Semiclassical approximation

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The true power of the Feynman path integral method can be seen when the *semi-classical limits* $\hbar \to 0$ of quantum theories are dealt with. This includes the situation in which a macroscopic objest being rest at a classical equilibrium position and the quantum fluctuations around it are asked. Here we shall learn the Feynman path integral method for treating a massive particle in a well, i.e., a simple harmonic oscillator.

I. STATIONARY PHASE APPROXIMATION TO THE PATH INTEGRAL [1]

We learned that the quantum probability amplitude for the particle to go from a space-time point (q_i, t_i) to (q_f, t_f) $\langle q_f, t_f | q_i, t_i \rangle$ can be obtained by *Feynman path integral*:

$$\begin{aligned} \langle q_f, t_f | q_i, t_i \rangle &= \int_{q_i}^{q_f} Dq \exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f} dt L(q,\dot{q})\right] \\ &= \int_{q_i}^{q_f} Dq \exp\left[\frac{i}{\hbar} S[q]\right], \end{aligned} \tag{1}$$

where $L(q, \dot{q})$ is the classical Lagrangian of a partical of mass m in a 1-dimensional potential $V(q)$,

$$L(q,\dot{q}) = \frac{1}{2}m\dot{q}^2 - V(q), \tag{2}$$

and

$$\int_{q_i}^{q_f} Dq = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} \int_{-\infty}^{\infty} dq_{N-1}\int_{-\infty}^{\infty} dq_{N-2}\cdots\int_{-\infty}^{\infty} dq_1. \tag{3}$$

is a infinite-dimensional path integral with $\{q_f, q_{N-1}, q_{N-2}, \cdots, q_1, q_i\}$ representing a single path (trajectory) of the particle in a coordinate space and $S[q]$ is the action. The true power of the Feynman path integral method can be seen when the *semi-classical limits* of quantum theories are dealt with.

To see how the solutions of classical equations of motion appear in the path integral, let us explore the *stationary phase (saddle-point) approximation* to the path integral. The first step is to find the solutions of the classical equation of motion associated with the Lagrangian $L(q, \dot{q})$, that is, the Euler-Lagrange equation;

$$\frac{d}{dt}\left(\frac{\partial L(q,\dot{q})}{\partial \dot{q}}\right) - \frac{\partial L(q,\dot{q})}{\partial q} = 0. \tag{4}$$

This follows from *Hamilton's principle*, which states that the unique classical path q_{cl} is determined by minimizing the action $S[q] = \int_{t_i}^{t_f} dt L(q, \dot{q})$. For $L(q, \dot{q})$ in Eq. (2) it is given by

$$m\ddot{q} + \frac{\partial V(q)}{\partial q} = 0. \tag{5}$$

As the second step, let q_{cl} be a only solution of Eq. (5) and set $q = q_{cl} + r$. The action $S[q] \equiv \int_0^t dt' L(q, \dot{q})$ in Eq. (1)

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can then be Taylor-expanded as

$$\begin{aligned} S[q] &= \int_0^t dt' L(q,\dot{q}) \\ &= S[q_{cl}] + \int_0^t dt' \underbrace{\frac{\delta S[q_{cl}]}{\delta q(t')}}_{0} r(t') + \frac{1}{2}\int_0^t dt' \int_0^t dt'' r(t') \frac{\delta^2 S[q_{cl}]}{\delta q(t')\delta q(t'')} r(t'') + \cdots \\ &\simeq S[q_{cl}] + \frac{1}{2}\int_0^t dt' \int_0^t dt'' r(t') \frac{\delta^2 S[q_{cl}]}{\delta q(t')\delta q(t'')} r(t''), \end{aligned} \tag{6}$$

where $\frac{\delta S[q_{cl}]}{\delta q(t')} = 0$ is ensured by the classical solution q_{cl}. Here $\frac{\delta S[q_{cl}]}{\delta q(t')}$ and $\frac{\delta^2 S[q_{cl}]}{\delta q(t')\delta q(t'')}$ are the *functional derivatives*. The meaning of the functional derivatives can be made clear latter on. Finally, by plugging Eq. (6) into Eq. (1) we have the *semiclassical (sationary phase, or, saddle-point) approximation* to the path integral:

$$\begin{aligned} \langle q_f, t_f | q_i, t_i \rangle &= \int_{q_i}^{q_f} Dq \exp\left[\frac{i}{\hbar} S[q]\right] \\ &= \underbrace{\exp\left[\frac{i}{\hbar} S[q_{cl}]\right]}_{\text{classical path}} \underbrace{\int_{q_i}^{q_f} Dr \exp\left[\frac{1}{2}\int_0^t dt' \int_0^t dt'' r(t') \frac{\delta^2 S[q_{cl}]}{\delta q(t')\delta q(t'')} r(t'')\right]}_{\text{quantum fluctuation}}. \end{aligned} \tag{7}$$

This semiclassical approximation, Eq. (7), appears to be very appealing: the classical path associated with the classical action $S[q_{cl}]$ are embellished with the quantum fluctuation. Note that the quantum fluctuation is now completely described by c-numbers as opposed to quantum operators.

