

PY 421/621 - Advanced Computing in Physics

Lecture notes.

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1 Project PI: path integral formulation of quantum mechanics.

We are interested in calculating the partition function of a quantum system (and related observables):

$$Z = \sum_n e^{-\beta E_n} \quad (1)$$

where we denoted by E_n the energy of the n^{th} quantum state and $\beta = 1/(k_T T)$.

In the basis of eigenstates of energy $|n\rangle$ the Hamiltonian operator H is diagonal with $\langle n|H|n\rangle = E_n$ and therefore

$$Z = \sum_n \langle n|e^{-\beta H}|n\rangle \quad (2)$$

[For the student not familiar with Dirac's bra ($\langle|$) and ket ($| \rangle$) notation, the expression $\langle m|A|n\rangle$ stands for the matrix element $A_{m,n}$ of an operator A in the basis formed by the vectors $|n\rangle$. If the space is finite dimensional, one can also think of bras and kets as row and column vectors, respectively.]

Equation 2 states that the partition function is the trace (i.e. the sum of the diagonal matrix elements) of the operator $\exp(-\beta H)$. But the trace of an operator is invariant in a change of basis. Thus, if we go from the basis of energy eigenstates $|n\rangle$ to the basis formed by the eigenstates of position $|x\rangle$, Z can also be written

$$Z = \int dx \langle x|e^{-\beta H}|x\rangle \quad (3)$$

where we have an integral rather than a sum because the eigenstates of position form a continuum.

[Again, for the student not familiar with Dirac's formalism, the best way to understand Eq. 3 is to imagine that we have discretized the x -axis, as we often do in computational applications. Thus we replace the continuum of values of x with the finite set $x = ia \quad i = -N/2 \dots N/2$. (Besides discretizing the axis, we also make the set of points finite by the restriction $-L \leq x \leq L$, with $L = Na/2$.) The eigenstates of energy, which in the continuum would be represented by wave functions $\psi^{(n)}(x)$, become now vectors $\psi_i^{(n)}$ and the trace of an operator A can be equivalently expressed as

$$\text{Tr}A = \sum_n A_{n,n} \quad (4)$$

with $A_{m,n} = \sum_{i,j} \psi_i^{(m)*} A_{i,j} \psi_j^{(n)}$, or

$$\text{Tr}A = \sum_i A_{i,i} \quad (5)$$

the equivalence of Eqs. 4 and 5 following from the fact that the vectors $\psi_i^{(n)}$ form an orthonormal basis. The “eigenstates” of position are now nothing else than the basis vectors

$$\hat{i} = (0, 0, \dots, 1 \text{ in the } i^{\text{th}} \text{ position}, \dots, 0) \quad (6)$$

However the continuum eigenstates of position $|x\rangle$ differ by a factor $1/\sqrt{a}$ in normalization: $|x\rangle = \hat{i}/\sqrt{a}$. With this convention, which is necessary to derive a continuum limit, Eq. 5 takes the form

$$\text{Tr}A = \sum_x a A_{x,x} \quad (7)$$

which becomes indeed $\text{Tr}A = \int dx \langle x|A|x\rangle$, as in Eq. 3, in the limits $a \rightarrow 0$ and $L \rightarrow \infty$.]

In order to calculate the trace in Eq. 3 we must make the Hamiltonian explicit. As quantum system we will consider a particle of mass m moving in one dimension with potential $V(x)$. Thus

$$H = -\frac{\hbar^2}{2m} \partial_x^2 + V(x) \quad (8)$$

We proceed now along lines similar to what we have done to solve the time dependent Schrödinger equation. We subdivide the exponential $\exp(-\beta H)$ in a product of N exponentials

$$e^{-\beta H} = e^{-H dt/\hbar} e^{-H dt/\hbar} \dots e^{-H dt/\hbar} \quad (9)$$

where, in order to push the analogy, we defined $dt = \hbar\beta/N$. (Notice that $\hbar\beta = \hbar/(k_T T)$ has indeed dimensions of time.)

Up to this point we have made no approximation. But now we approximate

$$e^{-H dt/\hbar} \simeq e^{(\hbar/2m)dt \partial_x^2} e^{-V dt/\hbar} = e^{-K dt/\hbar} e^{-V dt/\hbar} \quad (10)$$

with an error of order dt^2 .

