Because different modes are orthogonal upon t-integral, the action is

$$S = S_c + \sum_{n=1}^{\infty} \frac{m}{2} \left(\frac{(n\pi)^2}{t_f - t_i} - \omega^2 (t_f - t_i) \right) \frac{1}{2} a_n^2. \tag{58}$$

Therefore the path integral is an infinite number of Fresnel integrals over a_n using the measure in Eq. (41)

$$\begin{aligned}
\langle x_f, t_f | x_i, t_i \rangle &= e^{iS_c/\hbar} \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} \\
&\quad \times \prod_{n=1}^{\infty} \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} \frac{n\pi}{\sqrt{2}} \int da_n \exp \left[\frac{i}{\hbar} \frac{m}{2} \left(\frac{(n\pi)^2}{t_f - t_i} - \omega^2 (t_f - t_i) \right) \frac{1}{2} a_n^2 \right] \\
&= e^{iS_c/\hbar} \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} \prod_{n=1}^{\infty} \left(1 - \left(\frac{\omega(t_f - t_i)}{n\pi} \right)^2 \right)^{-1/2}.
\end{aligned} \tag{59}$$

Now we resort to the following infinite product representation of the sine function

$$\prod_{n=1}^{\infty} \left(1 - \frac{x^2}{n^2} \right) = \frac{\sin \pi x}{\pi x}. \tag{60}$$

We find

$$\begin{aligned}\langle x_f, t_f | x_i, t_i\rangle &= e^{iS_c/\hbar}\sqrt{\frac{m}{2\pi i\hbar(t_f-t_i)}}\sqrt{\frac{\omega(t_f-t_i)}{\sin\omega(t_f-t_i)}} \\ &= e^{iS_c/\hbar}\sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega(t_f-t_i)}} \end{aligned} \tag{61}$$

This agrees with the result from the more conventional method as given in Sakurai Eq. (2.5.18).

Again, we can pay closer attention to the normalization by going through the same steps as for a free particle using discretized time slices. The action is

$$S = \frac{1}{2}m\sum_{n=1}^{N-1}\frac{(x_{n+1}-x_n)^2}{\Delta t} - \frac{1}{2}m\omega^2\sum_{n=1}^{N-1}x_n^2 - \frac{1}{2}m\omega^2\left(\frac{1}{2}x_0^2+\frac{1}{2}x_N^2\right). \tag{62}$$

The last term is there to correctly acccount for all $N-1$ time slices for the potential energy term $-\int V dt$, but to retain the symmetry between the initial and final positions, we took their average. Once again, this is nothing but a big Fresnel (complex Gaussian) integral:

$$S = \frac{1}{2}\frac{m}{\Delta t}(x_N^2+x_0^2) - \frac{m}{\Delta t}(x_{N-1},x_{N-2},x_{N-3},\cdots,x_2,x_1)\begin{pmatrix} x_N \\ 0 \\ 0 \\ \vdots \\ 0 \\ x_0 \end{pmatrix} + \frac{1}{2}\frac{m}{\Delta t}\times$$

$$(x_{N-1},x_{N-2},x_{N-3},\cdots,x_2,x_1)\begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 \\ 0 & 0 & 0 & \cdots & -1 & 2 \end{pmatrix}\begin{pmatrix} x_{N-1} \\ x_{N-2} \\ x_{N-3} \\ \vdots \\ x_2 \\ x_1 \end{pmatrix}$$

$$-\frac{1}{2}m\omega^2(x_{N-1},x_{N-2},x_{N-3},\cdots,x_2,x_1)\begin{pmatrix} x_{N-1} \\ x_{N-2} \\ x_{N-3} \\ \vdots \\ x_2 \\ x_1 \end{pmatrix}\Delta t - \frac{1}{4}m\omega^2(x_N^2+x_0^2)\Delta t$$

(63)

