Introduction to Path Integrals

In the coordinate basis, motion of a quantum particle is described by the propagation amplitude

$$U(t_B,\mathbf{x}_B;t_A,\mathbf{x}_A) \;=\; \langle\mathbf{x}_B|\,e^{-i(t_B-t_A)\hat{H}/\hbar}\,|\mathbf{x}_A\rangle \tag{1}$$

for moving from point $\mathbf{x}_A$ at time t_A to point $\mathbf{x}_B$ at time t_B; this amplitude is also called the *evolution kernel.* In the semi-classical regime, this kernel is given by the WKB approximation

$$U(B;A) \;\approx\; \text{prefactor}\times\exp(iS[\mathbf{x}_{\rm cl}(t)]/\hbar) \tag{2}$$

where

$$S[\mathbf{x}(t)] \;=\; \int\limits_{t_A}^{t_B} L(\mathbf{x}(t),\dot{\mathbf{x}}(t))\,dt \tag{3}$$

is the action integral of the *classical mechanics* and $\mathbf{x}_{\rm cl}(t)$ is the classical path from A to B that obeys the Euler–Lagrange equations of motion. In action terms, this path minimizes the the functional $S[\mathbf{x}(t)]$ under conditions $\mathbf{x}(t_A)=\mathbf{x}_A$ and $\mathbf{x}(t_B)=\mathbf{x}_B$. If there are several classical paths from A to B, then $S[\mathbf{x}]$ has several *local minima*, they all contribute to the evolution kernel with appropriate phases, and we get interference:

$$U(B;A) \;\approx\; \sum_{\substack{\text{classical}\\ \text{paths } i}} \text{prefactor}_i\times\exp(iS[\mathbf{x}_i(t)]/\hbar). \tag{4}$$

In the exact quantum mechanics, a sum (4) over classical paths becomes an integral over all possible path from A to B,

$$U(B;A) \;=\; \iiint\limits_{\mathbf{x}(t_A)=\mathbf{x}_A}^{\mathbf{x}(t_B)=\mathbf{x}_B} \mathcal{D}[\mathbf{x}(t)]\,\exp\bigl(iS[\mathbf{x}(t)]/\hbar\bigr). \tag{5}$$

However, unlike the sum (4), the integral here is not limited to the classical paths that obey the Euler–Lagrange equations of motion. Instead, we integrate is over *all* differentiable paths $\mathbf{x}(t)$ from A to B, and they do not obey any equations of motion except by accident. But in the semiclassical $\hbar \to 0$ limit, the contributions of most paths to the integral is washed out by interference with similar paths whose action differs by only $O(\hbar)$. The only survivors of this wash-out are the stationary "points" of the functional $S[\mathbf{x}(t)]$, which are precisely the classical paths from A to B. This is how the WKB approximation (4) — and eventually the classical mechanics — emerge in the $\hbar \to 0$ limit.

The problem with the *path integral* (5) is how to define the integration measure $\mathcal{D}[\mathbf{x}(t)]$ for paths. The basic method is to discretize the time: Slice the continuous time interval $t_A \leq t \leq t_B$ into a large but finite set of discrete times

$$(t_0, t_1, t_2, \ldots, t_{N-1}, t_N), \quad t_n = t_A + n\Delta t, \quad \Delta t = \frac{t_B - t_A}{N}, \quad t_0 = t_A, \quad t_N = t_B, \tag{6}$$

but eventually take the $N \to \infty$ limit. This gives us

$$\mathcal{D}[\mathbf{x}(t)] \stackrel{\text{def}}{=} \lim_{N\to\infty} d^3\mathbf{x}_1\, d^3\mathbf{x}_2 \cdots d^3\mathbf{x}_{N-1} \times \text{normalization\_factor}, \qquad \text{where} \quad \mathbf{x}_n \equiv \mathbf{x}(t_n). \tag{7}$$

Note that we do not integrate over the $\mathbf{x}_0 \equiv \mathbf{x}(t_A)$ and $\mathbf{x}_N \equiv \mathbf{x}(t_B)$ because they are fixed by the boundary conditions in eq. (5).

The non-obvious part of eq. (7) is the normalization_factor. We shall see later in these notes that this factor depends on N, on the net time $T = t_B - t_A$, and even on the particle's mass, and the exact formula for this factor is not easy to guess. Fortunately, there is a different version of path integration that does not suffer from such normalization factors.

Let's consider paths in the phase space $(\mathbf{x}, \mathbf{p})$ rather than just the $\mathbf{x}$-space. In other words, let's treat $\mathbf{x}(t)$ and $\mathbf{p}(t)$ as independent variables and write the action integral (3) in the Hamiltonian language

$$S[\mathbf{x}(t), \mathbf{p}(t)] = \int_A^B \bigl[\mathbf{p}(t)\cdot d\mathbf{x}(t) \;-\; H(\mathbf{x}(t), \mathbf{p}(t))\, dt\bigr] \tag{8}$$

as a functional of both $\mathbf{x}(t)$ and $\mathbf{p}(t)$. A classical path is a minimax of this functional — a (local) minimum with respect to variations of the $\mathbf{x}(t)$ but a (local) maximum with respect to variations of the $\mathbf{p}(x)$. Also, the position $\mathbf{x}(t)$ is subject to boundary conditions at the start A and finish

B, but there are no boundary conditions for the momentum $\mathbf{p}(t)$. In the quantum mechanics,

$$U(B;A) \;=\; \iiint\limits_{\mathbf{x}(t_A)=\mathbf{x}_A}^{\mathbf{x}(t_B)=\mathbf{x}_B} \mathcal{D}'[\mathbf{x}(t)] \iiint \mathcal{D}[\mathbf{p}(t)] \, \exp\bigl(iS[\mathbf{x}(t),\mathbf{p}(t)]/\hbar\bigr) \tag{9}$$

where

$$\mathcal{D}'[\mathbf{x}(t)] \times \mathcal{D}[\mathbf{p}(t)] \;=\; \lim_{N\to\infty} \prod_{n=1}^{N-1} d^3\mathbf{x}_n \times \prod_{n=1}^{N} \frac{d^3\mathbf{p}_n}{(2\pi\hbar)^3}\,. \tag{10}$$

This time, there are no funny normalization factors: all we have is the $d^3\mathbf{p}/(2\pi\hbar)^3$ for each momentum variable, and that's standard convention in quantum mechanics. Note that for a given N, we integrate over N momenta but only $N-1$ positions because of the boundary conditions on both ends; to make this difference explicit, I have marked the $\mathcal{D}'[\mathbf{x}(t)]$ with a prime.

