Instantons and quantum tunneling

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We shall now learn how the Feynman path integral can be used to deal with a particle in an double-well potential with two minima. The particle in such a potential undergoes quantum tunnelings. To handle these tunnelings we introduce the instantons along with the Euclidean path integral. The instantons are playing important roles in modern physics and mathematics. The instanton living in a double-well potential we shall consider is the simplest among these.

I. DOUBLE-WELL POTENTIAL AND QUANTUM TUNNELINGS

Let us now try to apply the Feynman path integral method to the situation in which a particle of mass $m$ is placed in a 1-dimensional anharmonic potential with two minima at $q = \pm a$, that is, a double-well potential. Suppose that initially at $t = 0$ the particle is placed in the minimum $q = a$. There is a trivial stationary path, that is, $q(t) = a$. To be more specific, suppose that the double-well potential is symmetric and is written as

$$V(q) = \frac{k}{8a^6} (q^2 - a^2)^2$$

(1)

as shown in Fig. 1. Around the minima $q = \pm a$ the potential Eq. (1) can be approximated as harmonic potential characterized by the eigenfrequency $\omega = \sqrt{\frac{k}{m}}$.

Then we may conclude the quantum probability amplitude $\langle q = a, t | q = a, 0 \rangle$ for the particle is the same as the...
particle in a simple harmonic potential;
\[
G_{\text{HO}}(a,a;t) = \langle q = a, t|q = a, 0 \rangle = \langle q = a|\exp \left[ -\frac{i}{\hbar}H \right]|q = a \rangle \\
= \int Dq \exp \left[ \frac{i}{\hbar} \int_{0}^{t} dt' \left( \frac{m}{2} \dot{q}(t')^2 - V(q(t')) \right) \right]
\]
\[
= \int Dq \exp \left[ \frac{1}{\hbar} \int_{0}^{t} dt' \left( \frac{m}{2} \dot{q}(t')^2 - V(q(t')) \right) \right]
= \int Dq \exp \left[ -\frac{1}{\hbar} S[q] \right].
\]

This guess is in fact incorrect since we ignored the possible contributions to the path integral from the paths associated with the *quantum tunnelings* between two minima. Those paths associated with the quantum tunnelings are, however, classically forbidden. How can we incorporate those paths?

## II. EUCLIDEAN PATH INTEGRAL

[1] The new insight can be obtained by considering the path integral with imaginary time \( \tau = it \). Exchanging \( t \) with \( \tau = it \) (called the Wick rotation) enables us to deal with the Euclidean space spanned by \( \tau \) and \( q \) as opposed to the Minkowski space spanned by \( t \) and \( q \). We then define *Euclidean path integral* as
\[
G_{\text{E}}(a,a;\tau) = \langle q = a, \tau|q = a, 0 \rangle = \langle q = a|\exp \left[ -\frac{\tau}{\hbar}H \right]|q = a \rangle \\
= \int Dq \exp \left[ \frac{1}{\hbar} \int_{0}^{\tau} d\tau' \left( \frac{m}{2} \dot{q}(\tau')^2 - V(q(\tau')) \right) \right]
= \int Dq \exp \left[ -\frac{1}{\hbar} S[q] \right].
\]

The stationary phase (saddle-point) equation, that is, the Euler-Lagrange equation, with respect to the imaginary time \( \tau \) becomes
\[
-m\ddot{q}(\tau) + \frac{\partial V(q(\tau))}{\partial q(\tau)} = 0,
\]
and is corresponding to the one with respect to the real time \( t \) but with the *inverted* potential, \(-V(q)\)! Then indeed a path going from \( q = a \) to \( q = -a \) and then from there to \( q = a \) is allowed now. Moreover there are infinitely many paths going from \( q = a \) to \( q = -a \), going back and forth many times, and then returning to \( q = a \) are permitted. Those classical paths can be thought of emerging because of the quantum tunnelings.