Comapring to the identity Eq. (106),

$$\int \prod_{n=1}^{N} dx_n e^{-\frac{1}{2}\mathbf{x}^T A\mathbf{x}-\mathbf{x}^T\mathbf{y}} = (2\pi)^{N/2}(\det A)^{-1/2}e^{+\frac{1}{2}\mathbf{y}^T A^{-1}\mathbf{y}} \tag{64}$$

we identify

$$A = \frac{i}{\hbar}m\omega^2\Delta t I_{N-1} - \frac{i}{\hbar}\frac{2m}{\Delta t}\begin{pmatrix} 1 & -1/2 & 0 & \cdots & 0 & 0 \\ -1/2 & 1 & -1/2 & \cdots & 0 & 0 \\ 0 & -1/2 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1/2 \\ 0 & 0 & 0 & \cdots & -1/2 & 1 \end{pmatrix} \tag{65}$$

This is nothing but the matrix K_{N-1} in Eq. (106) up to an overall factor of

$$-\frac{i}{\hbar}\frac{2m}{\Delta t} + \frac{i}{\hbar}m\omega^2\Delta t = \frac{m}{i\hbar\Delta t}(2-\omega^2(\Delta t)^2) \tag{66}$$

with

$$a = \frac{1}{2}\frac{2m/\Delta t}{\frac{2m}{\Delta t} - m\omega^2\Delta t} = \frac{1}{2-\omega^2(\Delta t)^2}. \tag{67}$$

Using Eq. (111),

$$\lambda_\pm = \frac{1}{2}\left(1 \pm \sqrt{1 - \frac{4}{(2-\omega^2(\Delta t)^2)^2}}\right) \tag{68}$$

Therefore,

$$\det A = \left(\frac{m}{i\hbar\Delta t}\right)^{N-1}(2-\omega^2(\Delta t)^2)^{N-1}\frac{\lambda_+^N - \lambda_-^N}{\lambda_+ - \lambda_-}. \tag{69}$$

Therefore, the prefactor of the path integral is

$$\begin{aligned} &\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2}(2\pi)^{(N-1)/2}(\det A)^{-1/2} \\ &= \sqrt{\frac{m}{2\pi i\hbar\Delta t}}\left(2-\omega^2(\Delta t)^2\right)^{-(N-1)/2}\left(\frac{\lambda_+^N - \lambda_-^N}{\lambda_+ - \lambda_-}\right)^{-1/2}. \end{aligned} \tag{70}$$

Now we use the identity

$$\lim_{N\to\infty}\left(1+\frac{x}{N}\right)^N = e^x. \tag{71}$$

We find in the limit of $\Delta t = (t_f - t_i)/N$ and $N \to \infty$,

$$\lambda_\pm = \frac{1}{2}\left(1 \pm \sqrt{1 - \frac{4}{(2-\omega^2(\Delta t)^2)^2}}\right) = \frac{1}{2}(1 \pm i\omega\Delta t) + O(N^{-3}), \tag{72}$$

and hence

$$\begin{aligned}\frac{\lambda_+^N - \lambda_-^N}{\lambda_+ - \lambda_-} &\to \frac{1}{2^N}\frac{e^{i\omega(t_f-t_i)} - e^{-i\omega(t_f-t_i)}}{i\omega\Delta t} + O(N^{-1}) \\ &= \frac{N}{2^{N-1}}\frac{\sin\omega(t_f-t_i)}{\omega(t_f-t_i)} + O(N^{-1}).\end{aligned} \tag{73}$$

In the same limit,

$$\begin{aligned}\left(2-\omega^2(\Delta t)^2\right)^{-(N-1)/2} &= 2^{-(N-1)/2}\left(1 - \frac{1}{2}\omega^2(\Delta t)^2\right)^{-(N-1)/2} \\ &= 2^{-(N-1)/2} + O(N^{-1}).\end{aligned} \tag{74}$$

Therefore, the prefactor Eq. (70) is

$$\sqrt{\frac{m}{2\pi i\hbar\Delta t}}2^{-(N-1)/2}\left(\frac{N}{2^{N-1}}\frac{\sin\omega(t_f-t_i)}{\omega(t_f-t_i)}\right)^{-1/2} = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega(t_f-t_i)}}\,. \tag{75}$$