Deriving the Phase–Space Path Integral from the Hamiltonian QM

Let's derive the phase-space path integral (9) from the conventional formulation of quantum mechanics based on the Hamiltonian operator $\hat{H}$. First, we need a couple of lemmas.

Lemma 1: *for any operator $\hat{W}$ in the Hilbert space of $\Psi(\mathbf{x})$, and for any integer $N \geq 2$,*

$$\langle\mathbf{x}_B|\,\hat{W}^N\,|\mathbf{x}_A\rangle \;=\; \int\! d^3\mathbf{x}_1 \int\! d^3\mathbf{x}_2 \cdots \int\! d^3\mathbf{x}_{N-1} \prod_{n=1}^{N} \langle\mathbf{x}_n|\,\hat{W}\,|\mathbf{x}_{n-1}\rangle \tag{11}$$

where we identify $\mathbf{x}_0 = \mathbf{x}_A$ and $\mathbf{x}_N = \mathbf{x}_B$.

Proof: In the Hilbert space in question, the definite-position states $|\mathbf{x}\rangle$ form a complete orthogonal basis, hence

$$\int\! d^3\mathbf{x}\; |\mathbf{x}\rangle\,\langle\mathbf{x}| \;=\; \hat{1}. \tag{12}$$

Therefore, for $N = 2$

$$\begin{aligned}
\langle\mathbf{x}_B=\mathbf{x}_2|\,\hat{W}^2\,|\mathbf{x}_A=\mathbf{x}_0\rangle \;&=\; \langle\mathbf{x}_2|\,\hat{W}\times\hat{1}\times\hat{W}\,|\mathbf{x}_0\rangle \\
&=\; \langle\mathbf{x}_2|\,\hat{W}\times\Bigl(\int\! d^3\mathbf{x}_1\; |\mathbf{x}_1\rangle\,\langle\mathbf{x}_1|\Bigr)\times\hat{W}\,|\mathbf{x}_0\rangle \\
&=\; \iint\! d^3\mathbf{x}_1\; \langle\mathbf{x}_2|\,\hat{W}\,|\mathbf{x}_1\rangle \times \langle\mathbf{x}_1|\,\hat{W}\,|\mathbf{x}_0\rangle\,,
\end{aligned} \tag{13}$$

exactly as in eq. (11). As to the higher $N > 2$, the proof is by induction in N. We have the induction base for $N = 2$, so let's prove that IF Lemma 1 holds for some N THEN it also holds for $N + 1$. And indeed,

$$\begin{aligned}
\langle \mathbf{x}_{N+1}| \hat{W}^{N+1} |\mathbf{x}_0\rangle &= \langle \mathbf{x}_{N+1}| \hat{W} \times \hat{1} \times \hat{W}^N |\mathbf{x}_0\rangle \\
&= \langle \mathbf{x}_{N+1}| \hat{W} \times \left(\int d^3\mathbf{x}_N \; |\mathbf{x}_N\rangle \langle \mathbf{x}_N|\right) \times \hat{W}^N |\mathbf{x}_0\rangle \\
&= \int d^2\mathbf{x}_N \; \langle \mathbf{x}_{N+1}| \hat{W} |\mathbf{x}_N\rangle \times |\mathbf{x}_N\rangle \hat{W}^N |\mathbf{x}_0\rangle \\
&\qquad \langle\!\langle \text{ by the induction assumption } \rangle\!\rangle \\
&= \int d^2\mathbf{x}_N \; \langle \mathbf{x}_{N+1}| \hat{W} |\mathbf{x}_N\rangle \times \int d^3\mathbf{x}_1 \int d^3\mathbf{x}_2 \cdots \int d^3\mathbf{x}_{N-1} \prod_{n=1}^{N} \langle \mathbf{x}_n| \hat{W} |\mathbf{x}_{n-1}\rangle \\
&= \int d^3\mathbf{x}_1 \int d^3\mathbf{x}_2 \cdots \int d^3\mathbf{x}_{N-1} \int d^3\mathbf{x}_N \prod_{n=1}^{N+1} \langle \mathbf{x}_n| \hat{W} |\mathbf{x}_{n-1}\rangle ,
\end{aligned} \tag{14}$$

exactly as in eq. (11) for $N \to N + 1$. *Quod erat demonstrandum.*

Next, **Lemma 2:** *for any two operators $\hat{C}$ and $\hat{D}$ — regardless if they commute with each other or do not commute, — in the large N limit one has*

$$\lim_{N\to\infty} \left(e^{\hat{C}/N} \times e^{\hat{D}/N}\right)^N \;=\; e^{\hat{C}+\hat{D}}. \tag{15}$$

Proof:

$$e^{\hat{C}/N} \times e^{\hat{B}/N} \;=\; 1 \;+\; \frac{\hat{C}+\hat{D}}{N} \;+\; O(1/N^2), \tag{16}$$

and

$$\lim_{N\to\infty} \left(1 \;+\; \frac{\hat{C}+\hat{D}}{N} \;+\; O(1/N^2)\right)^N \;=\; e^{\hat{C}+\hat{D}} \tag{17}$$

regardless of the details of the $O(1/N^2)$ terms.

