Chapter 6

Semiclassical Euclidean functional amplitudes

We have already introduced Euclidean propagators through the substitution

$$t = -i\tau \,, \tag{6.1}$$

so we obtain the following Euclidean versions of the propagators:

$$\begin{aligned} K_E(x_b, \tfrac{1}{2}T; x_a, -\tfrac{1}{2}T) &= <x_a|e^{-\frac{1}{\hbar}HT}|x_a> = \int [\mathcal{D}_E x(\tau)] e^{-\frac{1}{\hbar}S_E[x(\tau)]} \\ &= \int \prod_j \frac{dx_j}{a} e^{-\frac{1}{\hbar}\sum_j [\frac{m}{2}\frac{(x_{j+1}-x_j)^2}{\eta} + \eta V(x_j)]} \end{aligned} \tag{6.2}$$

where $a = \sqrt{2\pi\hbar\eta/m}$.

Let us look now at the semiclassical Euclidean propagator for the simple Lagrangian : $L = m\dot{x}^2/2 - V(x)$, $t = -i\tau$,

$$S_E[x(\tau)] = \int_{-T/2}^{T/2} d\tau \left[\tfrac{1}{2} m \left(\frac{dx}{d\tau} \right)^2 + V(x) \right] .$$

Similarly as before the quantal trajectory is split into the "classical" trajectory $\bar{x}(\tau)$ and the quantal fluctuation $y(\tau)$ with the boundary conditions

$$\bar{x}\left(-\tfrac{1}{2}T\right) = x_a \,, \qquad \bar{x}\left(\tfrac{1}{2}T\right) = x_b \,, \qquad y\left(-\tfrac{1}{2}T\right) = y\left(\tfrac{1}{2}T\right) = 0 \,. \tag{6.3}$$

We approximate S_E through a sum of the "classical" action, $S_E[\bar{x}(\tau)]$, and the gaussian (quantal) action $S_E[y(\tau)]$ (the cross terms, linear in $y(\tau)$, do not contribute because $\bar{x}(\tau)$ is at the stationary point of $S_E[x(\tau)]$)

$$S_E[x(\tau)] \approx \int_{-T/2}^{T/2} d\tau \left[\tfrac{1}{2} m\dot{\bar{x}}^2 + V(\bar{x}) \right] + \int_{-T/2}^{T/2} d\tau \left[\tfrac{1}{2} m\dot{y}^2 + \tfrac{1}{2} \left. \frac{\partial^2 V}{\partial x^2} \right|_{\bar{x}} y^2 \right] . \tag{6.4}$$

Because of (6.3) we have

$$\int_{-T/2}^{T/2} d\tau\, \dot{y}^2 = \int_{-T/2}^{T/2} d\tau \left[\frac{d}{d\tau}(y\dot{y}) - y\ddot{y}\right] = -\int_{-T/2}^{T/2} d\tau\, y\frac{d^2y}{d\tau^2}\,,$$

hence

$$S_E[x(\tau)] \;=\; S_E[\bar{x}(\tau)] + \tfrac{1}{2}\int_{-T/2}^{T/2} d\tau\, y D_E(\tau) y \tag{6.5}$$

where

$$D_E(\tau) \;=\; -m\frac{d^2}{d\tau^2} + \left.\frac{\partial^2 V}{\partial x^2}\right|_{\bar{x}(\tau)}. \tag{6.6}$$

So, now we find the eigenvalues and eigenfunctions of the differential operator $D_E(\tau)$:

$$D_E y_n(\tau) = \lambda_n y_n(\tau)\,, \qquad \int_{-T/2}^{T/2} d\tau\, y_n(\tau) y'_n(\tau) = \delta_{nn'}\,, \quad y_n\left(-\tfrac{1}{2}T\right) = y_n\left(\tfrac{1}{2}T\right) = 0\,. \tag{6.7}$$

Expanding $y(\tau)$ into this orthonormal set of functions

$$y(\tau) = \sum_n a_n y_n(\tau)\,, \tag{6.8}$$

we get

$$S_E[x(\tau)] = S_E[\bar{x}(\tau)] + \tfrac{1}{2}\sum_n a_n^2 \lambda_n\,. \tag{6.9}$$

Hence, in the semiclassical approximation, we get

$$K_E(x_b, \tfrac{1}{2}T; x_a, -\tfrac{1}{2}T) \;\approx\; e^{-\frac{1}{\hbar}S_E[\bar{x}]}\mathcal{N}\int\prod_n \frac{da_n}{\sqrt{2\pi\hbar}}\, e^{-\frac{1}{2\hbar}\sum_n a_n^2\lambda_n}\,, \tag{6.10}$$

where $\mathcal{N}$ is to be determined. Since

$$\int_{-\infty}^{+\infty} \frac{da_n}{\sqrt{2\pi\hbar}}\, e^{-\frac{1}{2\hbar}a_n^2\lambda_n} = \lambda_n^{-1/2}$$

we obtain

$$K_E(x_b, \tfrac{1}{2}T; x_a, -\tfrac{1}{2}T) \;\approx\; e^{-\frac{1}{\hbar}S_E[\bar{x}]}\,\mathcal{N}\,[\det D_E]^{-1/2}\,, \tag{6.11}$$

where $\det D_E = \prod_n \lambda_n$.

A few comments are here in order. First, there are many similarities with the semiclassical approximation for the real (Minkowski) time: many operations are completely parallel to the ones we have done in the previous section. On the other hand, however, there are some important differences. Now we are dealing with real, not complex, quantities. Our present expressions are well defined only when all $\lambda_n > 0$. In the case of real time transitions through zero of $\lambda's$ were interpreted as an appearance of focal points (caustic points) in close analogy to what we have in optics. Thus the processes of diffraction were present there. Now, for the Euclidean time, diffraction is absent and the cases when $\lambda's$ go through zero need some other physical interpretation.

In order to fix $\mathcal{N}$ let us work out the same example which we had in the last section of a potential with just one minimum, now for the case of the Euclidean amplitudes. Similarly as in the case of the last section, we build the (Euclidean) amplitude around the classical trajectory $\bar{x}$ which we choose to be a constant coordinate of the minimum of $V(\bar{x} = 0) = 0$. Note that this choice of the classical trajectory is implied by e.g. the simulation procedure of Metropolis discussed in Section 2 ("Brownian motion, Euclidean time"): Indeed, the largest contributions to the propagator come from the trajectory of the particle sitting still at the bottom of $V(x)$, compare (6.12).

We have now in the semiclassical approximation

$$L_E = \tfrac{1}{2}m\dot{x}^2 + V(x) \;\approx\; \tfrac{1}{2}m\dot{x}^2 + \tfrac{1}{2}V''(0)\,x^2\,. \tag{6.12}$$

Setting $V''(0) = m\omega^2$ we can now write down the Euclidean propagator taking the result for K for the real time t , and replacing $t = -i\tau$.

$$\begin{aligned} K_E(x,\tfrac{1}{2}T;0,-\tfrac{1}{2}T) \;&=\; \left(\frac{m\omega}{2\pi i\hbar\sin(-i\omega T)}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}\frac{m\omega}{2\sin(-i\omega T)}x^2\cos(-i\omega T)} \\ &=\; \left(\frac{m\omega}{2\pi\hbar\sinh(\omega T)}\right)^{\frac{1}{2}} e^{-\frac{1}{\hbar}\frac{m\omega}{2\sinh(\omega T)}x^2\cosh(\omega T)}\,. \end{aligned} \tag{6.13}$$

From (6.11) and(6.13) we get

$$\mathcal{N}[\det D_E]^{-1/2} \;=\; \left(\frac{m\omega}{2\pi\hbar\sinh(\omega T)}\right)^{\frac{1}{2}}. \tag{6.14}$$

Further on we shall need the limit $T \to \infty$ of the above expressions. From (6.13) and (6.14) we get

$$\begin{aligned} K_E(x,\tfrac{1}{2}T;0,-\tfrac{1}{2}T)\Big|_{T\to\infty} \;&=\; e^{-\frac{1}{2}\omega T}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{m\omega}{2\hbar}x^2} \\ &=\; e^{-\frac{1}{\hbar}E_0 T}\phi_0(x)\phi_0^*(0)\,, \end{aligned} \tag{6.15}$$

where E_0 is the ground state energy and ϕ_0 the ground state wave function of our system (in the semiclassical approximation). Note that (6.15) gives us – in accordance with our expectations – the ground state energy of the harmonic oscillator, $E_0 = \frac{1}{2}\hbar\omega$, and the ground state wave function

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}\,.$$

6.1 Two minimum potential: instantons

The situation changes radically when $V(x)$ has two minima. We shall discuss now a symmetric double well potential which can be well approximated around each of the two minima by an oscillator potential. For instance the following functional form for $V(x)$ can be used for detailed analytic calculations

$$V(x) = \kappa(x^2 - a^2)^2\,, \qquad V''(\pm a) = \omega^2 = 8\kappa a^2\,. \tag{6.16}$$

Since the "Euclidean motion" takes place in the potential $-V(x)$ we can build the Euclidean propagator around the classical trajectories which take the particle from one minimum to the other one. For a justification of this step we may, again, recourse to the Metropolis simulations whose procedures prevent the quantal trajectories to get stuck in a *local* minimum.

