PATH INTEGRAL for the HARMONIC OSCILLATOR

In class, I have showed how to use path integral formalism to calculate the partition function of a quantum system. Formally,

$$\begin{aligned} Z(T) \;&=\; \mathrm{Tr}\left[e^{-iT\hat{H}} \;=\; \hat{\mathcal{U}}(T,0)\right] \;=\; \int dx_0\, U(x_0,T;x_0,0) \\ &= \int dx_0 \iint\limits_{x(0)=x_0}^{x(T)=x_0} \mathcal{D}'[x(t)]\, e^{iS[x(t)]} \;=\; \iint\limits^{x(T)=x(0)} \mathcal{D}[x(t)]\, e^{iS[x(t)]} \end{aligned} \tag{1}$$

where

$$S[x(t)] \;=\; \int_0^T dt\, \left(\tfrac{M}{2}\dot{x}^2 \;-\; V(x)\right) \tag{2}$$

is the Lagrangian action functional. Note the boundary conditions in the last path integral in eq. (1): $x(t)$ is required to be periodic in time, $x(T) = x(0)$ but there are no separate initial or final conditions.

In class, I evaluated the path integral (1) for the harmonic oscillator, but I was deliberately ignoring all issues of convergence and hoping that all the pre-exponential factors would somehow take care of themselves. In this note I take care of all those pesky pre-exponential factors.

Actually, there are two separate convergence problems. Formally, the path integral is defined via time discretization according to

$$\iint\limits^{x(T)=x(0)} \mathcal{D}[x(t)]\, e^{iS[x(t)]} \;=\; \lim_{N\to\infty} \left(\frac{MN}{2\pi i T}\right)^{N/2} \int dx_1 \cdots \int dx_N\, \exp\left(iS^{\mathrm{discr}}(x_1, x_2, \ldots, , x_N)\right), \tag{3}$$

so there is an obvious convergence problem of the continuum-time limit of $N \to \infty$. But even for finite N there is a separate convergence problem of an N–dimensional integral of a rapidly-oscillating but unimodular function e^{iS}. In fact, for $N \geq 2$ this integral does not converge, not even conditionally, so it must be re-defined via analytic continuation.

The usual analytic continuation keeps the $x_n = x(t_n)$ real but makes the time itself imaginary, $t = -it_E$ which runs from 0 to $T = -i\beta$. In field theory, t_E is called the Euclidean time because the 4D spacetime spanned by $(x_1, x_2, x_3, x_4 = t_E)$ is Euclidean rather than Minkowski. Going from the real Minkowski time t to the real Euclidean time $t_E = it$ turns the oscillating phase function

$$\exp\left[iS^{\rm discr} \;=\; \frac{iT}{N}\sum_{n=1}^{N}\left(\frac{M}{2}\,\left(\frac{x_n - x_{n-1}}{(T/N)}\right)^2 \;-\; V(x_n)\right)\right] \tag{4}$$

of the (discretized) path integral into a real narrowly peaked function

$$\exp\left[-S_E^{\rm discr} \;=\; -\frac{\beta}{N}\sum_{n=1}^{N}\left(\frac{M}{2}\,\left(\frac{x_n - x_{n-1}}{(\beta/N)}\right)^2 \;+\; V(x_n)\right)\right]. \tag{5}$$

Note that in the Euclidean action $S_E^{\rm discr}$ both kinetic-energy and potential-energy are positive, so for each finite N we have an absolutely convergent integral

$$\left(\frac{MN}{2\pi\beta}\right)^{N/2}\int dx_1\,\cdots\int dx_N\,\exp\left(-S_E^{\rm discr}(x_1, x_2, \ldots, , x_N)\right). \tag{6}$$

This is generally true for all kinds of quantum systems and not just for the Harmonic oscillator. The continuous-Euclidean-time limit $N \to \infty$ is also well-behaved in most cases. Therefore, *the technical definition of the Minkowski-time path integral is nothing but the analytic continuation of the Euclidean-time PI back to Minkowski time* $t = it_E$.

By the way, the continuous Euclidean-time action is

$$S_E[x(t_E)] \;=\int_0^\beta dt_E\,\left[\frac{M}{2}\,\left(\frac{dx}{dt_E}\right)^2 \;+\; V(x)\right], \tag{7}$$

and the Euclidean partiction function is

$$Z_E(\beta) \;=\; {\rm Tr}\left[e^{-\beta\hat{H}}\right] \;=\; \iint_{x(\beta)=x(0)} \mathcal{D}[x(t_E)]\,e^{-S_E[x(t_E)]}, \tag{8}$$

which looks exacly like a partition function in Statistical Mechanics. Regardless of the path integral, it is well worth calculating in its own right.