## III. INSTANTONS

[1, 2] The classical paths emerged after the Wick rotation can be viewed as the results of the creations and annihilations of *instantons*. Let us consider the contribution of these instantons to the path integral. The first integral of the equation of motion, Eq. (5), can be given by
\[
\int_{0}^{\tau} d\tau' \left( -m\ddot{q} \right) + \int_{0}^{\tau} d\tau' \left( \frac{\partial V(q)}{\partial q} \dot{q} \right) = 0.
\]

Now suppose the boundary condition at \( \tau = 0 \) as \( q_{cl}(0) = -a \) and \( \dot{q}_{cl}(0) = 0 \). Then the first term on the left hand side of Eq. (6) gives
\[
\int_{0}^{\tau} d\tau' \left( -m\ddot{q} \right) = \left[ -m\dot{q}^2 \right]_{0}^{\tau} - \int_{0}^{\tau} dt' \left( -m\ddot{q} \right)
\]

\[
-\frac{m\dot{q}(\tau)^2 + m\dot{q}(0)^2}{m\dot{q}(\tau)^2} = -m\dot{q}(\tau)^2
\]
and thus
\[ \int_0^\tau dt' \left( -\frac{m}{2} \dddot{q} \right) = -\frac{m}{2} q(\tau)^2. \] (8)

The second term on the left hand side of Eq. (6) gives
\[ \int_0^\tau dt' \left( \frac{\partial V(q)}{\partial q} \frac{dq}{dt'} \right) = \int_{-a}^{q(\tau)} dq \frac{dV(q)}{dq} = V(q(\tau)) - V(-a) = V(q(\tau)). \] (9)

Thus we have, from Eq. (6),
\[ \frac{m}{2} \dddot{q} = V(qcl). \] (10)

This leads to
\[ \tau = \tau_1 + \int_0^{q_{cl}} \frac{dq}{\sqrt{\frac{2V(q)}{m}}}, \] (11)

where \( \tau_1 \) is an integration constant, at which \( q_{cl} = 0 \).

The contribution of instantons (classical paths of quantum tunnelings) to the Euclidean action \( S[q] \) in Eq. (4) can then be given by
\[ S_{in} = \int_0^\tau dt' \left( \frac{m}{2} \dddot{q}_{cl}^2 + V(q_{cl}) \right) = \int_0^\tau dt' \frac{dq_{cl}}{dt'} \frac{dq_{cl}}{dt'} \frac{dq_{cl}}{dt'} \bigg|_{q_{cl}} = \int_{-a}^{q_{cl}(\tau)} dq_{cl} \sqrt{\frac{2mV(q_{cl})}{m}}. \] (12)

Note that this formula is the same form as the barrier-penetration formula obtained by the semiclassical Wentzel-Kramers-Brillouin (WKB) method [2].

We now proceed to explore the temporal features of instantons. The solution of Eq. (10) with the boundary condition, \( q_{cl}(\tau) = a \) at \( \tau \to \infty \), is obtained with the parameter \( \tau_1 \) appeared in Eq. (11) as
\[ q_{cl}(\tau) = a \tanh \left( \frac{\omega (\tau - \tau_1)}{2} \right). \] (13)

The solution, Eq. (13), reflects the time-translation invariance of the first integral Eq. (10), that is, \( \tau_1 \) assumes any positive value. This will indicate the existence of a zero mode around the saddle-point \( q_{cl} \). We will explain the implication of the zero mode in Appendix A. Note that the temporal extension of the instanton is of the order of \( \omega^{-1} \) around the kink at \( \tau_1 \) as shown in Fig. 2. Here and hereafter the temporal extension of the instanton \( \omega^{-1} \) is considered to be short with respect to \( \tau \to \infty \).