So, we are seeking the transition amplitudes taking us from $-a$ to a or *vice versa* an arbitrary number of times. Because of symmetry of the potential there are just two such amplitudes

$$\begin{aligned} <-a|e^{-\frac{1}{\hbar}HT}|-a> &= <a|e^{-\frac{1}{\hbar}HT}|a> \\ <-a|e^{-\frac{1}{\hbar}HT}|a> &= <a|e^{-\frac{1}{\hbar}HT}|-a>\;. \end{aligned} \tag{6.17}$$

The first pair are the amplitudes for the particle to remain at the original position. The second pair is for the process of tunnelling.

Let us have a look at the classical trajectories going from e.g. a to $-a$. The equations of motion following from (6.12) the energy $E = \frac{1}{2}m\dot{\bar{x}}^2 - V(x)$ is a constant of motion. In our case $E = 0$, hence the equation of motion can be written in either of the following forms:

$$\tfrac{1}{2}m\dot{\bar{x}}^2 - V(x) = 0\,, \qquad \dot{\bar{x}} = \left[\frac{2}{m}V(\bar{x})\right]^{\frac{1}{2}}, \qquad \frac{d\tau}{d\bar{x}} = \frac{1}{\sqrt{\frac{2}{m}V(\bar{x})}}\,. \tag{6.18}$$

Solving the last one we obtain

$$\tau = \tau_1 + \int_0^{\bar{x}} d\bar{x}\frac{1}{\sqrt{\frac{2}{m}V(\bar{x})}}\,, \tag{6.19}$$

where τ_1 is the constant of integration. Note that for $V(x)$ given by (6.16) one can do the integral in (6.19) and obtains $\bar{x} \sim \tanh(\mathrm{const}(\tau - \tau_1))$.

When the particle is right in between the two minima: $\bar{x} = 0$ and $\tau = \tau_1$. Thus τ_1 is the moment when the particle moves with maximal velocity. The classical trajectories from one minimum to the other one one calls *instantons* (say, from $-a$ to a) and *anti-instantons* (from a to $-a$). Since one transition takes a very, very long time, the constant τ_1 marks the position of an instanton (anti-instanton) in an essentially infinitely long segment of time from $-T/2$ to $T/2$. We shall use this constant to label instantons (anti-instantons).

We can have an idea about the general shape of instantons solving the differential equation (6.18) close to e.g. a. We expand $V(\bar{x})$ around a:

$$V(\bar{x}) \approx \tfrac{1}{2}V''(a)(\bar{x}-a)^2 .$$

Thus the equation in the neighborhood of a takes the form

$$\frac{d(\bar{x}-a)}{d\tau} = -\left[\frac{V''(a)}{m}\right]^{\frac{1}{2}}(\bar{x}-a)$$

where the sign is fixed such as to make $d\bar{x}/d\tau$ positive when $\bar{x}$ (hence the particle) is approaching a from the left. Thus

$$|\bar{x}-a| \sim e^{-\sqrt{\frac{V''(a)}{m}}\,\tau} = e^{-\omega\tau} \tag{6.20}$$

where $\omega = \sqrt{V''(a)/m}$. Thus the instantons and anti-instantons are well localized in time, and they are – in the commonly accepted terminalogy – *kinks* and *anti-kinks*. In the perspective of an infinite T they look like some well localized in time steps.

Now, we are going to build the amplitudes (6.17) from *superpositions* of many instantons and anti-instantons which *do not overlap*. This last condition is essential for such a procedure to be internally consistent because $V(\bar{x})$ is a non-linear function of $\bar{x}$, but the lack of overlap makes it to be a sum of contributions from all instantons and anti-instantons. On the scale of T the instantons (anti-instantons) are very narrow: most of the time the particle stays in the vicinity of the maxima of $-V(\bar{x})$ and it passes the minimum of $-V(\bar{x})$ in an "instant"(hence the name). Therefore, the classical action $S[\bar{x}]$ becomes a sum of the individual contributions from the instantons (anti-instantons). The action of one instanton (anti-instanton) is

$$S_E^0 = \int_{-T/2}^{+T/2} d\tau \left[\tfrac{1}{2}m\frac{2}{m}V(\bar{x}) + V(\bar{x})\right] = \int_{-a}^{+a} d\bar{x}\sqrt{2mV(\bar{x})} = \int_{-a}^{+a} d\bar{x}\, p(\bar{x}) \tag{6.21}$$

where $p(\bar{x}) = m\dot{\bar{x}} = m\sqrt{2V(\bar{x})/m}$. This is a special case (E=0) of the expression which appears in the so called transmission coefficients through a barrier.

Now we come to the construction of the amplitude $<\!-a|e^{-HT/\hbar}|-a\!>$. When we start from $-a$ the first comes instanton, then anti-instanton and we have to have an even number of them (we have to go back to $-a$). The trajectory with n instantons (anti-instantons) present is (for $T\to\infty$)

$$x(\tau) = \bar{x}_{\tau_1\ldots\tau_n}(\tau) + y(\tau) \approx \bar{x}_{\tau_1}(\tau) + \bar{x}_{\tau_2}(\tau) + \ldots + \bar{x}_{\tau_n}(\tau) + y(\tau)\,. \tag{6.22}$$

Here $y(\tau)$ represents the quantum fluctuations around the classical trajectory of n instantons (anti-instantons). $\tau_1, ..., \tau_n$ mark the positions of the well separated

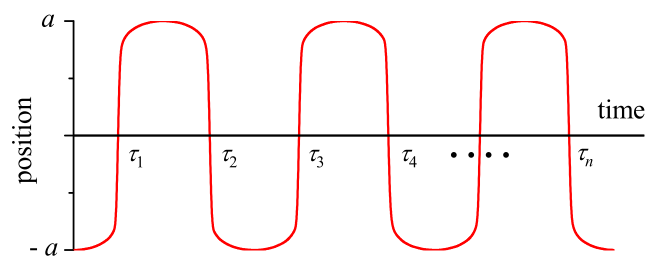

Figure 6.1: Chain of separated instanton–anti-instanton transitions.

in time instantons and anti-instantons.

$$<-a|e^{-\frac{1}{\hbar}HT}|-a> = \sum_{even\, n} \int\limits_{-T/2}^{+T/2} d\tau_1 ... \int\limits_{-T/2}^{\tau_{n-2}} d\tau_{n-1} \int\limits_{-T/2}^{\tau_{n-1}} d\tau_n \, e^{-\frac{1}{\hbar}S_E[\bar{x}_{\tau_1...\tau_n}(\tau)]}$$

$$\times \int_{y(-\frac{T}{2})=y(+\frac{T}{2})=0} [\mathcal{D}y_E(\tau)] \, e^{-\frac{1}{2\hbar}\int\limits_{-T/2}^{+T/2} d\tau y(-m\frac{d^2}{d\tau^2}+V''(\bar{x}))y} . \tag{6.23}$$

For a "dilute gas of instantons"

$$S_E[\bar{x}_{\tau_1...\tau_n}(\tau)] \approx nS_E^0 ,$$

where S_E^0 is given by (6.21).

Let us consider the path integral over the fluctuations $y(\tau)$

$$K_E(0, \tfrac{1}{2}T; 0, -\tfrac{1}{2}T) = \int_{y(-\frac{T}{2})=y(+\frac{T}{2})=0} [\mathcal{D}y_E(\tau)] \, e^{-\frac{1}{2\hbar}\int\limits_{-T/2}^{+T/2} d\tau y(-m\frac{d^2}{d\tau^2}+V''(\bar{x}))y} .$$

It can be represented as a convolution of n K_E's with the intermediate positions $T_1, ..., T_n$ set in between τ_j's

$$\int K_E(0, \tfrac{1}{2}T; y_n, T_n) \, dy_n \, ... \, dy_2 K_E(y_2, T_2; y_1, T_1) \, dy_1 K_E(y_1, T_1; 0, -\tfrac{1}{2}T) . \tag{6.24}$$

hence each T_j is, more or less, half way between two τ_j's, in the region where our system is very well approximated by a harmonic oscillator. In fact, apart from a flash of a kink (or anti-kink) in between of two T_j's the system behaves as an oscillator. So, if not for the kinks, the convolution (6.24) would produce K_E of the harmonic oscillator.

