

## 9 Instantons in Quantum Mechanics

### 9.1 General discussion

It has already been briefly mentioned that in quantum mechanics certain aspects of a problem can be overlooked in a perturbative treatment. One example occurs if we have a harmonic oscillator with a cubic anharmonic term:  $V(q) = \frac{1}{2}m\omega^2q^2 + \lambda q^3$  (Figure 15).

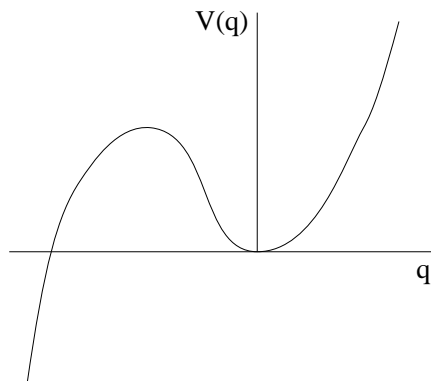


Figure 15:  $V(q) = \frac{1}{2}m\omega^2q^2 + \lambda q^3$ .

We can calculate corrections to harmonic oscillator wave functions and energies perturbatively in  $\lambda$ , to any desired order, blissfully ignorant of a serious pathology in the model. As can be seen from Figure 15, this model has no ground state: the potential energy is unbounded as  $q \rightarrow -\infty$ , a point completely invisible to perturbation theory.

A second example is the double-well potential,  $V(q) = \frac{\lambda}{4!}(q^2 - a^2)^2$  (Figure 16). There

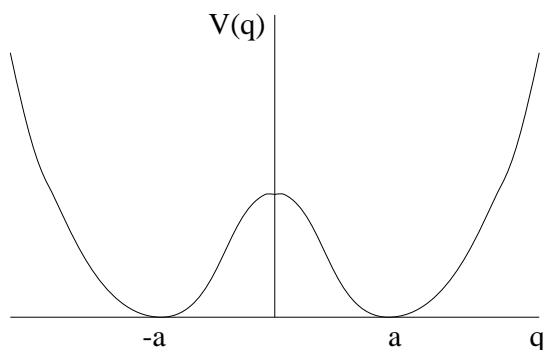


Figure 16:  $V(q) = \frac{\lambda}{4!}(q^2 - a^2)^2$ .

are two classical ground states. We can ignore this fact and expand  $V$  about one of the minima; it then takes the form of a harmonic oscillator about that minimum plus anharmonic terms (both cubic and quartic). We can then compute perturbative corrections to the wave functions and energies, and never see any evidence of the other minimum. Were we to expand about the other minimum, we would produce an identical set of perturbative corrections. By symmetry the ground state energies calculated perturbatively to *any order* will be the same

for the expansions about the two minima, so it appears that we have degenerate ground states. But in fact the ground state is not degenerate: a nonperturbative energy splitting separates the true ground state (an even function of  $q$ ) from the first excited state (an odd function); this splitting is not seen in perturbation theory.

We will examine this second example using PIs, the main goal being to calculate the energy splitting between the two candidate ground states.

Let us first recall the PI expression for the Euclidean propagator:

$$K_E(q', \frac{\beta}{2}; q, -\frac{\beta}{2}) = \langle q' | e^{-\beta H/\hbar} | q \rangle = \int \mathcal{D}q e^{-S_E/\hbar},$$

where

$$S_E = \int_{-\beta/2}^{\beta/2} d\tau \left( \frac{1}{2} m \dot{q}^2 + V(q) \right).$$

Henceforth, we will set  $m \rightarrow 1$ .  $K_E$  is useful because we can write it as

$$K_E = \sum_n \langle q' | n \rangle \langle n | q \rangle e^{-\beta E_n/\hbar}; \quad (53)$$

in the limit  $\beta \rightarrow \infty$ , this term will be dominated by the lowest-energy states. I say “states” here rather than “state” because we must calculate the two lowest-energy eigenvalues to get the splitting of the (perturbatively degenerate) lowest-energy states in the double-well potential.

We will evaluate the PI using an approximation known as the semiclassical approximation, or alternatively as the method of steepest descent. To illustrate it, consider the following integral

$$I = \int_{-\infty}^{\infty} dx e^{-S(x)/\hbar},$$

where  $S(x)$  is a function with several local minima (Figure 17).

