Lecture 3

Instantons – imaginary time

A. Introduction

Last lecture we reviewed the standard WKB approach from your quantum mechanics class. The key to making the approximation work is that at fixed E, and near some fixed x, the wavefunction locally must be of the form $\psi \sim Ae^{ipx} + Be^{-ipx}$, with $p^2/2m + V(x) = E$. This works fine in 1D, but what about 2D or 3D? Or what about the field theory version of things where you might be working in ∞D. The generic approach that has developed to deal with tunneling in these higher dimensions is *instantons*. In this chapter we will look at things from a thermodynamic perspective. In a later chapter we will take a dynamical view instead.

I'll assume everyone has seen path integrals, and just skim the details. [They are a standard part of the graduate quantum course, which is a prereq for this module.] If they are new to you, don't panic. As with most other mathematical constructs, the hardest part is learning what the notation means, and not feeling too uncomfortable when you realize that you do not actually know how to evaluate the expressions.

B. The partition function

B.1. Definitions

For concreteness we will once again consider the double well potential $V(x) = V_0 x^2(x^2 - a^2)$. We want to know the splitting between the two nearly degenerate ground states. The tact we will take here is thermodynamics. We will calculate the partition function

$$Z = \mathrm{Tr} e^{-\beta H}. \tag{3.1}$$

In the low temperature limit, Z is dominated by the two lowest energy states, and

$$Z \approx e^{-\beta E}\left(1+e^{-\beta\Delta}\right). \tag{3.2}$$

If all we care about is Δ, we just need the ratio of the first and second terms: hence one can often be pretty cavalier about multiplicative constants. I always like to dot my I's and cross my t's, so I'll try to be as careful as I can with them.

We will calculate the partition function through a path integral. This means we split up the trace in Eq. (3.1) into a product of N terms:

$$Z = \mathrm{Tr} e^{-H\delta\tau/\hbar} e^{-H\delta\tau/\hbar}\cdots e^{-H\delta\tau/\hbar} \tag{3.3}$$

There are N factors of $e^{-H\delta\tau/\hbar}$ and $\delta\tau = \hbar\beta/N$.

Many of you have seen this approach before, and may be a little complacent. Here, where we are going to take the "semiclassical limit" $\hbar \to 0$. If you are smart, this whole setup should smell a little fishy. Aside from being dimensional, $\hbar$ is a completely artificial parameter in this case. Why did we chose to put the $\hbar$'s where we did? If we were doing time dynamics the answer would be obvious: $\hbar$ is the conversion factor between energy and frequency. If we want τ to be a time, we need a $\hbar$. Here the Trotter expansion is largely a mathematical trick, and so far it is not obvious why we are doing this. As we continue on, follow the $\hbar$'s.

We now insert a resolution of the identity

$$1 = \int \frac{dx\,dp}{2\pi\hbar}\,|x\rangle\langle x|\,|p\rangle\langle p| \tag{3.4}$$

between each term in Eq. (3.3). A typical term will be

$$\begin{aligned}
\langle x_1|p_1\rangle\langle p_1|e^{-H\delta\tau/\hbar}|x_2\rangle &\approx \langle x_1|p_1\rangle\langle p_1|1-H\delta\tau/\hbar|x_2\rangle \qquad (3.5)\\
&= x\langle x_1|p_1\rangle\langle p_1|x_2\rangle\left(1-\frac{\delta\tau}{\hbar}\left(\frac{p_1^2}{2m}+V(x_2)\right)\right)\\
&\approx \exp\left(\frac{i}{\hbar}p_1(x_2-x_1)-\left(\frac{p_1^2}{2m}+V(x_2)\right)\frac{\delta\tau}{\hbar}\right)
\end{aligned}$$

Both terms in the exponent carry a $1/\hbar$. This is our reason for our choice of τ being a time variable. We want the same coefficient to be in front of each term. Taking the product of all these terms we get

$$\begin{aligned}
Z &= \int \frac{dx_1 dp_1}{2\pi\hbar}\cdot\frac{dx_N dp_N}{2\pi\hbar}\, e^{-\frac{1}{\hbar}\sum_j \delta\tau\left[-ip_j\frac{x_j-x_{j-1}}{\delta\tau}+\left(p_j/2m+V(x_j)\right)\right]} \qquad (3.6)\\
&\equiv \int \mathcal{D}x\mathcal{D}p \exp\frac{-1}{\hbar}\int_0^{\hbar\beta} d\tau\left[-ip\partial_\tau x + H\right], \qquad (3.7)
\end{aligned}$$

