

3) Path integral quantisation (from Sachs, Sen, Sexton, Modern stat. mech. CUP)

Consider the case of a quantum mechanical system confined to a one dimensional box of size L . The Hamiltonian for the system is taken to be

$$\hat{H} = T(\hat{p}) + V(\hat{q}) = \frac{1}{2m} \hat{p}^2 + V(\hat{q}).$$

\hat{H} , \hat{p} and \hat{q} are quantum mechanical operators, with \hat{p} and \hat{q} satisfying the usual commutation relation

$$[\hat{p}, \hat{q}] = -i\hbar.$$

In what follows we will work in the Heisenberg picture, where states are independent of time. Since the partition function we seek to evaluate involves a trace over all states of the system, we are at liberty to choose a basis for the operators and states which will be convenient for our purpose. Finally, we impose periodic boundary conditions on wave functions in our box. The basic idea underlying the path integral approach to quantum mechanics is to replace a calculation involving operators and states by an alternative but equivalent calculation involving just commuting numbers. The fundamental operators in our current problem are the momentum operator \hat{p} and the coordinate operator \hat{q} . We can always replace one of these operators with a commuting number if we arrange that the operator acts on one of its eigenvectors. For a particle confined to a one dimensional box of length L with periodic boundary conditions, the possible eigenvalues of the coordinate operator, \hat{q} , are the continuous numbers $q \in [-L/2, L/2]$, while the possible eigenvalues of the momentum operator, \hat{p} , are discrete, $p = 2\pi n\hbar/L$, with n an integer, as we have seen in 7. We have

$$\hat{q} |q\rangle = q |q\rangle \quad \hat{p} |p\rangle = p |p\rangle$$

with the following orthogonality and completeness relations,

$$\begin{aligned} \int dq |q\rangle \langle q| &= 1 & \langle q | q' \rangle &= \delta(q - q') \\ \frac{2\pi\hbar}{L} \sum_p |p\rangle \langle p| &= 1 & \langle p | p' \rangle &= \frac{L}{2\pi\hbar} \delta_{p,p'} \end{aligned}$$

The normalizations are chosen so that the discrete sum over p is correctly weighted to become an integral in the limit $L \rightarrow \infty$. In this same limit, the discrete δ function defining $\langle p | p' \rangle$ is also correctly weighted to become $\delta(p - p')$. The transition between complete basis vectors $|q\rangle$ and $|p\rangle$ is given by the scalar product

$$\langle q | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipq/\hbar}.$$

However, \hat{p} and \hat{q} do not commute, and it is thus not possible to have simultaneous eigenvectors and eigenvalues of \hat{p} and \hat{q} .

Consider now applying \hat{H} to a state $|p\rangle$ or a state $|q\rangle$. \hat{H} is a sum of two terms. The kinetic term depends on the operator \hat{p} only, so when applied to $|p\rangle$ this term becomes a commuting number term

$$\frac{1}{2m} \hat{p}^2 |p\rangle = \frac{1}{2m} p^2 |p\rangle$$

Similarly the potential term depends on the operator \hat{q} only, so when applied to $|q\rangle$ this term also becomes a commuting number term

$$V(\hat{q}) |q\rangle = V(q) |q\rangle$$

The commutation relation for \hat{q} and \hat{p} however implies that it is not possible to find a state which is simultaneously an eigenvector of both \hat{p} and \hat{q} . Thus although we can arrange that either the kinetic or potential term can be made into a commuting number term by acting either on $|p\rangle$ or $|q\rangle$ it is not possible that both simultaneously be made into commuting number terms.

