Path Integrals

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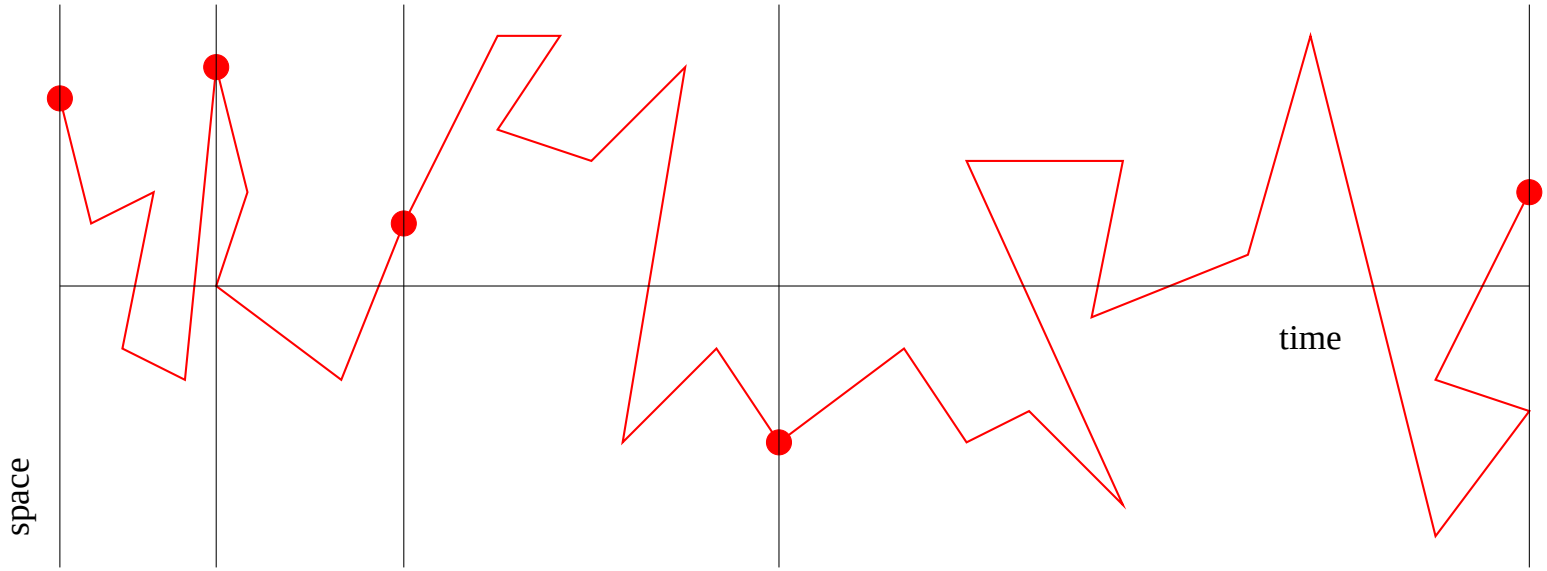
Post-colonial quantum mechanics

$$\langle x_i, t_i | x_f, t_f \rangle = \sum_{x_m} \langle x_i, t_i | x_m, t_m \rangle \langle x_m, t_m | x_f, t_f \rangle$$



Sum over all paths: path integral

Dirac (1933), Feynman (1948)

The unitary operator

When the Hamiltonian of a quantum system is H, then time evolution of any quantum state in the Hilbert space on which H acts is

$$|\psi(t)\rangle = U(t, t_0)\,|\psi(t_0)\rangle\,, \qquad U(t, t_0) = \exp[-iH(t - t_0)].$$

We have assumed, as everywhere in this course, that H is time-independent.
The evolution operator U is unitary, since H is Hermitean. Also, the evolution operators form a group, since

$$U(t, t) = 1, \quad U(t, t'') = U(t, t')U(t', t''), \quad U(t, t')^{-1} = U(t', t),$$

and multiplication of operators is associative. The generator of infinitesimal time evolution is H. Clearly U is block diagonal in the eigenbasis of H.

Slicing the time interval

Using the group property, we can write

$$U(t_f, t_i) = \prod_{i=0}^{N-1} U(t_i + \delta t, t_i), \qquad \text{where} \qquad \delta t = (t_f - t_i)/N.$$

If the state at time t_m is $|\psi_m\rangle$, then

$$\langle\psi(t_i)|\, U(t_f, t_i)\, |\psi(t_i)\rangle = \sum_{\{\psi_m\}} \prod_{m=0}^{N-1} \langle\psi_m|\, U(t_m + \delta t, t_m)\, |\psi_m\rangle\,,$$

where $|\psi(t_f)\rangle = |\psi_{N+1}\rangle$ and $|\psi(t_i)\rangle = |\psi_0\rangle$. The sum over all intermediate states is called a path integral.
If the states $|\psi_m\rangle$ are eigenstates of the Hamiltonian then the matrix elements on the right are pure phases. However, if we do not know the eigenstates of the Hamiltonian, then the path integral is non-trivial.