The exponent is given by

$$\frac{i}{\hbar}\frac{1}{2}\frac{im}{\hbar\Delta t}(x_N^2+x_0^2) - \frac{i}{\hbar}\frac{1}{4}m\omega^2(x_N^2+x_0^2) + \frac{1}{2}\left(\frac{im}{\hbar\Delta t}\right)^2(x_N,0,0,\cdots,0,x_0)A^{-1}\begin{pmatrix}x_N\\0\\0\\\vdots\\0\\x_0\end{pmatrix} \tag{76}$$

We need only $(1,1)$, $(N-1,N-1)$, $(1,N-1)$, and $(N-1,1)$ components of A^{-1}.

$$\begin{aligned}&(A^{-1})_{1,1} = (A^{-1})_{N-1,N-1} \\ &\quad= \frac{i\hbar\Delta t}{m}(2-\omega^2(\Delta t)^2)^{-1}\frac{\det K_{N-2}}{\det K_{N-1}} = \frac{i\hbar\Delta t}{m}(2-\omega^2(\Delta t)^2)^{-1}\frac{\lambda_+^{N-1}-\lambda_-^{N-1}}{\lambda_+^N-\lambda_-^N}\end{aligned} \tag{77}$$

On the other hand,

$$
\begin{aligned}
(A^{-1})_{1,N-1} &= (A^{-1})_{N-1,1} \\
&= \frac{i\hbar\Delta t}{m}(2-\omega^2(\Delta t)^2)^{-1}\frac{1}{\det K_{N-1}}(-1)^{N-2}\det\begin{pmatrix} -a & 1 & -a & \cdots & 0 \\ 0 & -a & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -a \end{pmatrix} \\
&= \frac{i\hbar\Delta t}{m}(2-\omega^2(\Delta t)^2)^{-1}\frac{\lambda_+ - \lambda_-}{\lambda_+^N - \lambda_-^N}a^{N-2} \\
&\to \frac{i\hbar\Delta t}{m}2^{-1}\frac{2^{N-1}}{N}\frac{\omega(t_f-t_i)}{\sin\omega(t_f-t_i)}\frac{1}{2^{N-2}} = \frac{i\hbar\Delta t}{Nm}\frac{\omega(t_f-t_i)}{\sin\omega(t_f-t_i)}.
\end{aligned} \tag{78}
$$

We hence find the exponent

$$
\begin{aligned}
&\frac{i}{\hbar}\left(\frac{1}{2}\frac{im}{\hbar\Delta t} - \frac{1}{4}m\omega^2\right)(x_N^2+x_0^2) + \frac{1}{2}\left(\frac{m}{\Delta t}\right)^2 (x_N, 0, 0, \cdots, 0, x_0)A^{-1}\begin{pmatrix} x_N \\ 0 \\ 0 \\ \vdots \\ 0 \\ x_0 \end{pmatrix} \\
&= \frac{i}{\hbar}\left(\frac{1}{2}\frac{im}{\hbar\Delta t} - \frac{1}{4}m\omega^2\right)(x_N^2+x_0^2) + \frac{1}{2}\left(\frac{im}{\hbar\Delta t}\right)^2\frac{i\hbar\Delta t}{m}\times \\
&\quad \left((2-\omega^2(\Delta t)^2)^{-1}\frac{\lambda_+^{N-1}-\lambda_-^{N-1}}{\lambda_+^N-\lambda_-^N}(x_N^2+x_0^2) + \frac{2}{N}\frac{\omega(t_f-t_i)}{\sin\omega(t_f-t_i)}x_N x_0\right)
\end{aligned} \tag{79}
$$

Taking the limit $N \to \infty$, the second term is obviously regular, and the last term in the parentheses is also:

$$
\frac{1}{2}\left(\frac{im}{\hbar\Delta t}\right)^2\frac{i\hbar\Delta t}{m}\frac{2}{N}\frac{\omega(t_f-t_i)}{\sin\omega(t_f-t_i)}x_N x_0 = -\frac{i}{\hbar}\frac{m\omega}{\sin\omega(t_f-t_i)}x_N x_0. \tag{80}
$$