11.1.1 Phase Space Path Integral

To address the problem just described we adopt an approach in which we act first on states $|p\rangle$ then on states $|q\rangle$. We begin by considering the operator $\exp(-\epsilon(\hat{T} + \hat{V}))$ which is the fundamental object of interest. We anticipate a little here by replacing β by ϵ which, as we shall see later, needs to be taken small. We would like now to act with this operator on either a state $|p\rangle$ or $|q\rangle$ and replace respectively either the operators \hat{p} or \hat{q} with their corresponding eigenvalues. This is not immediately possible however, since the exponential function is not a simple function as was the Hamiltonian. We can replace an operator with its eigenvalue only so long as it is the rightmost operator acting on the corresponding eigenvector. The exponential function (when expanded in power series) will give us many different orderings of operators, and only a few of the many terms which occur in this series will be in the correct rightmost positions. The simplest solution to this problem is to use the Baker-Cambel-Hausdorff formula which we generated in chapter 6 to reorder operators in the exponential. We express the result we require as a theorem

Theorem 11.1 The term $e^{-\epsilon(\hat{T} + \hat{V})}$ is given by

$$e^{-\epsilon(\hat{T} + \hat{V})} = e^{-\frac{\epsilon}{2}\hat{V}} e^{-\epsilon\hat{T}} e^{-\frac{\epsilon}{2}\hat{V}} + O(\epsilon^3)$$

Proof. ~~The proof follows along the same lines as the theorem proved in Chapter 6. We will thus not repeat it here.~~ **Exercise** \square

This theorem gives us a particular splitting of the exponential of the Hamiltonian where terms depending only on \mathbf{p} are cleanly separated from terms depending only on \mathbf{q} . The error we make in so separating terms is of $O(\epsilon^3)$. In order to make this error small we must make ϵ small. ~~Our basic goal is~~ ^{Suppose we won't} to evaluate $Z = \text{Tr} e^{-\beta\hat{H}}$. A direct splitting using the theorem is of no use since β is not necessarily small, and the error we make will also not necessarily be small. However we can proceed in steps. Define ϵ as

$$\epsilon = \frac{\beta}{n}$$

where n is an integer. Then

$$\begin{aligned} \text{Tr} e^{-\beta\hat{H}} &= \text{Tr} (e^{-\epsilon\hat{H}})^n \\ &= \text{Tr} (e^{-\frac{\epsilon}{2}\hat{V}} e^{-\epsilon\hat{T}} e^{-\frac{\epsilon}{2}\hat{V}})^n + nO(\epsilon^3) \\ &= \text{Tr} (e^{-\epsilon\hat{T}} e^{-\epsilon\hat{V}})^n + nO(\epsilon^3) \end{aligned}$$

These manipulations result in splitting the exponential $e^{-\beta\hat{H}}$ into an interleaved product of n factors $\exp(-\epsilon\hat{T})$ and n factors $\exp(-\epsilon\hat{V})$. The error we make in this process is $nO(\epsilon^3) = \beta^3 O(n^{-2})$. Since n is a free parameter in this procedure, we are free to take it as large as we like. In the limit $n \rightarrow \infty$ the error term will go to zero, and we have achieved a splitting of the original exponential operator

$$\text{Tr} e^{-\beta\hat{H}} = \lim_{n \rightarrow \infty} \text{Tr} \left(e^{-\frac{\beta}{n}\hat{T}} e^{-\frac{\beta}{n}\hat{V}} \right)^n$$

At this point we are still working with operators, but we can now insert a complete set of states between each two terms in the product and convert the problem to one with just commuting numbers. Immediately to the right of each factor $\exp(-\epsilon\hat{T})$ we insert the complete set of states

$$\frac{2\pi\hbar}{L} \sum_p |p\rangle\langle p|,$$

while immediately to the right of each factor $\exp(-\epsilon\hat{V})$ we insert the complete set of states,

$$\int_{-L/2}^{L/2} |q\rangle\langle q|.$$

Since we actually have n factors of each kind, we have to be careful to label the different insertions to the right of each different term,

$$\begin{aligned} \text{Tr } e^{-\beta \hat{H}} &= \left(\frac{2\pi\hbar}{L} \right)^n \sum_{p_1, \dots, p_{n-1}} \int_{-L/2}^{L/2} dq_1 \cdots dq_{n-1} \text{Tr} \left(e^{-\epsilon \hat{T}} | p_{n-1} \rangle \langle p_{n-1} | e^{-\epsilon \hat{V}} | q_{n-1} \rangle \right. \\ &\quad \left. \cdot \langle q_{n-1} | \cdots e^{-\epsilon \hat{T}} | p_0 \rangle \langle p_0 | e^{-\epsilon \hat{V}} | q_0 \rangle \langle q_0 | \right) \end{aligned}$$

To simplify the notation at this point, we introduce the quantity $\int [dpdq]$ as a shorthand way of indicating the integrations over complete sets of states which we have to perform,

$$\int \left[\frac{dpdq}{2\pi\hbar} \right] \equiv \prod_{k=0}^{n-1} \left(\frac{1}{L} \sum_{p_k} \int_{-L/2}^{L/2} dq_k \right)$$

The extra factor $1/2\pi\hbar$ included here for each pair p_k, q_k produces a dimensionless integration measure for that pair.

