Instantons and quantum tunneling

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(Dated: January 20, 2017)

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. INSTANTONS [1–4]

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

$$V(q) = \frac{k}{8a^2}\left(q^2 - a^2\right) \tag{1}$$

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

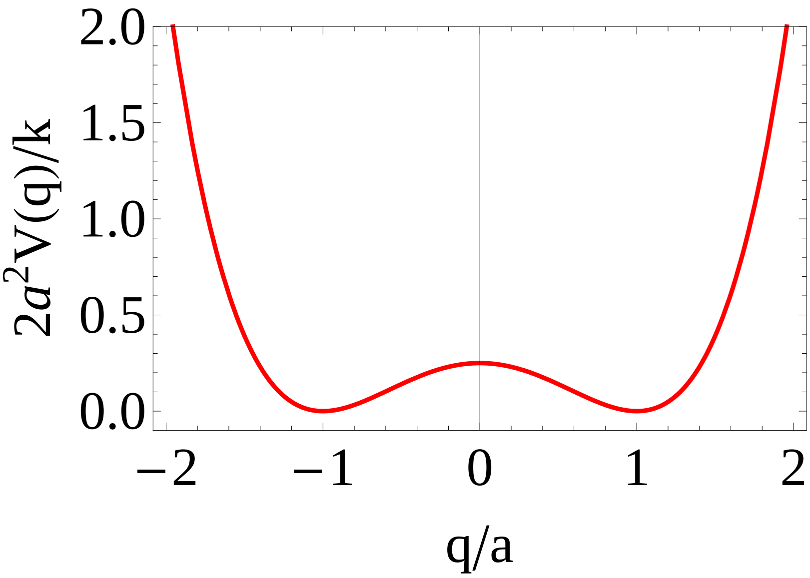

FIG. 1: A double-well potential.

Then we may conclude the quantum probability amplitude $\langle q = a, t | q = a, 0\rangle$ for the particle is the same as the

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particle in a simple harmonic potential;

$$
\begin{aligned}
G_{\mathrm{HO}}(a,a;t) = \langle q=a,t|q=a,0\rangle &= \langle q=a|\exp\left[-\frac{it}{\hbar}H\right]|q=a\rangle \\
&= \int Dq \exp\left[\frac{i}{\hbar}\int_0^t dt' \left(\frac{m}{2}\dot{q}(t')^2 - V(q(t'))\right)\right] \qquad (2)\\
&= \sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega t)}}\Theta(t). \qquad (3)
\end{aligned}
$$

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 mimima. Those paths associated with the quantum tunnelings are, however, classically forbidden. How can we incorporate those paths?

A. Euclidean path integral

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 τ and q as opposed to the Minkowski space spanned by t and q. We then define *Euclidean path integral* as

$$
\begin{aligned}
G_{\mathrm{E}}(a,a;\tau) = \langle q=a,\tau|q=a,0\rangle &= \langle q=a|\exp\left[-\frac{\tau}{\hbar}H\right]|q=a\rangle \\
&= \int Dq \exp\left[-\frac{1}{\hbar}\int_0^\tau d\tau' \left(\frac{m}{2}\dot{q}(\tau')^2 + V(q(\tau'))\right)\right] \\
&= \int Dq \exp\left[-\frac{1}{\hbar}S[q]\right]. \qquad (4)
\end{aligned}
$$

The stationary phase (saddle-point) equation, that is, the Euler-Lagrange equation, with respect to the imaginary time τ becomes

$$
-m\ddot{q}(\tau) + \frac{\partial V(q(\tau))}{\partial q(\tau)} = 0, \qquad (5)
$$

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.