To make things more explicit let us repeat the same calculation with the form $L(q,\dot{q})$ in Eq. (2). By expanding the action $S[q_{cl}]$ in $r(t)$ explicitly we have

$$\begin{aligned} S[q] &= \int_0^\infty dt' \left(\frac{1}{2} m\dot{q}^2 - V(q)\right) \\ &\simeq \int_0^t dt' \left[\frac{1}{2} m\left(\dot{q_{cl}}^2 + 2\dot{q_{cl}}\dot{r} + \dot{r}^2\right) - \left(V(q_{cl}) + \frac{\partial V(q_{cl})}{\partial q} r + \frac{1}{2}\frac{\partial^2 V(q_{cl})}{\partial q^2} r^2\right)\right] \\ &= \int_0^t dt' \left[\frac{1}{2} m\dot{q_{cl}}^2 - V(q_{cl})\right] + \int_0^t dt' \left[m\dot{q_{cl}}\dot{r} - \frac{\partial V(q_{cl})}{\partial q} r\right] + \int_0^t dt' \left[\frac{1}{2} m\dot{r}^2 - \frac{1}{2}\frac{\partial^2 V(q_{cl})}{\partial q^2} r^2\right] \\ &= S[q_{cl}] - \int_0^t dt' \underbrace{\left[m\ddot{q_{cl}} + \frac{\partial V(q_{cl})}{\partial q}\right]}_{0} r(t') - \frac{1}{2}\int_0^t dt' r(t') \left[m\frac{d^2}{dt'^2} + \frac{\partial^2 V(q_{cl})}{\partial q^2}\right] r(t') \\ &= S[q_{cl}] - \frac{1}{2}\int_0^t dt' r(t') \left[m\frac{d^2}{dt'^2} + \frac{\partial^2 V(q_{cl})}{\partial q^2}\right] r(t'), \end{aligned} \tag{8}$$

where, in the third line, we performed the integrations by part,

$$\int_0^t dt' m\dot{q_{cl}}\dot{r} = \underbrace{\left[m\dot{q_{cl}} r\right]_0^t}_{0} - \int_0^t dt' m\ddot{q_{cl}} r \tag{9}$$

$$\int_0^t dt' m\dot{r}^2 = \underbrace{\left[m\dot{r} r\right]_0^t}_{0} - \int_0^t dt' m\ddot{r} r. \tag{10}$$

By compared with Eq. (6) we obtain the following relation:

$$\frac{1}{2}\int_0^t dt' \int_0^t dt'' r(t') \frac{\delta^2 S[q_{cl}]}{\delta q(t')\delta q(t'')} r(t'') = -\frac{1}{2}\int_0^t dt' r(t') \left[m\frac{d^2}{dt'^2} + \frac{\partial^2 V(q_{cl})}{\partial q^2}\right] r(t'). \tag{11}$$

A. Example: quantum harmonic oscillator

Let us apply the above argument to a massive particle in a harmonic potential $V = \frac{1}{2}kq^2$, that is, a harmonic oscillator. The classical equation of motion is $m\ddot{q} + kq = 0$. Imposing the boundary conditions $q(0) = q(t) = 0$, the solution of the classical motion is obiously $q_{cl}=0$. We thus have

$$
\begin{aligned}
G_{\rm HO}(0,0;t)\equiv\langle q_f=0,t|q_i=0,0\rangle &= \int Dq\exp\left[\frac{i}{\hbar}S[q]\right]\\
&\simeq \underbrace{\exp\left[\frac{i}{\hbar}S[q_{cl}]\right]}_{1}\int Dr\exp\left[-\frac{i}{\hbar}\int_0^t dt'r(t')\left[\frac{1}{2}\left(m\frac{d^2}{dt'^2}+\frac{\partial^2V(q_{cl})}{\partial q^2}\right)\right]r(t')\right]\\
&= \int Dr\exp\left[-\frac{i}{\hbar}\int_0^t dt'r(t')\frac{m}{2}\left(\frac{d^2}{dt'^2}+\omega^2\right)r(t')\right], \qquad (12)
\end{aligned}
$$

where $\omega=\sqrt{\frac{k}{m}}$ is the eigenfrequency of the oscillator. This integral is again Gaussian form, so we can perform the Gaussian integration. To perform the integral let us tentatively assume the differential operator $-\frac{m}{2}\left(\frac{d^2}{dt'^2}+\omega^2\right)$ be a finite-dimensional matrix $\mathbf{A}$. The integral then becomes familiar one as Eq. (A3) and get

$$
G_{\rm HO}(0,0;t)=\mathcal{N}\frac{1}{\sqrt{\det\left[\mathbf{A}\right]}}, \qquad (13)
$$

with $\mathcal{N}$ absorbed several constants, which may be divergent after taking the continuum limit, though. Then the question is; what is $\det\left[\mathbf{A}\right]$? The answer can be found by expressing $\mathbf{A}$ in terms of eigenvalues, that is,

$$
\begin{aligned}
\mathbf{A}v_n &\equiv -\frac{m}{2}\left(\frac{d^2}{dt'^2}+\omega^2\right)v_n\\
&= \epsilon_n v_n. \qquad (14)
\end{aligned}
$$