Finally, we insert repeatedly in Eq. 3, which now reads

$$Z = \int dx \langle x | e^{-K dt/\hbar} e^{-V dt/\hbar} e^{-K dt/\hbar} e^{-V dt/\hbar} \dots e^{-K dt/\hbar} e^{-V dt/\hbar} | x \rangle, \quad (11)$$

the identity matrix in the form

$$I = \int dx |x\rangle \langle x| \quad (12)$$

Relabeling the original variable of integration $x \rightarrow x_0$ and being careful to use a different variable of integration for every insertion of the identity, we get

$$Z = \int dx_0 \int dx_1 \int dx_2 \dots \int dx_{N-1} \langle x_0 | e^{-K dt/\hbar} e^{-V dt/\hbar} | x_1 \rangle \langle x_1 | e^{-K dt/\hbar} \times \\ e^{-V dt/\hbar} | x_2 \rangle \langle x_2 | e^{-K dt/\hbar} \dots e^{-V dt/\hbar} | x_{N-1} \rangle \langle x_{N-1} | e^{-K dt/\hbar} e^{-V dt/\hbar} | x_0 \rangle \quad (13)$$

[Note that this possibly daunting expression takes a very familiar form in our discretized x -space. It reduces indeed to the standard formula for the product of matrices

$$Z = \sum_{i_0} \sum_{i_1} \sum_{i_2} \dots \sum_{i_{N-1}} \left(e^{-K dt/\hbar} e^{-V dt/\hbar} \right)_{i_0, i_1} \left(e^{-K dt/\hbar} e^{-V dt/\hbar} \right)_{i_1, i_2} \\ \dots \left(e^{-K dt/\hbar} e^{-V dt/\hbar} \right)_{i_{N-1}, i_0} \quad] \quad (14)$$

We must now calculate the matrix elements

$$f(x_i, x_{i+1}) = \langle x_i | e^{-K dt/\hbar} e^{-V dt/\hbar} | x_{i+1} \rangle \quad (15)$$

For the exponential $e^{-V(x)dt/\hbar}$ this is easy. $|x_{i+1}\rangle$ is an eigenstate of x , so we just replace the operator x in $V(x)$ with its eigenvalue x_{i+1} and take then the number $e^{-V(x_{i+1})dt/\hbar}$ out of the matrix element:

$$f(x_i, x_{i+1}) = \langle x_i | e^{-K dt/\hbar} | x_{i+1} \rangle e^{-V(x_{i+1}) dt/\hbar} \quad (16)$$

For the matrix element of the exponential of the kinetic part of the Hamiltonian, proceeding again in complete analogy with what we did for the time dependent Schrödinger equation, we perform a Fourier transform to go from x -space to momentum space. Formally, the transformation can be represented by inserting again the identity, but now in p -space

$$I = \int dp |p\rangle \langle p| \quad (17)$$

This gives

$$f(x_i, x_{i+1}) = \int dp \langle x_i | e^{-K dt/\hbar} | p \rangle \langle p | x_{i+1} \rangle e^{-V(x_{i+1}) dt/\hbar} \quad (18)$$

$|p\rangle$ is an eigenstate of K with eigenvalue $p^2/2m$ and thus

$$f(x_i, x_{i+1}) = \int dp \langle x_i | p \rangle \langle p | x_{i+1} \rangle e^{-p^2 dt/(2m\hbar)} e^{-V(x_{i+1}) dt/\hbar} \quad (19)$$

The integral can be made explicit by recalling that

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \quad (20)$$

[In the present context this is nothing else than a convenient way to express the Fourier transform.]

We thus get

$$\begin{aligned} f(x_i, x_{i+1}) &= \frac{1}{2\pi\hbar} e^{-V(x_{i+1}) dt/\hbar} \int dp e^{ip(x_i - x_{i+1})/\hbar} e^{-p^2 dt/(2m\hbar)} \\ &= \frac{1}{2\pi\hbar} e^{-V(x_{i+1}) dt/\hbar} \int dp e^{-dt[p - im(x_i - x_{i+1})/dt]^2/(2m\hbar)} e^{-m(x_i - x_{i+1})^2/(2\hbar dt)} \\ &= \sqrt{\frac{m}{2\pi\hbar dt}} e^{-m(x_i - x_{i+1})^2/(2\hbar dt)} e^{-V(x_{i+1}) dt/\hbar} \end{aligned} \quad (21)$$