which defines the symbol $\int \mathcal{D}x\mathcal{D}p$: the limit $N \to \infty$ is implicit. [The expression in the exponential is just the definition of the Riemann integral, so no new notation is being introduced there.] Equation (3.7) is the "imaginary time phase space path integral" with $H = p^2/2m + V(r)$. It turns out that the phase space path integral is poorly behaved, so almost everyone at this point integrates out the p variables. This is actually straightforward, as p only appears quadratically. Taking one time slice, and completing the square

$$\int dp\, e^{i\frac{\delta\tau}{\hbar}p\frac{\partial x}{\partial\tau}-\frac{\delta\tau}{\hbar}\frac{p}{m}} = \int dp\, e^{-\frac{\delta\tau}{m\hbar}(p-im\partial_\tau x)^2-\frac{m}{\hbar}(\partial_\tau x)^2}, \tag{3.8}$$

$$= \sqrt{\frac{2\pi m\hbar}{\delta\tau}}\, e^{-\frac{m}{\hbar}\partial_\tau x}. \tag{3.9}$$

one finds that

$$Z = \int \frac{dx_1}{\lambda}\cdots\frac{dx_N}{\lambda} e^{-\frac{1}{\hbar}\sum_j \delta\tau\left[\frac{m}{2}\frac{x_j-x_j}{\delta\tau}+V(x_j)\right]} \tag{3.10}$$

$$\equiv \int \mathcal{D}x\, e^{-S_E/\hbar} \tag{3.11}$$

where the Euclidian Action is

$$S_E = \int_0^\beta d\tau\, \left[\frac{1}{2}mv^2 + V(x)\right]. \tag{3.12}$$

The lengthscale in Eq. (3.10) is proportional to the thermal wavelength,

$$\lambda^2 = \frac{2\pi\hbar\delta\tau}{m} = \frac{\lambda_T^2}{N}. \tag{3.13}$$

We have absorbed this coefficient into the definition of the symbol $\int \mathcal{D}x$. Typically it is not important

There are good reasons for calling the S_E in Eq. (3.11) an "action", but its clearly better to think of it as βE, averaged over a trajectory. Recall that in quantum mechanics you can make virtual transitions, "violating energy conservation", as long as you do so for sufficiently short times.

B.2. Small Parameters

We want to consider the partition function defined by

$$Z = \int \mathcal{D}x\, \exp -\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, \left[\frac{1}{2}m\dot{x}^2 + V_0x^2(x^2-a^2)\right]. \tag{3.14}$$

As in the first lecture, we can rescale lengths and energies

$$x = ay$$
$$\tau = (\hbar/V_0a^4)t$$

to get

$$Z = \int \mathcal{D}y, \exp - \int_0^{\beta V_0 a^4} d\tau \left[\frac{1}{2} \frac{m V_0 a^6}{\hbar^2} \dot{y}^2 + y^2(y^2 - 1^2) \right]. \tag{3.15}$$

As before, the small semiclassical parameter is $\epsilon = \hbar^2/(2mV_0a^6)$. When ϵ is small, it is expensive for paths to bend. There is of course a second parameter $\beta V_0 a^4$, which tells us how the temperature compares to the barrier height. For our argument, we are in the low temperature limit. Thus we will always assume that this thermal parameter is large, meaning that the barrier is large compared to temperature.

To be honest it would drive me crazy to work in these rescaled units – so typically won't.

B.3. Numerical Approach

To continue in my honesty streak, I find most treatments of instantons quite obtuse. The problem being that the imaginary time path integral is quite abstract. The really clean way to think about them is to imagine doing a numerical experiment. Imagine writing a computer program that generated positions $\{x_1, x_2, \cdots x_N\}$, such that the probability of any particular configuration is given by

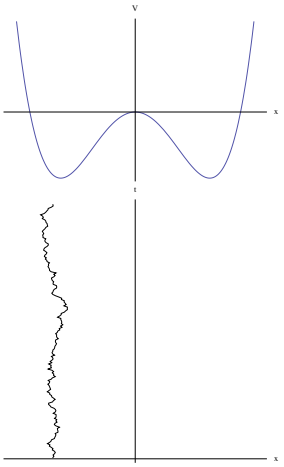
$$P(\{x_1, x_2, \cdots x_N\}) \frac{dx_1}{\lambda} \cdots \frac{dx_n}{\lambda} = e^{-\sum_j \left[\frac{m}{2} \frac{(x_{j+1} - x_j)^2}{\delta\tau} + V(x_j) \right]}. \tag{3.16}$$

I am not claiming it is trivial to write such a program, but it can be done: this will be the content of Cyrus Umrigar's module. On the other hand, once you have this program, you can learn about the quantum system by looking at the properties of this ensemble of configurations. For example, if you wanted to produce the probability that the particle is at position x, one just makes a histogram of the x_j across all of the ensembles.