Now we make the following approximation:

$$K_E(y_j, T_j; y_{j-1}, T_{j-1}) = \tilde{K} \, K_E^{\text{osc}}(y_j, T_j; y_{j-1}, T_{j-1}) \tag{6.25}$$

where $\tilde{K}$ is a constant to be determined later. Hence we assume that a renormalisation constant, $\tilde{K}$, takes care of the deviations of the fluctuations $y(\tau)$ from the ones one encounters in the harmonic oscillator. This implies that

$$K_E(0,\tfrac{1}{2}T,0,-\tfrac{1}{2}T)\Big|_{T\to\infty} = \tilde{K}^n \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\omega T}\,, \qquad \omega^2 = \frac{V''(\pm a)}{m}\,. \tag{6.26}$$

Since the integrand in (6.23) does not depend any more on $\tau_1, ..., \tau_n$ we can evaluate the integral over all τ 's:

$$\int\limits_{-T/2}^{+T/2} d\tau_1 ... \int\limits_{-T/2}^{\tau_{n-2}} d\tau_{n-1} \int\limits_{-T/2}^{\tau_{n-1}} d\tau_n = \frac{1}{n!} T^n\,. \tag{6.27}$$

So, our semiclassical amplitude, in the limit of a very large T becomes

$$\begin{aligned} <\!-a|e^{-\frac{1}{\hbar}HT}|-a\!> &\approx \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\omega T} \sum_{\text{even}\, n} \frac{1}{n!}\left(\tilde{K}e^{-S_E^0/\hbar}T\right)^n \qquad (6.28)\\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\omega T}\frac{1}{2}\left[e^{\tilde{K}e^{-S_E^0/\hbar}T} + e^{-\tilde{K}e^{-S_E^0/\hbar}T}\right]\\ &= \tfrac{1}{2}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}}\left[e^{-(\frac{1}{2}\omega-\tilde{K}e^{-S_E^0/\hbar})T} + e^{-(\frac{1}{2}\omega+\tilde{K}e^{-S_E^0/\hbar})T}\right]. \end{aligned}$$

Since we took the limit of very large T, we are left with the contributions of the states of the lowest energies. Eq. (6.28) tells us that the process of tunnelling removes the degeneracy of the ground state of the system with a potential energy with two identical minima. Instead of two degenerate states (the particle is either in the minimum $-a$ or in $+a$) the particle is either in the state (call it $|\,s\!>$) of the energy

$$E_s = \tfrac{1}{2}\hbar\omega - \hbar\tilde{K}e^{-S_E^0/\hbar}\,,$$

or in the state of somewhat higher energy (call it $|\,r\!>$)

$$E_r = \tfrac{1}{2}\hbar\omega + \hbar\tilde{K}e^{-S_E^0/\hbar}\,.$$

We get all amplitudes following the same steps and obtain

$$<\!\mp a|e^{-\frac{1}{\hbar}HT}|-a\!> \approx \tfrac{1}{2}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}}\left[e^{-(\frac{1}{2}\omega-\tilde{K}e^{-S_E^0/\hbar})T} \pm e^{-(\frac{1}{2}\omega+\tilde{K}e^{-S_E^0/\hbar})T}\right]. \tag{6.29}$$

What can we say about $|\,s>$ and $|\,r>$? From the general formula in the representation of eigenstates of energy

$$<\!\mp a|e^{-\frac{1}{\hbar}HT}|-a\!> = \sum_l <\!\mp a|l\!>\, e^{-E_l T/\hbar} <\!l|-a\!>\,,$$

in the limit of large T, just two lowest energy contributions remain

$$
\begin{aligned}
<\mp a|e^{-\frac{1}{\hbar}HT}|-a> \;\approx\; & <\mp a|s><s|-a>\, e^{-(\frac{1}{2}\omega-\tilde{K}e^{-S_E^0/\hbar})T} \\
& \pm\; <\mp a|r><r|-a>\, e^{-(\frac{1}{2}\omega+\tilde{K}e^{-S_E^0/\hbar})T} . \qquad (6.30)
\end{aligned}
$$

Comparing (6.30) with (6.29) we obtain

$$
\begin{aligned}
<\mp a|s><s|-a> &= \tfrac{1}{2}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \\
<\mp a|r><r|-a> &= \pm\tfrac{1}{2}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} . \qquad (6.31)
\end{aligned}
$$

On the other hand we know that, without tunnelling, we have two degenerate states of energy $\frac{1}{2}\hbar\omega$:

$$\Psi_0(x-a) \qquad \text{and} \qquad \Psi_0(x+a)$$

where

$$\Psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2} .$$

We also know that (in the first approximation) the states with removed degeneracies are linear combinations of the degenerate states. Indeed, it is fairly easy to find such combinations in our case. In the position representation

$$<\mp a|x> = \delta(x \pm a),$$

therefore

$$
\begin{aligned}
<\mp a|s> &= \int dx\, \frac{1}{\sqrt{2}}\left[\Psi_0(x+a)+\Psi_0(x-a)\right]\delta(x\pm a) \\
<\mp a|r> &= \int dx\, \frac{1}{\sqrt{2}}\left[\Psi_0(x+a)-\Psi_0(x-a)\right]\delta(x\pm a) .
\end{aligned}
$$

We get

$$
\begin{aligned}
<\mp a|s> &= \frac{1}{\sqrt{2}}[\Psi_0(\mp a+a)+\Psi_0(\mp a-a)] \;\approx\; \frac{1}{\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \\
<\mp a|r> &= \frac{1}{\sqrt{2}}[\Psi_0(\mp a+a)-\Psi_0(\mp a-a)] \;\approx\; \pm\frac{1}{\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} ,
\end{aligned}
$$

because $\Psi_0(\pm 2a) \ll \Psi_0(0)$. So we recover (6.31).

The fact that $|\,s>$ corresponds to lower and $|\,r>$ to higher energy follows from the oscillation theorem of the one dimensional Sturm–Liouville problem of the eigenfunctions and eigenvalues of the second order differential equations:

the eigefunction $\Psi_n(x)$ corresponding to the $(n+1)$'th eigenvalue E_n has (for finite x's) exactly n zeros $(n = 0, 1, 2, ...)$.

Therefore $|\, s>$ having no zeros has lower energy than $|\, r>$ which has one zero.

Analogous calculations one can perform for periodic potentials with predictable results that the infinitely degenerate system without tunnelling becomes a band of states when tunnelling is switched on. Let us go through similar steps as in the case of a double well.

We start with an infinitely degenerate state for a particle which may sit at any of the identical minima at

$$x_j(\tau) = ja \qquad j = ... -2, -1, 0, +1, +2, \ldots . \tag{6.32}$$

In the limit of very large T we evaluate the amplitude for transitions (in time T) from the initial position $j_- a$ to the position $j_+ a$. In the semiclassical approximation we build the amplitude around multi-instanton configurations. Let there be: n instantons and m anti-instantons. We have

$$\begin{aligned} <j_+|e^{-\frac{1}{\hbar}HT}|j_-> &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\omega T} \\ &\times \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{1}{n!\,m!}\left(\tilde{K}e^{-S_E^0/\hbar}T\right)^{n+m} \delta_{(n-m)(j_+-j_-)} \,. \end{aligned} \tag{6.33}$$

We use the following representation of the Kronecker delta

$$\delta_{(n-m)(j_+-j_-)} = \int_0^{2\pi} \frac{d\theta}{2\pi}\, e^{i\theta(n-m)} e^{i\theta(j_- - j_+)} \,, \tag{6.34}$$

and obtain

$$\begin{aligned} <j_+|e^{-\frac{1}{\hbar}HT}|j_-> &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\omega T} \int_0^{2\pi} \frac{d\theta}{2\pi}\, e^{i\theta(j_- - j_+)} \\ &\times \sum_{n=0}^{\infty} \frac{1}{n!}\left(\tilde{K}Te^{-S_E^0/\hbar + i\theta}\right)^n \sum_{m=0}^{\infty} \frac{1}{m!}\left(\tilde{K}Te^{-S_E^0/\hbar - i\theta}\right)^m \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\omega T} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{i\theta(j_- - j_+)} e^{\tilde{K}Te^{-S_E^0/\hbar + i\theta}} e^{\tilde{K}Te^{-S_E^0/\hbar - i\theta}} \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{1}{2}\omega T} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{i\theta(j_- - j_+)} e^{2\tilde{K}Te^{-S_E^0/\hbar}\cos\theta} \,. \end{aligned} \tag{6.35}$$

Thus, indeed, the ground state energy of the harmonic oscillator splits into a band of states:

$$\tfrac{1}{2}\hbar\omega \;\to\; E(\theta) = \tfrac{1}{2}\hbar\omega - 2\tilde{K}\hbar e^{-S_E^0/\hbar}\cos\theta \,. \tag{6.36}$$

Writing

$$<j_+|e^{-\frac{1}{\hbar}HT}|j_-> = \int_0^{2\pi} d\theta <j_+|\theta><\theta|e^{-HT/\hbar}|\theta><\theta|j_->$$

we get

$$<\theta|j> = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2\pi}} e^{i\theta j} .$$

Following similar steps as in the case of the double well potential we get the following spatial representation of the wave function of the band labelled by θ:

$$\Phi_\theta(x) = \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{+\infty} \Psi_0(x - ja)\, e^{i\theta j} , \tag{6.37}$$

where $\Psi_0(x)$ is the wave function of the particle sitting in the well whose minimum (zero) is at $x = 0$. Under the translation $\mathcal{T} : x \to x + a$, Φ_θ acquires a phase:

$$\begin{aligned} \Phi_\theta(x+a) &= \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{+\infty} \Psi_0(x-(j-1)a)\, e^{i\theta j} \\ &= e^{i\theta} \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{+\infty} \Psi_0(x-(j-1)a)\, e^{i\theta(j-1)} = e^{i\theta}\Phi_\theta(x) . \end{aligned}$$

Thus

$$\mathcal{T}\Phi_\theta(x) = e^{i\theta}\Phi_\theta(x) . \tag{6.38}$$

Introducing the wave vector k

$$\theta j = \frac{\theta}{a} ja = kx_j$$

we can write

$$\Phi_\theta(x) = \Phi_k(x) = \frac{1}{\sqrt{2\pi}} \sum_j \Psi_0(x - x_j)\, e^{ikx_j} . \tag{6.39}$$

$\Phi_k(x)$ are called the Bloch waves, and are commonly employed in descriptions of the band structure of solids.