A two-state path integral

For a two-state system take the Hamiltonian to be $H = \sum_i h_i \sigma_i$ with all four h_i real. Then the infinitesimal evolution operator is

$$U(\delta t) = 1 - iH\delta t + \mathcal{O}(\delta t^2) = \begin{pmatrix} 1 - i\delta t(h_0 + h_3) & -i\delta t(h_1 + ih_2) \\ -i\delta t(h_1 - ih_2) & 1 - i\delta t(h_0 - h_3) \end{pmatrix}.$$

Each of these elements is a phase factor associated with the path taken during the interval δt. A path contributing to the transition matrix element $\langle \alpha_0 | U(t_N, t_0) | \alpha_N \rangle$ is the sequence of intermediate states $|\alpha(t_i)\rangle$. The contribution of each path to the transition matrix element is

$$U_{\alpha_N, \alpha_0} = \sum_{\alpha_{N-1}, \cdots, \alpha_1} U_{\alpha_N \alpha_{N-1}} U_{\alpha_{N-1} \alpha_{N-2}} \cdots U_{\alpha_2 \alpha_1} U_{\alpha_1 \alpha_0}.$$

The sum over paths is a sum over intermediate states. This is exactly the same as doing the matrix multiplication needed to get the transition amplitude.

A different take on a two-state path integral

Another way of doing the two-state path integral is to introduce the unitary matrix V which diagonalizes the Hamiltonian, *i.e.*, $V^\dagger H V$ is diagonal. Then

$$U(\delta t) = V^\dagger \begin{pmatrix} e^{-iE_0\delta t} & 0 \\ 0 & e^{-iE_1\delta t} \end{pmatrix} V.$$

The sum over intermediate states is then diagonal, and the Vs act only on the initial and final states to give

$$\langle \alpha_N | \, U(t_N, t_0) \, | \alpha_0 \rangle = (\alpha_N^0)^* \alpha_0^0 e^{-iE_0 T} + (\alpha_N^1)^* \alpha_0^1 e^{-iE_1 T},$$

where $T = t_N - t_0$; therefore the path integral can be used to get the energy levels of the system. This is best done in Euclidean time, *i.e.*changing $t \to it$. Then the above expression becomes

$$\langle \alpha_N | \, U(t_N, t_0) \, | \alpha_0 \rangle \to (\alpha_N^0)^* \alpha_0^0 e^{-E_0 T},$$

when $E_1 > E_0$ and $T(E_1 - E_0) \gg 1$. This gives the lowest eigenvalue of H. The Euclidean U is the transfer matrix.

Using the path integral to compute energies

1. Choose δt and N ($T = N\delta t$). Fix $|\alpha_0\rangle$ and $|\alpha_N\rangle$.
2. Choose a random path in Hilbert space, *i.e.*, a random sequence of N quantum states $|\alpha_i\rangle$ for $1 \leq i < N$.
3. Compute the product of Euclidean factors $\delta_{\alpha_i,\alpha_{i+1}} - \delta t H_{\alpha_i,\alpha_{i+1}}$ along the path. Call this A.
4. Repeat the above two steps many times and find $\langle A \rangle$.
5. Increase N and repeat the above three steps until the exponential behaviour manifests itself.
6. The exponential slope gives the lowest energy eigenvalue, E_0.

This method is not the most efficient technique in quantum mechanics on finite dimensional Hilbert spaces (matrix multiplication is cheaper). However, for infinite dimensional Hilbert spaces, and in quantum field theory, often this is the best possible method. This is the foundational technique of quantum field theory.

Problem 16.1: Feynman diagrams

Take the Hamiltonian $H = H_0 + \lambda H_1$, and assume that the eigenvalues and eigenvectors of H_0 are non-degenerate and known. Now examine the evolution operator $U(t) = \exp(-iHt)$ in the eigenbasis of H_0.

For infinitesimal t, examine the relation between the unitary evolution operator and the perturbation of the wavefunction. Develop a diagrammatic expression in terms of the eigenstates of H_0 and this perturbation.

String together these infinitesimal operators to construct the evolution operator through an arbitrary time interval. Consider these matrix multiplications in terms of the diagrams you have developed.