The other terms are singular and we need to treat them carefully.

$$
\begin{aligned}
&\frac{i}{\hbar}\frac{1}{2}\frac{m}{\Delta t}(x_N^2+x_0^2) - \frac{1}{2}\frac{im}{\hbar\Delta t}(2-\omega^2(\Delta t)^2)^{-1}\frac{\lambda_+^{N-1}-\lambda_-^{N-1}}{\lambda_+^N-\lambda_-^N}(x_N^2+x_0^2) \\
&= \frac{im}{2\hbar\Delta t}\left(1-(2-\omega^2(\Delta t)^2)^{-1}\frac{\lambda_+^{N-1}-\lambda_-^{N-1}}{\lambda_+^N-\lambda_-^N}\right)(x_N^2+x_0^2).
\end{aligned} \tag{81}
$$

We need $O(N^{-1})$ term in the parentheses. The factor $(2-\omega^2(\Delta t)^2)^{-1} = 2^{-1}+O(N^{-2})$ is easy. Using Eq. (72), the next factor is

$$\frac{\lambda_+^{N-1}-\lambda_-^{N-1}}{\lambda_+^N-\lambda_-^N} = \frac{2^N}{2^{N-1}}\frac{(1+i\omega\Delta t)^{N-1}-(1-i\omega\Delta t)^{N-1}+O(N^{-2})}{(1+i\omega\Delta t)^N-(1-i\omega\Delta t)^N+O(N^{-2})} \quad (82)$$

Therefore, dropping $O(N^{-2})$ corrections consistently,

$$\begin{aligned} & 1-(2-\omega^2(\Delta t)^2)^{-1}\frac{\lambda_+^{N-1}-\lambda_-^{N-1}}{\lambda_+^N-\lambda_-^N} \\ &= \frac{(1+i\omega\Delta t)^N-(1-i\omega\Delta t)^N-(1+i\omega\Delta t)^{N-1}+(1-i\omega\Delta t)^{N-1}}{(1+i\omega\Delta t)^N-(1-i\omega\Delta t)^N} \\ &= i\omega\Delta t\frac{(1+i\omega\Delta t)^{N-1}+(1-i\omega\Delta t)^{N-1}}{(1+i\omega\Delta t)^N-(1-i\omega\Delta t)^N} \\ &= i\omega\frac{(t_f-t_i)}{N}\frac{2\cos\omega(t_f-t_i)}{2i\sin\omega(t_f-t_i)} = \frac{1}{N}\frac{\omega(t_f-t_i)\cos\omega(t_f-t_i)}{\sin\omega(t_f-t_i)}. \end{aligned} \quad (83)$$

Collecting all the terms, the exponent is

$$\begin{aligned} \frac{i}{\hbar}S_c &= -\frac{i}{\hbar}\frac{m\omega}{\sin\omega(t_f-t_i)}x_N x_0 + \frac{im}{2\hbar\Delta t}\frac{1}{N}\frac{\omega(t_f-t_i)\cos\omega(t_f-t_i)}{\sin\omega(t_f-t_i)}(x_N^2+x_0^2) \\ &= \frac{i}{\hbar}\frac{m\omega}{2}\frac{(x_N^2+x_0^2)\cos\omega(t_f-t_i)-2x_N x_0}{\sin\omega(t_f-t_i)} \end{aligned} \quad (84)$$

which is the same as the classical action Eq. (57).