Now let's go back to Quantum Mechanics of a particle living in 3 dimensions of space. For simplicity, assume the particle's Hamiltonian operator has form

$$\hat{H} \;=\; K(\hat{\mathbf{p}}) \;+\; V(\hat{\mathbf{x}}) \tag{18}$$

where the kinetic energy $\hat{K} \equiv K(\hat{\mathbf{p}})$ does not depend on the position $\hat{\mathbf{x}}$ and the potential energy $\hat{V} = V(\hat{\mathbf{x}})$ does not depend on the momentum $\hat{\mathbf{p}}$. Using lemma 2 for $\hat{C} = -i\hat{V}(t_B - t_A)/\hbar$ and

$\hat{D} = -i\hat{K}(t_B - t_A)/\hbar$, we have

$$\begin{aligned}
&\lim_{N\to\infty} \left(e^{-i\hat{V}\Delta t/\hbar} \times e^{-i\hat{K}\Delta t/\hbar}\right)^N \qquad \langle\!\langle \text{ where } \Delta t = (t_B - t_A)/N \,\rangle\!\rangle \\
&= \lim_{N\to\infty} \left(e^{\hat{C}/N} \times e^{\hat{D}/N}\right)^N \;=\; e^{\hat{C}+\hat{D}} \\
&= \exp\left(-i\frac{\hat{V}(t_B - t_A)}{\hbar} - i\frac{\hat{K}(t_B - t_A)}{\hbar} = -i\frac{\hat{H}(t_B - t_A)}{\hbar}\right) \\
&= \hat{U}(t_B - t_A), \quad \text{the evolution operator.}
\end{aligned} \tag{19}$$

In other words,

$$\begin{aligned}
\hat{U}(t_B - t_A) &= \lim_{N\to\infty} \hat{W}^N \\
\text{where } \hat{W} &= e^{-i\hat{V}\Delta t/\hbar} \times e^{-i\hat{K}\Delta t/\hbar}, \\
&\qquad \text{which implicitly depends on } N \text{ via } \Delta t = (t_B - t_A)/N.
\end{aligned} \tag{20}$$

Now let's apply Lemma 1 to the coordinate-space matrix elements of this evolution operator:

$$\begin{aligned}
\langle \mathbf{x}_B | \hat{U}(t_B - t_A) | \mathbf{x}_A \rangle &= \lim_{N\to\infty} \langle \mathbf{x}_B | \hat{W}^N | \mathbf{x}_A \rangle \\
&= \lim_{N\to\infty} \int d^3\mathbf{x}_1 \cdots \int d^3\mathbf{x}_{N-1} \prod_{n=1}^{N} \langle \mathbf{x}_n | \hat{W} | \mathbf{x}_{n-1} \rangle ,
\end{aligned} \tag{21}$$

where we have identified $\mathbf{x}_0 \equiv \mathbf{x}_A$ and $\mathbf{x}_N \equiv \mathbf{x}_B$. Furthermore, each Dirac bracket in this product evaluates to

$$\begin{aligned}
\langle \mathbf{x}_n | \hat{W} | \mathbf{x}_{n-1} \rangle &= \langle \mathbf{x}_n | e^{-i\hat{V}\Delta t/\hbar} \times e^{-i\hat{K}\Delta t/\hbar} | \mathbf{x}_{n-1} \rangle \\
&\quad \langle\!\langle \text{ since } \mathbf{x}_n \text{ is an eigenstate of } \hat{V} \text{ and hence of } e^{-i\hat{V}\Delta t/\hbar} \,\rangle\!\rangle \\
&= e^{-iV(\mathbf{x}_n)\Delta t/\hbar} \times \langle \mathbf{x}_n | e^{-i\hat{K}\Delta t/\hbar} | \mathbf{x}_{n-1} \rangle \\
&= e^{-iV(x_n)\Delta t/\hbar} \times \int \frac{d^3\mathbf{p}_n}{(2\pi\hbar)^3} \langle \mathbf{x}_n | \mathbf{p}_n \rangle \, e^{-iK(\mathbf{p}_n)\Delta t/\hbar} \langle \mathbf{p}_n | \mathbf{x}_{n-1} \rangle \\
&= \int \frac{d^3\mathbf{p}_n}{(2\pi\hbar)^3} e^{-iV(\mathbf{x}_n)\Delta t/\hbar} \times e^{i\mathbf{x}_n\cdot\mathbf{p}_n/\hbar} \times e^{-iK(\mathbf{p}_n)\Delta t/\hbar} \times e^{-i\mathbf{x}_{n-1}\cdot\mathbf{p}_n/\hbar} \\
&= \int \frac{d^3\mathbf{p}_n}{(2\pi\hbar)^3} \exp\left[\frac{i}{\hbar}\Big(\mathbf{p}_n\cdot(\mathbf{x}_n - \mathbf{x}_{n-1}) - V(\mathbf{x}_n)\Delta t - K(\mathbf{p}_n)\Delta t\Big)\right].
\end{aligned} \tag{22}$$

Plugging this formula back into eq. (21) and combining all the exponentials, we arrive at

$$U(B;A) \;=\; \lim_{N\to\infty}\int\!d^3\mathbf{x}_1\cdots\int\!d^3\mathbf{x}_{N-1}\int\!\frac{d^3\mathbf{p}_1}{(2\pi\hbar)^3}\cdots\int\!\frac{d^3\mathbf{p}_N}{(2\pi\hbar)^3}\,\exp\bigl(iS/\hbar\bigr), \tag{23}$$

where

$$S \;=\; \sum_{n=1}^N \mathbf{p}_n\cdot(\mathbf{x}_n-\mathbf{x}_{n-1}) \;-\; \Delta t\times\sum_{n=1}^N\Bigl(V(\mathbf{x}_n)\,+\,K(\mathbf{p}_n)\Bigr) \tag{24}$$

is the discretized action for a discretized path. Indeed, in the large N limit

$$\begin{aligned}\sum_{n=1}^N\Bigl[\mathbf{p}_n\cdot(\mathbf{x}_n-\mathbf{x}_{n-1}) \;-\; (V(\mathbf{x}_n)+K(\mathbf{p}_n))\times\Delta t\Bigr] \;\xrightarrow[N\to\infty]{}\; &\int_A^B\Bigl(\mathbf{p}(t)\cdot d\mathbf{x}(t) \;-\; H(\mathbf{x}(t),\mathbf{p}(t))\,dt\Bigr)\\ \equiv\;& S[\mathbf{x}(t),\mathbf{p}(t)].\end{aligned} \tag{25}$$

