

1 Imaginary Time Path Integral

For the so-called imaginary time path integral, the object of interest is

$$\exp(-\frac{\tau H}{\hbar})$$

There are two reasons for using imaginary time path integrals. One is that the application might be statistical mechanics. There one interprets τ usually denoted as β as proportional to the inverse temperature of the system ($kT = \hbar/\tau$). To obtain the partition function, it is necessary to set the final variables (coordinates) equal to the initial, and integrate over them. This takes the trace. So for a system of one particle in one dimension, we would write

$$Z = \int dx \langle x | \exp(-\frac{\tau H}{\hbar}) | x \rangle .$$

The second reason for using imaginary time path integrals is to obtain information about the ground state of a quantum system. The idea is to take large values of τ . To see what this does consider

$$\langle x | \exp(-\frac{\tau H}{\hbar}) | x' \rangle$$

Sandwich the identity in terms of energy eigenstates (assume for simplicity they are all bound states)

$$I = \sum_n |n\rangle \langle n|$$

We obtain

$$\begin{aligned} & \sum_n \langle x | n \rangle \exp(-\frac{\tau E_n}{\hbar}) \langle n | x' \rangle \\ &= \langle x | 0 \rangle \exp(-\frac{\tau E_0}{\hbar}) \langle 0 | x' \rangle + \langle x | 1 \rangle \exp(-\frac{\tau E_1}{\hbar}) \langle 1 | x' \rangle + \dots \end{aligned}$$

As τ increases more and more, the lowest energy state dominates more and more, so for large enough τ , information about the ground state is obtained.

Deriving the Path Integral The procedure for deriving the path integral expression is identical to what was done for the real time case. We split our interval τ up into N small intervals of length ϵ , with $\tau = N\epsilon$. For a large enough number of intervals or small enough ϵ , we can get a simple approximation to

$$\exp(-\frac{\epsilon H}{\hbar})$$

Writing the expression exactly first, we have

$$\langle x | \exp(-\frac{\tau H}{\hbar}) | x' \rangle$$

$$= \int_{-\infty}^{\infty} dx_1 dx_2 \dots dx_{N-1} \langle x | \exp(-\frac{\epsilon H}{\hbar}) | x_1 \rangle \langle x_1 | \exp(-\frac{\epsilon H}{\hbar}) | x_2 \rangle \dots \langle x_{N-1} | \exp(-\frac{\epsilon H}{\hbar}) | x' \rangle$$

This is simply an identity. The purpose of doing it is that for small ϵ , the individual factors become simple. Consider

$$\langle x_k | \exp(-\frac{\epsilon H}{\hbar}) | x_{k-1} \rangle .$$

For a Hamiltonian of the form

$$H = \frac{PP}{2m} + V(X),$$

we may split the kinetic energy and potential energy in the exponent making only an error of $O(\epsilon^2)$ in the exponent. We have

$$\begin{aligned} \langle x_k | \exp(-\frac{\epsilon H}{\hbar}) | x_{k-1} \rangle &\approx \langle x_k | \exp(-\frac{\epsilon PP}{2m\hbar}) \exp(-\frac{\epsilon V(X)}{\hbar}) | x_{k-1} \rangle \\ &= \langle x_k | \exp(-\frac{\epsilon PP}{2m\hbar}) | x_{k-1} \rangle \exp(-\frac{\epsilon V(x_k)}{\hbar}) \end{aligned} \quad (1)$$

Note that both terms have real quantities in the exponent. Let us concentrate on the first factor. This is just the imaginary time free propagator. We can determine it by inserting a complete set of momentum eigenstates and doing a Gaussian integral. However, there is a simpler way. Suppose we have

$$\exp(-\frac{itE}{\hbar})$$

where E is a real energy. We may convert this to

$$\exp(-\frac{\tau E}{\hbar})$$

by making the replacement $t \rightarrow -i\tau$, where τ is a real, positive number. Let us do this on our previous formula for the free propagator. We had

$$\langle x | \exp(-\frac{iP^2(t-t')}{2m\hbar}) | x' \rangle = \sqrt{\frac{m}{2\pi i\hbar(t-t')}} \exp(\frac{im(x-x')^2}{2\hbar(t-t')})$$