7 Partition Function

The path integral is useful also in statistical mechanics to calculate partition functions. Starting from a conventional definition of a partition function

$$Z = \sum_n e^{-\beta E_n}, \quad (85)$$

where $\beta = 1/(k_B T)$, we rewrite it in the following way using completeness relations in both energy eigenstates and position eigenstates.

$$\begin{aligned} Z &= \sum_n \langle n|e^{-\beta H}|n\rangle = \int dx \sum_n \langle n|x\rangle\langle x|e^{-\beta H}|n\rangle \\ &= \int dx \sum_n \langle x|e^{-\beta H}|n\rangle\langle n|x\rangle = \int dx \langle x|e^{-\beta H}|x\rangle. \end{aligned} \quad (86)$$

The operator $e^{-\beta H}$ is the same as $e^{-iHt/\hbar}$ except the analytic continuation $t \to -i\tau = -i\hbar\beta$. Therefore, the partition function can be written as a path integral for all *closed* paths, *i.e.*, paths with the same beginning and end points, over a "time" interval $-i\hbar\beta$. For a single particle in the potential $V(x)$, it is then

$$Z = \int \mathcal{D}x(\tau) \exp\left[\frac{-1}{\hbar}\oint_0^{\hbar\beta} d\tau \left(\frac{m}{2}\left(\frac{\partial x}{\partial \tau}\right)^2 + V(x)\right)\right]. \tag{87}$$

The position satisfies the periodic boundary condition $x(\hbar\beta) = x(0)$.

For example, in the case of a harmonic oscillator, we can use the result in the previous section

$$\begin{aligned}&\langle x_f, t_f | x_i, t_i\rangle \\ &= \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega(t_f - t_i)}} \exp\left[\frac{i}{\hbar}\frac{1}{2}m\omega\frac{(x_i^2 + x_f^2)\cos\omega(t_f - t_i) - 2x_i x_f}{\sin\omega(t_f - t_i)}\right],\end{aligned} \tag{88}$$

and take $x_f = x_i = x$, $t_f - t_i = -i\hbar\beta$

$$\langle x|e^{-\beta H}|x\rangle = \sqrt{\frac{m\omega}{2\pi\hbar \sinh\beta\hbar\omega}} \exp\left[-\frac{1}{\hbar}\frac{1}{2}m\omega x^2 \frac{2\cosh\beta\hbar\omega - 2}{\sinh\beta\hbar\omega}\right]. \tag{89}$$

Then integrate over x,

$$\begin{aligned} Z &= \int dx \langle x|e^{-\beta H}|x\rangle \\ &= \sqrt{\frac{m\omega}{2\pi\hbar\sinh\beta\hbar\omega}}\sqrt{\pi\hbar\frac{2}{m\omega}\frac{\sinh\beta\hbar\omega}{2\cosh\beta\hbar\omega - 2}} \\ &= \sqrt{\frac{1}{4\sinh^2\beta\hbar\omega/2}} \\ &= \frac{1}{2\sinh\beta\hbar\omega/2} \\ &= \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} \\ &= \sum_{n=0}^{\infty} e^{-\beta(n+\frac{1}{2})\hbar\omega}. \end{aligned} \tag{90}$$

Of course, we could have redone the path integral to obtain the same result. The only difference is that the classical path you expand the action around is now given by sinh rather than sin.

Let us apply the path-integral representation of the partition function to a simple harmonic oscillator. The expression is

$$Z = \int \mathcal{D}x(\tau) \exp \frac{-1}{\hbar} \oint_0^{\hbar\beta} d\tau \left(\frac{m}{2} \left(\frac{\partial x}{\partial \tau} \right)^2 + \frac{m}{2}\omega^2 x^2 \right). \tag{91}$$

We write all possible "paths" $x(\tau)$ in Fourier series as

$$x(\tau) = a_0 + \sum_{n=1}^{\infty} a_n \cos \frac{2\pi n}{\hbar\beta}\tau + \sum_{n=1}^{\infty} b_n \sin \frac{2\pi n}{\hbar\beta}\tau, \tag{92}$$

satisfying the periodic boundary condition $x(\hbar\beta) = x(0)$. Then the exponent of the path integral becomes

$$\begin{aligned} &\frac{-1}{\hbar} \oint_0^{\hbar\beta} d\tau \left(\frac{m}{2} \left(\frac{\partial x}{\partial \tau} \right)^2 + \frac{m}{2}\omega^2 x^2 \right) \\ &\quad = -\frac{\beta m}{2} \left[a_0^2 + \frac{1}{2} \sum_{n=1}^{\infty} \left(\left(\frac{2\pi n}{\hbar\beta} \right)^2 + \omega^2 \right) (a_n^2 + b_n^2) \right]. \end{aligned} \tag{93}$$