To summarize:

– without tunnelling the symmetry under $\mathcal{T}$ is broken,

– tunnelling restores it in the form given by (6.38).

6.2 Detailed calculations of $\tilde{K}$

A few comments are now in order. First let us re-write the equation of motion of one instanton:

$$\frac{d\bar{x}}{d\tau} = \left(\frac{2}{m}V(\bar{x})\right)^{\frac{1}{2}} \quad \to \quad \frac{d^2\bar{x}}{d\tau^2} = \frac{d}{d\bar{x}}\left[\left(\frac{2}{m}V(\bar{x})\right)^{\frac{1}{2}}\right]\frac{d\bar{x}}{d\tau} = \frac{1}{m}\frac{dV}{d\bar{x}}\,. \tag{6.40}$$

Another differentiation over τ gives

$$\left(-m\frac{d^2}{d\tau^2} + \frac{d^2V}{d\bar{x}^2}\right)\frac{d\bar{x}}{d\tau} = 0\,. \tag{6.41}$$

When we compare the above with our eigenvalue equation

$$\left(-m\frac{d^2}{d\tau^2} + \frac{d^2V}{d\bar{x}^2}\right)y_n(\tau) = \lambda_n y_n(\tau)\,, \tag{6.42}$$

we see that

$$y_1(\tau) = \left(S_E^0\right)^{-\frac{1}{2}}\sqrt{m}\,\frac{d\bar{x}}{d\tau} \tag{6.43}$$

is a normalized eigen solution corresponding to the eigenvalue $\lambda_1 = 0$. Indeed, since

$$S_E^0 = \int\limits_{-T/2}^{+T/2} d\tau\, 2V(\bar{x})\,, \tag{6.44}$$

we have

$$\int\limits_{-T/2}^{+T/2} d\tau y_1^2 \;=\; \left(S_E^0\right)^{-1} m \int\limits_{-T/2}^{+T/2} d\tau\,\frac{2V(\bar{x})}{m} = 1\,. \tag{6.45}$$

It would seem that we run into serious problem: the integral over da_1 is divergent! This is, nevertheless, not so. First, let us point out that $y_1(\tau)$ has *no zeros*. Hence λ_1 is the lowest of all λ's. In other words the oscillation theorem tells us that $\lambda_n > 0$, for all $n > 1$, hence the only problem is with λ_1. But it turns out that the integration over τ_1 made the integration over a_1 redundant. Indeed,

$$x(\tau) = \bar{x}(\tau) + y(\tau) = \bar{x}(\tau) + a_1 y_1(\tau) + \sum_{l>1} a_l\, y_l(\tau)\,. \tag{6.46}$$

Hence the the integration over $d\tau_1$ is equivalent to integration over da_1. In other words: the integration over da_1 is already done. Indeed, we can change the trajectory either by shifting τ_1 or a_1:

either
$$dx(\tau) \;=\; \frac{d\bar{x}}{d\tau_1}\,d\tau_1$$

or
$$dx(\tau) \;=\; y_1 da_1\,. \tag{6.47}$$

Equating the r.h.s. of (6.42) and employing the normalized y_1 we get

$$d\tau_1 = \left(S_E^0\right)^{-\frac{1}{2}} \sqrt{m}\, da_1\,. \tag{6.48}$$

Note that only the specific form of y_1 makes possible this simple equivalence of integrations over $d\tau_1$ and da_1.

Now we can find a formula for $\tilde{K}$. We calculate the contribution of the quantal fluctuations around *one instanton positioned anywhere between* $-T/2$ and $T/2$ in two ways: (a) using the general formula (6.10), and (b) the approximate formula with $\tilde{K}$ present and the fluctuations around the classical trajectory (one instanton) taken over from one oscillator. Then we equate (a) and (b) and get

$$\tilde{K} = \frac{K_{\text{one inst.},\lambda_1=0}(a, \frac{1}{2}T; -a, -\frac{1}{2}T)}{K_{\text{one inst.,harm.osc.}}(a, \frac{1}{2}T; -a, -\frac{1}{2}T)}\,. \tag{6.49}$$

Since

$$K_{\text{one inst.},\lambda_1=0}(a, \tfrac{1}{2}T, -a, -\tfrac{1}{2}T) = e^{-\frac{1}{\hbar}S_E^0[\bar{x}]}\mathcal{N}\int\prod_{n=1}\frac{da_n}{\sqrt{2\pi\hbar}}e^{-\frac{1}{2\hbar}\sum_n\lambda_n a_n^2}$$

$$= e^{-\frac{1}{\hbar}S_E^0[\bar{x}]}\mathcal{N}\,[\det{}'(-m\frac{d^2}{d\tau^2}+V''(\bar{x}))]^{-\frac{1}{2}}\int_{-\infty}^{+\infty}\frac{da_1}{\sqrt{2\pi\hbar}}$$

$$= e^{-\frac{1}{\hbar}S_E^0[\bar{x}]}\mathcal{N}\,[\det{}'(-m\frac{d^2}{d\tau^2}+V''(\bar{x}))]^{-\frac{1}{2}}\int_{-T/2}^{+T/2}d\tau_1\left(S_E^0\right)^{\frac{1}{2}}\frac{1}{\sqrt{m}}\frac{1}{\sqrt{2\pi\hbar}}$$

$$= e^{-\frac{1}{\hbar}S_E^0[\bar{x}]}\mathcal{N}\,[\det{}'(-m\frac{d^2}{d\tau^2}+V''(\bar{x}))]^{-\frac{1}{2}}\,T\left(S_E^0\right)^{\frac{1}{2}}\frac{1}{\sqrt{m}}\frac{1}{\sqrt{2\pi\hbar}}\,, \tag{6.50}$$

where

$$\det{}'(-m\frac{d^2}{d\tau^2}+V''(\bar{x})) = \prod_{n=2}\lambda_n\,.$$

On the other hand

$$K_{\text{one inst.,harm.osc.}}(a, \tfrac{1}{2}T, -a, -\tfrac{1}{2}T) = e^{-\frac{1}{\hbar}S_E^0[\bar{x}]}\mathcal{N}\,[\det(-m\frac{d^2}{d\tau^2}+m\omega^2))]^{-\frac{1}{2}}\,T$$

with $m\omega^2 = V''(\pm a)$. Thus we obtain

$$\tilde{K} = \left(\frac{S_E^0}{m2\pi\hbar}\right)^{\frac{1}{2}}\frac{[\det(-m\frac{d^2}{d\tau^2}+m\omega^2))]^{\frac{1}{2}}}{[\det{}'(-m\frac{d^2}{d\tau^2}+V''(\bar{x}))]^{\frac{1}{2}}}\,. \tag{6.51}$$

To obtain $\tilde{K}$ we have to have a method for calculating the determinants in (6.51). This can be done as follows [6.1]. The starting point is the eigevalue equation which we write in a simplified form (for simplicity sake we set $m = 1$, and write ∂_t in place of $\frac{\partial}{\partial t}$):

$$(-\partial_t^2 + W(t))\, y(t) = \lambda\, y(t) \tag{6.52}$$

where $W(t)$ is bounded for all t. Let $y(t)$ be the solution satisfying the following initial conditions:

$$y_\lambda\left(-\tfrac{1}{2}T\right) = 0\,, \qquad \partial_t y_\lambda\left(-\tfrac{1}{2}T\right) = 1\,. \tag{6.53}$$

The operator $(-\partial_t^2 + W)$ acting on functions $y_{\lambda_n}(t)$ has the eigenvalue λ_n only when $y_{\lambda_n}(+T/2) = 0$. Note that

$$(-\partial_t^2 + W - \lambda)\, y_{\lambda_n} = (\lambda_n - \lambda)\, y_{\lambda_n}\,, \tag{6.54}$$

thus y_{λ_n} diagonalize not only $(-\partial_t^2 + W)$ but also $(-\partial_t^2 + W - \lambda)$. Clearly :

$$\det(-\partial_t^2 + W) = \prod_n \lambda_n\,. \tag{6.55}$$

Let $W^{(1)}$, $W^{(2)}$ be two functions bounded for all t, and let $y^{(1)}$ and $y^{(2)}$ be two solutions of (6.52). One can show [6.1] that

$$\frac{\det[-\partial_t^2 + W^{(1)} - \lambda]}{\det[-\partial_t^2 + W^{(2)} - \lambda]} = \frac{y_\lambda^{(1)}\left(\frac{1}{2}T\right)}{y_\lambda^{(2)}\left(\frac{1}{2}T\right)} = \frac{\prod_n(\lambda_n^{(1)} - \lambda)}{\prod_n(\lambda_n^{(2)} - \lambda)}\,. \tag{6.56}$$

If so, then

$$\frac{\det[-\partial_t^2 + W^{(1)} - \lambda]}{y_\lambda^{(1)}\left(\frac{1}{2}T\right)} = \frac{\det[-\partial_t^2 + W^{(2)} - \lambda]}{y_\lambda^{(2)}\left(\frac{1}{2}T\right)} = 2\mathcal{N}^2\pi\hbar\,, \tag{6.57}$$

where $\mathcal{N}$ does not depend on W!

