Tunneling in asymmetric double well: instanton calculus

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Abstract

The level splitting formula of an asymmetric double well potential is calculated taking into account the multi-instanton contributions (dilute gas approximation). Results can be related with known semiclassical ones obtained with a truncated hamiltonian, and the symmetric case is easily recovered provided we consider the right limit.

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Instanton calculations when applied in Quantum Mechanics result powerful methods to build semiclassical approximations, see e.g. the lecture from Coleman [1]. Regretly, summation of all the multinstanton contributions in a problem can be hard work, and there are only a few examples in the literature, mainly for highly symmetrical potentials [3]. When the symmetry disappears, it is usually need a fully explicit path integral calculation, with no shorter ways. This could explain the minimal implementation this technique appears to have in more applied physics.

But focusing some less symmetrical potentials, simplified summation is also possible, if we assume the series to be enough kindly comported. We show here one possibility for the simplest asymmetric example, a double well

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with different values ω_0, ω_1, for V'' on the minima (see figure 1; think by example on the sextic potential $\lambda x^2(x-2)^4$). Here the fluctuations around the minima have different contributions, $\frac{1}{2}\omega_1 > \frac{1}{2}\omega_0$, so the n-instanton contribution can not be directly factorized as usually it is made, taking the integral on zero modes apart.

Our method will rearrange the n-instanton integrals in such form that a recursive definition can be given for all the family, then obtaining the summation from recurrence equations. Only the path between both minimum is calculated, as this is enough to show the general strategy. A graphical picture is suggested to follow more easily the discussion.

We are going first to calculate the contribution M_i of the multinstanton composed of $i+1$ instantons $\omega_0 \rightarrow \omega_1$ and i antinstantons $\omega_1 \rightarrow \omega_0$. Its integral is:

$$\begin{aligned} M_i &= N\ K^{2i+1} A^{2i+1} \int_{\frac{-T}{2}}^{\frac{T}{2}} dt_1 \int_{t_1}^{\frac{T}{2}} dt_2 ... \qquad (1) \\ & ... \int_{t_{2i}}^{\frac{T}{2}} dt_{2i+1} e^{-\frac{1}{2}\omega_0(t_1-(-\frac{T}{2}))} e^{-\frac{1}{2}\omega_1(t_2-t_1)} e^{-\frac{1}{2}\omega_0(t_3-t_2)} ... e^{-\frac{1}{2}\omega_1(\frac{T}{2}-t_{2i+1})} \end{aligned}$$

where as usual N is the normalization constant, K is the one-instanton contribution, and A is the exponential of the classical action for one instanton.

Note that N and K are usually calculated (or pulled away) by relating them to the harmonic oscillator solution. This is unimportant for our discussion and we are going to leave out N in the following. Note also that we have taken equal contributions for instanton and antinstanton, as we have put the relevant differences in the integral term.

The integrand in (1) being factorizable, we could try to solve the integral going to complex variable, as it is indicated in any handbook (by example, [2]) but no garantees are given. Now if we put $B \equiv KA,\ t \equiv (t_1-t_2)+(t_3-t_4)+...+t_{2i+1}$ we can see the integral in a more suitable form

$$M_i = B^{2i+1} \int_{-T/2}^{T/2} dt_1 \int_{t_1}^{T/2} dt_2 ... \int_{t_{2i}}^{T/2} dt_{2i+1} e^{\omega_0(T/2+t)} e^{\omega_1(t-T/2)} \qquad (2)$$

in which we can rearrange limits and sum up some integrals (see again [2], 3.3.4), so it rest:

$$M_i = B^{2i+1} e^{-\frac{1}{2}\frac{\omega_0+\omega_1}{2}T} \int_{\frac{-T}{2}}^{\frac{T}{2}} dt\ e^{\frac{\omega_0-\omega_1}{2}t} \frac{(T/2+t)^i}{i!} \frac{(T/2-t)^i}{i!} \qquad (3)$$

For the symmetrical well $\frac{\omega_0-\omega_1}{2} \to 0$ and (3) is simply Euler' Beta function, which evaluates to $\frac{T^{2i+1}}{2i+1!}$, the expected zero-mode contribution. Of course, (3) could be postulated on physical asumptions, $(T/2{+}t)$ and $(T/2{-}t)$ being the time the instanton stays at each vacuum; but we found useful to point out the derivation process.