Consider now the integrand. This still involves operators, but now each operator acts on an eigenstate immediately to its right. We can therefore replace each operator with its corresponding eigenvalue.

$$\begin{aligned} \text{Tr } e^{-\beta \hat{H}} &= (2\pi\hbar)^n \int \left[\frac{dpdq}{2\pi\hbar} \right] \\ &\quad \times \text{Tr} \left(e^{-\epsilon T(p_{n-1})} | p_{n-1} \rangle \langle p_{n-1} | e^{-\epsilon V(q_{n-1})} | q_{n-1} \rangle \langle q_{n-1} | \right. \\ &\quad \left. \cdots e^{-\epsilon T(p_0)} | p_0 \rangle \langle p_0 | e^{-\epsilon V(q_0)} | q_0 \rangle \langle q_0 | \right) \end{aligned}$$

Since the exponentials in the integrand are now just numbers we can collect them into a single exponential $\exp[\sum_{k=0}^{n-1} T(p_k) + V(q_k)]$. In addition we substitute the scalar product for the brackets $\langle p_i | q_j \rangle$. This then leads to the simple expression

$$\text{Tr } e^{-\beta \hat{H}} = \int \left[\frac{dpdq}{2\pi\hbar} \right] e^{-\epsilon \sum_{k=0}^{n-1} (T(p_k) + V(q_k))} e^{\frac{i}{\hbar} p_{n-1}(q_0 - q_{n-1})} \cdots e^{\frac{i}{\hbar} p_0(q_1 - q_0)}$$

The factor $(2\pi\hbar)^n$ has cancelled with the denominator of the in the scalar product $\langle p_i | q_j \rangle$. It is convenient to introduce a new redundant variable $q_n \equiv q_0$, so that we can rewrite the above expression in the compact form

$$\text{Tr } e^{-\beta \hat{H}} = \int \left[\frac{dpdq}{2\pi\hbar} \right] e^{\sum_{k=0}^{n-1} \left(\frac{i}{\hbar} p_k (q_{k+1} - q_k) - \epsilon H(p_k, q_k) \right)}$$

In generating this form for the partition function we have fulfilled our basic aim to replace a problem involving operators and states with a problem involving commuting numbers. Our calculation of the partition function is now seen to reduce to that of evaluating a large multidimensional integral, and we find that the quantum problem we began with is now reduced to a problem in the same basic form as that of evaluating a canonical partition function for a classical system.

11.1.2 Feynman-Kac Formula

If the volume of our quantum mechanical system tends to infinity, so that the sum over the momenta p_k can be replaced by integrals, we can further simplify the above expression for the partition function. Indeed since $T(p) = \frac{1}{2m}p^2$, the p_k integral is just a Gaussian integral of the form

$$\int \frac{dx}{2\pi\hbar} e^{-\frac{a}{2}x^2 - ibx} = \frac{1}{\sqrt{2\pi\hbar^2 a}} e^{-\frac{b^2}{2a}},$$

for each p_k , with a and b real numbers and $a > 0$. This formula follows directly from the Gauss integral formula by a shift $x \rightarrow x + \frac{i}{a}b$. Thus we can perform the p_k integral explicitly for each k leading to

$$\text{Tr } e^{-\beta H} = \left(\frac{m}{2\pi\epsilon\hbar^2} \right)^{\frac{n}{2}} \int [dq] e^{-\sum_{k=0}^{n-1} \left(\frac{m}{2\epsilon\hbar^2} (q_{k+1} - q_k)^2 + \epsilon V(q_k) \right)}$$

This is the celebrated *Feynman-Kac formula* for the path integral representation of the partition sum.

