Instantonic approach to triple well potential

Soo-Young Lee\textsuperscript{a}, Jae-Rok Kahng\textsuperscript{a}, Sahng-Kyoon Yoo\textsuperscript{b}, D.K.Park\textsuperscript{c}, C.H.Lee\textsuperscript{d}, Chang Soo Park\textsuperscript{e}, Eui-Soon Yim\textsuperscript{f}

\textsuperscript{a} Department of Physics, College of Science, Korea University, Seoul 136-701, Korea
\textsuperscript{b} Department of Physics, Seonam University, Namwon, Chunbuk 590-170, Korea
\textsuperscript{c} Department of Physics, Kyungnam University, Masan 631-701, Korea
\textsuperscript{d} D\&S Dept., R\&D Center, Anam Industrial CO., LTD, Seoul 133-120, Korea
\textsuperscript{e} Department of Physics, Dankook University, Cheonan 330-180, Korea
\textsuperscript{f} Department of Physics, Semyung University, Cheonan 390-230, Korea

(February 7, 2022)

Abstract

By using a usual instanton method we obtain the energy splitting due to quantum tunneling through the triple well barrier. It is shown that the term related to the midpoint of the energy splitting in propagator is quite different from that of double well case, in that it is proportional to the algebraic average of the frequencies of the left and central wells.
I. INTRODUCTION

The Euclidean time formalism of path integral has been applied successfully to the problems in which quantum tunneling occurs \[1,2\]. In most cases, their results are consistent with the WKB approximation \[3\] as well as numerical calculations \[4\]. Recently much attention has been paid to periodic instanton method \[5,6\] which can be applied to high-energy quantum tunneling and has a possibility to explore the baryon- and lepton-number violation in electroweak theory. Furthermore, there is another approach called valley instanton method that allows exploration of the quantum tunneling from false to true vacua \[7,8\].

In general the Euclidean time formalism gives the information about the ground state, i.e., the ground state wavefunction and the ground state energy. In the case of double well, it allows applications of path integral by opening a possibility of finding a classical path in Euclidean space, and explains quantum tunneling through the barrier between wells resulting in an energy splitting of the degenerate ground states. This energy splitting was also investigated through the WKB approximation and numerical calculation as well as through the path integral with Euclidean time(instanton method). These results are consistent with each other and it was conjectured that the instanton method may give more exact result than the WKB approximation\[3\].

We here consider a triple well potential on the ground of the instanton method. For simplicity, we take the triple well potential in the following form;

$$V(\phi) = \alpha \phi^2 (\phi - \beta)^2 (\phi + \beta)^2.$$  \hspace{1cm} (1.1)

This potential has three wells among which two side wells have topologically identical vacua, and central well is rather broader as shown in Fig. 1. This potential form may be realized by designing supperlattices with different compound compositions whose applications might come true in electronic devices such as laser without inversion \[9\]. Therefore, understanding the structure of the energy level, which influences the dynamics of electrons, is essential in constructing electronic devices.

Compared with the double well case, there are two different aspects. Firstly, the energy spectrum forms discrete blocks, each of which is composed of three levels. The level located in the middle of each block has different symmetry; for example, energy levels in the lowest block is arranged in the order of even, odd and even states in energy. Secondly, the central vacuum is not identical with the others locating at the sides. This indicates that the structure of the block can be adjusted by changing the curvature of the central vacuum. This aspect might be important in practical electronic engineering.

In this paper we obtain the central position and width of the lowest block, i.e., energy splitting, and partial information about the wavefunctions of the lowest block using the instanton method. The term related to the midpoint of energy splitting turns out to be proportional to algebraic average of the frequencies of the left and central wells. In Sec.II, we find out what physical quantities are related to the propagator with large Euclidean time. One instanton contribution to the propagator is calculated in Sec.III, and in order to obtain a desired form of the propagator we use the dilute gas approximation for the configurations composed of multi-instantons and anti-instantons in Sec.IV. In Sec.V a brief conclusion is given. Throughout this paper, we take $\hbar = 1$ and the mass $m = 1$ for simplicity.
II. PROPAGATOR AT LARGE EUCLIDEAN TIME

We consider a triple well problem in which barriers are so high that at least one discrete eigenvalue can exist below the barrier height. Generally in the case of triple well potential, an energy level is split into three levels with slightly different energy values due to the quantum tunneling through barriers.