Let us apply this relation to the case of simple harmonic oscillator and check (6.57) on a well known case:

$$\lambda = 0 \quad \to \quad (-\partial_t^2 + \omega^2)\, y_0(t) = 0\,, \tag{6.58}$$

and its solution

$$y_0(t) = \frac{1}{2\omega}\left(e^{\omega(t+\frac{1}{2}T)} - e^{-\omega(t+\frac{1}{2}T)}\right), \tag{6.59}$$

satify the initial conditions (6.53). Thus

$$y_0\left(\tfrac{1}{2}T\right) = \frac{1}{2\omega}\left(e^{\omega T} - e^{-\omega T}\right)\,, \tag{6.60}$$

and

$$\frac{\det(-\partial_t^2 + \omega^2)}{\frac{1}{2\omega}(e^{\omega T} - e^{-\omega T})} = 2\pi\hbar\mathcal{N}^2\,. \tag{6.61}$$

In the limit of very large T , taking square roots of both sides of (6.61) we obtain the formula we are very familiar with:

$$\mathcal{N}\left[\det(-\partial_t^2 + \omega^2)\right]^{-\frac{1}{2}} = \sqrt{\frac{\omega}{\pi\hbar}}\, e^{-\frac{1}{2}\omega T}\,. \tag{6.62}$$

The arguments in support of (6.56) go along the following lines [6.1]. Both sides of (6.56) are some *meromorphic functions* of λ in the complex plane and tend to 1 when $\lambda \to \infty$ (except along the positive real axis) with poles and zeros at the same values of λ. Moreover, they are the same functions. (Incidentally: when all the singularities of a function in a given region of the complex plane are *poles*, the function is meromorphic in this region). Be it as it may, (6.56) gives us a handle to compute (6.51). We know $\det(-\partial_t^2+\omega^2)$, now we compute $\det{}'(-\partial_t^2+V''(\bar{x}))$ following these steps:

1. First we compute

$$\det(-\partial_t^2+V''(\bar{x})) \;=\; 2\pi\hbar\mathcal{N}^2 y_{\lambda=0}\left(\tfrac{1}{2}T\right)\,, \tag{6.63}$$

$$y_{\lambda=0}\left(-\tfrac{1}{2}T\right)=0\,,\qquad \partial_t y_{\lambda=0}\left(-\tfrac{1}{2}T\right)=1$$

   where we set $\lambda=0$ in (6.52).

2. Then, we compute $\lambda_1(T)$ *for finite but large* T (which must be such that $\lim_{T\to\infty}\lambda_1(T)=0$) and calculate

$$\det{}'(-\partial_t^2+V''(\bar{x})) \;=\; \lim_{T\to\infty}\frac{\det(-\partial_t^2+V''(\bar{x}))}{\lambda_1(T)}\,. \tag{6.64}$$

We construct $y_{\lambda=0}(t)$ from two independent solutions of $(-\partial_t^2+V''(\bar{x}))\,y=0$ of which we already know one

$$y_1(t) \;=\; \left(S_E^0\right)^{-\frac{1}{2}}\sqrt{m}\,\frac{d\bar{x}}{dt}\,. \tag{6.65}$$

Thus we take a linear combination of y_1 and a linearly independent solution $\tilde{y}_1$ to form $y_{\lambda=0}$ satisfying the initial conditions (6.53)

$$y_{\lambda=0}(t) \;=\; a y_1(t) + b\,\tilde{y}_1(t)\,. \tag{6.66}$$

The condition for $\tilde{y}_1$ to be linearly independent of y_1 is to have their Wronskian different from zero:

$$y_1(t)\,\partial_t\tilde{y}_1(t) \;-\; \tilde{y}_1(t)\,\partial_t y_1(t) \;\neq\; 0\,. \tag{6.67}$$

Since we attempt to construct $\det{}'(...)$ for very large times $|t|$ close to $|\frac{1}{2}T|$ it will be enough to employ the asymptotic forms of the solutions $y_1(t)$ and $\tilde{y}_1(t)$. We already know it for y_1:

$$y_1(t) = A\,e^{-|t|\omega}\,,\qquad \omega=\sqrt{V''(\pm a)}\,. \tag{6.68}$$

It is easy to guess the asymptotic form of $\tilde{y}_1$:

$$\tilde{y}_1(t) = \pm A\,e^{|t|\omega}\,,\qquad t\to\pm\infty\,. \tag{6.69}$$

Indeed, we find that

$$y_1(t)\,\partial_t\tilde{y}_1(t) \;-\; \tilde{y}_1(t)\,\partial_t y_1(t) \;=\; 2A^2\omega\,. \tag{6.70}$$

This means that $y_1(t)$ and $\tilde{y}_1(t)$ are two independent solutions, and we can now construct the solution $y_{\lambda=0}(t)$ choosing a and b such that the initial conditions (6.53) are satisfied. Choosing (since ω =const we can, without loosing anything, set $\omega = 1$)

$$y_{\lambda=0}(t) \;=\; \frac{1}{2A}\left(e^{\frac{1}{2}T} y_1(t) \;+\; e^{-\frac{1}{2}T}\tilde{y}_1(t)\right), \tag{6.71}$$

we see that indeed

$$y_{\lambda=0}(-\tfrac{1}{2}T) = 0 \qquad \text{and} \qquad \partial_t y_{\lambda=0}(-\tfrac{1}{2}T) = 1\,. \tag{6.72}$$

Note that we also find

$$y_{\lambda=0}(\tfrac{1}{2}T) \;=\; \frac{1}{2A}\left(e^{\frac{1}{2}T}Ae^{-\frac{1}{2}T} \;+\; e^{-\frac{1}{2}T}Ae^{\frac{1}{2}T}\right) = 1\,, \tag{6.73}$$

which we shall presently need to calculate the determinant (for large T) from (6.63):

$$\det(-\partial_t^2 + V''(\bar{x})) \;=\; 2\pi\hbar\mathcal{N}^2 y_{\lambda=0}\left(\tfrac{1}{2}T\right) \;=\; 2\pi\hbar\mathcal{N}^2\,. \tag{6.74}$$

Now, in order to obtain $\lambda_1(T)$, we have to solve

$$(-\partial_t^2 + V''(\bar{x}))\, y_T(t) \;=\; \lambda_1(T)\, y_T(t) \tag{6.75}$$

for *finite* (but large !) T. Thus $\lambda_1(T)$ must be *small* because for $T \to \infty$ it is zero.

First, we convert (6.75) into an integral equation. It is an exercise in mathematical physics that

$$y_T(t) = y_{\lambda=0}(t) - \lambda_1(T)\,\frac{1}{2A^2}\int_{-T/2}^{t} dt'\left\{\tilde{y}_1(t)\, y_1(t') - y_1(t)\,\tilde{y}_1(t')\right\} y_T(t') \tag{6.76}$$

is the integral equation we are looking for. Note that

$$y_T\left(-\tfrac{1}{2}T\right) = y_{\lambda=0}\left(-\tfrac{1}{2}T\right) = 0 \qquad \text{and} \qquad (-\partial_t^2 + V''(\bar{x}))\, y_{\lambda=0} = 0\,. \tag{6.77}$$

In order to check that $y_T(t)$ of (6.76) is a solution of (6.75) we employ the familiar equations

$$\partial_t^2 y_1(t) = V''(\bar{x}) y_1(t) \qquad \text{and} \qquad \partial_t^2 \tilde{y}_1(t) = V''(\bar{x})\tilde{y}_1(t)\,, \tag{6.78}$$

and note that

$$\int_{-T/2}^{t} dt'\,\left\{\tilde{y}_1(t)\, y_1(t') - y_1(t)\,\tilde{y}_1(t')\right\} y_T(t') =$$

$$= \int_{-T/2}^{T/2} dt'\,\theta(t-t')\left\{\tilde{y}_1(t)\, y_1(t') - y_1(t)\,\tilde{y}_1(t')\right\} y_T(t')\,. \tag{6.79}$$

With the help of eqs.(6.78) and (6.70) we get (remember that $\partial_t\theta(t-t') = \delta(t-t')$, $\partial_t^2\theta(t-t') = \delta'(t-t')$ and $\int dt'\delta'(t-t')f(t') = \partial_t f(t)$.)

$$(-\partial_t^2 + V'') \int_{-T/2}^{T/2} dt'\, \theta(t-t') \left\{\tilde{y}_1(t)\, y_1(t') - y_1(t)\, \tilde{y}_1(t')\right\} y_T(t') \;=\; -2A^2 y_T(t)\,, \tag{6.80}$$

thus it is clear that (6.76) leads to (6.75).