Taking $t - t'$ to $-i(\tau - \tau')$, we obtain

$$\langle x | \exp(-\frac{P^2(\tau - \tau')}{2m\hbar}) | x' \rangle = \sqrt{\frac{m}{2\pi\hbar(\tau - \tau')}} \exp(-\frac{m(x-x')^2}{2\hbar(\tau - \tau')})$$

Returning to Eq.(1) we now have

$$\langle x_k | \exp(-\frac{\epsilon PP}{2m\hbar}) | x_{k-1} \rangle = \sqrt{\frac{m}{2\pi\hbar\epsilon}} \exp(-\frac{m(x_k - x_{k-1})^2}{2\hbar\epsilon})$$

Putting all the terms together, we finally have

$$\langle x | \exp(-\frac{\tau H}{\hbar}) | x' \rangle = \int \sqrt{\frac{m}{2\pi\hbar\epsilon}} \prod_{j=1}^{N-1} \sqrt{\frac{m}{2\pi\hbar\epsilon}} dx_j \exp\left(-\frac{1}{\hbar} \left(\sum_k m \left(\frac{x_k - x_{k-1}}{\epsilon}\right)^2 + V(x_k)\right)\epsilon\right),$$

where the limit $N \rightarrow \infty$ is assumed. More symbolically, we may write the result as follows

$$\langle x | \exp(-\frac{\tau H}{\hbar}) | x' \rangle = \int \mathcal{D}(x(\tau_1)) \exp(-\frac{\tilde{S}}{\hbar})$$

where

$$\tilde{S} = \int_{\tau'}^{\tau} d\tau_1 \left(\frac{m}{2} \left(\frac{dx}{d\tau_1} \right)^2 + V(x(\tau_1)) \right)$$

This expression has some similarities as well as some crucial differences compared to the real time path integral. Here just as in the real time case, the integral is over all paths connecting the initial point x' to the final point x . The quantity \tilde{S} has the dimensions of action and is the integral of a Lagrangian-like quantity. The differences are (i) that the quantity in the exponent is *real*, and (ii) in the Lagrangian-like quantity whose integral gives \tilde{S} the kinetic energy term and potential energy term have the *same* sign, unlike the real time Lagrangian. Defining

$$\tilde{L} = \frac{m}{2} \left(\frac{dx}{d\tau} \right)^2 + V(x(\tau)),$$

we may write

$$\tilde{S}(x, \tau; x', \tau') = \int_{\tau'}^{\tau} d\tau_1 \tilde{L}(x(\tau_1))$$

Example of the Harmonic Oscillator Here we want

$$\langle x_a | \exp(-\frac{H\tau}{\hbar}) | x_b \rangle,$$

where $\tau = \tau_a - \tau_b$. Using the $t \rightarrow -i\tau$ prescription, we may obtain the result from the real time expression for the harmonic oscillator. We have

$$\langle x_a | \exp(-\frac{H\tau}{\hbar}) | x_b \rangle = \sqrt{\frac{m\omega}{2\pi\hbar \sinh \omega\tau}} \exp(-\frac{\tilde{S}}{\hbar})$$

where

$$\tilde{S} = \frac{m\omega}{2 \sinh \omega\tau} \left((x_a^2 + x_b^2) \cosh \omega\tau - 2x_a x_b \right)$$