Let $|L_0 >$, $|C_0 >$, and $|R_0 >$ denote the normalized lowest energy eigenstates of the isolated left, central, and right well, respectively. When barriers are appropriately high and wide, the three lowest eigenstates in triple well can be obtained as following through a variational method [10],

$|E'_0 > \approx \frac{1}{\sqrt{2 + a_+^2}}(|L_0 > + a_+|C_0 > + |R_0 >)$ (2.1)

$|E'_1 > \approx \frac{1}{\sqrt{2}}(|L_0 > - |R_0 >)$ (2.2)

$|E'_2 > \approx \frac{1}{\sqrt{2 + a_-^2}}(|L_0 > - a_-|C_0 > + |R_0 >)$ (2.3)

where

$a_\pm \equiv \frac{1}{2} \left[ \pm \frac{H_{LL} - H_{CC}}{|H_{LC}|} + \sqrt{\left( \frac{H_{LL} - H_{CC}}{|H_{LC}|} \right)^2 + 8} \right]$ (2.4)

Here,

$H_{LL} \equiv < L_0 | H | L_0 >$, $H_{CC} \equiv < C_0 | H | C_0 >$, $H_{LC} \equiv < L_0 | H | C_0 >$, (2.5)

where $H$ is the total Hamiltonian. In getting these states, we use the fact that the ground state wavefunctions of each well are taken to be almost separated due to large potential barriers and there is a two-fold symmetry. The lowest three eigenstates in Eqs.(2.1-2.3) are orthogonal to each other and have following eigenvalues:

$< E'_0 | H | E'_0 > \equiv E'_0 \approx \frac{2H_{LL} + a_+^2H_{CC} - 4a_+|H_{LC}|}{2 + a_+^2}$ (2.6)

$< E'_1 | H | E'_1 > \equiv E'_1 \approx H_{LL}$ (2.7)

$< E'_2 | H | E'_2 > \equiv E'_2 \approx \frac{2H_{LL} + a_-^2H_{CC} + 4a_-|H_{LC}|}{2 + a_-^2}$ (2.8)

If the curvatures of the potential with three vacua are equivalent, then this problem is reduced to three-fold degenerate one. In this case, $H_{LL} = H_{CC}$ and $a_\pm = \sqrt{2}$. Thus the lowest energy eigenstate is split into three eigenstates having equal spacing $\Delta E = \sqrt{2}|H_{LC}|$ between the eigenvalues.

It is well known that for a large Euclidean time interval the propagator gives the information of the ground state energy. In the triple well case, the propagator from left($\phi_i$) to central vacuum($\phi_f$) is approximately described as follows:

$< \phi_f | e^{-2HT} | \phi_i > \approx \sum_{j=0}^{2} < \phi_f | E'_j > < E'_j | \phi_i > e^{-2E'_j T}$. (2.9)
Here, since the wave function of the state $|E'_1\rangle$ is odd, $<\phi_f|E'_1\rangle$ vanishes, and the coefficients of the terms corresponding to $j = 0$ and $j = 2$ in the Eq.(2.9) are equal, that is,

$$\frac{2a_+}{2 + a_+^2} = \frac{2a_-}{2 + a_-^2} = \frac{2}{\sqrt{(H_{LL} - H_{CC})^2 + 8}}. \tag{2.10}$$

Then, the propagator becomes

$$<\phi_f|e^{-2HT}|\phi_i> \simeq \frac{2}{\sqrt{(H_{LL} - H_{CC})^2 + 8}} <\phi_f|C_0><L_0|\phi_i>e^{-2ET}\sinh 2\Delta ET, \tag{2.11}$$

where

$$E \equiv \frac{E'_0 + E'_2}{2}, \quad \Delta E \equiv \frac{E'_2 - E'_0}{2}. \tag{2.12}$$

This result shows that, in the case of triple well, the propagator for large Euclidean time $T$ tells us about the width and the central position of the lowest energy block.

In the following sections we will calculate the propagator by using the instanton method, and show that the propagator with the dilute instanton gas approximation takes the same form as Eq.(2.11).

### III. ONE-INSTANTON CONTRIBUTION

In the present section we will calculate the one-instanton contribution to the propagator. The Euclidean propagator from $(\phi_i, -T)$ to $(\phi_f, T)$ is written as

$$<\phi_f|e^{-2HT}|\phi_i> = \int_{\phi_i}^{\phi_f,T} D\phi e^{-S_E[\phi]}, \tag{3.1}$$

where the Euclidean action is

$$S_E[\phi] = \int_{-T}^{T} d\tau \left[ \frac{1}{2}\dot{\phi}^2 + V(\phi) \right]. \tag{3.2}$$