Since we expect $\lambda_1(T)$ to be very small (T very large) we solve (6.76) in the first approximation setting under the integral

$$y_T(t') = y_{\lambda=0}(t')\,. \tag{6.81}$$

Our $y_T(t)$ satisfies one boundary condition: $y_T(-T/2) = 0$. In order to have an *eigensolution* we have to have also $y_T(T/2) = 0$. Demanding this amounts to imposing the relation

$$0 = 1 - \lambda_1(T)\, \frac{1}{2A^2} \int_{-T/2}^{T/2} dt' \left\{\tilde{y}_1(\tfrac{1}{2}T)\, y_1(t') - y_1(\tfrac{1}{2}T)\, \tilde{y}_1(t')\right\} y_{\lambda=0}(t')\,, \tag{6.82}$$

which, for large T ($\tilde{y}_1(t) \to Ae^t$, $y_1(t) \to Ae^{-t}$) and after inserting (6.71), becomes

$$0 = 1 - \lambda_1(T)\, \frac{1}{4A^2} \int_{-T/2}^{T/2} dt' \left(e^T y_1^2(t') - e^{-T}\tilde{y}_1^2(t')\right)\,. \tag{6.83}$$

Now, since $y_1(t)$ is normalized

$$\int_{-T/2}^{T/2} dt' e^T y_1^2(t') = e^T \qquad \text{and} \qquad \int_{-T/2}^{T/2} dt' e^{-T}\tilde{y}_1^2(t') < \infty\ ,$$

we can neglect the second term in (6.83) relative to e^T. Thus our final equation is

$$0 = 1 - \lambda_1(T)\, \frac{1}{4A^2}\, e^T\,, \tag{6.84}$$

hence our final formula for the eigenvalue $\lambda_1(T)$ for *finite* but large T is

$$\lambda_1(T) \;=\; 4A^2 e^{-T}\,. \tag{6.85}$$

Indeed, it goes to zero as $T \to \infty$.

Thus

$$\mathcal{R} = \frac{\det{}'[-\partial_t^2 + V''(\bar{x})]}{\det[-\partial_t^2 + \omega^2]} \;=\; \frac{\frac{2\pi\hbar\mathcal{N}^2}{4A^2e^{-T}}}{2\pi\hbar\mathcal{N}^2\frac{1}{2}e^T} \;=\; \frac{1}{2A^2}\,, \tag{6.86}$$

and the problem of calculation of $\tilde{K}$ is reduced to determination of the asymptotic coefficient A of

$$y_1(t) \;=\; \sqrt{\frac{m}{S_E^0}}\, \frac{d\bar{x}}{dt}\bigg|_{t\ \text{large}} \;=\; Ae^{-|t|}\,, \tag{6.87}$$

that is to say for $\bar{x}$ close to a. One can show that

$$A = \frac{1}{\sqrt{S_E^0}} |\bar{x} - a| \, e^{\int_0^{\bar{x}} dx \frac{1}{\sqrt{2V(x)}}} , \tag{6.88}$$

with $S_E^0 = \int_{-a}^{a} dx \sqrt{2mV(x)}$. An alternative expression is

$$\int_0^{\bar{x}} dx \frac{1}{\sqrt{2V(x)}} = -\ln\left((S_E^0)^{-\frac{1}{2}} A^{-1} |\bar{x} - a|\right) . \tag{6.89}$$

So, A can be found numerically from one of these formulae by taking $\bar{x}$ close to a.

6.2.1 The amplitude for decay processes

Our last application of the semiclassical approximations to tunnelling is a brief outline of construction of the amplitude for decay processes.

In this case the potential is such that it cannot contain the particle for ever around its minimum. Let us take $V(x)$ such that $V(x) \to \pm\infty$ as $x \to \mp\infty$, $V(0) = 0$ is its local minimum, V has one finite maximum at some positive x and $V(x_b) = 0$ for $x_b > 0$. Now the "elementary" Euclidean trajectory from which we shall built the amplitude is one "bounce": the motion, as before, is in the potential $-V(x)$. It starts at $x = 0$ (the total energy is again zero), goes through the minimum of $-V(x)$ (where it has the maximal kinetic energy), stops at x_b and immediately goes back to $x = 0$. Since the total energy is zero, it takes an infinitely long time T to complete one "bounce".

The classical trajectory is now a sequence of an arbitrary number of "bounces". The energy is a constant of motion and gives the equation of motion:

$$\dot{\bar{x}} = \pm\sqrt{\frac{2V(\bar{x})}{m}} \tag{6.90}$$

which, in turn, gives the action for one bounce

$$\begin{aligned} S_E^0 \equiv B &= \int d\tau \left(\tfrac{1}{2} m \frac{2}{m} V + V\right) = \int_0^{x_b} d\bar{x} \frac{2V(\bar{x})}{\sqrt{2V(\bar{x})/m}} + \int_{x_b}^0 d\bar{x} \frac{V(\bar{x})}{-\sqrt{2V(\bar{x})/m}} \\ &= 2\int_0^{x_b} d\bar{x} \, \sqrt{2mV(\bar{x})} \, . \end{aligned} \tag{6.91}$$

Summing over an arbitrary number of bounces we get the amplitude for the particle to remain at $x = 0$:

$$<0|e^{-\frac{1}{\hbar}HT}|0> = \sqrt{\frac{m\omega}{\pi\hbar}} \, e^{-\frac{1}{2}\omega T} \sum_{n=0}^{\infty} \frac{(\tilde{K} e^{-B/\hbar} T)^n}{n!} = \sqrt{\frac{m\omega}{\pi\hbar}} \, e^{(-\frac{1}{2}\omega + \tilde{K} e^{-B/\hbar})T} . \tag{6.92}$$

Therefore, the ground state energy is

$$E_0 = \tfrac{1}{2}\omega\hbar - \hbar\tilde{K} e^{-\frac{B}{\hbar}} . \tag{6.93}$$

However, we know that

$$\tilde{K} \sim \prod_l (\lambda_l)^{-\frac{1}{2}} .$$

On the other hand going through similar steps as before we can convince ourselves that we have again the eigenvalue $\lambda_1 = 0$ whose eigenfunction is proportional to $\frac{d\bar{x}}{d\tau}$, $\bar{x}$ being this time the trajectory of one bounce. $\lambda_1 = 0$ itself does not bother us any more because we know that the integration over the position of a bounce on the time axis gets rid of the problem, but $\frac{d\bar{x}}{d\tau}$ has exactly one zero! (Because it has one maximum at the time when it reaches x_b). Therefore, the oscillation theorem tells us that there exist an eigevalue $\lambda_0 < 0$ whose eigenfunction has no zeros. But that means that $\tilde{K}$ is purely imaginary, hence E_0 of (6.93) is complex. So we may expect that the width of the ground state is

$$\Gamma = |\tilde{K}| \, e^{-\frac{B}{\hbar}} . \tag{6.94}$$

That this indeed is the case takes some additional arguments because an unstable state cannot be an eigenvalue of H. One has to perform a process of analytic continuation. Instead of going into this we suggest reading some classic contributions to this subject [6.1]-[6.4].

====> This part is completely redone

6.3 Explicit calculation of the instanton propagator

6.3.1 Classical trajectory

In this section we shall calculate explicitly ratio of two determinants $\mathcal{R}$ defined in eq. (6.86) for a motion of a particle of a unit mass $m = 1$ in the double well potential (6.16):

$$V(x) = \frac{1}{8a^2}(a^2 - x^2)^2 \tag{6.95}$$

where for simplicity we have set $\kappa = 1/8a^2$. Most of the material presented here is based on Ref.[6.5].

From general considerations of the previous section we know that

$$\mathcal{R} = \frac{1}{2A^2} \tag{6.96}$$

where A is normalization factor of the classical solution $\overline{x}(\tau)$, defined for example, by eq. (6.89):

$$\tau \to -\ln\left(\frac{1}{A\sqrt{S_0^E}}(a - \bar{x})\right) . \tag{6.97}$$

for large τ. The classical trajectory can be calculated from eq. (6.19):

$$\tau - \tau_1 = \int_0^{\bar{x}(\tau)} \frac{dx}{\sqrt{2V(x)}} = \ln\frac{a + \bar{x}}{a - \bar{x}} \tag{6.98}$$

which yields:

$$\bar{x}(\tau) = a \tanh \frac{\tau - \tau_1}{2}. \tag{6.99}$$

The classical action along the trajectory (6.99) is given by eq. (6.21):

$$S_E^0 = \int_{-a}^{+a} dx \sqrt{2V(x)} = \frac{1}{2a} \int_{-a}^{+a} dx \left(a^2 - x^2\right) = \frac{2}{3} a^2. \tag{6.100}$$

From eqs. (6.97), (6.98) and (6.100) we find:

$$A = \frac{2a}{\sqrt{S_E^0}} = \sqrt{6}. \tag{6.101}$$

Hence the ratio $\mathcal{R} = 1/12$ for the potential (6.95).