We now substitute back into Eq. 13, combining all exponential factors into a single exponential. We thus obtain

$$Z = \left[\sqrt{\frac{m}{2\pi\hbar dt}} \right]^N \int dx_0 \int dx_1 \int dx_2 \dots \int dx_{N-1} \times \\ \exp \left\{ -\frac{1}{\hbar} \left[m \frac{(x_0 - x_1)^2}{2dt} + V(x_1) dt + m \frac{(x_1 - x_2)^2}{2dt} + V(x_2) dt + \right. \right. \\ \left. \left. \dots + m \frac{(x_{N-2} - x_{N-1})^2}{2dt} + V(x_{N-1}) dt + m \frac{(x_{N-1} - x_0)^2}{2dt} + V(x_0) dt \right] \right\} \quad (22)$$

This formula has a beautiful interpretation! We can consider x_0, x_1, \dots, x_{N-1} , x_0 as the coordinates along a discretized trajectory $x = x(t)$ which begins at x_0 for $t = 0$ and returns to x_0 at $t_F = \hbar\beta$. The argument in the exponential of Eq. 22 can be thought of as the discretized form of $-S_E/\hbar$, where the “Euclidean action” S_E (see later for the name) is the integral

$$S_E = \int_0^{\hbar\beta} \left\{ \frac{m}{2} \left[\frac{dx(t)}{dt} \right]^2 + V(x(t)) \right\} dt \quad (23)$$

Thus, the partition function Z can be thought of as an integral over all periodic trajectories (i.e. trajectories that begin and end at the same point) of the weight factor $\exp(-S_E/\hbar)$. This “integral” over all trajectories is called a path integral and is often denoted by the special symbol $\int \mathcal{D}x(t)$:

$$Z = \int \mathcal{D}x(t) e^{(-S_E/\hbar)} \quad (24)$$

Of course, however suggestive, Eq. 24 has only formal significance: the path integral $\int \mathcal{D}x(t)$ must be given a precise mathematical meaning and this is found precisely in Eq. 22. The path integral is the limit for $N \rightarrow \infty$ of the integral in the l.h.s. of Eq. 22 (inclusive of the measure factor $(m/2\pi\hbar dt)^{N/2}$). The reinterpretation of quantum mechanical expressions in terms of path integrals over trajectories is due to Feynman.

We should be careful not to think of the trajectories in the path integral as smooth classical trajectories. Normally, when we visualize a possible classical trajectory of a particle, we think of a function $x(t)$ with well a defined derivative $\dot{x}(t) = dx(t)/dt$. The existence of \dot{x} implies that the distance between two neighboring points along the trajectory, $x(t+dt) - x(t)$, goes to 0 like dt for $dt \rightarrow 0$ and, consequently, that $[x(t+dt) - x(t)]^2 \sim dt^2$. But for

the trajectories that give the dominant contribution to the path integral the expectation value of $[x(t + dt) - x(t)]^2$ goes to zero like dt (rather than dt^2). Thus the trajectories in the path integral are much more “rugged” than the classical trajectories we normally would think of. The numerical simulation of the path integral shows this fact very vividly. However, we can also see that $\langle [x(t + dt) - x(t)]^2 \rangle \sim dt$ in the path integral through the following, rather elaborated, analytical argument.

Let us calculate the thermodynamical average of the energy of our quantum system. It is given by

$$\langle E \rangle = \frac{1}{Z} \sum_n E_n e^{-\beta E_n} = -\frac{\partial \log(Z)}{\partial \beta} \quad (25)$$

Let us calculate the derivative of $\log(Z)$ using the expression for Z given by Eq. 22. The dependence of Z on β in that equation occurs only through the dependence of its r.h.s. on dt and the relation $dt = \hbar\beta/N$. Thus

$$-\frac{\partial \log(Z)}{\partial \beta} = -\frac{\hbar}{N} \frac{\partial \log(Z)}{\partial dt} \quad (26)$$

(in this equation dt should be thought of as a finite, albeit small variable, and not as a differential). Equation 22 gives

$$\log Z = -\frac{N}{2} \log(dt) + \log \left(\int dx_0 \dots \int dx_{N-1} e^{-S_E/\hbar} \right) + c \quad (27)$$

where we denoted by c terms which do not depend on dt . We have

$$S_E = \sum_i \frac{m(x_{i+1} - x_i)^2}{2dt} + \sum_i V(x_i) dt \quad (28)$$

and thus

$$\frac{\partial S_E}{\partial dt} = -\sum_i \frac{m(x_{i+1} - x_i)^2}{2dt^2} + \sum_i V(x_i) \quad (29)$$