B. Instantons

The classical paths emerged after the Wick rotaion can be viewed as the results of the creations and annihilations of a *instanton*. 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

$$
\int_0^\tau d\tau' \left(-m\ddot{q}\dot{q}\right) + \int_0^\tau d\tau' \left(\frac{\partial V(q)}{\partial q}\dot{q}\right) = 0. \qquad (6)
$$

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

$$
\int_0^\tau d\tau' \left(-m\ddot{q}\dot{q}\right) = \underbrace{\left[-m\dot{q}^2\right]_0^\tau}_{-m\dot{q}(\tau)^2 + m\dot{q}(0)^2 = -m\dot{q}(\tau)^2} - \int_0^\tau dt' \left(-m\ddot{q}\dot{q}\right) \qquad (7)
$$

and thus

$$
\int_0^\tau d\tau' \left(-m\ddot{q}\dot{q}\right) = -\frac{m}{2}\dot{q}(\tau)^2. \qquad (8)
$$

The second term on the left hand side of Eq. (6) gives

$$\int_0^\tau d\tau' \left(\frac{\partial V(q)}{\partial q}\frac{dq}{d\tau'}\right) = \int_{-a}^{q(\tau)} dq \frac{dV(q)}{dq} = V(q(\tau)) - \underbrace{V(-a)}_{0} = V(q(\tau)). \tag{9}$$

Thus we have, from Eq. (6),

$$\frac{m}{2}\dot{q_{cl}}^2 = V(q_{cl}). \tag{10}$$

The instanton action can then be given by

$$S_{\rm in} = \int_0^\tau d\tau' \left(\frac{m}{2}\dot{q_{cl}}^2 + \underbrace{V(q_{cl})}_{\frac{m}{2}\dot{q_{cl}}^2}\right) = \int_0^\tau d\tau' \frac{dq_{cl}}{d\tau'} m\dot{q_{cl}} = \int_{-a}^{q_{cl}(\tau)} dq_{cl}\sqrt{2mV(q_{cl})}. \tag{11}$$

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

We then proceed to explore the *temporal* features of the instantons. The solution of Eq. (10) with the boundary condition, $q_{cl}(\tau) = a$ at $\tau \to \infty$, is obtained by introducing a parameter τ_1 as

$$q_{cl}(\tau) = a \tanh\left(\frac{\omega(\tau - \tau_1)}{2}\right). \tag{12}$$

The solution, Eq. (12), reflects the time-translation invariance of the first integral Eq. (10), that is, τ_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 ω^{-1} around the *kink* at τ_1 as shown in Fig. 2. Here and hereafter the *temporal* extension of the instanton ω^{-1} is considered to be *short* with respect to $\tau \to \infty$.

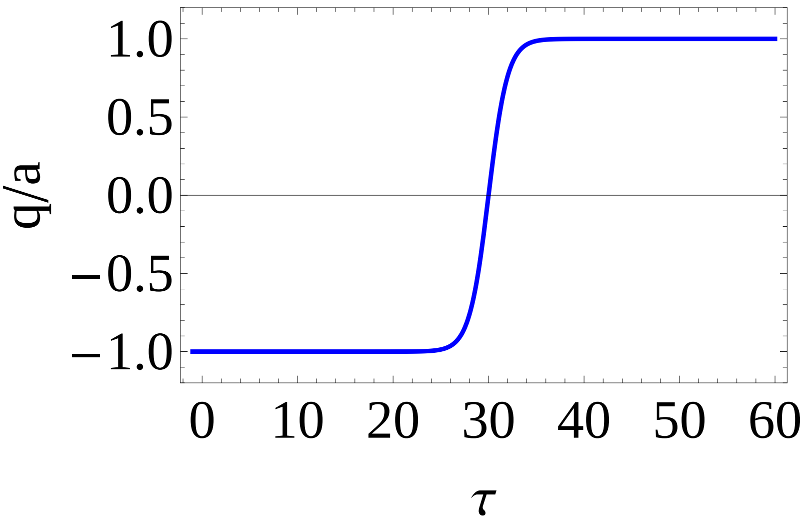

FIG. 2: A single instanton. Here the solution Eq. (12) with $\omega = 1$ and $\tau_1 = 30$ is shown.