Let us now take the large τ limit, using

$$\cosh \omega\tau = \frac{1}{2} \exp(\omega\tau) (1 + \exp(-2\omega\tau)) \rightarrow \frac{1}{2} \exp(\omega\tau),$$

and corresponding expressions for $\sinh \omega\tau$. Keeping only the biggest terms,

$$\tilde{S} \rightarrow \frac{m\omega}{2}(x_a^2 + x_b^2)$$

We finally have

$$\langle x_a | \exp(-\frac{H\tau}{\hbar}) | x_b \rangle \rightarrow \exp(-\frac{\omega\tau}{2}) \left(\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp(-\frac{m\omega x_a^2}{2\hbar}) \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp(-\frac{m\omega x_b^2}{2\hbar}) \right).$$

But the right hand side of this expression is just

$$\exp(-\frac{\tau E_0}{\hbar}) \langle x_a | 0 \rangle \langle 0 | x_b \rangle$$

for the harmonic oscillator. Again, we note that we can obtain the ground state energy and wave function by doing a purely classical calculation, then going to imaginary time. The terms in excited states can be obtained as well by retaining the terms $O(\exp(-2\omega\tau))$ in $\sinh(\omega\tau)$ and $\cosh \omega\tau$.

Possibility of Stationary \tilde{S} In the semiclassical approximation for the real time path integral, the answer is dominated by the action for a classical path (one satisfying $F = ma$) which goes from initial to final points. It is worth asking if and when stationary values of \tilde{S} occur. The answer is that they do occur when there is tunneling present. Penetration of a particle through a potential barrier is on the one hand a purely quantum phenomenon, but on the other hand can be treated using the imaginary time path integral. A typical example is for a so-called two well potential, for example

$$V(x) = \lambda(x^2 - x_0^2)^2 \quad (2)$$

This potential has minima at $x = \pm x_0$, and the minima are separated by a barrier of height λx_0^4 . A stationary value for \tilde{S} requires that the equation

$$m \frac{d^2 x}{d\tau^2} = \frac{\partial V(x)}{\partial x} \quad (3)$$

be satisfied. (Note the different sign of the right hand side vs the real time equations.)

Exercise 1 For the potential in Eq.(2) show that there must exist a solution of Eq.(3). This can be done using conservation of 'energy'. Computing the value of \tilde{S} for this solution can also be done in a surprisingly elementary way. Draw a picture involving the potential appropriate for Eq.(3) to get insight. (Not part of the exercise-To continue on and get the splitting between the 'even parity' and 'odd parity' levels in this potential, multiple tunnelings must be considered.)

The Partition Function Given our expression for the imaginary time propagator for the harmonic oscillator, we may get the partition function by setting $x_a = x_b$ and integrating. We have

$$\begin{aligned} Z &= \sqrt{\frac{m\omega}{2\pi\hbar \sinh \omega\tau}} \int dx_a \exp\left(-\frac{m\omega}{2\hbar \sinh \omega\tau} 2x_a^2 (\cosh \omega\tau - 1)\right) \\ &= \sqrt{\frac{1}{2(\cosh \omega\tau - 1)}} = \frac{1}{2 \sinh \omega\tau/2} = \frac{e^{-\omega\tau/2}}{1 - e^{-\omega\tau}} \\ &= e^{-\omega\tau/2} + e^{-3\omega\tau/2} + e^{-5\omega\tau/2} + \dots \end{aligned}$$

which is the correct result. Physically this is the partition function for a harmonic oscillator surrounded by a heat bath.

Use of Imaginary Time Path Integrals Imaginary time path integrals are practically useful in problems in condensed matter physics and particle physics. Numerical techniques involving random numbers (so-called Monte Carlo methods) are available for evaluating high dimensional real integrals. A typical system might be a quantum liquid, such as He^4 , or the electron 'gas'. The system is typically uniform and composed of like particles, numbering a few hundred. An example where imaginary time path integrals would not be appropriate would be a system of complicated, non-symmetric molecules. This could only be handled if the molecules were modeled in some way. Building the molecules from scratch and then having them interact involves too many energy scales to allow practical use of imaginary time path integrals. However for uniform systems of identical particles, imaginary time path integrals have become the dominant method.