11.1.1: Derivation of the Discretized Path Integral

We begin our discussion of the Feynman path integral with the canonical ensemble. The expressions for the partition function and expectation value of an observable A are, respectively

$$Q(N,V,T) = \mathrm{Tr}(e^{-\beta H})$$

$$\langle A \rangle = \frac{1}{Q}\mathrm{Tr}(Ae^{-\beta H})$$

It is clear that we need to be able to evaluate traces of the type appearing in these expressions. We have already derived expressions for these in the basis of eigenvectors of H. However, since the trace is basis independent, let us explore carrying out these traces in the coordinate basis. We will begin with the partition function and treat expectation values later.

Consider the ensemble of a one-particle system. The partition function evaluated as a trace in the coordinate basis is

$$Q(\beta) = \int dx \langle x|e^{-\beta H}|x\rangle$$

We see that the trace involves the diagonal density matrix element $\langle x|e^{-\beta H}|x\rangle$. Let us solve the more general problem of *any* density matrix element $\langle x|e^{-\beta H}|x'\rangle$.

If the Hamiltonian takes the form

$$H = \frac{P^2}{2m} + U(X) \equiv K + U$$

then we cannot evaluate the operator $exp(-\beta H)$ explicitly because the operators for kinetic (T) and potential energies (U) do not commute with each other, being, respectively, functions of momentum and position, i.e.,

$$[K,U] \neq 0$$

In this instance, we will make use of the Trotter theorem, which states that given two operators A and B, such that $[A,B] \neq 0$, then for any number λ,

$$e^{\lambda(A+B)} = \lim_{P\to\infty}\left[e^{\lambda B/2P}e^{\lambda A/P}e^{\lambda B/2P}\right]^P$$

Thus, for the Boltzmann operator,

$$e^{-\beta(K+U)} = \lim_{P\to\infty}\left[e^{-\beta U/2P}e^{-\beta K/P}e^{-\beta U/2P}\right]^P$$

and the partition function becomes

$$Q(\beta) = \lim_{P\to\infty}\int dx\langle x|\left[e^{-\beta U/2P}e^{-\beta K/P}e^{-\beta U/2P}\right]^P|x\rangle$$

Define the operator in brackets to be Ω:

$$\Omega = e^{-\beta U/2P}e^{-\beta K/P}e^{-\beta U/2P}$$

Then,

$$Q(\beta) = \lim_{P\to\infty}\int dx\langle x|\Omega^P|x\rangle$$

In between each of the P factors of Ω, the coordinate space identity operator

$$I = \int dx|x\rangle\langle x|$$

is inserted. Since there are P factors, there will be $P-1$ such insertions. the integration variables will be labeled $x_2,\ldots,x_P$. Thus, the expression for the matrix element becomes

$$\langle x|\Omega|x'\rangle = \int dx_2 \cdots dx_P \langle x|\Omega|x_2\rangle\langle x_2|\Omega|x_3\rangle\langle x_3|\ldots|x_P\rangle\langle x_P|\Omega|x'\rangle$$

$$\int dx_2 \cdots dx_P \prod_{i=1}^{P} \langle x_i|\Omega|x_{i+1}\rangle|_{x_1=x,x_{P+1}=x'}$$

The next step clearly involves evaluating the matrix elementx

$$\langle x_i|\Omega|x_{i+1}\rangle = \langle x_i|e^{-\beta U(x)/2P}e^{-\beta P^2/2mP}e^{-\beta U(X)/2P}|x_{i+1}\rangle$$

Note that in the above expression, the operators involving the potential $U(X)$ act on their eigenvectors and can thus be replaced by the corresponding eigenvalues:

$$\langle x_i|\Omega|x_{i+1}\rangle = e^{-\beta(U(x_i)+U(x_{i+1})/2}\langle x_i|e^{-\beta P^2/2mP}|x_{i+1}\rangle$$