To illustrate how the path integral works let us apply it to the by now familiar one-dimensional harmonic oscillator with Hamiltonian $H = \frac{1}{2m}p^2 + \frac{\kappa^2}{2}q^2$. Substituting this Hamiltonian into the phase space path integral expression for the partition sum and performing the Gaussian integral over the momenta p_k we end up with

$$\text{Tr } e^{-\beta H} = \left(\frac{m}{2\pi\epsilon\hbar^2} \right)^{\frac{n}{2}} \int [dq] e^{-\frac{m}{2} \sum_{k=0}^{n-1} \left(\frac{1}{\epsilon\hbar^2} (q_{k+1} - q_k)^2 + \epsilon\omega^2 q_k^2 \right)},$$

where $\omega^2 = \frac{\kappa^2}{m}$. Since this action is quadratic in q_k we can write it as a bilinear form in a \mathbf{R}^n . For this we introduce the vector $q = (q_0, \dots, q_{n-1})$ and a $n \times n$ matrix

$$\mathbf{M} = \frac{m}{\epsilon\hbar^2} \begin{pmatrix} a & -1 & 0 & \dots & \dots & \dots & 0 & -1 \\ -1 & a & -1 & 0 & \dots & \dots & 0 & 0 \\ 0 & -1 & a & -1 & 0 & \dots & 0 & 0 \\ \cdot & & & & & & & \\ \cdot & & & & & & & \\ 0 & 0 & \dots & \dots & 0 & -1 & a & -1 \\ -1 & 0 & \dots & \dots & \dots & 0 & -1 & a \end{pmatrix}$$

with

$$a = 2 + \epsilon^2 \hbar^2 \omega^2$$

The path integral representation of the partition sum of the one-dimensional harmonic oscillator is thus just the multidimensional Gauss integral

$$\text{Tr } e^{-\beta H} = \left(\frac{m}{2\pi\epsilon\hbar^2} \right)^{\frac{n}{2}} \int d^n q e^{-\frac{m}{2\epsilon\hbar^2} (\mathbf{q}, \mathbf{M} \mathbf{q})}$$

This integral can be evaluated along the same way as the usual Gauss integral. Here we prove a slightly more general formula which will be used in the sequel.

Result 11.2

$$\begin{aligned} I(\mathbf{M}, \mathbf{B}) &= \int_{-\infty}^{\infty} \frac{d^n x}{\sqrt{(2\pi)^n}} e^{-\frac{1}{2}(\mathbf{x}, \mathbf{M} \mathbf{x}) + (\mathbf{B}, \mathbf{x})} \\ &= (\det \mathbf{M})^{-\frac{1}{2}} e^{\frac{1}{2}(\mathbf{B}, \mathbf{M} \mathbf{B})} \end{aligned}$$

where $M_{ij} = M_{ji}$ and M_{ij} is assumed to be real.

Proof. The volume element $dx_1 \dots dx_n$ and the scalar product will remain unchanged if the vectors \mathbf{x}, \mathbf{y} undergo an orthogonal transformation $\mathbf{x} \rightarrow \mathbf{x}' = \mathbf{R} \mathbf{x}$, where the matrix \mathbf{R} satisfies the condition $\mathbf{R}^T \mathbf{R} = \mathbf{I}$ where \mathbf{R}^T is the transpose of \mathbf{R} . Since the matrix \mathbf{M} in the problem is symmetric there's a matrix \mathbf{R} such that

$\mathbf{R}^T \mathbf{M} \mathbf{R} = \mathbf{D}$ with \mathbf{D} diagonal. We suppose all the diagonal entries of \mathbf{D} are non-zero. Then,

$$I(\mathbf{M}, \mathbf{B}) = \prod_{i=1}^n \left(\int \frac{dx'_i}{\sqrt{2\pi}} e^{-\frac{\lambda_i}{2} (x'_i)^2 + B'_i x'_i} \right)$$

where $B'_i = \sum_j R_{ij} B_j$, $x'_i = \sum_j R_{ij} x_j$ and $\lambda_i = 1, \dots, n$ are the eigenvalues of \mathbf{M} . But we have already seen that

$$\int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2 \lambda + Bx} \frac{dx}{\sqrt{2\pi}} = \frac{1}{\sqrt{\lambda}} e^{\frac{1}{2} B^2 \frac{1}{\lambda}}$$