The path giving major contribution is determined by the classical equation of motion, i.e., $\delta S_E/\delta \dot{\phi} = 0$. For the triple well potential in Eq.(1.1) whose central well is wider than the side wells, the equation of motion becomes

$$\ddot{\phi} = \frac{\partial V(\phi)}{\partial \phi} = 2\alpha\phi(3\phi^4 - 4\beta^2\phi^2 + \beta^4). \tag{3.3}$$

The classical solution of this equation of motion, so-called instanton, is

$$\phi_{cl}(\tau) = \frac{-\beta}{\sqrt{1 + e^{2\beta^2\sqrt{2\alpha}(\tau - \tau_0)}}}. \tag{3.4}$$

We here take a boundary condition as $\phi_i = -\beta$ and $\phi_f = 0$ (from left to central vacuum). Substituting the solution into Eq.(3.2), and taking a $T \to \infty$ limit, we obtain
\[
\lim_{T \to \infty} S_E[\phi_{cl}] = \frac{\sqrt{2}\alpha \beta^4}{4}.
\]

(3.5)

In order to evaluate the contribution of paths neighboring on the instanton solution to the propagator, we define

\[
\phi(\tau) = \phi_{cl}(\tau) + \eta(\tau),
\]

(3.6)

where \( \eta(\tau) \) is an arbitrary function satisfying a boundary condition:

\[
\eta(-T) = \eta(T) = 0.
\]

(3.7)

Now the action can be divided into the two parts: one from instanton and the other from the paths neighboring on the instanton. Therefore, the total action becomes

\[
S_E = S_E[\phi_{cl}] + \int_{-T}^{T} d\tau \left[ \frac{1}{2} \dot{\eta}^2 + \alpha Y(\tau) \eta^2 \right],
\]

(3.8)

where

\[
Y(\tau) \equiv 15\phi_{cl}^4(\tau) - 12\beta^2 \phi_{cl}^2(\tau) + \beta^4.
\]

(3.9)

In Eq.(3.8), we keep up to the second order terms of \( \eta \). Then the propagator can be written as

\[
<0|e^{-\frac{1}{2}HT} - \beta|0> = e^{-S_E[\phi_{cl}]} I(T),
\]

(3.10)

where

\[
I(T) = \int_{(-T,0)}^{(T,0)} D\eta e^{-\int d\tau M\eta},
\]

(3.11)

and

\[
\dot{M} = -\frac{1}{2} \frac{d^2}{d\tau^2} + \alpha Y(\tau).
\]

(3.12)

Our next task is to calculate the functional integral \( I(T) \) which has approximated to a Gaussian form. This is, however, not simple because it contains a zero mode, which is easily seen from the fact,

\[
\dot{M}\phi_{cl}(\tau) = 0.
\]

(3.13)

It indicates that \( \dot{\phi}_{cl}(\tau) \) is the eigenvector corresponding to zero eigenvalue of \( \dot{M} \). Therefore, the zero mode should be treated carefully in calculating \( I(T) \). Here we follow the method used by Gildener and Patrascioiu [3] in performing the functional integral.

Let the eigenfunctions and corresponding eigenvalues of \( \dot{M} \) be \( \psi_m \) and \( \varepsilon_m \), respectively,

\[
\dot{M}\psi_m = \varepsilon_m \psi_m.
\]

(3.14)

Then the small fluctuating path \( \eta(\tau) \) can be expanded as a linear combination of the eigenfunctions:
\[ \eta(\tau) = \sum_m c_m \psi_m(\tau). \] (3.15)

In the Gaussian functional integral \( I(\tau) \), the integral variable \( \eta \) can now be changed to the coefficients \( c_m \), which gives a formal solution including the Jacobian in the form

\[ I(T) = | \frac{\partial \eta}{\partial c_n} | \int \prod_m dc_m e^{-\sum_m \varepsilon_m c_m^2} \]
\[ = | \frac{\partial \eta}{\partial c_n} | \prod_{m=0}^{\infty} \sqrt{\frac{\pi}{\varepsilon_m}}. \] (3.16)

To surmount the difficulty of the zero mode, one can use the collective coordinate method, which gives

\[ I(T) = 2T \sqrt{S_E[\phi_{cl}]} I_0, \] (3.17)

where

\[ I_0 \equiv | \frac{\partial \eta}{\partial c_n} | \prod_{m=1}^{\infty} \sqrt{\frac{\pi}{\varepsilon_m}}. \] (3.18)