Consequently, we should interpret the product of coordinate and momentum integrals in eq. (23) as the discretized integral over the paths in the momentum space,

$$\int\!d^3\mathbf{x}_1\cdots\int\!d^3\mathbf{x}_{N-1}\int\frac{d^3\mathbf{p}_1}{(2\pi\hbar)^3}\cdots\int\frac{d^3\mathbf{p}_N}{(2\pi\hbar)^3}\;\xrightarrow[N\to\infty]{}\;\iiint\!\mathcal{D}'[\mathbf{x}(t)]\iiint\!\mathcal{D}[\mathbf{p}(t)] \tag{26}$$

in perfect agreement with eq. (10). And eq. (23) itself is the proof of the path-integral formula

$$U(B;A) \;=\; \iiint\limits_{\mathbf{x}(t_A)=\mathbf{x}_A}^{\mathbf{x}(t_B)=\mathbf{x}_B}\mathcal{D}'[\mathbf{x}(t)]\iiint\!\mathcal{D}[\mathbf{p}(t)]\,\exp\bigl(iS[\mathbf{x}(t),\mathbf{p}(t)]/\hbar\bigr). \tag{9}$$

A note on discretization. Interpreting the sum $\sum_n\mathbf{p}_n\cdot(\mathbf{x}_n-\mathbf{x}_{n-1})$ as the discretized integral $\int\mathbf{p}\cdot d\mathbf{x}$ calls for assigning the momenta $\mathbf{p}_n$ to mid-point discrete times with respect to the coordinates $\mathbf{x}_n$:

$$\mathbf{x}_n \;\equiv\; \mathbf{x}(t=t_A+n\Delta t) \quad \textbf{but} \quad \mathbf{p}_n \;\equiv\; \mathbf{p}(t=t_A+(n-\tfrac12)\Delta t). \tag{27}$$

As long as the Hamiltonian can be split into separate kinetic and potential energies according to eq. (18), such different discrete times for the $\mathbf{x}_n$ and $\mathbf{p}_n$ are OK because

$$\int\!H(\mathbf{x},\mathbf{p})\,dt \;=\; \int\!V(\mathbf{x})\,dt \;+\int\!K(\mathbf{p})\,dt \;\to\; \Delta t\sum_{n=1}^N V(\mathbf{x}_n) \;+\; \Delta t\sum_{n=1}^N K(\mathbf{p}_n) \tag{28}$$

and the details of the discretization do not matter in the large N limit. However, *when the classical Hamiltonian is more complicated than a sum of kinetic and potential energies, the path* *integral formalism suffers from the discretization ambiguity.* For example, for

$$H(\mathbf{x},\mathbf{p}) \;=\; \frac{\mathbf{p}^2}{2M(\mathbf{x})} \tag{29}$$

we could discretize the action as

$$\begin{aligned} S \;\to\;& \sum_n \mathbf{p}_n\cdot(\mathbf{x}_n-\mathbf{x}_{n-1}) \;-\; \Delta t\sum_n \frac{\mathbf{p}_n^2}{2M(\mathbf{x}_n)}\,,\\ \text{or}\to\;& \sum_n \mathbf{p}_n\cdot(\mathbf{x}_n-\mathbf{x}_{n-1}) \;-\; \Delta t\sum_n \frac{\mathbf{p}_n^2}{2M(\mathbf{x}_{n-1})}\,,\\ \text{or}\to\;& \sum_n \mathbf{p}_n\cdot(\mathbf{x}_n-\mathbf{x}_{n-1}) \;-\; \Delta t\sum_n \frac{\mathbf{p}_n^2}{M(x_n)+M(\mathbf{x}_{n-1})}\,,\\ \text{or}\to\;& \text{something else,} \end{aligned} \tag{30}$$

all these options lead to different evolution kernels, and there are no general rules how to resolve such ambiguities. Instead, *the discretization ambiguities of the path-integral formalism correspond to the operator-ordering ambiguities of the Hilbert-space formalism of quantum mechanics.* For example, given the classical Hamiltonian of the form (29), we can take the quantum Hamiltonian operators to be

$$\begin{aligned} \hat{H} \;&=\; \frac{1}{2M(\hat{\mathbf{x}})}\,\hat{\mathbf{p}}^2, \quad \text{or } \hat{H} \;=\; \hat{\mathbf{p}}^2\,\frac{1}{2M(\hat{\mathbf{x}})}\,, \quad \text{or } \hat{H} \;=\; \hat{\mathbf{p}}\,\frac{1}{2M(\hat{\mathbf{x}})}\hat{\mathbf{p}}\,, \quad \text{or}\\ \hat{H} \;&=\; \frac{1}{2M(\hat{\mathbf{x}})}\,\hat{\mathbf{p}}M(\hat{\mathbf{x}})\hat{\mathbf{p}}\,\frac{1}{M(\hat{\mathbf{x}})}\,, \quad \text{or something else.} \end{aligned} \tag{31}$$

The Lagrangian Path Integral

In this section, I shall reduce the Hamiltonian path integrals over both $\mathbf{x}(t)$ and $\mathbf{p}(t)$ to the Lagrangian path integrals over the $\mathbf{x}(t)$ alone by integrating over the paths in momentum space. *This works only when the kinetic energy is quadratic in the momentum,*

$$H(\mathbf{p},\mathbf{x}) \;=\; \frac{\mathbf{p}^2}{2M} \;+\; V(\mathbf{x}) \quad\Longrightarrow\quad \hat{H} \;=\; \frac{\hat{\mathbf{p}}^2}{2M} \;+\; V(\hat{\mathbf{x}}). \tag{32}$$