A. Single instanton

Within the saddle-point approximation, the single instanton contribution to the path integral \( G(a, -a; \tau) \) can be obtained by integrating the paths with a single instanton (occurred at \( \tau = \tau_1 \)) over \( \tau_1 \)
\[ G^{(1)}(a, -a; \tau) = \int_0^\tau d\tau_1 A_{1,cl}(\tau_1) \times A_{1,q}(\tau_1), \] (14)

where \( A_{1,cl}(\tau_1) \) and \( A_{1,q}(\tau_1) \) are the classical and quantum contributions, respectively.

To proceed, let us consider the following 4 contributions separately. First, consider the contribution from the classical part \( A_{1,cl}(\tau_1) \) that stems from the non-kink region where the particle rests on \( q_{cl} = \pm a \). This is in fact negligible as in the case of a harmonic oscillator. The classical contribution from the instanton, that is, from the kink region, is non-zero and given, from Eq. (12), by
\[ A_{1,q}(\tau_1) = \exp \left[ -\frac{S_{in}}{\hbar} \right] = \exp \left[ -\frac{1}{\hbar} \left( \int_{-a}^{a} dq \sqrt{2mV(q)} \right) \right], \] (15)
which completely dictates the classical action. Note that this contribution is independent on $\tau_1$. Third contribution is from the quantum fluctuation accompanying with the instanton at $\tau_1$, which appears within $\Delta \tau \sim \omega^{-1}$. But this can be considered to be negligible since $\Delta \tau$ is too short for this to be significant as compared to the quantum contribution from the non-kink region. The latter constitutes the forth contribution, which can be viewed as coming from the Euclidean version of the action for a harmonic oscillator. From the Minkowski path integral given in Eq. (3), we can infer the Euclidean version (for $\tau \rightarrow \infty$) as

$$G_q = \langle q = 0, \tau | q = 0, 0 \rangle = \langle q = a | \exp \left[ -\frac{\tau}{\hbar} H \right] | q = 0 \rangle = \sum_n \langle q = 0 | n \rangle \langle n | q = 0 \rangle e^{-\frac{E_n}{\hbar}} \sqrt{\frac{m \omega}{\sinh (\omega \tau)}},$$

where $K$ is a constant to make sense the single instanton contribution [2]. We will evaluate $K$ in Appendix A.

**B. Dilute instanton gas**

There are paths with $n$ (odd) instantons which contributes to $G(a, -a; \tau)$. Here we make the *dilute instanton gas* approximation, where each interaction can be treated independently. We will comment on the validity of dilute
The instanton gas approximation in Appendix B. We can then extend Eq. (19) to the one with n instantons as

$$G(n, a, -a; \tau) = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{x}{\hbar}} \left( K^ne^{-\frac{\pi}{\hbar}} \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n \right),$$

(20)

where the classical instanton contribution becomes $e^{-\frac{\pi}{\hbar}}$ while the contribution from the quantum fluctuation is the same as for the single instanton case within the dilute instanton gas approximation. By summing up all the contributions with $n = 1, 3, \cdots$ instantons, we have finally

$$G(a, -a; \tau) = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{x}{\hbar}} \sum_{n \text{ odd}} K^n e^{-\frac{\pi}{\hbar}} \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{x}{\hbar}} \sum_{n \text{ odd}} \frac{1}{n!} \left( \tau K e^{-\frac{\pi}{\hbar}} \right)^n$$

(21)

$$= \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{x}{\hbar}} \sinh \left( \tau K e^{-\frac{\pi}{\hbar}} \right),$$

(22)

where in the first line we use the diluteness assumption and

$$\int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n = \frac{1}{n!} \left( \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n \right)$$

$$= \frac{\tau^n}{n!},$$

(23)

that is, out of all possible $n!$ arrangements of $\{\tau_1, \tau_2, \cdots, \tau_n\}$ in $\int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n$ in the right-hand-side of Eq. (23) one particular arrangement realizes the order suggested in the left-hand-side of Eq. (23).