In order to find an explicit expression for \( I_0 \) we use the method of changing variables [11]. Then the functional integral \( I(T) \) can be represented as

\[ I(T) = \left( 2\pi N(T) N(-T) \int_{-T}^{T} \frac{d\tau}{N^2(\tau)} \right)^{-1/2}, \] (3.19)

where

\[ N(\tau) = \dot{\phi}_{cl} = \frac{\beta^3 \sqrt{2\alpha} e^{2\beta^2 \sqrt{2\alpha} \tau}}{(1 + e^{2\beta^2 \sqrt{2\alpha} \tau})^{3/2}}. \] (3.20)

For large \( T \), this becomes

\[ I(T) = \beta \left( \frac{2}{\pi} \sqrt{2\alpha} \right)^{1/2} e^{-\frac{1}{2} \beta^2 \sqrt{2\alpha} T}. \] (3.21)

Comparing Eq.(3.21) with Eq.(3.16) and Eq.(3.18), we obtain

\[ I_0 = \frac{\beta}{\pi} (2\beta^2 \sqrt{2\alpha} \varepsilon_0)^{1/2} e^{-\frac{1}{2} \beta^2 \sqrt{2\alpha} T}. \] (3.22)

Imposing the boundary condition, \( \psi_n(-T) = \psi_n(T) = 0 \), yields the lowest energy \( \varepsilon_0 \) in WKB approximation at large \( T \)[3] as

\[ \varepsilon_0 = 8\alpha \beta^4 e^{-2\beta^2 \sqrt{2\alpha} T}. \] (3.23)

Inserting this into Eq.(3.22), we get

\[ I_0 = \frac{4\beta^3}{\pi} (\alpha \sqrt{2\alpha})^{1/2} e^{-\frac{1}{2} \beta^2 \sqrt{2\alpha} T}. \] (3.24)
From Eq.(3.17), therefore, the final form of the functional integral $I(T)$ is expressed in the form

$$I(T) = \frac{8}{\pi} \beta^3 T \sqrt{S_E[\phi_{cl}]} (\alpha \sqrt{2 \alpha})^{1/2} e^{-\frac{1}{2} \beta^2 \sqrt{2 \alpha} T}.$$  \hspace{1cm} (3.25)

In the case of double well, it is well known that the exponent in the exponential function is closely related to the curvature of vacuum, that is, if the second derivative of the double well potential at vacuum positions is $\omega^2$, then the exponential function is given by $e^{-\omega T}$. However, in our triple well potential the curvature of the side vacua is different from that of the central vacuum (Fig.1). Note that in this case the exponent is also related to the potential curvatures at the vacuum positions in a way of algebraic averaging, that is,

$$\omega \equiv \frac{\omega_1 + \omega_2}{2} = \frac{3}{2} \beta^2 \sqrt{2 \alpha} \hspace{1cm} (3.26)$$

where

$$\omega_1 \equiv V''(-\beta) = 8 \alpha \beta^4, \quad \omega_2 \equiv V''(0) = 2 \alpha \beta^4. \hspace{1cm} (3.27)$$

As will be seen shortly, $\omega/2$ is the central position of the energy block composed of three almost degenerate lowest levels.

From Eq.(3.10), the contribution of one instanton to the propagator becomes

$$<0|e^{-2HT}|-\beta> = 2\kappa T \sqrt{S_E[\phi_{cl}]} \sqrt{\frac{\omega}{\pi}} e^{-S_E[\phi_{cl}]} e^{-\omega T}, \hspace{1cm} (3.28)$$

where

$$\kappa \equiv 4 \beta^4 \sqrt{\frac{2 \alpha}{3 \pi}}. \hspace{1cm} (3.29)$$

In the next section the contribution of multi-instanton to the propagator will be explored.

**IV. MULTI-INSTANTON CONTRIBUTION**

In the previous section we consider the contribution of the stationary solution(instanton) and its neighboring paths. However, since the path integral in Eq.(3.11) includes all possible paths starting from $(-\beta, -T)$ and ending at $(0, T)$, let us consider the paths consisting of $n_1$ instantons and $n_2$ anti-instantons which are located at large distance with each other in Euclidean time so that the interaction between them can be ignored. In order to satisfy the boundary condition, the number of instanton must be one larger than that of anti-instanton. Furthermore, since the total number of possible configurations is $2^{n_2}$, the multi-instanton contribution to the propagator is

$$<0|e^{-2HT}|-\beta>$$

$$= \sum_{n_1=1}^{\infty} \sum_{n_2=0}^{\infty} c_{n_1-n_2,1} \frac{2^{n_2}}{(n_1 + n_2)!} e^{-(n_1+n_2)S_E[\phi_{cl}]} (2\kappa T \sqrt{S_E[\phi_{cl}]})^{n_1+n_2} \sqrt{\frac{\omega}{\pi}} e^{-\omega T}$$