For such Hamiltonians,

$$\begin{aligned}\mathbf{p}\cdot\dot{\mathbf{x}} - H(\mathbf{p},\mathbf{x}) &= \mathbf{p}\cdot\dot{\mathbf{x}} - \frac{\mathbf{p}^2}{2M} - V(\mathbf{x}) = -\frac{(\mathbf{p}-M\dot{\mathbf{x}})^2}{2M} + \frac{M\dot{\mathbf{x}}^2}{2} - V(\mathbf{x}) \\ &= L(\dot{\mathbf{x}},\mathbf{x}) - \frac{(\mathbf{p}-M\dot{\mathbf{x}})^2}{2M}\end{aligned} \tag{33}$$

and consequently

$$S^{\mathrm{Ham}}[\mathbf{x}(t),\mathbf{p}(t)] = S^{\mathrm{Lagr}}[\mathbf{x}(t)] - \frac{1}{2M}\int dt\,(\mathbf{p}-M\dot{\mathbf{x}})^2\,. \tag{34}$$

Therefore, in the path integral formalism,

$$\begin{aligned}U(B;A) &= \iiint_A^B \mathcal{D}'[\mathbf{x}(t)] \iiint \mathcal{D}[\mathbf{p}(t)]\, \exp\left(\frac{i}{\hbar}\, S^{\mathrm{Ham}}[\mathbf{x}(t),\mathbf{p}(t)]\right) \\ &= \iiint_A^B \mathcal{D}'[\mathbf{x}(t)]\, \exp\left(\frac{i}{\hbar}\, S^{\mathrm{Lagr}}[\mathbf{x}(t)]\right) \times \iiint \mathcal{D}[\mathbf{p}(t)]\, \exp\left(\frac{-i}{2M\hbar}\int dt\,(\mathbf{p}-M\dot{\mathbf{x}})^2\right).\end{aligned} \tag{35}$$

On the second line here, we integrate over the coordinate-space paths $\mathbf{x}(t)$ after integrating over the momentum-space paths $\mathbf{p}(t)$, so as far as $\iiint \mathcal{D}[\mathbf{p}(t)]$ is concerned, we can treat the coordinate-space path $\mathbf{x}(t)$ as a constant. Also, the path-integral measure is linear so we may shift the integration variable by a constant, thus

$$\begin{aligned}\iiint \mathcal{D}[\mathbf{p}(t)]\, \exp\left(\frac{-i}{2M\hbar}\int dt\,(\mathbf{p}-M\dot{\mathbf{x}})^2\right) &= \iiint \mathcal{D}[\mathbf{p}(t)-M\dot{\mathbf{x}}(t)]\, \exp\left(\frac{-i}{2M\hbar}\int dt\,(\mathbf{p}-M\dot{\mathbf{x}})^2\right) \\ &= \iiint \mathcal{D}[\mathbf{p}'(t)]\, \exp\left(\frac{-i}{2M\hbar}\int dt\,\mathbf{p}'^2(t)\right) \\ &= \text{const.}\end{aligned} \tag{36}$$

Plugging this formula back into eq. (35) gives us the Lagrangian path integral

$$U(B;A) = \text{const} \times \iiint_{\mathbf{x}(t_A)=\mathbf{x}_A}^{\mathbf{x}(t_B)=\mathbf{x}_B} \mathcal{D}'[\mathbf{x}(t)]\, \exp\left(\frac{i}{\hbar}\, S^{\mathrm{Lagr}}[\mathbf{x}(t)]\right). \tag{37}$$

In this formalism there is no independent momentum-space path $\mathbf{p}(t)$, we integrate only over the coordinate-space path $\mathbf{x}(t)$, and the action is given by the Lagrangian formula (3). However, the price of this simplification is the un-known overall constant multiplying the path integral (37).

To calculate this constant we should first discretize the time and only then integrate out the discrete momenta $\mathbf{p}_n$. For finite N, the discretized Hamiltonian-formalism action (24) can be written as

$$\begin{aligned} S^{\text{Ham}}_{\text{discr}}(\mathbf{x}_0,\ldots,\mathbf{x}_N;\mathbf{p}_1,\ldots,\mathbf{p}_N) \;&=\; \sum_n \mathbf{p}_n\cdot(\mathbf{x}_n-\mathbf{x}_{n-1}) \;-\; \frac{\Delta t}{2M}\sum_n \mathbf{p}_n^2 \;-\; \Delta t\sum_n V(\mathbf{x}_n) \\ &=\; -\frac{\Delta t}{2M}\sum_n \left(\mathbf{p}_n \;-\; M\frac{\mathbf{x}_n-\mathbf{x}_{n-1}}{\Delta t}\right)^2 \\ &\quad+\;\frac{M}{2\Delta t}\sum_n(\mathbf{x}_n-\mathbf{x}_{n-1})^2 \;-\; \Delta t\sum_n V(\mathbf{x}_n) \\ &=\; -\frac{\Delta t}{2M}\sum_n \left(\mathbf{p}_n \;-\; M\frac{\mathbf{x}_n-\mathbf{x}_{n-1}}{\Delta t}\right)^2 \;+\; S^{\text{Lagr}}_{\text{discr}}(\mathbf{x}_0,\ldots,\mathbf{x}_N) \end{aligned} \tag{38}$$

where

$$\begin{aligned} S^{\text{Lagr}}_{\text{discr}}(\mathbf{x}_0,\ldots,\mathbf{x}_N) \;&=\; \Delta t\sum_n \left[\frac{M}{2}\left(\frac{\mathbf{x}_n-\mathbf{x}_{n-1}}{\Delta t}\right)^2 \;-\; V(\mathbf{x}_n)\right] \\ &\xrightarrow[N\to\infty]{} \int\! dt\left[\frac{M}{2}\left(\frac{d\mathbf{x}}{dt}\right)^2 \;-\; V(\mathbf{x})\right] \;=\; S^{\text{Lagr}}[\mathbf{x}(t)] \end{aligned} \tag{39}$$