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So, after all these preliminaries, let is calculate the Euclidean path integral for the harmonic oscillator. The Euclidean action of the oscillator

$$S_E \;=\int_0^\beta dt_E\,\frac{M}{2}\left[\left(\frac{dx}{dt_E}\right)^2 \;+\; \omega^2 x^2\right] \tag{9}$$

discretizes to

$$S_E^{\rm discr}(x_1,\ldots,x_N) \;=\; \frac{NM}{2\beta}\sum_{n=1}^{N}\left[(x_n-x_{n-1})^2 \;+\; \frac{\omega^2\beta^2}{N^2}x_n^2\right]. \tag{10}$$

which is a quadratic function of the integration variables $x_1,\ldots,x_N$. Consequently, the discretized path integral

$$Z(\beta,N) \;=\; \left(\frac{MN}{2\pi\beta}\right)^{N/2}\int d^N x\,\exp\bigl(-S_E^{\rm discr}(x_1,\ldots,x_N)\bigr) \tag{11}$$

is Gaussian and may be evaluated exactly. Unfortunately, the determinant of the quadratic form (10) is rather formidable, so the best way to evaluate the integral (11) is to diagonalize the action as a quadratic form.

The continuum-time Euclidean action is diagonalized via Fourier transform

$$\begin{aligned} x(t_E) \;&=\; \sum_{k=-\infty}^{+\infty}\;\beta^{-1/2}\,e^{-2\pi i k t_e/\beta}y_k\,, \\ S_E[x] \;&=\; \frac{M}{2}\sum_k\left(\omega^2 \;+\; \frac{(2\pi k)^2}{\beta^2}\right)\,|y_k|^2\text{:} \end{aligned} \tag{12}$$

note that the frequencies here are discrete because the Euclidean time is periodic; also, $y_k^* = y_{-k}$. For the discretized action (10) however, we need the discrete Fourier transform

$$x_n \;=\; \frac{1}{\sqrt{N}}\sum_{k=1}^{N} e^{-2\pi i k n/N}y_k \tag{13}$$

where the discrete frequencies k are defined modulo N, *i.e.* $y_0 \equiv y_N$, $y_{-k} \equiv y_{N-k}$, *etc.*, *etc.*; again, the frequency modes y_k are complex, but the complete set of $y_1,\ldots y_N$ is self-conjugate

as $y_k^* = y_{-k}$. The key formula of the discrete Fourier transform is

$$\sum_n e^{-2\pi i(k-\ell)n/N} \;=\; N\delta^{\mathrm{mod}\,N}(k-\ell). \tag{14}$$

Consequently,

$$\sum_n^{\mathrm{mod}\,N} x_n^2 \;=\; \sum_n^{\mathrm{mod}\,N} x_n^* x_n \;=\; \sum_k^{\mathrm{mod}\,N} y_k^* y_k \tag{15}$$

and likewise

$$\sum_n^{\mathrm{mod}\,N} (x_n - x_{n-1})^2 \;=\; \sum_k^{\mathrm{mod}\,N} \left|1 - e^{2\pi ik/N}\right|^2 y_k^* y_k \tag{16}$$

where the latter follows from

$$x_n - x_{n-1} \;=\; \sum_k^{\mathrm{mod}\,N} N^{-1/2} e^{-2\pi ikn/N} \left(1 - e^{2\pi ik/N}\right) y_k \,.$$

Thus

$$S_E^{\mathrm{discr}}[y_k] \;=\; \frac{MN}{2\beta} \sum_k^{\mathrm{mod}\,N} \left(4\sin^2\frac{\pi k}{N} \,+\, \frac{\omega^2\beta^2}{N^2}\right) |y_k|^2, \tag{17}$$

and therefore

$$\begin{aligned} Z(\beta,\omega,N) \;&=\; \left(\frac{MN}{2\pi\beta}\right)^{N/2} \times J(N) \times \int d^N y\, e^{-S_E^{\mathrm{discr}}(y)} \\ &=\; J(N) \times \prod_k^{\mathrm{mod}\,N} \left(4\sin^2\frac{\pi k}{N} \,+\, \frac{\omega^2\beta^2}{N^2}\right)^{-1/2} \end{aligned} \tag{18}$$

where $J(N)$ is the Jacobian of the discrete Fourier transform (13). To evaluate this Jacobian, we perform the Fourier transform twice:

$$y_k \;=\; \sum_m^{\mathrm{mod}\,N} N^{-1/2} e^{-2\pi imk/N} z_m, \qquad x_n \;=\; \sum_k^{\mathrm{mod}\,N} N^{-1/2} e^{-2\pi ikn/N} y_k \;=\; (-1)^n z_n \,, \tag{19}$$

which immediately tells us that

$$\left[\det \frac{\partial x_n}{\partial y_k}\right]^2 \;=\; \det \frac{\partial x_n}{\partial z_m} \;=\; \pm 1.$$