Using position eigenstates

Choose to work with the position basis states $|x_i\rangle$. Then the sum over intermediate states becomes integrals over the positions—

$$\langle x(t_{fin})|\, U(t_{fin}, t_{in})\, |x(t_{in})\rangle = \int \left\{ \prod_{i=1}^{N-1} dx_i\, \langle x_{i+1}|\, \mathrm{e}^{-iT\delta t}\, |x_i\rangle\, \mathrm{e}^{-iV(x)\delta t} \right\}.$$

We have used the decomposition, $H = T + V$. One way to evaluate the matrix element involving the kinetic energy is to insert complete sets of eigenvectors of momentum. Then

$$\langle x|'\, \mathrm{e}^{-iT\delta t}\, |x\rangle = \int dp \mathrm{e}^{-\frac{i\delta t}{2m}\left(p^2 - 2mp\frac{x-x'}{\delta t}\right)} \propto \exp\left[\frac{im\delta t}{2}\left(\frac{\delta x}{\delta t}\right)^2\right].$$

The Gaussian integral can be performed after completing squares and shifting. The only dependence on x and x' is in the factor shown.

Expression in terms of the action

Putting all this together, the transition matrix element becomes

$$\int \left\{ \prod_{i=1}^{N-1} dx_i \right\} \prod_{i=0}^{N-1} \exp \left[i\delta t \left\{ \frac{m}{2} \left(\frac{dx_i}{dt} \right)^2 - V(x_i) \right\} \right].$$

The expression within braces is the Lagrangian of the system. The product of exponentials is just the Riemann integral when the time step is taken to zero,

$$\prod_{i=0}^{N-1} \exp\left[i\delta t L(x_i) \right] \longrightarrow \exp\left\{ i \int dt L[x(t)] \right\} = \mathrm{e}^{iS[x]},$$

where the action is defined to be $S[x] = \int dt L[x(t)]$. Feynman's path integral is then

$$Z = \langle x(t_i) | \, U(t_f, t_i) \, | x(t_i) \rangle = \int \mathcal{D}x \mathrm{e}^{iS[x]},$$

where the paths join the given points $x(t_i)$ and $x(t_f)$.

Classical from quantum

... if we move the path ... by a small amount δx, *small on the classical scale*, the change in S is likewise small on the classical scale, but not when measured in the tiny unit $\hbar$. These small changes in path will, generally, make enormous changes in phase, and our cosine or sine will oscillate exceedingly rapidly between plus and minus values. The total contribution will then add to zero; for if one makes a positive contribution, another infinitesimally close (on a classical scale) makes an equal negative contribution, so that no net contribution arises.
... But for the special path $\overline{x}$, for which S is an extremum, a small change in path produces, in the first order at least, no change in S. All the contributions from the paths in this region are nearly in phase, at phase S_{cl}, and do not cancel out. Therefore, only for paths in the vicinity of $\overline{x}$ can be get important contributions, and in the classical limit we need only consider this particular trajectory as being of importance.
(from "Quantum mechanics and Path Integrals", (1965) by R. P. Feynman and A. R. Hibbs, p 30)

Problem 16.2: Evaluating a path integral

1. Evaluate the Gaussian integral over momenta carefully and find the normalization of Feynman's path integral.
2. For a free particle show that the action S_{cl} corresponding to the classical motion is $S_{cl} = m(x_{fin} - x_{in})^2/2(t_{fin} - t_{in})$.
3. For a harmonic oscillator with $T = t_{fin} - t_{in}$ show that

$$S_{cl} = \frac{m\omega}{2\sin\omega T}\left[(x_{in}^2 + x_{fin}^2)\cos\omega T - 2x_{in}x_{fin}\right].$$

4. Find S_{cl} for a particle moving under a constant force F.
5. Formulate the problem of many particles in the path integral language.
6. How would you find the lowest energy bound state in a potential using a Monte Carlo computation of the path integral in Euclidean time?

Time slicing

The path integral for the free particle is

$$Z = \int \mathcal{D}x \exp\left[i\frac{m}{2} \int_{t_{in}}^{t_{fin}} dt \left(\frac{dx}{dt}\right)^2 \right]$$

Again divide the time interval into pieces of length δt and use the coordinates x_i at $t_i = t_0 + i\delta t$ to write the derivative as a finite difference. The resulting integral is quadratic in the x_i, and hence the problem reduces to a set of Gaussian integrals. One can perform each integral separately using Gauss' formula

$$\int_{-\infty}^{\infty} dx \mathrm{e}^{-x^2/(2a^2)} = \sqrt{(2\pi)}a.$$

Does this integral converge for all complex a?
The multivariate version of Gauss' formula can be written down most compactly in the form

$$\int \prod dx_{i=1}^{N} \exp\left[-\frac{1}{2}\mathbf{x}^T A\mathbf{x} \right] = (2\pi)^{N/2} \left(\mathrm{Det}\, A\right)^{-1/2}.$$