Now, we choose not to evaluate this integral, and we make a simultaneous study of integrals of the kind

$$I(n,m) = B^{n+m+1} e^{-\frac{1}{2}\frac{\omega_0+\omega_1}{2}T} \int_{-T/2}^{T/2} dt\; e^{\delta t} \frac{(T/2+t)^n}{n!} \frac{(T/2-t)^m}{m!} \tag{4}$$

Integrating by parts we can give the following recursive definition for all the family:

$$I(0,0) = \frac{B}{\delta}[e^{\frac{1}{2}\delta T} - e^{-\frac{1}{2}\delta T}] \tag{5}$$

$$I(n,0) = \frac{B}{\delta}[e^{\frac{1}{2}\delta T}\frac{(BT)^n}{n!} - I(n-1,0)] \tag{6}$$

$$I(0,m) = \frac{B}{\delta}[I(0,m-1) - e^{-\frac{1}{2}\delta T}\frac{(BT)^m}{m!}] \tag{7}$$

$$I(n,m) = \frac{B}{\delta}[I(n,m-1) - I(n-1,m)] \tag{8}$$

which can be seen in a pictorial form by putting the integrals in a triangle (figure 2), such that each integral is obtained by substracting the two above it and putting an additional factor B/δ.

So, $I(n,m)$ can be directly calculated by inspecting the triangle, counting and weighting the number of paths from each term in the sides. The result is:

$$\begin{aligned} I(n,m) &= e^{-\frac{1}{2}\omega_0 T} \sum_{i=0}^{i=n} \binom{m+n-i}{m} (-1)^{n-i} (\frac{B}{\delta})^{n+m-i+1} \frac{(BT)^i}{i!} + \\ &+ e^{-\frac{1}{2}\omega_1 T} \sum_{j=0}^{j=m} \binom{m+n-j}{n} (-1)^{n+1} (\frac{B}{\delta})^{n+m-j+1} \frac{(BT)^j}{j!} \end{aligned} \tag{9}$$

We could again be tempted, now of using (9) to sum all the multinstanton contributions. But it results that we can avoid it by newly inspecting the triangle and fixing our attention on sums of columns, which must, as everything in these combinatorial triangles, own some interesting properties.

Let $S(n,m)$ be the sum of a column $\sum_{i=0} I(n+i,m+i)$, and let $S_j^{\pm}(n,m)$ be the coefficient of $S(n,m)$ associated to the term $\frac{(BT)^j}{j!}e^{\pm\delta T/2}$. Grafically (see figure 3) we find some relations between sums:

$$
\begin{aligned}
S_i(n,m) = & \quad \frac{B}{\delta}[S_i(n,m-1) - S_i(n-1,m)] && (10)\\
S_i^+(n,m) = & \quad S_{i+1}^+(n+1,m) && (11)\\
n < i \Rightarrow S_i^+(n,m) = & \quad S_i^+(i, m+(i-n)) && (12)\\
S_i^+(i,m) = & \quad \frac{B}{\delta}[S_i^+(i,m-1) - S_i^(i,m+1)] = && (13)\\
= & \quad \frac{B}{\delta}[S_{i-1}^+(i-1,m-1) - S_{i+1}^(i+1,m+1)]
\end{aligned}
$$

In particular, this last rule (13), when applied to the central column, lets us to formulate a recurrence equation for the coefficients $a_i^{\pm} \equiv S_i^{\pm}(i,i)$ of the series of powers in $\frac{(BT)^j}{j!}$. Symply put, we get:

$$
a_{i+1}^{\pm} = a_{i-1}^{\pm} \mp \frac{\delta}{B} a_i^{\pm} \tag{14}
$$

which corresponds to the series produced by a lineal combination of two exponentials $C_+e^{\alpha_+} + C_-e^{\alpha_-}$.

