Path integrals (2)

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Outline

Time slicing

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

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

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

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

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

We find

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

As a result, the commutator $[\Delta, \nabla] = 0$.
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

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

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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

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

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

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

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.

Outline

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).

Outline

References

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