Expansion in quantum fluctuations

The classical path is

$$\frac{d^2x_c}{dt^2} = 0, \qquad \text{giving} \qquad x_c(t) = x_{in} + \frac{x_{fin} - x_{in}}{t_{fin} - t_{in}}(t - t_{in}).$$

Decompose an arbitrary path in the form $x(t) = x_c(t) + q(t)$, where $q(t_{in}) = q(t_{fin}) = 0$. The quantity $q(t)$ corresponds to quantum fluctuations of the path around its classical value. Since the classical path is an extremum of the action, one can show that

$$S = S_{cl} + \frac{m}{2}\int_{t_{in}}^{t_{fin}} dt \left(\frac{dq}{dt}\right)^2.$$

As a result, the partition function factors into the form $Z = Z_c Z_q$. Since Z_q again contains only quadratic integrals, one can use the Gaussian integration formula all over again. Note that the quadratic form is diagonalized through Fourier transformation.

The result

For a free particle, the partition function is

$$Z = \sqrt{\frac{m}{2\pi i(t_{fin} - t_{in})}} \exp\left[\frac{im}{2}\frac{(x_{fin} - x_{in})^2}{t_{fin} - t_{in}}\right].$$

The exponential comes from factor Z_c and the square root in the prefactor is the result of performing the integral over the quantum fluctuations.

The Euclidean continuation describes a random walk. When a random walker is released from x_{in} at time t_{in} and its position, x_{fin} is measured at time t_{fin}, the probability distribution of x_{fin} is given by

$$\sqrt{\frac{D}{2\pi(t_{fin} - t_{in})}} \exp\left[-\frac{D}{2}\frac{(x_{fin} - x_{in})^2}{t_{fin} - t_{in}}\right].$$

The mean distance travelled by the random walker grows as $\sqrt{t_{fin} - t_{in}}$. This correspondence reflects the fact that the Schrödinger's equation in imaginary time is the diffusion equation.

Time slicing

The path integral for the free particle is $Z = Z_c Z_q$, where

$$Z_q = \int \mathcal{D}q \exp\left[i\frac{m}{2} \int_{t_{in}}^{t_{fin}} dt \left(\frac{dq}{dt}\right)^2 \right],$$

and $q(t_{in}) = q(t_{fin}) = 0$. The quantum part of the action (above) can be simplified through integration by parts—

$$\int_{t_{in}}^{t_{fin}} dt \left(\frac{dq}{dt}\right)^2 = q\frac{dq}{dt}\Big|_{t_{in}}^{t_{fin}} - \int_{t_{in}}^{t_{fin}} dtq \left(\frac{d^2}{dt^2}\right) q.$$

This is quadratic in q and hence can be integrated. The integral involves the determinant of the second derivative operator. This determinant can be computed either by Fourier transformation or by discretization. We introduce the discretized derivatives—

$$\Delta q_i = \frac{1}{\delta t}(q_{i+1} - q_i) \qquad \text{and} \qquad \nabla q_i = \frac{1}{\delta t}(q_i - q_{i-1}).$$

The algebra of discretized derivatives

The commutator $[\Delta, \nabla] = 0$ since

$$\Delta\nabla q_i = \frac{1}{(\delta t)^2}(q_{i+1} - 2q_i + q_{i-1}) = \nabla\Delta q_i.$$

One also has a formula for summation by parts—

$$\sum_{i=1}^{N} x_i \nabla y_i = \frac{1}{\delta t}(x_N y_N - x_0 y_0) - \sum_{i=0}^{N-1} (\Delta x_i) y_i.$$

This can be proven by explicitly writing out the differences and sums. When $x_N = x_0 = 0$ (or $y_N = y_0 = 0$), this can be rewritten in the form

$$\sum_{i=1}^{N} x_i \nabla y_i = -\sum_{i=0}^{N-1} (\Delta x_i) y_i = -\sum_{i=1}^{N} (\Delta x_i) y_i.$$

Matrices for discretized derivatives

The matrix form of the derivatives are

$$\Delta = \frac{1}{\delta t}\begin{pmatrix} \cdots & \vdots & \vdots & \vdots & \cdots \\ \cdots & -1 & 1 & 0 & \cdots \\ \cdots & 0 & -1 & 1 & \cdots \\ \cdots & \vdots & \vdots & \vdots & \cdots \end{pmatrix} = \nabla^\dagger,$$

although, in the limit $\delta t \to 0$, both go to the continuum derivative. Also

$$\Delta\nabla = \frac{1}{(\delta t)^2}\begin{pmatrix} \cdots & \vdots & \vdots & \vdots & \cdots \\ \cdots & -2 & 1 & 0 & \cdots \\ \cdots & 1 & -2 & 1 & \cdots \\ \cdots & 0 & 1 & -2 & \cdots \\ \cdots & \vdots & \vdots & \vdots & \cdots \end{pmatrix} = \nabla\Delta.$$

We have to find the determinant of this matrix.