Let us to make it explicitly for the S^+ terms. In this case the coefficients in the exponentials are:

$$
\alpha_{\pm} = -\frac{\delta}{2B} \pm \sqrt{(\frac{\delta}{2B})^2 + 1} \tag{15}
$$

and it rests to fix C_+, C_-; we can made it from the two first terms of the serie, which obviusly fulfill:

$$
\begin{aligned}
a_0 = & \quad C_+ + C_- && (16)\\
a_1 = & \quad -(C_+ + C_-)\frac{\delta}{2B} + (C_+ - C_-)\sqrt{(\frac{\delta}{2B})^2 + 1} && (17)
\end{aligned}
$$

So, we finally need to sum two series,

$$
\begin{aligned}
a_0 = \sum_{i=0} \binom{2i}{i} (-1)^i \left(\frac{B}{\delta}\right)^{2i+1} &= \frac{B}{\delta} \sum_{i=0} \frac{1}{2} .. \frac{2i-1}{2} (-1)^i \frac{(2B/\delta)^{2i}}{i!} && (18)\\
a_1 = \sum_{i=0} \binom{2i-1}{i-1} (-1)^{i-1} \left(\frac{B}{\delta}\right)^{2i} &= \sum_{i=1} \frac{1}{2} .. \frac{2i-1}{2} (-1)^{i-1} 2^{2i-1} \frac{(2B/\delta)^{2i}}{i!} && (19)
\end{aligned}
$$

but we can acomplish it by simply browsing across any handbook and remembering the expansion of $(1+x)^{-1/2}$, and we obtain:

$$a_0 = \frac{1}{2\sqrt{1+(\frac{\delta}{2B})^2}} \tag{20}$$

$$a_1 = \frac{1}{2} - \frac{1}{2\sqrt{1+(\frac{2B}{\delta})^2}} \tag{21}$$

And from here we get $C_- = 0$ and $C_+ = \frac{1}{2\sqrt{1+(\frac{\delta}{2B})^2}}$.

Now, for the S^- part we see, by symmetry of the triangle, that the calculus is similar, and we get the same coefficients $C_+, C-$, but interchanged and with a sign changed.

The final result is, thus,

$$\sum_{i=0} M_i = \frac{1}{2\sqrt{1+(\frac{\delta}{2B})^2}}[e^{-E_+T} - e^{-E_-T}] \tag{22}$$

with

$$E_\pm = \frac{\omega_0+\omega_1}{4} \mp \sqrt{\frac{\delta^2}{4}+B^2} \tag{23}$$

And expanding, we have that the gap between the first two levels is:

$$\Delta = \sqrt{\frac{(\omega_1-\omega_0)^2}{4} + 4K^2 e^{-2S_{inst}}} \tag{24}$$

As a consistency check, we observe that when we go back to the symmetrical case, $\delta \to 0$, equation (23) gives us the well known formula for the energy splitting. And of course, when the instanton contribution is negligible, $B \to 0$, we get two separated wells with same energy levels.

We can compare this result with the "ancient" semiclassical method, merely diagonalization of the truncated hamiltonian matrix

$$H = \begin{pmatrix} \omega_0/2 & B' \\ B' & \omega_1/2 \end{pmatrix} \tag{25}$$

and we obtain again (23), only replacing B by B'. Then also in the asymmetrical case we can use the instanton method to estimate the barrier penetration factor B'.

The method can be complicated in two directions: we can add more minima with different curvature, which force us to leave off the plain-triangle and obscures the method; or we can use it to treat potentials with more minima but only two curvatures, as by example the polynomical x^6 triple well, which add some instantons more to calculate, but doesn't add other different summations.

Finally, note that this operation method implies some rearrangements of power series, some care of the convergency conditions must be put when working on a more general case. Apart from this, a strong asymmetry can force the breakdown described by Jona Lasinio et al., see [5],[4].

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