Thus the result holds with $\sqrt{\det \mathbf{M}} = \sqrt{\lambda_1 \dots \lambda_n}$ and $(\mathbf{B} \mathbf{M}^{-1} \mathbf{B}) = \sum_{i=1}^n (B_i)^2 \frac{1}{\lambda_i}$. \square

To complete our calculation we need to evaluate the determinant of M . For this we expand the determinant in the first column

$$\det M = a \det l_{n-1} - 2 \det l_{n-2} - 2,$$

where l_{n-p} is obtained from M by deleting the first p rows and columns. Let us begin by calculating $\det l_k$, $k \leq n-1$. For this we expand $\det l_k$ in the first row which leads to the recursion relation $\det l_k = a \det l_{k-1} - \det l_{k-2}$ with initial conditions $\det l_0 = 1$ and $\det l_1 = a$. This relation is solved by

$$\det l_{n-1} = \frac{\sinh\left(\frac{n\mu}{2}\right)}{\sinh\left(\frac{\mu}{2}\right)}, \quad \text{where} \quad \cosh\frac{\mu}{2} = \frac{a}{2}.$$

Substituting this result into the expression for $\det M$ and using the identity $2 \cosh a \sinh b = \cosh(a+b) + \sinh(b-a)$, we then end up with the simple result

$$\det M = 4 \sinh^2\left(\frac{n\mu}{4}\right).$$

We are now ready to evaluate the path integral completely. Performing the Gaussian integral it is not hard to see the factors of ϵ , \hbar , m and 2π all cancel out so that the final result reads simply

$$\text{Tr} e^{-\beta \hat{H}} = \frac{1}{2 \sinh\left(\frac{n\mu}{4}\right)}.$$

However, we can bring this result in a more familiar form by expressing μ in terms of a . We have

$$\cosh\frac{\mu}{2} \simeq 1 + \frac{\mu^2}{8} = 1 + \frac{\epsilon^2 \hbar^2 \omega^2}{2}$$

and thus

$$\begin{aligned} \text{Tr} e^{-\beta \hat{H}} &= \frac{1}{2 \sinh\left(\frac{\hbar\omega\beta}{2}\right)} \\ &= \frac{e^{-\frac{\hbar\omega\beta}{2}}}{1 - e^{-\hbar\omega\beta}} \\ &= \sum_{n=0}^{\infty} e^{-\hbar\omega\beta(n+\frac{1}{2})}, \end{aligned}$$

which is the correct result for the partition sum of a harmonic oscillator. This then shows that the path integral although, somewhat formal in its derivation produces the correct result.

We have seen in the example of the harmonic oscillator that although it is not clear how to define the path integral measure in the continuum limit the final result is perfectly well defined when $n \rightarrow \infty$ (or $\epsilon \rightarrow 0$). In what follows we will give a formal definition of the continuum limit. To do so we first focus on the first argument of the exponential. According to what we have just said the difference

$(q_{k+1} - q_k)/i\epsilon\hbar$ becomes to the derivative of $q(t)$ with respect to imaginary time as ϵ tends to zero ($n \rightarrow \infty$). Similarly $\epsilon\hbar \sum_k \rightarrow \int_0^{\hbar\beta} d\tau$ as $\epsilon \rightarrow 0$. Thus the path integral expression for $\text{Tr} e^{-\beta\hat{H}}$ takes the simple form

$$\text{Tr} e^{-\beta\hat{H}} = \mathcal{C} \int [dq] e^{-\frac{1}{\hbar} S_E[q(\tau)]}$$

where

$$S_E[q(\tau)] = \int_0^{\hbar\beta} \left(\frac{m}{2} \dot{q}(\tau)^2 + V(q(\tau)) \right) d\tau$$

is the action of the point particle in imaginary time $t = -i\tau$. As an illustration we can again refer to the harmonic oscillator treated above. The Lagrange function for this system is found as usual via the Legendre transform

$$\begin{aligned} \mathcal{L}(q, \dot{q}) &= H(p, q) - p\dot{q} \\ &= \frac{m}{2} (-\dot{q}^2 + \omega^2 q^2) \end{aligned}$$