1. *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 τ_1

$$G^{(1)}(a, -a; \tau) = \int_0^\tau d\tau_1 A_{1,cl}(\tau_1) \times A_{1,q}(\tau_1), \tag{13}$$

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 contibution 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 by

$$A_{1,q}(\tau_1) = \exp\left[-\frac{S_{\rm in}}{\hbar}\right] = \exp\left[-\frac{1}{\hbar}\left(\int_{-a}^{a} dq\sqrt{2mV(q)}\right)\right], \tag{14}$$

which completely dictates the classical action. Note that this contribution is independent on τ_1. Third contribution is from the quatum fluctuation accompanying with the instanton at τ_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 $\tau \to \infty$) as

$$\begin{aligned} G_{\rm q} &= \langle q=0,\tau|q=0,0\rangle \\ &= \langle q=a|\exp\left[-\frac{\tau}{\hbar}H\right]|q=0\rangle = \sum_n \langle q=0|n\rangle\langle n|q=0\rangle e^{-\frac{E_n\tau}{\hbar}} \\ &= \sqrt{\frac{m\omega}{2\pi i\hbar\sin(-i\omega\tau)}} = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega\tau)}} \\ &\cong \sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{\omega\tau}{2}}, \end{aligned} \tag{15}$$

Here we recognize that the lowest (ground-state, i.e., $n=0$) energy contribution becomes dominant as $\tau\to\infty$ and the grand-state wave function and the energy can be given by

$$|\langle q=0|n=0\rangle|^2 = \sqrt{\frac{m\omega}{\pi\hbar}} \tag{16}$$

$$E_0 = \frac{\hbar\omega}{2}, \tag{17}$$

respectively. Summing up all the contributions with a single instanton, the Euclidean path integral Eq. (13) becomes

$$G^{(1)}(a,-a;\tau) = \sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{\omega\tau}{2}}\left(Ke^{-\frac{S_{\rm in}}{\hbar}}\int_0^{\tau} d\tau_1\right), \tag{18}$$

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

2. *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 instanton gas approximation in Appendix B. We can then extend Eq. (18) to the one with n instantons as

$$G^{(n)}(a,-a;\tau) = \sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{\omega\tau}{2}}\left(K^n e^{-\frac{nS_{\rm in}}{\hbar}}\int_0^{\tau} d\tau_1\int_0^{\tau_1} d\tau_2\cdots\int_0^{\tau_{n-1}} d\tau_n\right), \tag{19}$$

where the classical instanton contribution becomes $e^{-\frac{nS_{\rm in}}{\hbar}}$ 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

$$G(a,-a;\tau) = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{\omega\tau}{2}} \sum_{n:\mathrm{odd}} K^n e^{-\frac{nS_{\mathrm{in}}}{\hbar}} \underbrace{\int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n}_{\frac{\tau^n}{n!}}$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{\omega\tau}{2}} \sum_{n:\mathrm{odd}} \frac{1}{n!} \left(\tau K e^{-\frac{S_{\mathrm{in}}}{\hbar}}\right)^n \tag{20}$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{\omega\tau}{2}} \sinh\left(\tau K e^{-\frac{S_{\mathrm{in}}}{\hbar}}\right). \tag{21}$$

II. REMARKS

A. 1-dimentional Ising magnets

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

$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta H}\right] = \int D\phi \exp\left[\underbrace{-\beta \int_0^L dx \left(\underbrace{\frac{1}{2}\left(\frac{\partial\phi(x)}{\partial x}\right)^2}_{\text{exchange interaction}} + \underbrace{\frac{r}{2}\phi(x)^2 + g\phi(x)^4}_{\text{double}-\text{well potential}} + \underbrace{f\phi(x)}_{\text{bias}}\right)}_{S[\phi]}\right]. \tag{22}$$

This is indeed the celebrated *Ginzburg-Landau* model of the 1-dimensional Ising systems of length L [1]. The action $S[\phi]$ is called ϕ^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 importnat roles in modern physics and mathematics.