Consequently, $J = |\det(\partial x_n/\partial y_k)| = 1$ and

$$Z(\beta,\omega,N) \;=\; \prod_{k}^{\mathrm{mod}\,N} \left(4\sin^2\frac{\pi k}{N} \,+\, \frac{\omega^2\beta^2}{N^2}\right)^{-1/2}. \tag{20}$$

At this point, let me use without proof a somewhat obscure mathematical formula

$$\prod_{k=1}^{N-1} \left(2\sin\frac{\pi k}{N}\right) \;=\; N, \tag{21}$$

which allows me to re-write the discretized partition function as

$$\begin{aligned} Z(\beta,\omega,N) \;&=\; \frac{N}{\omega\beta} \times \prod_{k=1}^{N-1} \left(4\sin^2\frac{\pi k}{N} \,+\, \frac{\omega^2\beta^2}{N^2}\right)^{-1/2} \\ &=\; \frac{1}{\omega\beta} \times \prod_{k=1}^{N-1} \left(1 \,+\, \frac{\omega^2\beta^2}{4N^2\sin^2\frac{\pi k}{N}}\right)^{-1/2} \end{aligned} \tag{22}$$

To evaluate the large N limit of this partition function (physically, the continuous time limit), we approximate $4N^2\sin^2(\pi k/N) \approx (2\pi k)^2$ for $k \ll N$, and likewise $4N^2\sin^2(\pi k/N) \approx (2\pi(N-k))^2$ for $(N-k) \ll N$, while for the remaining modes $\sin^2(\pi k/N) = O(1)$ and hence

$$1 \,+\, \frac{\omega^2\beta^2}{4N^2\sin^2\frac{\pi k}{N}} \;\approx 1.$$

Consequently,

$$\begin{aligned} Z(\beta,\omega,N) \;&\xrightarrow[N\gg 1]{}\; \frac{1}{\omega\beta} \times \prod_{1\le k\ll N} \left(1 \,+\, \frac{\omega^2\beta^2}{(2\pi k)^2}\right)^{-1/2} \times \prod_{1\le (N-k)\ll N} \left(1 \,+\, \frac{\omega^2\beta^2}{(2\pi(N-k))^2}\right)^{-1/2} \\ &\xrightarrow[N\to\infty]{}\; \frac{1}{\omega\beta} \times \prod_{k=1}^{\infty} \left(1 \,+\, \frac{\omega^2\beta^2}{(2\pi k)^2}\right)^{-1}. \end{aligned} \tag{23}$$

It remains to evaluate the infinite product in the last formula. Consider $Z(\omega\beta)$ as an analytic function of a complex argument. Whenever any factor of on the right hand side has

a zero in the complex $(\omega\beta)$ plane, $Z(\omega\beta)$ has a zero and ditto for the poles. Also, the product converges, so these are the only poles and zeroes of the $Z(\omega\beta)$ The individual factors at hand are $1/(\omega\beta)$ and

$$\frac{1}{1+\frac{\omega^2\beta^2}{(2\pi k)^2}} \;=\; \frac{(2\pi k)^2}{(\omega\beta+2\pi ki)\times(\omega\beta-2\pi ki)}$$

for $k=1,2,3,\ldots$. Thus, the $Z(\omega\beta)$ function has no zeroes and it has poles at $\omega\beta=2\pi ki$ for all integers k (positive, negative and zero). In other words, it has the same poles and zeroes as the $1/\sinh(\omega\beta/2)$ function and indeed, there is a well known formula

$$\sinh(z) \;=\; z\prod_{k=1}^{+\infty}\left(1+\frac{z^2}{(\pi k)^2}\right).$$

Thus, at the end of the long path-integral calculation, we arrive at a rather simple formula

$$Z_E(\beta) \;=\; \frac{1}{2\sinh(\omega\beta/2)} \tag{24}$$

in Euclidean time, and by analytic continuation to Minkowski time

$$Z_M(T) \;=\; \frac{1}{2i\sin(\omega T/2)}\,. \tag{25}$$

Expanding the latter partition function into a sum of e^{-iET} phases, we have

$$\frac{1}{2i\sin(\omega T/2)} \;=\; \frac{e^{-i\omega T/2}}{1-e^{-i\omega T}} \;=\; \sum_{n=0}^{\infty}1\times\exp\bigl(-iT\times(n+\tfrac{1}{2})\omega\bigr), \tag{26}$$

which immediately tells us that the harmonic oscillator has non-degenerate energy spectrum with eigenvalues $E_n=(n+\frac{1}{2})\omega$. Of course, we new *that* long before this calculation, but it confirms that (properly applied) path-integral formalism does yield the correct spectrum.