Path integrals

Sourendu Gupta

TIFR Graduate School

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Outline

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

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

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. The group is the group $U(1)$, since the action on each eigenstate of H is to multiply it by a phase. These eigenstates carry irreducible representations.

Slicing the time interval

Using the group property, we can write

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

If the state at time t_i is $|\psi_i\rangle$, then

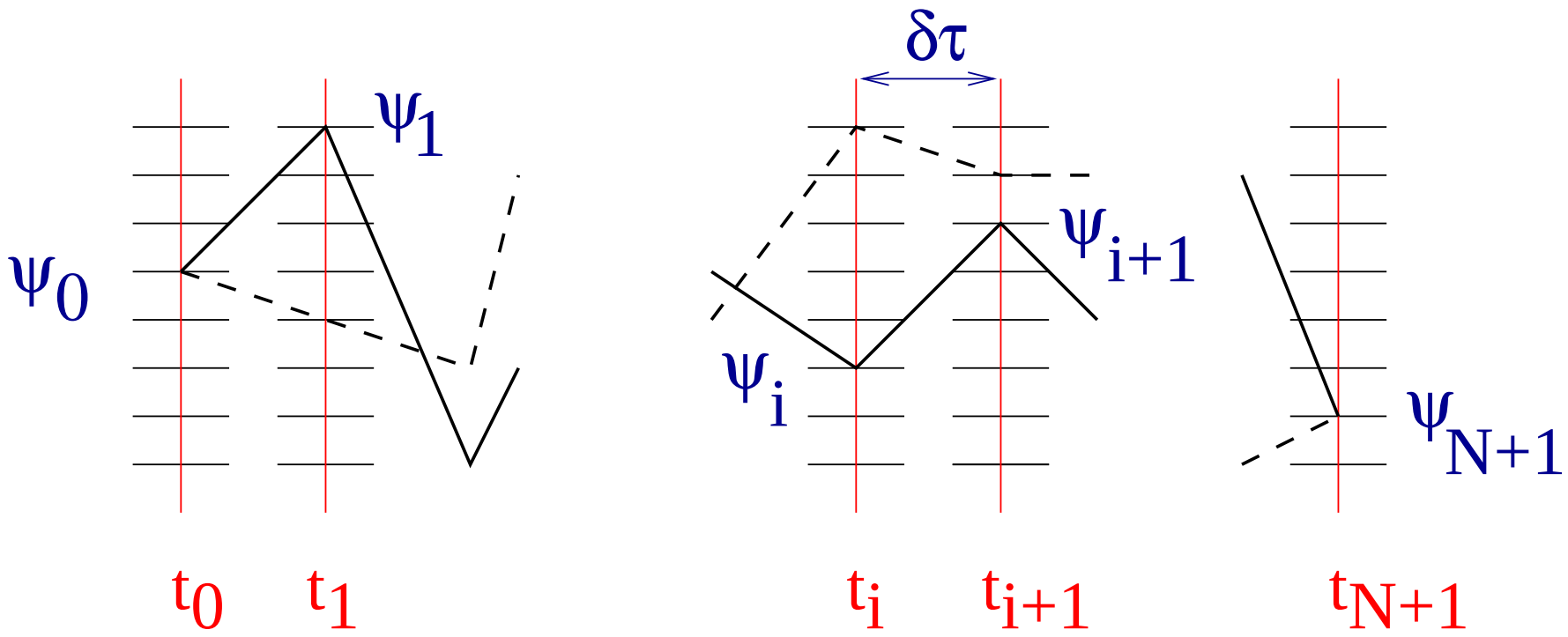
$$\langle\psi(t_{fin})|U(t_{fin}, t_{in})|\psi(t_{in})\rangle = \sum_{\{\psi_i\}} \prod_{i=0}^{N-1} \langle\psi_{i+1}|U(t_i + \delta t, t_i)|\psi_i\rangle,$$

where $|\psi(t_{fin})\rangle = |\psi_{N+1}\rangle$ and $|\psi(t_{in})\rangle = |\psi_0\rangle$. The sum over all intermediate states is called a path integral.
If the states $|\psi_i\rangle$ are eigenstates of the Hamiltonian then

$$\langle\psi_{i+1}|U(t_i + \delta t, t_i)|\psi_i\rangle = \mathrm{e}^{-iE_i\delta t/\hbar}\delta_{\psi_{i+1},\psi_i}.$$

However, if we choose a complete set of states which does not coincide with the eigenstates of the Hamiltonian, then the path integral may be non-trivial.

A path integral



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

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

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 $\langle \alpha_N | U(t_N, t_0) | \alpha_0 \rangle$ is the sequence of intermediate states $|\alpha(t_i)\rangle$. The contribution of each path to the transition matrix element is

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

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.

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

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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

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

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

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

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

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

when $E_1 > E_0$ and $T(E_1 - E_0) \gg \hbar$. This gives the lowest eigenvalue of H.

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 $\delta_{\alpha_i,\alpha_{i+1}} - \delta t H_{\alpha_i,\alpha_{i+1}}/\hbar$ 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 one of the techniques of lattice quantum theory.

Outline

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—-

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

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

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

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

Expression in terms of the action

Putting all this together, the transition matrix element turns out to be

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

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,

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

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

$$Z = \langle x(t_{fin}) | U(t_{fin}, t_{in}) | x(t_{in}) \rangle = \int \mathcal{D}x \mathrm{e}^{iS[x]/\hbar},$$

where the paths join the given points $x(t_{in})$ and $x(t_{fin})$.

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)

Problems

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?

Outline

Time slicing

The path integral for the free particle is

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

The most straightforward method for doing this is to use the route we have taken before. Divide the time interval into pieces of length δt and use the coordinates x_i at $t_i = t_{in} + i\delta t$ 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

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

Note that this result can also be obtained from Schrödinger's equation. One can check that 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 of this result ($t \to it$) shows that the distribution is exactly that which results from 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 is closely related to the fact that Schrödinger's equation goes to the diffusion equation with this analytic continuation of the time.

Outline

References

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