III. PROBLEM

A. Tunnel splitting

We shall now see that the above instanton method can predict the tunnel splitting of the enegy 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 $\frac{\hbar\omega}{2}$ if there were no tunneling, but, as a result of the tunneling, the energies are *tunnel splitting* to become

$$\epsilon_S = \frac{\hbar\omega}{2} - \frac{\Delta\epsilon}{2} \tag{23}$$

$$\epsilon_A = \frac{\hbar\omega}{2} + \frac{\Delta\epsilon}{2}, \tag{24}$$

where $\Delta\epsilon$ stand for the tunnel splitting. Try calculate

$$G(a,-a;\tau) = \langle a| \left(\exp\left[-\frac{\tau}{\hbar}H\right]\right)(|S\rangle\langle S| + |A\rangle\langle A|)\,|a\rangle, \tag{25}$$

with $\langle a|S\rangle\langle S|-a\rangle = \frac{C}{2}$ and $\langle a|A\rangle\langle A|-a\rangle|^2 = -\frac{C}{2}$. Here $C = \sqrt{\frac{m\omega}{\pi\hbar}}$, the spread of the ground-state wave function appeared in Eq. (16). Compare the result with Eq. (21) and show that the tunneling splitting can be expressed as

$$\Delta\epsilon = 2\hbar K \exp\left[-\frac{S_{\rm in}}{\hbar}\right]. \tag{26}$$

Appendix A: Evaluation of K [2]

The constant K appeared in Eq. (18) 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

$$q(\tau) = q_{cl}(\tau) + \sum_n r_n x_n(\tau), \tag{A1}$$

where $q_{cl}(\tau)$ is the classical path and $r_n(\tau)$s are the quantum fluctuations around $q_{cl}(\tau)$. Here x_ns are a complete set of real orthonormal functions and vanish at the boundaries, that is,

$$\int_0^\tau d\tau' x_n(\tau')x_m(\tau') \;=\; \delta_{nm}, \tag{A2}$$

$$x_n(0) = x_n(\tau) \;=\; 0. \tag{A3}$$

Then, the Euclidean path integral Eq. (18) can be rewritten as

$$G_{\rm q} \cong e^{-\frac{S_{\rm in}}{\hbar}}\mathcal{N}\int\prod_n \frac{dr_n}{\sqrt{2\pi\hbar}}\exp\left[-\frac{1}{\hbar}\int_0^\tau d\tau' r_n\left(-m\left(\frac{d}{d\tau'}\right)^2 + \frac{\partial^2 V(q_{cl})}{\partial q^2}\right)r_n\right], \tag{A4}$$

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 $-\left(m\frac{d}{d\tau}\right)^2 + \frac{\partial^2 V(q_{cl})}{\partial q^2}$ is positive. However we saw that there is a zero mode with eigenvalue 0 (see Eq. (12)). To see more explicitly let us differentiate the saddle-point equation (5) once more to give

$$\left(-m\left(\frac{d}{d\tau}\right)^2 + \frac{\partial^2 V(q_{cl})}{\partial q^2}\right)\frac{dq_{cl}}{d\tau} = 0. \tag{A5}$$

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

$$x_1(\tau) = \sqrt{\frac{m}{S_{\rm in}}}\frac{dq_{cl}(\tau)}{d\tau}. \tag{A6}$$

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

$$\int_0^\tau d\tau' x_1(\tau')x_1(\tau') = \frac{1}{S_{in}}\underbrace{\int_0^\tau m\left(\frac{dq_{cl}(\tau)}{d\tau}\right)^2}_{S_{\rm in}} = 1, \tag{A7}$$

where we used Eq. (11). We cannot then perferm the gaussian integration without encountering a *disastrous infinity*.