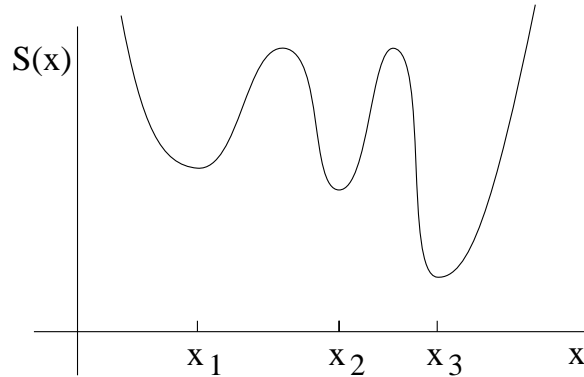


Figure 17: Potential with several minima.

Suppose we are interested in this integral as  $\hbar \rightarrow 0$ . Then the integral will be dominated by the minima of  $S$ ; we can approximate it by a series of Gaussian integrations, one for each minimum of  $S$ . If  $x_i$  is such a minimum, then in its vicinity  $S(x) \simeq S(x_i) + \frac{1}{2}(x - x_i)^2 S''(x_i)$ ; we can write

$$I \simeq I_1 + I_2 + I_3 + \dots, \quad (54)$$

where

$$\begin{aligned} I_i &= \int_{-\infty}^{\infty} dx \exp -[S(x_i) + \frac{1}{2}(x - x_i)^2 S''(x_i)]/\hbar \\ &= e^{-S(x_i)/\hbar} \sqrt{\frac{2\pi\hbar}{S''(x_i)}}. \end{aligned}$$

Anharmonicities of  $S$  appear as corrections of order  $\hbar$  to  $I$ . (This can be easily seen, for example, by considering a specific case such as  $S(x) = ax^2 + bx^4$ .)

We will compute the PI (53) in the semi-classical approximation, where the analog of the  $x_i$  in the above example will be classical paths (extremum of the action  $S_E[q]$ ).

Suppose, then, that  $q_c(\tau)$  is the classical solution to the problem

$$\frac{d^2}{d\tau^2}q = \frac{\partial V(q)}{\partial q}, \quad q(-\beta/2) = q, \quad q(\beta/2) = q'.$$

We can write  $q(\tau) = q_c(\tau) + y(\tau)$ ; the action is

$$\begin{aligned} S_E[q_c + y] &= \int_{-\beta/2}^{\beta/2} d\tau \left( \frac{1}{2}\dot{q}_c + \dot{y}^2 + V(q_c + y) \right) \\ &= \int_{-\beta/2}^{\beta/2} d\tau \left( \frac{1}{2}\dot{q}_c^2 + V(q_c) \right) + (\text{linear in } y) \\ &\quad + \int_{-\beta/2}^{\beta/2} d\tau \left( \frac{1}{2}\dot{y}^2 + \frac{1}{2}V''(q_c)y^2 \right) + \dots \end{aligned} \quad (55)$$

The term linear in  $y$  vanishes for the usual reason, and the higher order terms not written down are of cubic or higher order in  $y$ . Neglecting these (which give order  $\hbar$  corrections to the PI), the propagator becomes

$$K_E = \int \mathcal{D}q e^{-S_E/\hbar} = e^{-S_E[q_c]/\hbar} \int \mathcal{D}y \exp - \int d\tau \left( \frac{1}{2}\dot{y}^2 + \frac{1}{2}V''(q_c)y^2 \right) / \hbar.$$

The functions  $y(\tau)$  over which we integrate satisfy the boundary conditions  $y(-\beta/2) = y(\beta/2) = 0$ . The PI, being Gaussian, can be done exactly; it is not as straightforward as the harmonic oscillator PI since  $V''(q_c)$  depends on  $\tau$ . While we have often managed to *avoid* evaluating PIs, here we must evaluate it. (Unfortunately, this is rather difficult.)