$$= 2\kappa T \sqrt{S_E[\phi_{cl}]} \sqrt{\frac{\omega}{\pi}} e^{-\omega T} e^{-S_E[\phi_{cl}]} \sum_{n=0}^{\infty} \frac{[2e^{-2S_E[\phi_{cl}]} (2\kappa T \sqrt{S_E[\phi_{cl}]})^2]^n}{(2n+1)!}.$$  \hspace{1cm} (4.1)
Using the identity,
\[ \sum_{n=0}^{\infty} \frac{x^n}{(2n+1)!} = \frac{1}{\sqrt{x}} \sinh \sqrt{x}, \]
the infinite sum in Eq.(4.1) is represented by a hyperbolic sine function. Therefore, the final result is of the following form,

\[ <0| e^{-2HT} | - \beta > = \sqrt{\frac{\omega}{2\pi}} e^{-\omega T} \sinh (2\sqrt{2\kappa T} \sqrt{S_E[\phi_{cI}] e^{-S_E[\phi_{cI}]}}). \] (4.3)

Comparing this result with Eq.(2.11), we get the central position \( E \) and the width \( 2\Delta E \) of the lowest energy block in terms of potential parameters, \( \alpha \) and \( \beta \), which are

\[ E = \frac{3}{4} \beta^2 \sqrt{2\alpha} \] (4.4)

and

\[ \Delta E = \sqrt{\frac{8}{3\pi}} (2\alpha)^{3/4} \beta^4 e^{-\frac{1}{4} \beta^4 \sqrt{2\alpha}}. \] (4.5)

For sufficiently large \( \beta \), in other words, both large well separation and high potential barrier, the energy splitting decreases exponentially as expected. Moreover, the product of the amplitudes of the ground state wavefunction at vacuum positions is expressed as

\[ <0| E'_0 | - \beta > = \frac{\beta}{4} \left( \frac{3}{\pi} \sqrt{2\alpha} \right)^{1/2}. \] (4.6)

V. CONCLUSION

The quantum tunneling for the triple well potential case is investigated by means of the instanton method. Unlike the case of double well potential, the curvature of the central well is topologically different from those of the others, which results in the fact that the midpoint of energy splitting is proportional to the algebraic average of the frequencies of the left and central wells. We also obtained the energy splitting \( \Delta E \) of the lowest block. Although this kind of approach can be extended to the \( n \)-tuple \((n > 3)\) well, much complication in counting the possible configuration gets involved. In the case of quadruple well, for example, two different types of instanton and anti-instanton solutions should be considered carefully. The study about this subject is in progress.

ACKNOWLEDGEMENT

This work was supported in part by Nondirected Research Fund, Korea Research Foundation, 1995 and by Korea Science and Engineering Foundation (961-0201-005-1).
REFERENCES

[1] S.Coleman, "The uses of Instantons", in The why's of subnuclear physics, ed. A.Zichichi (Plenum, New York, 1979).
[2] R.Rajaraman, Solitons and Instantons, (North-Holland, the Netherlands, 1987).
[3] E.Gildener and A.Patrascioiu, Phys. Rev. D16, 423 (1977).
[4] K.Banerjee and S.P.Bhatnagar, Phys. Rev. D18, 4767 (1978).
[5] S.Yu.Khlebnikov, V.A.Rubakov, and P.G.Tinyakov, Nucl. Phys. B367, 334 (1991).
[6] J.Q.Liang and H.J.W.Müller-Kirsten, Phys. Rev. D50, 6519 (1994); 51, 718 (1995).
[7] H.Aoyama, T.Harano, M.Sato, and S.Wada, Nucl. Phys. B466, 127 (1996).
[8] H.Aoyama, T.Harano, H.Kikuchi, M.Sato, and S.Wada, hep-th/9606159.
[9] S.E.Harris, Phys. Rev. Lett. 62, 1033 (1989).
[10] R.L.Liboff, Introductory Quantum Mechanics, (Addison-Wesley Publishing Company, Inc. 1992).
[11] R.F.Dashen, B.Hasslacher, and A.Neveu, Phys. Rev. D10, 4114 (1974).
FIGURES

FIG. 1. Triple well potential as a function of position.
\[ V(\phi) = \frac{4\alpha\beta^6}{27} \]

The diagram shows the potential function \( V(\phi) \) as a function of \( \phi \), with critical points at \( -\beta \), \( -\beta/3^{1/2} \), \( 0 \), \( \beta/3^{1/2} \), and \( \beta \). The value of the potential function at these points is labeled.