is the discretized action for of the Lagrangian formalism. In light of eq. (38) we may write the discretized path integral (23) as

$$\begin{aligned} &\int\! d^3\mathbf{x}_1\cdots\!\int\! d^3\mathbf{x}_{N-1}\int\!\frac{d^3\mathbf{p}_1}{(2\pi\hbar)^3}\cdots\!\int\!\frac{d^3\mathbf{p}_N}{(2\pi\hbar)^3}\,\exp\left(\frac{i}{\hbar}\,S^{\text{Ham}}_{\text{discr}}(\mathbf{x}_0,\ldots,\mathbf{x}_N;\mathbf{p}_1,\ldots,\mathbf{p}_N)\right) \;= \\ &\qquad=\int\! d^3\mathbf{x}_1\cdots\!\int\! d^3\mathbf{x}_{N-1}\,\exp\left(\frac{i}{\hbar}\,S^{\text{Lagr}}_{\text{discr}}(\mathbf{x}_0,\ldots,\mathbf{x}_N)\right)\times \\ &\qquad\qquad\times\prod_{n=1}^{N}\int\!\frac{d^3\mathbf{p}_n}{(2\pi\hbar)^3}\,\exp\left(\frac{-i\Delta t}{2M\hbar}\left(\mathbf{p}_n \;-\; M\frac{\mathbf{x}_n-\mathbf{x}_{n-1}}{\Delta t}\right)^2\right) \end{aligned} \tag{40}$$

where we integrate over all the momenta $\mathbf{p}_n$ before we integrate over the coordinates. Consequently, in each integral on the last line of eq. (40) we may shift the integration variable from $\mathbf{p}_n$ to $\mathbf{p}'_n = \mathbf{p}_n - M\Delta\mathbf{x}_n/\Delta t$, thus

$$\begin{aligned} \int\!\frac{d^3\mathbf{p}_n}{(2\pi\hbar)^3}\,\exp\left(\frac{-i\Delta t}{2M\hbar}\left(\mathbf{p}_n \;-\; M\frac{\mathbf{x}_n-\mathbf{x}_{n-1}}{\Delta t}\right)^2\right) \;&=\; \int\!\frac{d^3\mathbf{p}'_n}{(2\pi\hbar)^3}\,\exp\left(\frac{-i\Delta t}{2M\hbar}\,\mathbf{p}'^2_n\right) \\ &=\; \left(\frac{M}{2\pi i\hbar\Delta t}\right)^{3/2}. \end{aligned} \tag{41}$$

Plugging this formula back into eq. (40), we arrive at the Lagrangian path integral

$$\begin{aligned} U(B;A) &= \lim_{N\to\infty} \left(\frac{MN}{2\pi i\hbar(t_B-t_A)}\right)^{3N/2} \times \int d^3\mathbf{x}_1 \cdots \int d^3\mathbf{x}_{N-1}\, \exp\left(\frac{i}{\hbar}\, S^{\rm Lagr}_{\rm discr}(\mathbf{x}_0,\ldots,\mathbf{x}_N)\right) \\ &\equiv \iiint\limits_{\mathbf{x}(t_A)=\mathbf{x}_A}^{\mathbf{x}(t_B)=\mathbf{x}_B} \mathcal{D}'[\mathbf{x}(t)]\, \exp\left(\frac{i}{\hbar}\, S^{\rm Lagr}[\mathbf{x}(t)]\right). \end{aligned} \tag{42}$$

Note however that in the Lagrangian formalism, the $\mathcal{D}'[\mathbf{x}(t)]$ is not just the limit of $d^{3(N-1)}\mathbf{x} \equiv d^3\mathbf{x}_1 \cdots d^3\mathbf{x}_{N-1}$ but also includes the normalization factor

$$C(N, M, t_B - t_A) \;=\; \left(\frac{MN}{2\pi i\hbar(t_B-t_A)}\right)^{3N/2}. \tag{43}$$

This normalization factor depends on N, on the net time $T = t_B - t_A$, and on the particle's mass M, but it does not depend on the potential $V(x)$ or the initial and final points x_A and x_B. Consequently, *without discretizing time, a Lagrangian path integral calculation yields the amplitude $U(B;A)$ up to an unknown overall factor $F(M,T)$.* However, we may obtain this factor by comparing with a similar path integral for a free particle: the overall $F(M,T)$ factor is the same in both cases, and the free amplitude is known to be

$$U_{\rm free}(B;A) \;=\; \left(\frac{M}{2\pi i\hbar T}\right)^{3/2} \times \exp\left(\frac{iM(x_B-x_A)^2}{2\hbar T}\right). \tag{44}$$

Alternatively, all kind of quantities can be obtained from the ratios of path integrals, and such ratios do not depend on the overall normalization of the $\mathcal{D}[x(t)]$; this is the method most commonly used in the quantum field theory.