To this end, we can use a generalization of the Fourier expansion technique mentioned in Section 2.2.2. We can rewrite the action as

$$S_E = \int d\tau \left( \frac{1}{2}\dot{y}^2 + \frac{1}{2}V''(q_c)y^2 \right) = \frac{1}{2} \int d\tau y \left( -\frac{d^2}{d\tau^2} + V''(q_c) \right) y. \quad (56)$$

The Schroedinger-like equation

$$\left( -\frac{d^2}{d\tau^2} + V''(q_c) \right) y = \lambda y, \quad y(-\beta/2) = y(\beta/2) = 0$$

has a complete, orthonormal set of solutions; let the solutions and eigenvalues be  $y_k(\tau)$  and  $\lambda_k$ , respectively. The orthonormality relation is

$$\int_{-\beta/2}^{\beta/2} d\tau y_k(\tau) y_l(\tau) = \delta_{kl}.$$

Then we can substitute  $y(\tau) = \sum_k a_k y_k(\tau)$  in (56), giving

$$S_E = \frac{1}{2} \int d\tau \sum_k a_k y_k \left( -\frac{d^2}{d\tau^2} + V''(q_c) \right) \sum_l a_l y_l = \frac{1}{2} \sum_{k,l} a_k a_l \lambda_l \int d\tau y_k y_l = \frac{1}{2} \sum_k a_k^2 \lambda_k.$$

The PI can now be written as an integral over all possible values of the coefficients  $\{a_k\}$ . This gives

$$K_E = J' \int \prod_k da_k e^{-\sum_k a_k^2 \lambda_k / 2\hbar}, \quad (57)$$

where  $J'$  is the Jacobian of the transformation from  $y(\tau)$  to  $\{a_k\}$ . (57) is a product of uncoupled Gaussian integrals; the result is

$$K_E = J' \prod_k \left( \frac{2\pi\hbar}{\lambda_k} \right)^{1/2} = J' \prod_k (2\pi\hbar)^{1/2} (\prod_k \lambda_k)^{-1/2} = J' \prod_k (2\pi\hbar)^{1/2} \det^{-1/2} \left( -\frac{d^2}{d\tau^2} + V''(q_c) \right),$$

where we have written the product of eigenvalues as the determinant of the Schrodinger operator on the space of functions vanishing at  $\pm\beta/2$ .

We can write  $J = J' \prod_k (2\pi\hbar)^{1/2}$ , giving

$$K_E = J \det^{-1/2} \left( -\frac{d^2}{d\tau^2} + V''(q_c) \right) (1 + o(\hbar)),$$

where the  $o(\hbar)$  corrections can in principle be computed from the neglected beyond-quadratic terms in (55). We will not be concerned with these corrections, and henceforth we will drop the  $(1 + o(\hbar))$ .

## 9.2 Single Well in the Semiclassical Approximation

Before looking at the double well, it is worthwhile examining the single well, defined be

$$V(q) = \frac{1}{2} \omega^2 q^2 + \frac{\lambda}{4!} q^4.$$

The classical equation is

$$\frac{d^2}{d\tau^2} q = V'(q).$$

Note that this is the equation of motion for a particle moving in a potential  $-V(q)$ . If we choose the initial and final points  $q = q' = 0$ , then the classical solution is simply  $q_c(\tau) = 0$ ; furthermore,  $V''(q_c) = V''(0) = \omega^2$ , and

$$K_E = J \det^{-1/2} \left( -\frac{d^2}{d\tau^2} + \omega^2 \right).$$

The evaluation of the determinant is not terribly difficult (the eigenvalues can be easily found; their product can be found in a table of mathematical identities); the result, for large  $\beta$ , is

$$K_E = \left( \frac{\omega}{\pi \hbar} \right)^{1/2} e^{-\beta \omega / 2}.$$

From (5.3), we can extract the ground state energy since, for large  $\beta$ ,  $K_E \sim \exp -E_0 \beta / \hbar$ . We find  $E_0 = \hbar \omega / 2$  up to corrections of order  $\lambda \hbar^2$ . We have discovered an incredibly complicated way of calculating the ground state energy of the harmonic oscillator!

### 9.3 Instantons in the Double Well Potential

Let us now study a problem of much greater interest: the double well. We will see that configurations known as “instantons” make a non-perturbative correction to the energies. We wish to evaluate the PI

$$K_E = \int_{q, -\beta/2}^{q', \beta/2} \mathcal{D}q e^{-S_E},$$

where

$$S_E = \int d\tau \left( \frac{1}{2} \dot{q}^2 + \frac{\lambda}{4!} (q^2 - a^2)^2 \right),$$

for  $\beta \rightarrow \infty$ . As explained above, the PI is dominated by minima of  $S_E$ , *i.e.*, by classical solutions. The classical equation corresponds to a particle moving in the potential  $-V(q)$  (Figure 18); the “energy”  $E = \frac{1}{2} \dot{q}^2 - V(q)$  is conserved.