Finally, let us calculate the velocity of the instanton:

$$\frac{d\bar{x}(\tau)}{d\tau} = \frac{a}{2} \frac{1}{\cosh^2\left(\frac{\tau - \tau_0}{2}\right)} \tag{6.102}$$

which we shall need later in sect.6.3.4.

6.3.2 Euclidean harmonic oscillator

Before proceeding with the instanton case, let us for completeness consider the case of a harmonic oscillator with unit mass and unit frequency $m = \omega = 1$. The classical trajectory of an Euclidean oscillator is simply zero, hence the classical action is also zero. What remains to be calculated is a determinant of the Sturm-Liouville operator:

$$D(\tau) = -\frac{d^2}{d\tau^2} + V''[\bar{x}(\tau)]. \tag{6.103}$$

To calculate the determinant we have to solve the eigenproblem for $D(\tau)$ and calculate a product of all nonzero eigenvalues. For the case of a harmonic oscillator the eigenequation takes the following form:

$$\left[-\frac{d^2}{d\tau^2} + 1\right] y_n(\tau) = \lambda_n \, y_n(\tau). \tag{6.104}$$

Since eq.(6.104) has a continuous spectrum we have to close system in a box $-T/2 < \tau < T/2$ and impose boundary conditions on the functions y_n

$$y_n\left(-\frac{T}{2}\right) = y_n\left(\frac{T}{2}\right) = 0. \tag{6.105}$$

Defining $k_n^2 = \lambda_n - 1$ we get by elementary differential equation theory

$$y_n(\tau) = \text{const} \sin\left(k_n \tau\right), \quad k_n = \frac{\pi n}{T} \tag{6.106}$$

with $n = 1, 2, 3 \dots$.

Now we shall calculate determinant of $D(\tau)$:

$$\det\left[-\frac{d^2}{d\tau^2}+1\right] = \prod_{n=1}^{\infty}\lambda_n = \prod_{n=1}^{\infty}\left(1+k_n^2\right) = \prod_{n=1}^{\infty}\left(1+\left(\frac{\pi n}{T}\right)^2\right) \tag{6.107}$$

This expression can be explicitly evaluated. For that purpose let us restore the frequency ω :

$$\prod_{n=1}^{\infty}\left(\omega+\left(\frac{\pi n}{T}\right)^2\right) = \prod_{n=1}^{\infty}\left(\frac{\pi n}{T}\right)^2\prod_{n=1}^{\infty}\left(1+\left(\frac{\omega T}{\pi n}\right)^2\right) = \text{const}\,\frac{\sinh(\omega T)}{\omega T}. \tag{6.108}$$

Here const corresponds to the first product in Eq.(6.108) which does not depend on ω and combines with the Jacobian and other factors into a single constant which can be determined from the propagator of a free particle. Indeed for this case the determinant of a Sturm-Liouville operator reads:

$$\det\left[-\frac{d^2}{d\tau^2}\right] = \prod_{n=1}^{\infty}\lambda_n = \prod_{n=1}^{\infty}k_n^2 = \prod_{n=1}^{\infty}\left(\frac{\pi n}{T}\right)^2. \tag{6.109}$$

6.3.3 Sturm-Liouville equation for the instanton

For the potential (6.95) and the instanton centered around $\tau_1 = 0$ the Sturm-Liouville equation (6.103) takes the following form:

$$\left[-\frac{d^2}{d\tau^2}-\frac{3}{2}\frac{1}{\cosh^2\left(\frac{\tau}{2}\right)}\right]y_n(\tau) = (\lambda_n-1)\;y_n(\tau). \tag{6.110}$$

This is a Schrödinger equation for a motion in a potential $1/\cosh^2(\tau/2)$ which is discussed, for example, in Ref. [6.6]. The spectrum of the eigenenergies $\varepsilon_n = (\lambda_n - 1)$ for this potential consists from a finite number of discrete levels with $\varepsilon_n < 0$ and a continuous spectrum with $\varepsilon_n > 0$. Therefore in the case of $\varepsilon_n < 0$ we can push $T \to \infty$, whereas for $\varepsilon_n > 0$ we have to work in a finite box with the boundary conditions (6.105).

Since the asymptotics of eq.(6.110) is exponential, let us substitute:

$$y_n(\tau) = e^{\alpha\tau}w_n(\tau). \tag{6.111}$$

This substitution leads to the following equation

$$\left[-\frac{d^2}{d\tau^2}-2\alpha\frac{d}{d\tau}-\left[\alpha^2-(1-\lambda_n)\right]-\frac{3}{2}\left(1-\tanh^2\left(\frac{\tau}{2}\right)\right)\right]w_n(\tau)=0 \tag{6.112}$$

where we have used

$$\frac{1}{\cosh^2\left(\frac{\tau}{2}\right)} = 1-\tanh^2\left(\frac{\tau}{2}\right).$$

To satisfy (6.111) we have to choose:

$$\alpha = \pm\sqrt{-\varepsilon_n} = \pm\sqrt{1-\lambda_n}. \tag{6.113}$$

For the discrete levels $\varepsilon_n < 0$ and we have to make sure that the solutions have proper asymptotics, by choosing the right sign in eq.(6.113). For the continuous spectrum α is imaginary and both solutions (6.113) will contribute.

Let us introduce a new variable

$$z = \tanh\left(\frac{\tau}{2}\right), \quad \frac{d}{d\tau} = \frac{1}{2}\left(1 - z^2\right)\frac{d}{dz}$$

with $-1 < z < 1$. In this new variable eq.(6.110) reads:

$$\left[\left(1 - z^2\right)\frac{d^2}{dz^2} + 2(2\alpha - z)\frac{d}{dz} + 6\right] w_n(z) = 0. \tag{6.114}$$

It is convenient to change variables once more

$$u = \frac{1}{2}(1 + z), \quad \frac{d}{dz} = \frac{1}{2}\frac{d}{du}$$

with $0 < u < 1$ and rewrite eq.(6.114) as

$$\left[u(1-u)\frac{d^2}{du^2} + (2\alpha + 1 - 2u)\frac{d}{du} + 6\right] w_n(u) = 0. \tag{6.115}$$

This a hypergeometric equation of the form

$$u(1-u)\, w''(u) + \{c - (a + b + 1)\, u\}\; w'(u) - ab\, w(u) = 0 \tag{6.116}$$

with

$$c = 2\alpha + 1,\ a = 3,\ b = -2.$$

Let us recall that the general solution of eq.(6.116) is given as a power series:

$$F(a, b, c; u) = 1 + \frac{ab}{c}\frac{u}{1!} + ... + \frac{a(a+1)...(a+n)\, b(b+1)...(b+n)}{c(c+1)...(c+n)}\,\frac{u^{n+1}}{(n+1)!} + ... \tag{6.117}$$

and therefore the solution for $w_n(u) = AF(3, -2, c; u)$ is a polynomial [1]. Coming back to the original variables, and choosing the normalization factor to be $A = c(c+1) = 2(\alpha+1)(2\alpha+1)$ we arrive at

$$y_n(\tau) = \mathcal{N}\left(3\tanh^2\left(\frac{\tau}{2}\right) - 6\alpha\tanh\left(\frac{\tau}{2}\right) + \left(4\alpha^2 - 1\right)\right)e^{\alpha\tau}. \tag{6.118}$$

Note that these are in fact two solutions depending on the sign of α (see eq.(6.113)).

6.3.4 Discrete spectrum

Let us denote $\kappa = \sqrt{-\varepsilon_n} > 0$. Consider the first case $\alpha = +\kappa$:

$$y_n^{(+)}(\tau) = \mathcal{N}\left(3\tanh^2\left(\frac{\tau}{2}\right) - 6\kappa\tanh\left(\frac{\tau}{2}\right) + \left(4\kappa^2 - 1\right)\right)e^{\kappa\tau}. \tag{6.119}$$

[1] We thank T. Romańczukiewicz for pointing out this simple form of the solution to us.

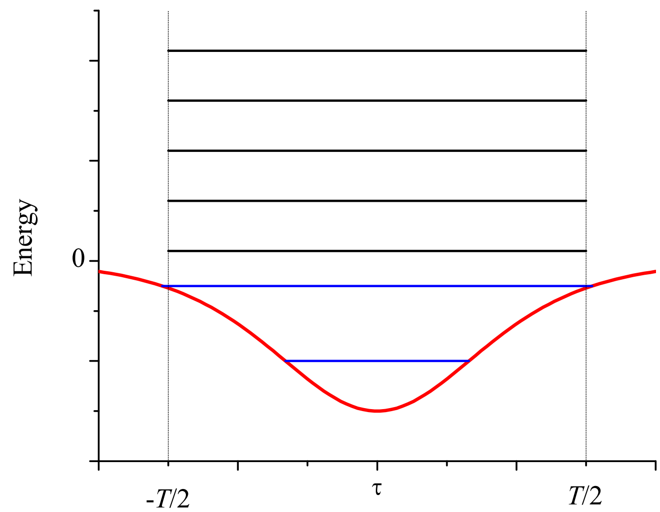

Figure 6.2: Schematic spectrum of energy levels of eq. (6.110). Continuous levels of positive energy are discretized by imposing boundary conditions (6.127).