At this juncture let us remember that we have already performed the strange integration over τ_1, the location of the instanton, in Eqs. (13) and (18). There is a relation between x_1 and τ_1. On the one hand, the change of the path $q(\tau)$ induced by a change in the location of the kink τ_1 by $d\tau_1$ is

$$dq(\tau) = \frac{dq_{cl}}{d\tau}d\tau_1. \tag{A8}$$

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

$$dq(\tau) = x_1 dr_1 = \underbrace{\sqrt{\frac{m}{S_{\rm in}}}\frac{dq_{cl}}{d\tau}}_{x_1} dr_1. \tag{A9}$$

Thus, we had effectively traded the disastrous integration over r_1 for the integration over τ_1 by setting

$$\frac{1}{\sqrt{2\pi\hbar}} dr_1 = \sqrt{\frac{S_{\rm in}}{2\pi\hbar m}} d\tau_1. \tag{A10}$$

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

$$\begin{aligned} G^{(1)}(a,-a;\tau) &= e^{-\frac{S_{\rm in}}{\hbar}} \underbrace{\sqrt{\frac{S_{\rm in}}{2\pi\hbar m}}\int_0^\tau d\tau_1}_{\text{zero mode}} \mathcal{N}\int\prod_{n=2}^{\infty}\frac{dr_n}{\sqrt{2\pi\hbar}}\exp\left[-\frac{1}{\hbar}\int_0^\tau d\tau' r_n\left(-m\left(\frac{d}{d\tau'}\right)^2 + \frac{\partial^2 V(q_{cl})}{\partial q^2}\right) r_n\right] \\ &= e^{-\frac{S_{\rm in}}{\hbar}} \sqrt{\frac{S_{\rm in}}{2\pi\hbar m}}\tau\mathcal{N}\frac{1}{\sqrt{\det'\left[-m\left(\frac{d}{d\tau'}\right)^2 + \frac{\partial^2 V(q_{cl})}{\partial q^2}\right]}}, \end{aligned} \tag{A11}$$

where by $\det'$ we mean the determinant does not contain the contibution from the zero mode. On the other hand, the same formula with K, Eq. (18), can be rewritting as

$$\begin{aligned} G^{(1)}(a,-a;\tau) &= e^{-\frac{S_{\rm in}}{\hbar}}\tau\left(\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{\omega\tau}{2}}\right)K \\ &= e^{-\frac{S_{\rm in}}{\hbar}}\tau\left(\mathcal{N}\frac{1}{\sqrt{\det\left[-m\left(\frac{d}{d\tau'}\right)^2 + m\omega^2\right]}}\right)K. \end{aligned} \tag{A12}$$

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

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

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 instanton can be given, from Eq. (20), by

$$P_n = \frac{\frac{1}{n!}\left(\tau K e^{-\frac{S_{\rm in}}{\hbar}}\right)^n}{\sum_{n:\rm odd}\frac{1}{n!}\left(\tau K e^{-\frac{S_{\rm in}}{\hbar}}\right)^n}. \tag{B1}$$

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

$$\langle n\rangle = \sum_{n:\rm odd} nP_n = \frac{\sum_{n:\rm odd}\frac{n}{n!}\left(\tau K e^{-\frac{S_{\rm in}}{\hbar}}\right)^n}{\sum_{n:\rm odd}\frac{1}{n!}\left(\tau K e^{-\frac{S_{\rm in}}{\hbar}}\right)^n} = \tau K e^{-\frac{S_{\rm in}}{\hbar}}. \tag{B2}$$

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

$$\frac{\langle n\rangle}{\tau} = K e^{-\frac{S_{\rm in}}{\hbar}}. \tag{B3}$$

Since $\hbar$ is small the density is exponentially small; the average separation between instantons are indeed enormous.

[1] A. Altland and B. D. Simons, *Condensed Matter Field Theory*, 2nd ed. (Cambridge University Press, Cambridge, 2010).
[2] Sidney Coleman, *Aspect of Symmetry*, (Cambridge University Press, Cambridge 1985), Chapter 7.
[3] Xiao-Gang Wen, *Quantum Field Theory of Many-Body Systems*, (Oxford University Press, Oxford, 2004).
[4] A. Zee, *Quantum Field Theory in a Nutshell*, (Princeton University Press, Princeton, 2003).