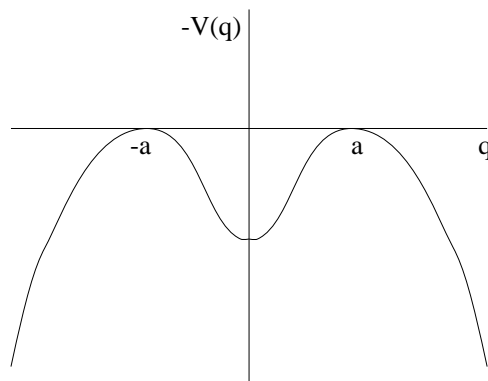


Figure 18: Inverted double-well potential.

Let us examine classical solutions, taking the boundary values  $q, q'$  of the classical solution corresponding to the maxima of  $-V$ ,  $\pm a$ . In the limit  $\beta \rightarrow \infty$ , these will be solutions of zero “energy”, since as  $\tau \rightarrow \pm\infty$  both the kinetic and potential “energy” vanish.

First, if  $q = q' = a$  (an identical argument applies if  $q = q' = -a$ ), the obvious classical solution is  $q(\tau) = a$ ; a quadratic approximation about this constant solution would be identical to the single-well case discussed above.

But what if  $q = -a$  and  $q' = a$  (or vice-versa)? Then the obvious classical solution corresponds to the particle initially sitting atop the maximum of  $-V$  at  $-a$ , rolling towards

$q = 0$  after a very long (infinite, in the limit  $\beta \rightarrow \infty$ ) time, and ending up at rest at the other maximum of  $-V$  as  $\tau \rightarrow \infty$  (Figure 19).

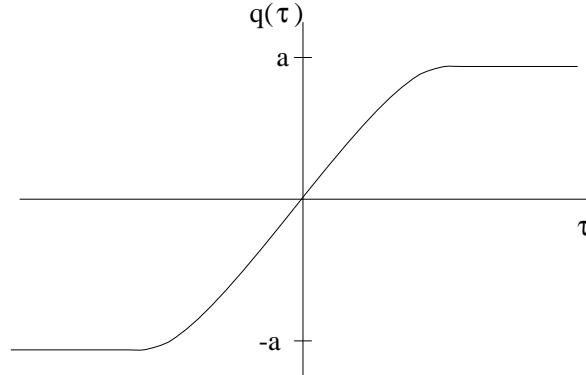


Figure 19: Instanton in the double-well potential.

We can get the analytical form of this solution: setting  $E \rightarrow 0$ , we have

$$\frac{1}{2}\dot{q}^2 = V(q), \quad \text{or} \quad \frac{dq}{d\tau} = \pm\sqrt{\frac{\lambda}{12}}(q^2 - a^2).$$

There are a family of solutions interpolating between  $-a$  and  $a$ :

$$q(\tau) = a \tanh \frac{\omega}{2}(\tau - \tau_0), \quad (58)$$

where  $\omega = \sqrt{\lambda a^2/3}$  and where  $\tau_0$  is an integration constant which corresponds to the time at which the solution crosses  $q = 0$ .

This solution is much like a topological soliton in field theory, except that it is localized in time rather than in space. One could argue that the solution doesn't appear to be localized:  $q$  goes to different values as  $\tau \rightarrow \pm\infty$ . But these are just different, but physically equivalent, ground states, so we can say that the instanton is a configuration which interpolates between two ground states; the system is in a ground state except for a brief time – an “instant”. For this reason, the solution is known as an *instanton*.