The Partition Function

In statistical mechanics, the partition function of a quantum system is

$$Z(\beta) \;=\; \sum_{\substack{\text{energy}\\ \text{eigenvalues}}} e^{-\beta E} \times \text{multiplicity}(E) \tag{45}$$

where β is the inverse temperature, or rather

$$\beta \;=\; \frac{1}{k_B \times \text{temperature}}\,. \tag{46}$$

Formally, the sum in eq. (45) is the *trace*

$$Z(\beta) \;=\; \mathrm{tr}\big(\exp(-\beta\hat{H})\big). \tag{47}$$

Aside: the trace of a matrix is defined as the sum of its diagonal elements,

$$\mathrm{tr}\big(\|M_{ij}\|\big) \;=\; \sum_i M_{ii}\,, \tag{48}$$

and for any diagonalizable matrix, the sum of its eigenvalues always equals to its trace,

$$\sum \mathrm{eigenvalues}(M) \;=\; \mathrm{tr}(M). \tag{49}$$

For the linear operators in a Hilbert space, we have a similar definition: the trace of an operator is the sum of its diagonal matrix elements in an orthonormal basis,

$$\mathrm{tr}(\hat{A}) \;=\; \sum_n \langle n|\,\hat{A}\,|n\rangle\,. \tag{50}$$

Note: the trace of an operator does not depend on the basis we use to calculate it. In any discrete basis $|n\rangle$ we get exactly the same trace (50), an even in a continuous basis a suitable generalization of eq. (50) yields the same trace,

$$\int d^3\mathbf{x}\;\langle\mathbf{x}|\,\hat{A}\,|\mathbf{x}\rangle \;=\; \int\frac{d^3\mathbf{p}}{(2\pi\hbar)^3}\;\langle\mathbf{p}|\,\hat{A}\,|\mathbf{p}\rangle \;=\; \text{same}\;\;\mathrm{tr}(\hat{A}). \tag{51}$$

In particular, if the operator $\hat{A}$ is diagonalizable, then taking the trace in its own eigenbasis we get

$$\mathrm{tr}(\hat{A}) \;=\; \sum_n A_n \times \mathrm{multiplicity}(A_n). \tag{52}$$

Thus, the partition function (45) is indeed the trace of the operator $\exp(-\beta\hat{H})$ as in eq. (47).

The partition function is related to the evolution operator $\hat{U}(t_B - t_A)$ by analytically continuing $Z(\beta)$ to imaginary

$$\beta \;\to\; \beta' \;=\; i\frac{t_B - t_A}{\hbar}\,, \tag{53}$$

hence

$$Z(i\beta') \;=\; \operatorname{tr}\exp\left(-i\frac{(t_B - t_A)}{\hbar}\hat{H}\right) \;=\; \operatorname{tr}\hat{U}(t_B - t_A) \tag{54}$$

Equivalently, we may say that the partition function for a real β is the trace of evolution operator over an imaginary time interval

$$T \;\equiv\; (t_B - t_A) \;\to\; -i\hbar\beta \;=\; \frac{-i\hbar}{k_B \times \text{Temperature}}\,. \tag{55}$$

Evolution in the imaginary time — especially in the context of path integrals — is explained in some details in my notes from the QFT class on the Euclidean time, but for the present purposes let's go back to the real time and re-define

$$Z(T) \;=\; \operatorname{tr}\bigl(\exp(-iT\hat{H}/\hbar)\bigr) \;=\; \operatorname{tr}\bigl(\hat{U}(T,0)\bigr) \;=\; \sum_{\substack{\text{energy}\\ \text{eigenstates}}} \exp(-iTE/\hbar) \times \text{multiplicity}(E). \tag{56}$$

In the coordinate basis, the trace of the evolution operator is

$$\operatorname{tr}(\hat{U}(T,0)) \;=\; \int d^3\mathbf{x}\, \langle\mathbf{x}|\,\hat{U}(T,0)\,|\mathbf{x}\rangle \;=\; \int d^3\mathbf{x}\, U(T,\mathbf{x};0,\mathbf{x}), \tag{57}$$

where $U(T,\mathbf{x};0,\mathbf{x})$ is the evolution kernel for propagation from $\mathbf{x}$ at time $t_0 = 0$ to exactly same point $\mathbf{x}$ at a later time T. In the path integral formulation,

$$U(T,\mathbf{z};0,\mathbf{y}) \;=\; \iiint\limits_{\mathbf{x}(0)=\mathbf{y}}^{\mathbf{x}(T)=\mathbf{z}} \mathcal{D}'[\mathbf{x}(t)]e^{iS[\mathbf{x}(t)]/\hbar}, \tag{42}$$

hence

$$\begin{aligned} Z(T) \;&=\; \operatorname{tr}\bigl(\hat{U}(T,0)\bigr) \;=\; \int d^3\mathbf{y}\, U(T,\mathbf{y};0,\mathbf{y}) \\ &=\; \int d^3\mathbf{y} \iiint\limits_{\mathbf{x}(0)=\mathbf{y}}^{\mathbf{x}(T)=\mathbf{y}} \mathcal{D}'[\mathbf{x}(t)]e^{iS[\mathbf{x}(t)]/\hbar} \\ &=\; \iiint\limits_{\substack{\mathbf{x}(T)=\mathbf{x}(0)\\ \text{whatever that is}}} \mathcal{D}[\mathbf{x}(t)]e^{iS[\mathbf{x}(t)]/\hbar}. \end{aligned} \tag{58}$$

Note no prime over $\mathcal{D}$ because the paths $\mathbf{x}(t)$ are subject to only one boundary condition — periodicity in time, $\mathbf{x}(T)=\mathbf{x}(0)$.

Without discretizing time, the path integral (58) can be calculated up to an overall normalization constant. Consequently, when we extract the Hamiltonian's spectrum $\{E_n\}$ from the partition function $Z(T)$, the multiplicity of all the eigenvalues can be determined only up to some unknown overall factor.