From Eqs. 26, 27 and 29 we conclude

$$\langle E \rangle = \frac{\hbar}{2dt} + \frac{\int dx_0 \dots \int dx_{N-1} \left(-\sum_i \frac{m(x_{i+1} - x_i)^2}{2dt^2} + \sum_i V(x_i) \right) e^{-S_E/\hbar}}{N \int dx_0 \dots \int dx_{N-1} e^{-S_E/\hbar}} \quad (30)$$

Symmetry implies that the averages

$$\langle (x_{i+1} - x_i)^2 \rangle = \frac{\int dx_0 \dots \int dx_{N-1} (x_{i+1} - x_i)^2 e^{-S_E/\hbar}}{\int dx_0 \dots \int dx_{N-1} e^{-S_E/\hbar}} \quad (31)$$

are all equal. Similarly the averages

$$\langle V(x_i) \rangle = \frac{\int dx_0 \dots \int dx_{N-1} V(x_i) e^{-S_E/\hbar}}{\int dx_0 \dots \int dx_{N-1} e^{-S_E/\hbar}} \quad (32)$$

cannot depend on the index i . Thus

$$\langle E \rangle = \frac{\hbar}{2dt} - \frac{m}{2dt^2} \langle (x_{i+1} - x_i)^2 \rangle + \langle V(x_i) \rangle \quad (33)$$

where the value of i is arbitrary. This is a very interesting formula. Its most striking feature is the factor of $1/dt$ in the first term, which diverges as $dt \rightarrow 0$. Since Eq. 33 must reduce to the exact value of $\langle E \rangle$ in the limit $N \rightarrow \infty$, $dt \rightarrow 0$, that divergence must be canceled by a compensating divergence in another term. But the expectation value of the potential energy $V(x_i)$ in general will not diverge for $dt \rightarrow 0$ (indeed, V could be bounded below and above, or even 0, and the argument would still apply). Thus the divergence must be canceled by the term $m \langle (x_{i+1} - x_i)^2 \rangle / 2dt^2$. But this requires $\langle (x_{i+1} - x_i) \rangle \sim dt$ or $\langle [x(t+dt) - x(t)]^2 \rangle \sim dt$, precisely as we stated above.

Another inference from Eq. 33 is a caution against using “intuitive” arguments too lightly, when dealing with path integrals. While the path integral formulation does provide a beautiful intuitive picture of quantum mechanics in terms of sums over trajectories, the intuition should be guided by a deep understanding of the underlying mathematics. In the specific case of $\langle E \rangle$, a simplistic intuition could lead us to conclude that $\langle E \rangle$ should be given by the sum of the expectation values of $m(x_{i+1} - x_i)^2 / 2dt^2$ and $V(x_i)$, since the two terms have an obvious interpretation of kinetic energy and potential energy along the trajectory. But, as Eq. 33 shows, that conclusion would be quite wrong. Indeed, it would lead to a divergent $\langle E \rangle$ in the limit $dt \rightarrow 0$, where, to the contrary, the expression ought to become exact. Apart from the route we followed above, the correct way to derive the expectation value of E as well as of other observables is to insert them in the original expression for the partition function, for example

$$\langle E \rangle = \frac{1}{Z} \text{Tr} (H e^{-\beta H}) \quad (34)$$

Casting $\text{Tr}(He^{-\beta H})$ into the form of a path integral, following the line we used for Z , would produce then the same expression for $\langle E \rangle$ as in Eq. 33 or a mathematically equivalent expression.

The path integral formulation can be applied also to the evolution of a quantum mechanical system in time. Indeed, this is the context in which it was originally developed by Feynman. The time evolution is given by the unitary operator

$$U(t) = e^{-\imath Ht/\hbar} \quad (35)$$

The matrix elements of U in configuration space

$$G(x, x', t) = \langle x|U(t)|x' \rangle = \langle x|e^{-\imath Ht/\hbar}|x' \rangle \quad (36)$$

constitute the Green's function for the time dependent Schrödinger equation. $G(x, x', t)$ allows us to express $\psi(x, t)$ as function of $\psi(x, 0)$ by