I called the two solutions  $q(\tau) = a$  and  $q(\tau) = a \tanh \frac{\omega}{2}(\tau - \tau_0)$  the *obvious* classical solutions because there are an infinite number of approximate classical solutions which are potentially important in the PI. Since the instanton is localized in time, and since the total time interval  $\beta$  is very large (in particular, much larger than the instanton width), a series of widely-separated instantons and anti-instantons (configurations interpolating between  $+a$  and  $-a$ ) is also a solution, up to exponentially small interactions between neighbouring instantons and anti-instantons. Such a configuration is shown in Figure 20, where the horizontal scale has been determined by the duration of imaginary time  $\beta$ ; on this scale the instanton and anti-instanton appear as step functions.

It is clear than an instanton must be followed by an anti-instanton, and that if the asymptotic values of the position are  $+a$  and  $+a$  the classical solution must contain anti-instanton-instanton pairs whereas if they are  $-a$  and  $+a$  we need an extra instanton at the beginning.

Let us choose first limiting values  $q(-\beta/2) = q(+\beta/2) = +a$ . Then we are interested in

$$K_E = \int_{a, -\beta/2}^{a, \beta/2} \mathcal{D}q e^{-S_E}.$$

In the spirit of (54), in the steepest-descent approximation  $K_E$  is equal to the sum of PIs evaluated about *all* classical solutions. The classical solutions are:  $q_c(\tau) = a$ ;  $q_c = \text{anti-instanton-instanton} \equiv AI$ ;  $q_c = AIAI$ ; *etc.*, where the positions of the *As* and *Is* are not determined, and must be integrated over. Schematically, we may write

$$K_E = K_E^0 + K_E^2 + K_E^4 + \dots, \quad (59)$$

where the superscript denotes the total number of *Is* or *As*. Let us discuss the first couple of contributions in some detail.

$q_c = a$ : This case is essentially equivalent to the single-well case discussed above, and we get

$$K_E^0 = \sqrt{\frac{\omega}{\pi\hbar}} e^{-\beta\omega/2},$$

where  $\omega = (\lambda a^2/3)^{1/2}$  is the frequency of small oscillations about the minimum of  $V$ .

$q_c = AI$ : This case is rather more interesting (that is to say, complicated!). Let us suppose that the classical solution around which we expand consists of an anti-instanton at time  $\tau_1$  and an instanton at  $\tau_2$  (Figure 21); clearly  $\tau_2 > \tau_1$ .

Then we can write  $q = q_c + y$ , and

$$S_E[q] = S_E[q_c] + S_E^{\text{quad}}[y].$$

We can evaluate  $S_E[q_c]$ : it is twice the action of a single instanton (assuming the *I* and *A* are sufficiently far apart that any interaction is negligible):  $S_E[q_c] = 2S_E^{\text{inst}}$ . The one-instanton action  $S_E^{\text{inst}}$  is

$$S_E^{\text{inst}} = \int d\tau \left( \frac{1}{2} \dot{q}^2 + V(q) \right) \Big|_{\text{inst}} = 2 \int d\tau V(q) \Big|_{\text{inst}}.$$

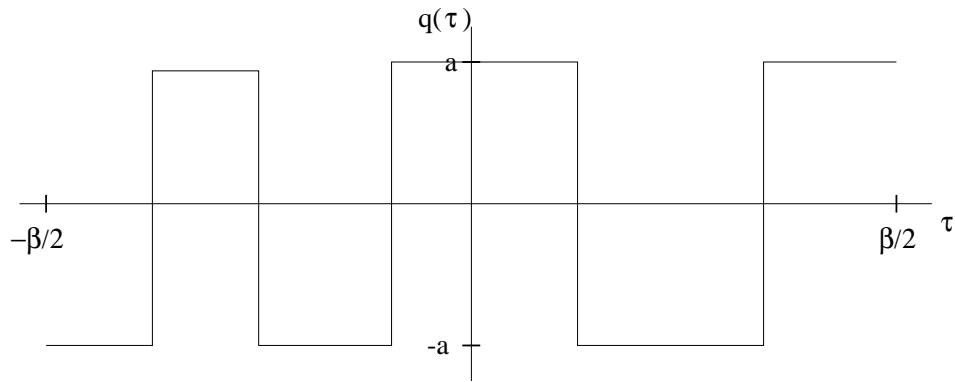


Figure 20: Multi-instanton configuration.

With the instanton profile given by (58), the result is

$$S_E^{\text{inst}} = \sqrt{\frac{\lambda}{3}} \frac{2a^3}{3}.$$

To evaluate the PI with the action  $S_E^{\text{quad}}[y]$ , let us divide the imaginary time interval into two semi-infinite regions  $I$  and  $II$ , where the boundary between the two regions is between and well away from the  $A$  and the  $I$  (Figure 22).