For example, consider a harmonic oscillator with action

$$S[x(t)] \;=\; \frac{M}{2}\int\!dt\,\left(\dot{x}^2(t)\;-\;\omega^2x^2(t)\right). \tag{59}$$

This action is a quadratic functional of the $x(t)$, and it can be diagonalized via Fourier transform,

$$x(t) \;=\; \sum_{n=-\infty}^{+\infty} y_n\times e^{2\pi int/T}, \qquad y_n^* \;=\; y_{-n}\,, \tag{60}$$

$$S[x(t)] \;=\; \sum_{n=-\infty}^{+\infty} C_n y_n^* y_n\,, \tag{61}$$

$$C_n \;=\; C_{-n} \;=\; \frac{MT}{2}\times\left(\left(\frac{2\pi n}{T}\right)^2\;-\;\omega^2\right). \tag{62}$$

Note that the discrete frequencies $2\pi n/T$ of the Fourier transform (60) are completely determined by the periodicity condition $x(T)=x(0)$ and have nothing to do with the oscillator's frequency ω. By linearity of the transform (60),

$$\begin{aligned}\iiint\limits_{\text{periodic}}\mathcal{D}[x(t)] \;&=\; \prod_{n=-\infty}^{+\infty}\int\!dy_n\times\text{a constant}\text{Jacobian}\\ &=\; J\times\int\!dy_0\prod_{n=1}^{\infty}\int\!d\,\mathrm{Re}\,y_n\int\!d\,\mathrm{Im}\,y_n\,.\end{aligned} \tag{63}$$

To be precise, the Jacobian J here depends on T and on the mass M via the normalization of the Lagrangian path integral, but it does not depend on any of the y_n variables, and it does not depend on the oscillator's frequency ω.

In terms of the Fourier variables y_n, the path integral (58) becomes

$$\begin{aligned} Z &= J \times \int dy_0 \prod_{n=1}^{\infty} \int d\,\mathrm{Re}\, y_n \int d\,\mathrm{Im}\, y_n \,\exp\left(\frac{i}{\hbar} S = \frac{iC_0}{\hbar}\, y_0^2 + \sum_{n=1}^{\infty} \frac{2iC_n}{\hbar}\, |y_n|^2\right) \\ &= J \times \int dy_0 \,\exp\bigl(-(C_0/i\hbar) y_0^2\bigr) \times \prod_{i=1}^{\infty} \int d^2 y_n \,\exp\bigl(-(2C_n/i\hbar)|y_n|^2\bigr) \\ &= J \times \sqrt{\frac{\pi i\hbar}{C_0}} \times \prod_{n=1}^{\infty} \frac{\pi i\hbar}{2C_n}\,. \end{aligned} \tag{64}$$

The coefficients C_n are spelled out in eq. (62), but it's convenient to rewrite them as

$$C_0 \;=\; -\frac{M}{2T} \times (\omega T)^2, \qquad C_{n>0} \;=\; \frac{2\pi^2 M n^2}{T} \times \left(1 - \left(\frac{\omega T}{2\pi n}\right)^2\right). \tag{65}$$

Consequently, the partition function (64) becomes

$$Z(T) \;=\; J \times \frac{\sqrt{-2\pi i\hbar T/M}}{\omega T} \times \prod_{n=1}^{\infty} \frac{(i\hbar T)/(4\pi n^2 M)}{1 - \left(\frac{\omega T}{2\pi n}\right)^2} \;=\; \frac{-iF}{(\omega T) \prod_{n=1}^{\infty} \left(1 - \left(\frac{\omega T}{2\pi n}\right)^2\right)} \tag{66}$$

where

$$F \;=\; J \times \sqrt{\frac{-2\pi i\hbar T}{M}} \times \prod_{n=1}^{\infty} \frac{i\hbar T}{4\pi M n^2} \tag{67}$$

combines all the factors that do not depend on the oscillator's frequency ω. *A priori,* F could be a function of M or T, but by the non-relativistic dimensional analysis, a dimensionless function $F(M, T, \hbar)$ which does not depend on anything else must be a constant.

Unfortunately, this argument does not tell us whether this constant F is finite or infinite: it contains an infinite product over n that is badly divergent, and the Jacobian J is also badly divergent, but the two divergences might somehow cancel each other. As it happens, they do and F is finite; in fact $F = 1$, unless there are some extra degrees of freedom besides $x(t)$. But alas, showing this takes more work than I am capable of doing in one extra lecture.

If you are interested, you can read my notes on convergence issue in path integrals. Those notes where written for my QFT class last year, so the second half (about the functional integrals in Euclidean spacetime) is way beyond the scope of this quantum mechanics class; but the first half (the first 9 pages) deals with a harmonic oscillator so you should be able to follow it.

Meanwhile, let's take finite F for granted and rewrite eq. (66) as

$$Z(T) = \frac{-iF}{2\pi} \times s(x) \tag{68}$$

$$\text{for } x = \frac{\omega T}{2\pi} \tag{69}$$

$$\text{and } s = \frac{1}{x} \times \prod_{n=1}^{\infty} \left(\frac{1}{1-(x/n)^2} = \frac{n}{n-x} \times \frac{n}{n+x} \right). \tag{70}$$

and focus on the remaining infinite product in this formula. Fortunately, this product is absolutely convergent and may be evaluated just by looking at its poles and zeroes. Specifically, $s(x)$ has no zeroes, it has simple poles at all integers (positive, negative, and zero), it does not have any worse-than-pole singularities in the complex x plane, and it does not grow when $\operatorname{Im} x \to \pm\infty$. These facts completely determine the $s(x)$ function to be

$$\frac{1}{x} \times \prod_{n=1}^{\infty} \frac{1}{1-(x/n)^2} = \frac{\pi}{\sin(\pi x)} \tag{71}$$

where the normalization comes from the residue of the pole at $x = 0$. Hence, the partition function $Z(T)$ of the harmonic oscillator turns out to be

$$Z(T) = \frac{-iF/2}{\sin(\omega T/2)}. \tag{72}$$

To extract the oscillator's eigenvalues from this partition function, we expand it as

$$\begin{aligned} Z(T) &= \frac{F}{2i\sin(\omega T/2)} = \frac{F}{e^{i\omega T/2} - e^{-i\omega T/2}} \\ &= \frac{Fe^{-i\omega T/2}}{1-e^{-i\omega T}} = F \times \sum_{n=0}^{\infty} e^{-i\omega T(n+\frac{1}{2})}. \end{aligned} \tag{73}$$

Comparing this series to eq. (56), we immediately see that the eigenvalues are $E_n = \hbar\omega(n+\frac{1}{2})$ and they all have the same multiplicity F. Of course, we all new those facts back in the undergraduate school (if not earlier), but now we know how to derive them in the path-integral formalism.