In order to evaluate the remaining matrix element, we introduce the momentum space identity operator

$$I = \int dp|p\rangle\langle p|$$

Letting $K = \frac{P^2}{2m}$, the matrix remaining matrix element becomes

$$\begin{aligned}\langle x_i|e^{-\beta K/P}|x_{i+1}\rangle &= \int dp\langle x_i|p\rangle\langle p|e^{-\beta P^2/2mP}|x_{i+1}\rangle \\ &= \int dp\langle x_i|p\rangle\langle p|x_{i+1}\rangle e^{-\beta p^2/2mP}\end{aligned}$$

Using the fact that

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$$

it follows that

$$\langle x_i|e^{-\beta K/P}|x_{i+1}\rangle = \frac{1}{2\pi\hbar}\int dp e^{ip(x_i-x_{i+1})/\hbar}e^{-\beta p^2/2mP}$$

The remaining integral over P can be performed by completing the square, leading to the result

$$\langle x_i|e^{-\beta K/P}|x_{i+1}\rangle = \left(\frac{mP}{2\pi\beta\hbar^2}\right)^{1/2}\exp\left(-\frac{mP}{2\beta\hbar^2}(x_{i+1}-x_i)^2\right)$$

Collecting the pieces together, and introducing the $P\rightarrow\infty$ limit, we have for the density matrix

$$\langle x|e^{-\beta H}|x'\rangle = \lim_{P\rightarrow\infty}\left(\frac{mp}{2\pi\beta\hbar^2}\right)^{1/2}\int dx_2\cdots dx_P exp\left[-\sum_{i=1}^{P}\left(\frac{mP}{2\beta\hbar^2}(x_{i+1}-x_i)^2+\frac{\beta}{2P}(U(x_i)+U(x_{i+1})\right)\right]$$
$$|_{x_1=x,x_{P+1}=x'}$$

The partition function is obtained by setting $x = x'$, which is equivalent to setting $x_1 = x_{P+1}$ and integrating over x, or equivalently x_1. Thus, the expression for $Q(\beta)$ becomes

$$Q(\beta) = \lim_{P\rightarrow\infty}\left(\frac{mP}{2\pi\beta\hbar^2}\right)^{1/2}\int dx_1\cdots dx_P exp\left[-\beta\sum_{i=1}^{P}\left(\frac{1}{2}m\omega_P^2(x_{i+1}-x_i)^2+\frac{1}{P}U(x_i)\right)\right]|_{x_{P+1}=x_1}$$

where we have introduced a "frequency"

$$\omega_P = \frac{\sqrt{P}}{\beta\hbar}$$

When expressed in this way, the partition function, for a finite value of P, is *isomorphic* to a classical configuration integral for a P-particle system, that is a cyclic chain of particles, with harmonic nearest neighbor interactions and interacting with an *external*

potential $\frac{U(x)}{P}$. That is, the partition function becomes

$$Q(\beta) \sim \int dx_1 \cdots dx_P e^{-\beta U_{\text{eff}}(x_1,\ldots,x_P)}$$

where

$$U_{\text{eff}}(x_1,\ldots,x_P) = \sum_{i=1}^{P} \left[\frac{1}{2} m\omega_P^2 (x_{i+1} - x_i)^2 + \frac{1}{P} U(x_i) \right]$$

Thus, for finite (if large) P the partition function in the discretized path integral representation can be treated as any ordinary classical configuration integral. Consider the integrand of $Q(\beta)$ in the limit that all P points on the cyclic chain are at the same location x. Then the harmonic nearest neighbor coupling (which is due to the quantum kinetic energy) vanishes and $(1/P)\sum_{i=1}^{P} U(x_i) \to U(x)$, and the integrand becomes

$$e^{-\beta U(x)}$$

which is just the true classical canonical position space distribution function. Therefore, the greater the spatial spread in the cyclic chain, the more "quantum" the system is, since this indicates a greater contribution from the quantum kinetic energy. The spatially localized it is, the more the system behaves like a classical system.

It remains formally to take the limit that $P \to \infty$. There we will see an elegant formulation for the density matrix and partition function emerges.

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