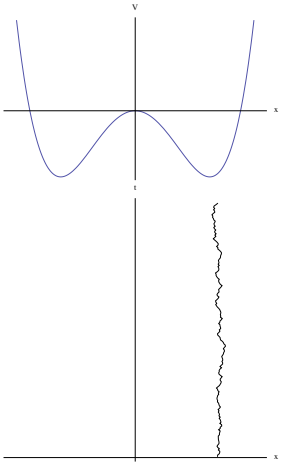
The way this is usually expressed is that the path integral maps quantum thermodynamics onto the classical thermodynamics of a collection of masses and springs. We know how to numerically sample the configurations of such classical systems.

Group Activity: What is the most probable trajectory?

One reason I bring this numerical approach up is that this numerical procedure gives a nice visual picture of what is going on. Below is a sketch of a typical trajectory that your black box spits out

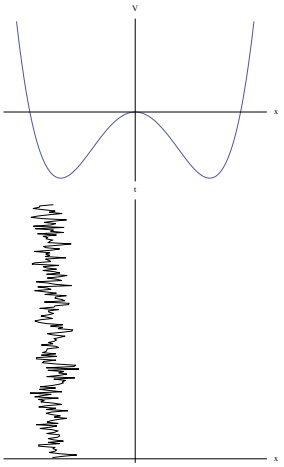


It stays near the energy minimum, undergoing some sort of random walk. Another, equally likely path is



The distance that the particle strays from the minimum (on average) is related to the parameter $\beta V_0 a^4$.

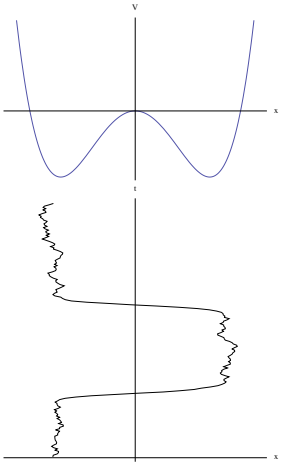
If we make ϵ larger, the "correlation time" drops. The RMS displacement of the path from the minimum is unchanged, but it moves around more rapidly:



Thus the semiclassical limit $\epsilon \to 0$ is the limit in which the correlation time is very long: ie. paths become smooth.

Another way to think about the correlation time is that there is a characteristic frequency of small oscillations about each minimum, ω_0. The correlation time must be something like $1/\hbar\omega_0$.

From what we know about tunneling, we expect the splitting between the two lowest energy states to have something to do with paths that visit both minima. A typical one of these looks like



It features relatively sudden "jumps" from one minimum to the other. These are short because it costs a lot of weight to spend much time away from the minimum. These jumps are known as instantons. As we will argue in the next two section, we can relate the probability of an instanton to the level splitting of the ground state.

Crudely speaking, there is a minimum action S_0 associated with an instanton

event. As we will show, this action is essentially $S_0 = \int dx \sqrt{-mV(x)}$, taken on the contour from one well to the other. We will find that $\Delta \sim e^{-S/\hbar}$. In higher dimensions, you just find the path which minimizes this action, and that gives you the level splitting. The hard part is finding the coefficient of in front of the exponential.

C. Calculating the path integral

Here I use an approach that is a variation on one I learned from John Shumway at ASU [who uses path integrals in a professional context, as opposed to my hobbyist approach]. It is similar to what Kleinert does in his book. The idea is you break the partition function into two parts: $Z = Z_s + Z_a$, where Z_s comes from all the symmetric states, and Z_a from all the antisymmetric states. Explicitly,

$$Z_s = \frac{1}{2}\int_0^\infty dx\,(\langle x| + \langle -x|)e^{-\beta H}(|x\rangle + |-x\rangle) = Z_+ + Z_- \quad (3.17)$$

$$Z_a = \frac{1}{2}\int_0^\infty dx\,(\langle x| - \langle -x|)e^{-\beta H}(|x\rangle - |-x\rangle) = Z_+ - Z_- \quad (3.18)$$

where we have introduced two more "partition functions"

$$Z_+ = Z = \int dx\,\langle x|e^{-\beta H}|x\rangle \quad (3.19)$$

$$Z_- = \int dx\,\langle x|e^{-\beta H}|-x\rangle. \quad (3.20)$$

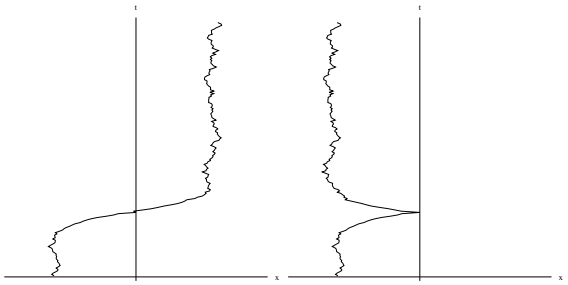
At low temperatures, the partition functions Z_s and Z_a are dominated by the lowest energy symmetric and antisymmetric states. Let E_2 be the energy of the *second* excited state – assumed to be well separated from the ground and first excited states. If $\beta E_2 \gg 1$

$$e^{-\beta\Delta} \approx \frac{Z_a}{Z_s} = \frac{1 - Z_-/Z_+}{1 + Z_-/Z_+}. \quad (3.21)$$