The integration over all possible "paths" can be done by integrating over the Fourier coefficients a_n and b_n. Therefore the partition function is

$$Z = c \int da_0 \prod_{n=1}^{\infty} da_n db_n \exp \frac{-\beta m}{2} \left[\omega^2 a_0^2 + \frac{1}{2} \sum_{n=1}^{\infty} \left(\left(\frac{2\pi n}{\hbar\beta} \right)^2 + \omega^2 \right) (a_n^2 + b_n^2) \right]. \tag{94}$$

This is an infinite collection of Gaussian integrals and becomes

$$Z = c \sqrt{\frac{2\pi}{\beta m \omega^2}} \prod_{n=1}^{\infty} \frac{4\pi}{\beta m} \left(\left(\frac{2\pi n}{\hbar\beta} \right)^2 + \omega^2 \right)^{-1}. \tag{95}$$

Here, c is a normalization constant which can depend on β because of normalization of Fourier modes, but not on Lagrangian parameters such as m or ω. Now we use the infinite product representation of the hyperbolic function

$$\prod_{n=1}^{\infty} \left(1 + \frac{x^2}{n^2} \right) = \frac{\sinh \pi x}{\pi x}. \tag{96}$$

The partition function Eq. (95) can be rewritten as

$$
\begin{aligned}
Z &= c\sqrt{\frac{2\pi}{\beta m\omega^2}}\prod_{n=1}^{\infty}\frac{\hbar^2\beta}{\pi m n^2}\left(1+\left(\frac{\hbar\beta\omega}{2\pi n}\right)^2\right)^{-1} \\
&= c'\frac{2}{\sinh \hbar\beta\omega/2} \\
&= c'\frac{e^{-\hbar\beta\omega/2}}{1-e^{-\hbar\beta\omega}}, \qquad (97)
\end{aligned}
$$

where c' is an overall constant, which does not depend on ω, is not important when evaluating various thermally averages quantities. If you drop c', this is exactly the partition function for the harmonic oscillator, including the zero-point energy.

A Path Integrals in Phase Space

As we saw above, the normalization of the path integral is a somewhat tricky issue. The source of the problem was when we did p integral in Eq. (9), that produced a singular prefactor $\sqrt{m/2\pi i\hbar\Delta t}$. On the other hand, if we do not do the p integral, and stop at

$$
\begin{aligned}
\langle x_1, t+\Delta t|x_0, t\rangle &= \int \frac{dp}{2\pi\hbar} e^{ipx_1/\hbar} e^{-i(px_0+\frac{p^2}{2m}\Delta t+V(x_0)\Delta t+O(\Delta t)^2)/\hbar} \\
&= \int \frac{dp}{2\pi\hbar} e^{i(p\frac{x_1-x_0}{\Delta t}-\frac{p^2}{2m}-V(x_0))\Delta t}, \qquad (98)
\end{aligned}
$$

we do not obtain any singular prefactor except $1/2\pi\hbar$ for every momentum integral. The path integral can then be written as

$$
\langle x_f, t_f|x_i, t_i\rangle = \int \mathcal{D}x(t)\mathcal{D}p(t) e^{iS[x(t),p(t)]/\hbar}, \qquad (99)
$$

where the action is given in the phase space

$$
S[x(t), p(t)] = \int_{t_i}^{t_f} (p\dot{x} - H(x,p))\, dt. \qquad (100)
$$

The expression (99) is an integral over all paths in the phase space (x,p). It is understood that there is one more p integral than the x integral (albeit both infinite) because of the number of times the completeness relations are inserted.