C. Tunnel splitting

We shall now see that the above instanton method can predict the tunnel splitting of the energy of the particle in the double well potential. Let us again calculate $G(a, -a; \tau)$ for a particle in the double-well potential Eq. (1) under the assumption that the particle has low energy and we only need to consider the lowest two levels, that is, symmetric and anti-symmetric eigenstates, $|S\rangle$ and $|A\rangle$, respectively. Suppose that these states have a degenerate energy $\frac{h\omega}{2}$ if there were no tunneling, but, as a result of the tunneling, the energies are tunnel splitting to become

$$\epsilon_S = \frac{h\omega}{2} - \frac{\Delta\epsilon}{2}$$

$$\epsilon_A = \frac{h\omega}{2} + \frac{\Delta\epsilon}{2},$$

(24)

(25)

where $\Delta\epsilon$ stand for the tunnel splitting. We then have

$$G(a, -a; \tau) = \langle a\lvert \left( \exp \left[ -\frac{\tau}{\hbar} H \right] \right) (\langle S\lvert + |A\rangle |A\rangle) \lvert -a\rangle$$

$$= \langle a\lvert S \rangle \left( \exp \left[ -\frac{\tau}{\hbar} \epsilon_S \right] \right) \langle S \lvert -a\rangle + \langle a\lvert A \rangle \left( \exp \left[ -\frac{\tau}{\hbar} \epsilon_A \right] \right) \langle A \lvert -a\rangle$$

$$= C \left( e^{-\frac{\tau}{\hbar} \epsilon_S} - e^{-\frac{\tau}{\hbar} \epsilon_A} \right)$$

(26)

$$= C e^{-\frac{\tau}{\hbar} \epsilon_S} \sinh \left( \frac{\Delta\epsilon \tau}{2\hbar} \right)$$

where $\langle a\lvert S\rangle \langle S\lvert -a\rangle = \frac{C}{2}$ and $\langle a\lvert A\rangle \langle A\lvert -a\rangle = -\frac{C}{2}$ with $C = \sqrt{\frac{\omega}{\hbar}}$ being the spread of the ground-state wave function appeared in Eq. (17). Comparing the result with Eq. (22) the tunneling splitting can be found to be

$$\Delta\epsilon = 2\hbar K \exp \left[ -\frac{S\omega}{\hbar} \right].$$

(27)

This result could have been derived by a WKB-type method. But, there are several reasons to acquire the instanton method: 1) the instantons are non-perturbative objects with well-controlled parameters 2) the extensions to the higher-dimensional field theories lead to a variety of interesting physics [1].
IV. REMARKS

A. 1-dimentional Ising magnets

The Euclidean path integral Eq. (4) can be viewed as the partition function by \( \frac{1}{h} \Rightarrow \beta = \frac{1}{k_B T} \), \( \tau \Rightarrow L \), \( \tau' \Rightarrow x \), and \( q(\tau') \Rightarrow \phi(x) \), that is,

\[ Z = \text{Tr} \left[ e^{-\beta H} \right] = \int D\phi \exp \left[ -\beta \int_0^L dx \left( \frac{1}{2} \left( \frac{\partial \phi(x)}{\partial x} \right)^2 + \frac{r}{2} \phi(x)^2 + g\phi(x)^4 + f\phi(x)^6 \right) \right]. \]  
\[ (28) \]

This is indeed the celebrated Ginzburg-Landau model of the 1-dimensional Ising systems of length \( L \). The action \( S[\phi] \) is called \( \phi^4 \)-action. We can use the instanton technique to deal with this model beyond the perturbative approach. We can, for instance, show that there is no ferromagnetic phase in 1-dimensional Ising systems in the thermodynamic limit by using the instanton technique [1].

B. Instantion and topology

The instanton we discussed is a kind of topological excitation in 1-dimensional space, called kink. By topological we mean that e.g., the classical path with 1 instanton and the path with 3 instantons are not connected by smooth deformation of the paths. So the paths with different instantons are topologically distinct. The higher dimensional topological excitations are called vortices(2D), monopoles(3D), and instantons(4D) [4]. These are playing important roles in modern physics and mathematics.