Then we can write

$$K_E^2 = \frac{\beta^2}{2} e^{-2S_E^{\text{inst}}} \int_{I+II} \mathcal{D}y e^{-S_E^{\text{quad}}/\hbar}. \quad (60)$$

Here the first factor represents integration over the positions of the  $A$  and  $I$  (remember that the  $A$  must be to the left of the  $I$ !). The quadratic action can be written

$$S_E^{\text{quad}} = S_E^{\text{quad}}{}_I + S_E^{\text{quad}}{}_{II},$$

where  $S_E^{\text{quad}}{}_I$  is the quadratic action in the presence of an anti-instanton and  $S_E^{\text{quad}}{}_{II}$  is that in the presence of an instanton.

Then the PI separates into two factors:

$$\int_{I+II} \mathcal{D}y e^{-S_E^{\text{quad}}/\hbar} = \int_I \mathcal{D}y e^{-S_E^{\text{quad}}{}_I/\hbar} \cdot \int_{II} \mathcal{D}y e^{-S_E^{\text{quad}}{}_{II}/\hbar}, \quad (61)$$

where there is an implied integration over the intermediate position at the boundary of the two regions. The quadratic no-instanton PI also separates into two factors:

$$\int \mathcal{D}y e^{-S_E^{\text{quad},0}/\hbar} = \int_I \mathcal{D}y e^{-S_E^{\text{quad},0}{}_I/\hbar} \times \int_{II} \mathcal{D}y e^{-S_E^{\text{quad},0}{}_{II}/\hbar}, \quad (62)$$

where the superscript “0” denotes that this is the PI about a no-instanton (constant) background. We can combine (61) and (62) to give:

$$\int_{I+II} \mathcal{D}y e^{-S_E^{\text{quad}}/\hbar} = \int \mathcal{D}y e^{-S_E^{\text{quad},0}/\hbar} \frac{\int_I \mathcal{D}y e^{-S_E^{\text{quad}}{}_I/\hbar}}{\int_I \mathcal{D}y e^{-S_E^{\text{quad},0}{}_I/\hbar}} \frac{\int_{II} \mathcal{D}y e^{-S_E^{\text{quad}}{}_{II}/\hbar}}{\int_{II} \mathcal{D}y e^{-S_E^{\text{quad},0}{}_{II}/\hbar}}. \quad (63)$$

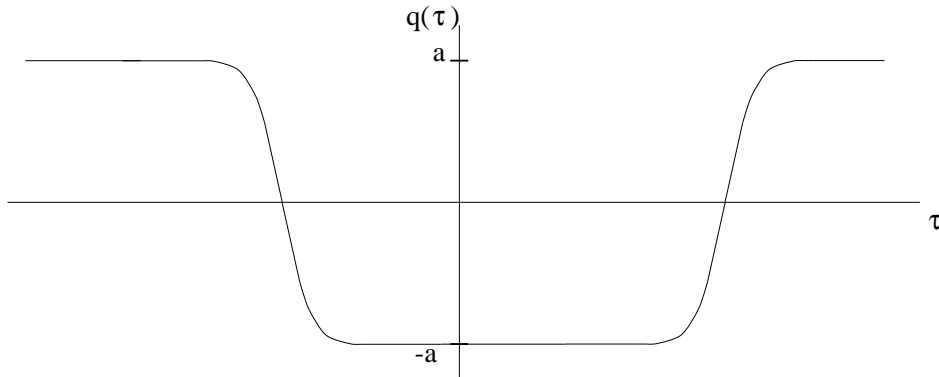


Figure 21: Anti-instanton-instanton.