A recursion for the determinant

When $N = 1$ we find $-(\delta t)^2 \Delta\nabla|_{N=1} = 2$ and the determinant is 2. When $N = 2$, we have

$$-(\delta t)^2 \Delta\nabla|_{N=2} = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix},$$

so the determinant is 3. A recursion relation is obtained by expanding the determinant by the first row—

$$\mathrm{Det}\left[-(\delta t)^2 \Delta\nabla|_N\right] = 2\mathrm{Det}\left[-(\delta t)^2 \Delta\nabla|_{N-1}\right] - \mathrm{Det}\left[-(\delta t)^2 \Delta\nabla|_{N-2}\right].$$

The initial conditions above can be used to solve this recursion to get

$$\mathrm{Det}\left[-(\delta t)^2 \Delta\nabla|_N\right] = N + 1.$$

Using this determinant, we can perform the integral

$$Z_q^N = \left(\frac{m}{2\pi i \delta t}\right)^{N/2} \int \left\{\prod_{i=1}^{N-1} dq_i\right\} \mathrm{e}^{iS_q}.$$

The integral to be performed

By considering fluctuations around the classical path one finds, as before, $Z = Z_c Z_q$. For Z_c one uses the previously evaluated value of S_{cl} for the harmonic oscillator. The integral over quantum fluctuations is written down in a way very similar to that for the free particle. Finally, for this problem we find

$$Z_q^{HO} = Z_q^{FP} \sqrt{\frac{\mathrm{Det}\,\{-(\delta t)^2 \Delta\nabla\}}{\mathrm{Det}\,\{-(\delta t)^2[\Delta\nabla + \omega^2]\}}},$$

where HO means harmonic oscillator and FP stands for free particle. This gives the result

$$Z_q^{HO} = \sqrt{\frac{m}{2\pi i(t_{fin} - t_{in})}} \sqrt{\frac{\omega(t_{fin} - t_{in})}{\sin\omega(t_{fin} - t_{in})}}.$$

Diagonalizing the discretized derivatives

Going to the discrete Fourier basis for q_i (since $q_0 = q_N = 0$),

$$q_i = \sum_n \mathrm{e}^{-i\omega_n t_i} q(\omega_n), \qquad \omega_n = \frac{\pi n}{N\delta t}.$$

we find that

$$\Delta q_i = \sum_n \frac{1}{\delta t}(\mathrm{e}^{-i\omega_n \delta t} - 1)\mathrm{e}^{-i\omega_n t_i} q(\omega_n).$$

Therefore, in the Fourier basis Δ is diagonal, and in the limit $\delta t \to 0$ it goes over to $-i\omega$. ∇ is also diagonal in the same basis, and its eigenvalues are complex conjugate to this. As a result

$$\Delta\nabla q(\omega_n) = \frac{2}{(\delta t)^2}(1 - \cos\omega_n \delta t).$$

This representation gives us another way of handling the determinants needed to evaluate the path integrals over the quantum fluctuations.

What have we gained?

Quadratic actions give Gaussian integrals and can be solved. Anything else is unsolvable. What have we gained?

1. The power of this method can be seen when solving interacting multi-particle problems. Since the number of coordinates to be handled is very large, reducing the problem to differential equations is highly unsatisfactory. The equations can hardly ever be made tractable. Path integrals give us new techniques.
2. Quantum statistical mechanics and quantum mechanics can be handled in exactly the same way. Path integrals connect quantum mechanics with the theory of probability.
3. If the non-quadratic parts of the action are "small" then we can set up approximation methods. One such method is perturbation theory. Perturbation theory in many-particle physics and quantum field theory is most easily set up using path integrals.
4. We have reduced the general problem to doing integrals. We have efficient numerical methods for evaluating integrals. So we have a method even when perturbation fails (which is almost always).

Keywords and References

Keywords

Time evolution, evolution operator, path integral, Euclidean time, transfer matrix, diagrammatic method, action, Feynman's path integral, Gaussian integrals, classical limit, quantum fluctuations.

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