Appendix A: Evaluation of \( K \) [2]

The constant \( K \) appeared in Eq. (19) takes care of the subtlety of the zero mode accompanying the instanton when executing the path integral. \( K \) can be evaluated in the following way. First, notice that within the saddle-point approximation the path can be written as

\[ q(\tau) = q_d(\tau) + \sum_n r_n x_n(\tau), \]  
\[ \text{(A1)} \]

where \( q_d(\tau) \) is the classical path and \( r_n(\tau) \)s are the quantum fluctuations around \( q_d(\tau) \). Here \( x_n \)'s are a complete set of real orthonormal functions and vanish at the boundaries, that is,

\[ \int_0^\tau d\tau' x_n(\tau') x_m(\tau') = \delta_{nm}, \]  
\[ \text{(A2)} \]

\[ x_n(0) = x_n(\tau) = 0. \]  
\[ \text{(A3)} \]

Then, the Euclidean path integral Eq. (19) within the saddle-point approximation for can be rewritten as

\[ G^{(1)}(a, -a; \tau) \equiv e^{-\frac{\sqrt{2}}{\pi} \mathcal{N}} \int \prod_n \frac{dr_n}{\sqrt{2\pi h}} \exp \left[ -\frac{1}{h} \int_0^\tau d\tau' r_n \left( -m \left( \frac{d}{d\tau'} \right)^2 + \frac{\partial^2 V(q_d)}{\partial q^2} \right) r_n \right], \]  
\[ \text{(A4)} \]

where \( \mathcal{N} \) is the normalization factor introduced for using the more convenient measure, which in the end does not need to be evaluated [2]. When we perform the gaussian integration the tacit assumption is that the eigenvalues of the differential operator \( \left( m \frac{d}{d\tau} \right)^2 + \frac{\partial^2 V(q_d)}{\partial q^2} \) is positive. However we saw that there is a zero mode with eigenvalue 0 (see Eq. (13)). To see more explicitly let us differentiate the saddle-point equation (5) once more to give

\[ \left( -m \left( \frac{d}{d\tau} \right)^2 + \frac{\partial^2 V(q_d)}{\partial q^2} \right) \frac{dq_d}{d\tau} = 0. \]  
\[ \text{(A5)} \]
This suggests the second derivative appeared in the saddle-point approximation of the path integral Eq. (A4), that is, \(-m \left( \frac{d}{d\tau} \right)^2 + \frac{\partial^2 V(q_{cl})}{\partial q^2} \) has a zero mode, whose eigenfunction can be written as

\[ x_1(\tau) = \sqrt{\frac{m}{S_{in}}} \frac{dq_{cl}(\tau)}{d\tau}. \] (A6)

Here the normalization factor \( \sqrt{\frac{m}{S_{in}}} \) comes from Eq. (A2), that is

\[ \int_0^\tau d\tau' x_1(\tau') x_1(\tau') = \frac{1}{S_{in}} \int_0^\tau m \left( \frac{dq_{cl}(\tau)}{d\tau} \right)^2 = 1, \] (A7)

where we used Eq. (12). We cannot then perform the gaussian integration without encountering a disastrous infinity.

At this juncture let us remember that we have already performed the strange integration over \( x_1 \), the location of the instanton, in Eqs. (14) and (19). There is a relation between \( x_1 \) and \( \tau_1 \). On the one hand, the change of the path \( q(\tau) \) induced by a change in the location of the kink \( \tau_1 \) by \( d\tau_1 \) is

\[ dq(\tau) = \frac{dq_{cl}}{d\tau} d\tau_1. \] (A8)

On the other hand, from Eq. (A1), we have

\[ dq(\tau) = x_1 dr_1 = \frac{m}{S_{in}} \frac{dq_{cl}}{d\tau} dr_1. \] (A9)