Note that we have defined the action with a global minus sign compared to the usual convention. This is just for later convenience and does not affect the dynamics of the system. Next we analytically continue the time variable to the negative imaginary axis, $t = -i\tau$. Using the identity $\frac{d}{d\tau} = -i\frac{d}{dt}$, the imaginary time Lagrange function is then given by

$$\mathcal{L}(q, \dot{q}) = \frac{m}{2} (\dot{q}^2 + \omega^2 q^2),$$

where the dot now symbolizes the derivative with respect to τ which, in turn, ranges for 0 to $\hbar\beta$. In order to recover the discrete version of the path integral we discretize the parameter τ into n steps with step size $\epsilon = \frac{\hbar\beta}{n}$. The action functional $S_E[q] = \int d\tau \mathcal{L}(q, \dot{q})$ then takes the form of a discrete sum

$$S[q] = \frac{m}{2} \sum_{k=0}^{n-1} \left(\frac{1}{\epsilon\hbar^2} (q_{k+1} - q_k)^2 + \epsilon\omega^2 q_k^2 \right)$$

The constant \mathcal{C} in the continuum version of the path integral is formally infinite but can be absorbed in the measure $[dq]$ as we have seen in the example of the harmonic oscillator.

10.3 Real Time Path Integral

So far we have presented the path integral representation of the finite temperature partition sum $\text{Tr} e^{-\beta\hat{H}}$. On the other hand, in our presentation of quantum field theory we saw that the partition sum can be written as the trace of the evolution operator $U(T, 0)$ evaluated for imaginary time $T = -i\hbar\beta$. The question which we will now address is whether there is a path integral expression for this evolution operator for real T . On a formal level this is easily seen to be the case. Indeed starting from the phase space path integral expression we can implement evolution in real time simply by "rotating" ϵ by a phase $e^{i(\frac{\pi}{2}-\delta)}$, where $\delta > 0$ and small ensures the convergence of the Gaussian integrals. It is clear that the transformed operator $e^{-i\epsilon\hat{H}}$ describes an infinitesimal evolution in real time. On the other hand we can substitute $\epsilon \rightarrow i\epsilon$ in the path integral formulas. This has the effect of multiplying the exponential by an overall factor i and furthermore changes the sign of the kinetic term since this term involves two time derivatives. Thus we end up with the expression

$$\mathcal{C} \int [dq] e^{\frac{i}{\hbar} S[q(\tau)]},$$

where $S[q(\tau)] = \int dt \left(\frac{m}{2} \dot{q}^2 - V(q) \right)$ is the familiar classical action for a point particle. A new issue that arises in the real time path integral concerns the boundary conditions for $q(t)$. Indeed for a real time evolution periodic boundary conditions are not a natural choice. Rather one would fix the initial and final position of the particle, $q(0)$ and $q(T)$. The interpretation of the path integral with these boundary condition is now clear: It corresponds to matrix elements of the evolution operator $U(T, 0)$, that is

$$\langle q_f | U(T, 0) | q_i \rangle = \mathcal{C} \int_{q(0)=q_i}^{q(T)=q_f} [dq] e^{\frac{i}{\hbar} \int_0^T dt \mathcal{L}(q, \dot{q})}.$$

In order to develop a geometric interpretation of the Feynman path integral we recall that $\epsilon = \beta/n$ where n is the number of steps introduced to discretize the 1-parameter family of operator $e^{-\beta H}$. We have seen in section 9.8 that β can be interpreted as "imaginary time" through the identification $T = i\beta\hbar$. If we carry this interpretation over to our path integral expression we would identify $\epsilon\hbar$ with an infinitesimal imaginary time while q_k is interpreted as the value of $q(t)$ at $t_k = -ik\epsilon\hbar$. The above representation of the partition sum can thus be interpreted as integrating over all possible discretized periodic paths, $q(t)$, in imaginary time. This then explains the usage of word *path integral*.