The eigestates v_n are given by

$$
v_n=\sin\left(\frac{n\pi t'}{t}\right) \qquad (15)
$$

with the eigenvalues

$$
\epsilon_n=\frac{m}{2}\left(-\omega^2+\left(\frac{n\pi}{t}\right)^2\right) \qquad (16)
$$

for $n=1,2,\cdots\infty$. Thus the determinant of $\mathbf{A}$ is given by

$$
\det\left[\mathbf{A}\right]=\prod_{n=1}^{\infty}\epsilon_n=\prod_{n=1}^{\infty}\frac{m}{2}\left(-\omega^2+\left(\frac{n\pi}{t}\right)^2\right). \qquad (17)
$$

We then notice that $\frac{1}{\sqrt{\det\left[\mathbf{A}\right]}}$ is obtained from the infinite product of $\left(-\omega^2+\left(\frac{n\pi}{t}\right)^2\right)^{-\frac{1}{2}}$, each of which is divergent for $\frac{n\pi}{t}=\omega$, a very alarming situation!

To circumvent the calculation of the dangerous determinant explicitly, we can exploit the well-behaved result obtained for a free particle. Indeed, $G_{\rm free}(0,0;t)$ is the special case of $G_{\rm HO}(0,0;t)$ for $V(q)=0$, that is, $\omega=0$. Let us evaluate the following quantity,

$$
G_{\rm HO}(0,0;t)=\left(\frac{G_{\rm HO}(0,0;t)}{G_{\rm free}(0,0;t)}\right)G_{\rm free}(0,0;t). \qquad (18)
$$

The quantity inside the parentheses in Eq. (18) gives

$$
\begin{aligned}
\frac{G_{\rm HO}(0,0;t)}{G_{\rm free}(0,0;t)} &= \frac{\mathcal{N}\prod_{n=1}^{\infty}\left[\frac{m}{2}\left(-\omega^2+\left(\frac{n\pi}{t}\right)^2\right)\right]^{-\frac{1}{2}}}{\mathcal{N}\prod_{n=1}^{\infty}\left[\frac{m}{2}\left(\frac{n\pi}{t}\right)^2\right]^{-\frac{1}{2}}}\\
&= \prod_{n=1}^{\infty}\left[1-\left(\frac{\omega t}{n\pi}\right)^2\right]^{-\frac{1}{2}}=\sqrt{\frac{\omega t}{\sin(\omega t)}}. \qquad (19)
\end{aligned}
$$

Thus, with Eq.(18), $G_{\rm HO}(0,0;t)$ bocomes

$$G_{\rm HO}(0,0;t)=\sqrt{\frac{\omega t}{\sin(\omega t)}}G_{\rm free}(0,0;t)=\sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega t)}}\Theta(t), \tag{20}$$

where we used

$$G_{\rm free}(q_f,q_i;t)=\sqrt{\frac{1}{4\pi\left(\frac{i\hbar}{2m}\right)t}}\exp\left[-\frac{(q_f-q_i)^2}{4\left(\frac{i\hbar}{2m}\right)t}\right]\Theta(t), \tag{21}$$

which we obtained previously.

Appendix A: Gaussian integration

First, some mathematics. The most fundamental Gaussian integration is

$$\int_{-\infty}^{\infty}dxe^{-\frac{1}{2}ax^2}=\sqrt{\frac{2\pi}{a}}. \tag{A1}$$

An interesting and useful Gaussian integration is

$$\int_{-\infty}^{\infty}dxe^{-\frac{1}{2}ax^2+bx}=\sqrt{\frac{2\pi}{a}}e^{\frac{b^2}{2a}}. \tag{A2}$$

The Multi-dimensional expansion of Eq. (A1) is

$$\int_{-\infty}^{\infty}d\boldsymbol{v}e^{-\frac{1}{2}\boldsymbol{v}^T\mathbf{A}\boldsymbol{v}}=(2\pi)^{\frac{N}{2}}\frac{1}{\sqrt{\det\left[\mathbf{A}\right]}}, \tag{A3}$$

and that of Eq. (A2) is

$$\int_{-\infty}^{\infty}d\boldsymbol{v}e^{-\frac{1}{2}\boldsymbol{v}^T\mathbf{A}\boldsymbol{v}+\boldsymbol{j}\cdot\boldsymbol{v}}=(2\pi)^{\frac{N}{2}}\frac{1}{\sqrt{\det\left[\mathbf{A}\right]}}e^{\frac{1}{2}\boldsymbol{j}^T\mathbf{A}^{-1}\boldsymbol{j}}, \tag{A4}$$

[1] A. Altland and B. D. Simons, *Condensed Matter Field Theory*, 2nd ed. (Cambridge University Press, Cambridge, 2010).