Thus, we had effectively traded the disastrous integration over \( \tau_1 \) for the integration over \( \tau_1 \) by setting

\[ \frac{1}{\sqrt{2\pi\hbar}} dr_1 = \sqrt{\frac{S_{in}}{2\pi\hbar m}} d\tau_1. \] (A10)

With this identification of zero mode the path integral Eq. (A4) should have been written as

\[
G^{(1)}(a, -a; \tau) = e^{-\frac{\hbar}{2\pi}} \sqrt{\frac{S_{in}}{2\pi\hbar m}} \int_0^\tau d\tau_1 N \prod_{n=2}^\infty \frac{dr_n}{\sqrt{2\pi\hbar}} \exp \left[ \frac{1}{\hbar} \int_0^\tau d\tau' r_n \left( -m \left( \frac{d}{d\tau'} \right)^2 + \frac{\partial^2 V(q_{cl})}{\partial q^2} \right) r_n \right]
\]

\[ = e^{-\frac{\hbar}{2\pi}} \sqrt{\frac{S_{in}}{2\pi\hbar m}} N \frac{1}{\sqrt{\det' \left[ -m \left( \frac{d}{d\tau} \right)^2 + \frac{\partial^2 V(q_{cl})}{\partial q^2} \right]}}. \] (A11)

where by \( \det' \) we mean the determinant does not contain the contribution from the zero mode. On the other hand, the same formula with \( K \), Eq. (19), can be rewriting as

\[
G^{(1)}(a, -a; \tau) = e^{-\frac{\hbar}{2\pi}} \frac{m \omega}{\pi \hbar} e^{-\frac{\omega}{\hbar}} K
\]

\[ = e^{-\frac{\hbar}{2\pi}} \frac{1}{\sqrt{\det \left[ -m \left( \frac{d}{d\tau} \right)^2 + m\omega^2 \right]}} K. \] (A12)

Comparing Eqs (A11) and (A12), we have

\[ K = \sqrt{\frac{S_{in}}{2\pi\hbar m}} \left( \frac{\det' \left[ -m \left( \frac{d}{d\tau} \right)^2 + m\omega^2 \right]}{\det -m \left( \frac{d}{d\tau} \right)^2 + \frac{\partial^2 V(q_{cl})}{\partial q^2}} \right). \] (A13)

The factor of \( \hbar^{-\frac{1}{2}} \) is coming from the zero mode [2].
Appendix B: Validity of the dilute instanton gas approximation [1, 2]

We have argued that the instatons are all widely separated. We can verify this by the following argument. The strategy is to evaluate the typical number of instantons \( \langle n \rangle \) and to show that the number is indeed small with respect to the time \( \tau \to \infty \).

First the probability of having \( n \) instantons can be given, from Eq. (21), by

\[
P_n = \frac{1}{n!} (\tau Ke^{-\frac{2\pi n}{h}})^n \sum_{n, \text{odd}} \frac{1}{n!} (\tau Ke^{-\frac{2\pi n}{h}})^n.
\]

Thus the typical number of instantons \( \langle n \rangle \) can be evaluated as

\[
\langle n \rangle = \sum_{n, \text{odd}} n P_n = \frac{\sum_{n, \text{odd}} n \left( \tau Ke^{-\frac{2\pi n}{h}} \right)^n}{\sum_{n, \text{odd}} \frac{1}{n!} \left( \tau Ke^{-\frac{2\pi n}{h}} \right)^n} = \tau Ke^{-\frac{2\pi n}{h}}.
\]

Here we used for \( \langle n \rangle \gg 1 \) the even/odd distinction in the sum can be ignored. Then the density of the instatanton can be given by

\[
\frac{\langle n \rangle}{\tau} = Ke^{-\frac{2\pi n}{h}}.
\]

Since \( h \) is small the density is exponentially small; the average separation between instantons are indeed enormous.