Using the path integral in the phase space, we can work out the precise normalization of path integrals up to numerical constants that depend on t, but not on m, or any other parameters in the Lagrangian. For instance, for the harmonic oscillator, we expand

$$x(t) = x_c(t) + \sqrt{\frac{2}{t_f - t_i}} \sum_{n=1}^{\infty} x_n \sin \frac{n\pi}{t_f - t_i}(t - t_i), \tag{101}$$

$$p(t) = p_c(t) + \sqrt{\frac{1}{t_f - t_i}} p_0 + \sqrt{\frac{2}{t_f - t_i}} \sum_{n=1}^{\infty} p_n \cos \frac{n\pi}{t_f - t_i}(t - t_i). \tag{102}$$

The action is then

$$S = S_c - \frac{p_0^2}{2m} - \frac{1}{2} \sum_{n=1}^{\infty} (p_n, x_n) \begin{pmatrix} \frac{1}{m} & \frac{n\pi}{t_f - t_i} \\ \frac{n\pi}{t_f - t_i} & m\omega^2 \end{pmatrix} \begin{pmatrix} p_n \\ x_n \end{pmatrix}, \tag{103}$$

where S_c is the action for the classical solution Eq. (57). Using the integration volume

$$\int \mathcal{D}x(t)\mathcal{D}p(t) = c(t_f - t_i) \int \frac{dp_0}{2\pi\hbar} \prod_{n=1}^{\infty} \frac{dx_n dp_n}{2\pi\hbar}, \tag{104}$$

we find the path integral to be

$$\begin{aligned} \langle x_f, t_f | x_i, t_i \rangle &= e^{iS_c/\hbar} c(t_f - t_i) \frac{1}{2\pi\hbar} \left(\frac{2\pi m\hbar}{i} \right)^{1/2} \\ &\quad \times \prod_{n=1}^{\infty} \frac{1}{2\pi\hbar} \left(\frac{2\pi m\hbar}{i} \right)^{1/2} \left(\frac{2\pi\hbar}{im} \frac{1}{\omega^2 - (n\pi/(t_f - t_i))^2} \right)^{1/2}. \end{aligned} \tag{105}$$

Up to an overall constant $c(t_f - t_i)$ that depends only on $t_f - t_i$, both m and ω dependences are obtained correctly.

B A Few Useful Identities

To carry out the integral, a few identities would be useful. For $N-1$-dimensional column vectors $\mathbf{x}$, $\mathbf{y}$, and a symmetric matrix A,

$$\int \prod_{n=1}^{N} dx_n e^{-\frac{1}{2}\mathbf{x}^T A \mathbf{x} - \mathbf{x}^T \mathbf{y}} = (2\pi)^{N/2} (\det A)^{-1/2} e^{+\frac{1}{2}\mathbf{y}^T A^{-1} \mathbf{y}} \tag{106}$$

It is easy to prove this equation first without the linear term $\mathbf{y}$ by diagonalizatin the matrix $A = O^T D O$, where O is a rotation matrix and $D = \text{diag}(\lambda_1, \cdots, \lambda_N)$ has N eigenvalues. Under a rotation, the measure $\prod dx_n$ is invariant because the Jacobian is $\det O = 1$. Therefore, after rotation of the integration variables, the integral is

$$\prod_{n=1}^{N} \int dx_n e^{\lambda_n x_n^2/2} = \prod_{n=1}^{N} \sqrt{\frac{2\pi}{\lambda_n}} = (2\pi)^{N/2} (\prod_{n=1}^{N} \lambda_n)^{-1/2} \tag{107}$$

The product of eigenvalues is nothing but the determinant of the matrix $\det A = \det O^T \det D \det O = \prod_{n=1}^N \lambda_n$, and hence

$$\int \prod_{n=1}^{N} dx_n e^{-\frac{1}{2}\mathbf{x}^T A\mathbf{x}} = (2\pi)^{N/2}(\det A)^{-1/2}. \tag{108}$$

In the presence of the linear term, all we need to do is to complete the square in the exponent,

$$-\frac{1}{2}\mathbf{x}^T A\mathbf{x} - \mathbf{x}^T\mathbf{y} = -\frac{1}{2}(\mathbf{x}^T - \mathbf{y}^T A^{-1})A(\mathbf{x} - A^{-1}\mathbf{y}) + \frac{1}{2}\mathbf{y}^T A^{-1}\mathbf{y}, \tag{109}$$

and shift $\mathbf{x}$ to eliminate $A^{-1}\mathbf{y}$, and diagonalize A. This proves the identity Eq. (106).