But

$$\frac{\int_I \mathcal{D}y e^{-S_E^{\text{quad}}/ \hbar}}{\int_I \mathcal{D}y e^{-S_E^{\text{quad},0}/ \hbar}} = \frac{\int \mathcal{D}y e^{-S_E^{\text{quad}}/ \hbar}}{\int \mathcal{D}y e^{-S_E^{\text{quad},0}/ \hbar}} \quad (64)$$

and similarly for the last factor in (63), so we obtain

$$\int_{I+II} \mathcal{D}y e^{-S_E^{\text{quad}}/ \hbar} = \sqrt{\frac{\omega}{\pi \hbar}} e^{-\beta \omega / 2} R^2,$$

where  $R$  is the ratio of the PI in the presence and absence of an instanton (or, equivalently, anti-instanton) given in (64). Substituting this into (60),

$$K_E^2 = e^{-2S_E^{\text{inst}}/ \hbar} \sqrt{\frac{\omega}{\pi \hbar}} e^{-\beta \omega / 2} R^2 \frac{\beta^2}{2}.$$

A similar argument gives

$$K_E^4 = e^{-4S_E^{\text{inst}}/ \hbar} \sqrt{\frac{\omega}{\pi \hbar}} e^{-\beta \omega / 2} R^4 \frac{\beta^4}{4!},$$

and so on for subsequent terms in the expansion (59).

Summing these contributions, we get

$$\begin{aligned} K_E &= \sqrt{\frac{\omega}{\pi \hbar}} e^{-\beta \omega / 2} \left( 1 + \frac{(\beta R e^{-S_E^{\text{inst}}/ \hbar})^2}{2!} + \frac{(\beta R e^{-S_E^{\text{inst}}/ \hbar})^4}{4!} + \dots \right) \\ &= \sqrt{\frac{\omega}{\pi \hbar}} e^{-\beta \omega / 2} \cosh(\beta R e^{-S_E^{\text{inst}}/ \hbar}) \\ &= \frac{1}{2} \sqrt{\frac{\omega}{\pi \hbar}} e^{-\beta \omega / 2} \left( e^{\beta R e^{-S_E^{\text{inst}}/ \hbar}} + e^{-\beta R e^{-S_E^{\text{inst}}/ \hbar}} \right). \end{aligned}$$

Now we must recall why we're calculating this object in the first place. The propagator can be written as in (53):

$$K_E = \sum_n \langle a | n \rangle \langle n | a \rangle e^{-\beta E_n / \hbar}.$$

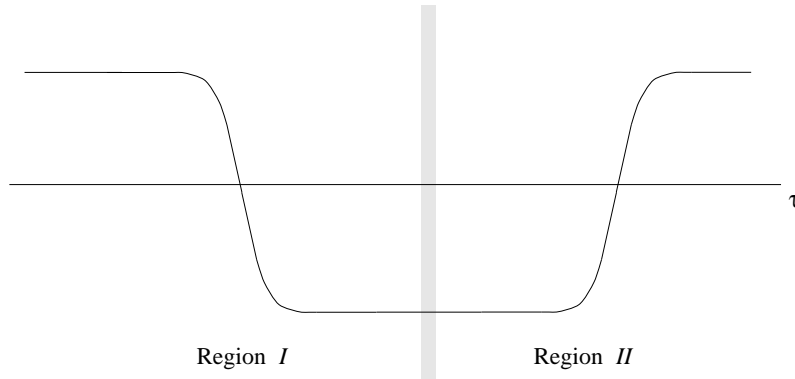


Figure 22: Division of imaginary time into two regions, one containing the anti-instanton, the other containing the instanton.

By comparing these two expressions we see that the lowest two energies are

$$\frac{\hbar\omega}{2} - \hbar Re^{-S_E^{\text{inst}}/\hbar} \quad \text{and} \quad \frac{\hbar\omega}{2} + \hbar Re^{-S_E^{\text{inst}}/\hbar}.$$

So the energy splitting is given by

$$\boxed{\Delta E = 2\hbar Re^{-S_E^{\text{inst}}/\hbar}}. \quad (65)$$

$\Delta E$  is clearly non-perturbative: it cannot be expanded as a power series in  $\hbar$  (or, equivalently, in  $\lambda$ ).

In principle, we should calculate the ratio

$$R = \frac{(\text{instanton background PI})}{(\text{constant background PI})} \sim \text{ratio of determinants},$$

but I don't know how to compute it other than by doing a very arduous, technical calculation; luckily, time will not permit it. The interested reader can consult the book by Sakita for a discussion of this calculation.

As a final note, we have calculated the PI with  $q = q' = a$ ; a good exercise is to do the analogous calculation for  $q = -a$ ,  $q' = a$ .