This solution vanishes for $\tau \to -\infty$, however it explodes for $\tau \to \infty$ unless the coefficient in the bracket vanishes in this limit:

$$2 - 6\kappa + 4\kappa^2 = 2(2\kappa - 1)(\kappa - 1) = 0. \tag{6.120}$$

Two solutions $\kappa_1 = 1$ and $\kappa_2 = 1/2$ translate into the following two values of λ:

$$\lambda_1 = 0, \ \lambda_2 = \frac{3}{4}. \tag{6.121}$$

For $\alpha = -\kappa$ the solution reads

$$y_n^{(-)}(\tau) = \mathcal{N}\left(3\tanh^2\left(\frac{\tau}{2}\right) + 6\kappa\tanh\left(\frac{\tau}{2}\right) + \left(4\kappa^2 - 1\right)\right)e^{-\kappa\tau}. \tag{6.122}$$

This time the coefficient in bracket has to vanish for $\tau \to -\infty$ which leads again to the condition (6.120).

We see, as anticipated from the general discussion in the previous section, that the instanton determinant has one zero mode corresponding to $\lambda_1 = 0$, which cannot be treated in the Gaussian approximation. The exact treatment of this mode corresponds to the integration over the center of the instanton. For the purpose of the present calculation we simply drop $\lambda_1 = 0$ from the formula for the determinant. It is interesting to rewrite the zero mode solution (6.119) for $\kappa = 1$ (or (6.122) for $\kappa = -1$) as:

$$y_1(\tau) = 3\mathcal{N}\left(\tanh\left(\frac{\tau}{2}\right) - 1\right)^2 e^{\tau} = 6\mathcal{N}\frac{1}{\cosh^2\frac{\tau}{2}}$$

which, up to the normalization factor $\mathcal{N}$, coincides with the classical velocity (6.102). This is an illustration of the general property of the zero mode solution (6.43).

6.3.5 Continuous spectrum

For $\varepsilon_n > 0$ we have two solutions $\alpha = \pm ik$ (with $k = \sqrt{\varepsilon_n} > 0$):

$$y_k^{(\pm)}(\tau) = \mathcal{N}\left(3\tanh^2\left(\frac{\tau}{2}\right) \mp i6k\tanh\left(\frac{\tau}{2}\right) - \left(4k^2+1\right)\right)e^{\pm ik\tau} \tag{6.123}$$

corresponding to the right (+) or left (−) moving waves. Note that there is no reflection in the present potential; the solutions (6.123) remain left or right moving on the both sides of the potential:

$$\begin{aligned} 2\mathcal{N}(1+ik)(1+2ik)e^{ik\tau} \underset{\tau\to-\infty}{\longleftarrow} y_k^{(+)} \underset{\tau\to\infty}{\longrightarrow} 2\mathcal{N}(1-ik)(1-2ik)e^{ik\tau}, \\ 2\mathcal{N}(1-ik)(1-2ik)e^{-ik\tau} \underset{\tau\to-\infty}{\longleftarrow} y_k^{(-)} \underset{\tau\to\infty}{\longrightarrow} 2\mathcal{N}(1+ik)(1+2ik)e^{-ik\tau}. \end{aligned} \tag{6.124}$$

The only effect of the potential is the phase shift:

$$e^{i\delta_k} = \frac{1+ik}{1-ik}\frac{1+2ik}{1-2ik}. \tag{6.125}$$

Indeed:

$$\begin{aligned} 2\mathcal{N}(1-ik)(1-2ik)e^{i(k\tau+\delta_k)} \underset{\tau\to-\infty}{\longleftarrow} y_k^{(+)} \underset{\tau\to\infty}{\longrightarrow} 2\mathcal{N}(1-ik)(1-2ik)e^{ik\tau}, \\ 2\mathcal{N}(1+ik)(1+2ik)e^{-i(k\tau+\delta_k)} \underset{\tau\to-\infty}{\longleftarrow} y_k^{(-)} \underset{\tau\to\infty}{\longrightarrow} 2\mathcal{N}(1+ik)(1+2ik)e^{-ik\tau}. \end{aligned} \tag{6.126}$$

(Note that $\delta_{-k} = -\delta_k$).

In order to calculate the determinant ratio $\mathcal{R}$ we shall proceed as in the case of the of the harmonic oscillator, namely we shall consider a general solution

$$Y_k(\tau) = A\,y_k^{(+)}(\tau) + B\,y_k^{(-)}(\tau),$$

close the system in a box $-T/2 < \tau < T/2$ and impose the boundary conditions:

$$\begin{aligned} Y_k(\frac{T}{2}) = A\,y_k^{(+)}(\frac{T}{2}) + B\,y_k^{(-)}(\frac{T}{2}) = 0, \\ Y_k(-\frac{T}{2}) = A\,y_k^{(+)}(-\frac{T}{2}) + B\,y_k^{(-)}(-\frac{T}{2}) = 0. \end{aligned} \tag{6.127}$$

Eqs.(6.127) imply that:

$$k_n\,T - \delta_k = \pi\,n \tag{6.128}$$

where $n = 0, 1, ...$ Let us denote the solution of this equation as k_n^I, to be distinguished from $k_n = \pi n$ corresponding to the harmonic oscillator (6.106).

We shall now compute the continuum contribution to $\mathcal{R}$:

$$\mathcal{R}_{\text{cont}} = \frac{\det_{\text{cont}}\left(-\frac{d^2}{d\tau^2} + V''[\bar{x}(\tau)]\right)}{\det\left(-\frac{d^2}{d\tau^2} + 1\right)} \tag{6.129}$$

which is the ratio of the instanton determinant over the one of the harmonic oscillator. We have:

$$\mathcal{R}_{\text{cont}} = \frac{\prod \lambda_n^I}{\prod \lambda_n} = \frac{\prod \left(1 + k_n^{I\,2}\right)}{\prod \left(1 + k_n^2\right)} = \exp\left\{\sum_n \ln \frac{1 + k_n^{I\,2}}{1 + k_n^2}\right\}. \tag{6.130}$$

In order to calculate (6.130) we shall transform the sum over n to an integral over dk, and make use of the fact that in the limit of large T, k_n and k_n^I differ by a small quantity δ_k/T. Therefore we shall keep only terms linear in δ_k/T. This is done in the following way:

$$\begin{aligned}
\mathcal{R}_{\text{cont}} &= \exp\left\{\sum_n \ln \frac{1 + k_n^2 + k_n^{I\,2} - k_n^2}{1 + k_n^2}\right\} = \exp\left\{\sum_n \ln\left(1 + \frac{k_n^{I\,2} - k_n^2}{1 + k_n^2}\right)\right\} \\
&\simeq \exp\left\{\sum_n \frac{k_n^{I\,2} - k_n^2}{1 + k_n^2}\right\} \simeq \exp\left\{\sum_n \frac{2k_n\left(k_n^I - k_n\right)}{1 + k_n^2}\right\} \\
&= \exp\left\{\frac{1}{T}\sum_n \frac{2k_n \delta_k}{1 + k_n^2}\right\}.
\end{aligned} \tag{6.131}$$

Now we shall transform the sum over n into an integral over dk:

$$\sum_n = \int dn = \frac{T}{\pi}\int dk \tag{6.132}$$

With this substitution we have

$$\mathcal{R}_{\text{cont}} = \exp\left\{\frac{1}{\pi}\int_0^\infty dk \frac{2k\,\delta_k}{1 + k^2}\right\} = \exp\left\{\frac{1}{\pi}\int_0^\infty dk \frac{d\delta_k}{dk} \ln\left(1 + k^2\right)\right\}. \tag{6.133}$$

The derivative of δ_k over k can be calculated from eq.(6.125)

$$\frac{d\delta_k}{dk} = \frac{6\left(1 + 2k^2\right)}{\left(1 + k^2\right)\left(1 + 4k^2\right)} = 2\left(\frac{1}{1 + k^2} + \frac{1}{1 + 4k^2}\right). \tag{6.134}$$

What remains to be calculated is the integral

$$-\frac{2}{\pi}\int_0^\infty dk \left(\frac{1}{1 + k^2} + \frac{1}{1 + 4k^2}\right) \ln\left(1 + k^2\right) = -\ln 9. \tag{6.135}$$

The last equality follows from the general formula given in Ref.[6.7]

$$\int_0^\infty dk \frac{1}{c^2 + g^2 k^2} \ln\left(a^2 + b^2 k^2\right) = \frac{\pi}{cg} \ln \frac{ag + bc}{g}. \tag{6.136}$$

So we finally arrive at

$$\mathcal{R}_{\text{cont}} = \frac{1}{9} \tag{6.137}$$

and the final answer for $\mathcal{R}$ consists in multiplying $\mathcal{R}_{\rm cont}$ by $\lambda_2 = 3/4$ calculated in sect. (6.3.4):

$$\mathcal{R} = \frac{1}{12} \tag{6.138}$$

as anticipated in the beginning of this section.

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