For a $N \times N$ matrix of the form

$$K_N = \begin{pmatrix} 1 & -a & 0 & \cdots & 0 & 0 \\ -a & 1 & -a & \cdots & 0 & 0 \\ 0 & -a & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -a \\ 0 & 0 & 0 & \cdots & -a & 1 \end{pmatrix}, \tag{110}$$

one can show

$$\det K_N = \frac{\lambda_+^{N+1} - \lambda_-^{N+1}}{\lambda_+ - \lambda_-}, \qquad \lambda_\pm = \frac{1}{2}(1 \pm \sqrt{1-4a^2}). \tag{111}$$

This is done by focusing on the top two-by-two block. The determinant that picks the $(1,1)$ element "1" comes with the determinant of remaining $(N-1)\times(N-1)$ block, namely $\det K_{N-1}$. If you pick the $(1,2)$ element "$-a$", it is necessary to also pick the $(2,1)$ element which is also $-a$ and the rest comes from the remaining $(N-2)\times(N-2)$ block, namely $\det K_{N-2}$. Therefore, we find a recursion relation

$$\det K_N = \det K_{N-1} - a^2 \det K_{N-2}. \tag{112}$$

We rewrite this recursion relation as

$$\begin{pmatrix} \det K_N \\ \det K_{N-1} \end{pmatrix} = \begin{pmatrix} 1 & -a^2 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \det K_{N-1} \\ \det K_{N-2} \end{pmatrix}. \tag{113}$$

The initial conditions are $\det K_1 = 1$, $\det K_2 = 1 - a^2$. Using the recursion relation backwards, it is useful to define $\det K_0 = 1$. We diagonalize the matrix

$$\begin{pmatrix} 1 & -a^2 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} \lambda_+ & \lambda_- \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} \begin{pmatrix} 1 & -\lambda_- \\ -1 & \lambda_+ \end{pmatrix} \frac{1}{\lambda_+ - \lambda_-}. \tag{114}$$

Hence,

$$\begin{pmatrix} \det K_N \\ \det K_{N-1} \end{pmatrix} = \begin{pmatrix} \lambda_+ & \lambda_- \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}^{N-1} \begin{pmatrix} 1 & -\lambda_- \\ -1 & \lambda_+ \end{pmatrix} \frac{1}{\lambda_+ - \lambda_-} \begin{pmatrix} \det K_1 \\ \det K_0 \end{pmatrix}$$

$$
\begin{aligned}
&= \frac{1}{\lambda_+ - \lambda_-}\begin{pmatrix} \lambda_+ & \lambda_- \\ 1 & 1 \end{pmatrix}\begin{pmatrix} \lambda_+^{N-1} & 0 \\ 0 & \lambda_-^{N-1} \end{pmatrix}\begin{pmatrix} 1-\lambda_- \\ -1+\lambda_+ \end{pmatrix} \\
&= \frac{1}{\lambda_+ - \lambda_-}\begin{pmatrix} \lambda_+^{N} & \lambda_-^{N} \\ \lambda_+^{N-1} & \lambda_-^{N-1} \end{pmatrix}\begin{pmatrix} \lambda_+ \\ -\lambda_- \end{pmatrix} \\
&= \frac{1}{\lambda_+ - \lambda_-}\begin{pmatrix} \lambda_+^{N+1} - \lambda_-^{N+1} \\ \lambda_+^{N} - \lambda_-^{N} \end{pmatrix}. \qquad (115)
\end{aligned}
$$