$$\psi(x, t) = \int G(x, x', t) \psi(x', 0) dx' \quad (37)$$

The matrix elements $\langle x|e^{-\imath Ht/\hbar}|x' \rangle$ can clearly be calculated following the same procedure we used earlier to calculate $\langle x_0|e^{-Ht/\hbar}|x_0 \rangle$ (with $t = \hbar\beta$). The only modifications are that our former dt should now be replaced with $\imath dt$, that the end coordinates $x_0 = x$ and $x_N = x'$ are now not identical and that there is now no integration over x_0 or x_N . With this in mind, it is straightforward to derive

$$\begin{aligned} G(x, x', t) = & \left[\sqrt{\frac{m}{2\pi\hbar\imath dt}} \right]^N \int dx_1 \int dx_2 \dots \int dx_{N-1} \times \\ & \exp \left\{ \frac{\imath}{\hbar} \left[m \frac{(x_0 - x_1)^2}{2dt} - V(x_1) dt + m \frac{(x_1 - x_2)^2}{2dt} - V(x_2) dt + \right. \right. \\ & \left. \left. \dots + m \frac{(x_{N-2} - x_{N-1})^2}{2dt} - V(x_{N-1}) dt + m \frac{(x_{N-1} - x_N)^2}{2dt} - V(x_N) dt \right] \right\} \quad (38) \end{aligned}$$

[A slightly more accurate expression is obtained by using the symmetric approximation $\exp(-\imath H dt/\hbar) = \exp(-\imath V dt/2\hbar) \exp(-\imath K dt/\hbar) \exp(-\imath V dt/2\hbar) \times [1 + O(dt^3)]$. This gives

$$\begin{aligned} G(x, x', t) = & \left[\sqrt{\frac{m}{2\pi\hbar\imath dt}} \right]^N \int dx_1 \int dx_2 \dots \int dx_{N-1} \times \\ & \exp \left\{ \frac{\imath}{\hbar} \left[-\frac{V(x_0) dt}{2} + m \frac{(x_0 - x_1)^2}{2dt} - V(x_1) dt + \dots \right. \right. \\ & \left. \left. + m \frac{(x_{N-2} - x_{N-1})^2}{2dt} - V(x_{N-1}) dt + m \frac{(x_{N-1} - x_N)^2}{2dt} - \frac{V(x_N) dt}{2} \right] \right\} \quad (39) \end{aligned}$$

Now the expression in the exponent is $\imath S/\hbar$ where S is the discretized form of the ordinary action

$$S(x(t), t) = \int \left[\frac{m}{2} \dot{x}(t)^2 - V(x(t)) \right] dt \quad (40)$$

calculated along the trajectory $x = x(t)$. We are now in the position of explaining the term “Euclidean action” encountered above. The analytic continuation $dt \rightarrow -\imath dt$ that converts the formula of Eq. 38 (for quantum mechanical evolution in ordinary time) into the formula of Eq. 22 (for the calculation of the quantum mechanical partition function) is tantamount to changing the metric of ordinary space-time $dx^2 - dt^2$ (with units where the speed of light $c = 1$) to the Euclidean metric $dx^2 + dt^2$. Correspondingly, in the action, the relative negative sign between the kinetic and potential energy terms becomes positive, and the action in Euclidean space-time takes the form of Eq. 23.

Formally, Eq. 38 can be cast in the form

$$G(x, x', t) = \int \mathcal{D}x(t) e^{\imath S/\hbar} \quad (41)$$

where the integral is extended over all trajectories that take the system from x to x' in time t . Equation 41 has again a beautiful interpretation. It states that the Green’s function, or amplitude, for the propagation of a quantum mechanical particle from x to x' can be obtained by averaging over all possible trajectories the phase factor $\exp \imath S/\hbar$, where S is the classical action calculated along the trajectory. The classical limit of quantum mechanics also follows immediately from this formulation. Since one averages phase factors, in general there will be destructive interference, unless a whole bundle of trajectories have phases which add up coherently. This destructive interference will be the more pronounced the smaller \hbar is, since the variation of the phase for a definite change of trajectory is inversely proportional to \hbar . When $\hbar \rightarrow 0$, the only trajectories that will contribute to the amplitude will be those where an infinitesimal change of trajectory will produce no change of action, namely the trajectories that satisfy

$$\frac{\delta S[x(t)]}{\delta x(t)} = 0 \quad (42)$$

But this is precisely the principle of stationary action, which in classical mechanics determines the trajectories followed by the system in its classical evolution.