We can make further approximation if either $\beta\Delta \gg 1$ or $\beta\Delta \ll 1$. We get insight by thinking of each of these.

C.1. Case 1: $\beta\Delta \gg 1$

Conceptually cleanest is the very very very low temperature limit, where the temperature is much smaller than the level spacing Δ. Then the left hand side of Eq. (3.21) is very close to zero. That must mean that Z_+ and Z_- are very close to eachother. How does this come about? It turns out that for every path in Z_- we can find a path in Z_+ with the same energy. Here is an example:



The path on the left is a contributor to Z_-, while the path on the right is a standard path which is periodic in imaginary time. Thus Z_- can be interpreted as the sum of all paths in Z which at some point hit the origin.

The difference $(Z_+ - Z_-)/Z$ is then the probability that a given path in our ensemble does *not* touch the origin.

Group Activity: Lets take some chunk of imaginary time τ_0 which is long compared to the "correlation time". Let p_0 be the probability that a path does not touch the origin in time τ_0. What is the probability that the path does not touch the origin in time $2\tau_0$?

Group Activity: Lets take some chunk of imaginary time τ_0 which is long compared to the "correlation time". Let p_0 be the probability that a path does not touch the origin in time τ_0. Can one determine how many times a path should touch the origin in time τ?

Let $dp/d\tau$ be the probability per unit time that a path touches the origin. In other words

$$\frac{dp}{d\tau} = \frac{\langle \text{number of times path crosses/touches the origin} \rangle}{\beta} \tag{3.22}$$

Assuming β is large compared to the "correlation time", $\delta\tau$, the probability of having no touches in time β is then

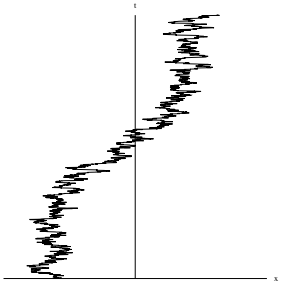
$$p_{\text{no}} = \left(1 - \frac{dp}{d\tau}\delta\tau\right)^{\hbar\beta/\delta\tau} = e^{-\hbar\beta\frac{dp}{d\tau}}. \tag{3.23}$$

Comparing this to our previous expression, we see that for $\beta\Delta \gg 1$,

$$e^{-\beta\Delta} = \frac{Z_+ - Z_-}{Z_+ + Z_-} = \frac{1}{2}e^{-\hbar\beta\frac{dp}{d\tau}}, \tag{3.24}$$

which to leading order in β gives $\Delta = \hbar dp/d\tau$. Or in words, **Δ is the probability per unit imaginary time that the path reaches the origin. In a simulation one can calculate Δ from Eq. (3.22).**

Of course, we have cheated a little bit. For sufficiently large N, the zero crossings presumably come in "avalanches" like this:



That is the path actually crosses the origin many times in an instanton event. If we count each "avalanche" as a single crossing/touching, then in the limit the events are sufficiently largely spaced our previous argument holds. The semiclassical limit is exactly the one in which the instanton spacing becomes large compared to its duration, making this approach sensibe.

The $\beta \gg 1$ limit gives us a nice physical picture of Δ, and it gives us a pretty good numerical approach to calculate it. For analytics, however, the opposite limit $\beta\Delta \ll 1$ is better.

It is also worth noting that in this limit, where $1/\beta$ is the largest energy scale in the problem, our algorithm is better formulated in terms of "diffusion Monte Carlo" instead of "path integral Monte Carlo". Essentially what we want to do is generate a sequence $x_1, x_2, \cdots$ such that the probability distribution $P(x_j) \propto \langle x_0|e^{-jH\delta\tau/\hbar}|x_0\rangle$. We then look at instanton events in this sequence. The average density of instanton events in imaginary time is exactly Δ. Again, Cyrus Umrigar will explain in his module how to construct such a sequence. After you have attended his module, I would encourage you to write a diffusion Monte Carlo program to calculate the level splitting.

C.2. Case 2: $\beta\Delta \ll 1$

Lets now consider the limit $\beta\Delta \ll 1$, for which a typical path contains no instantons. In this case $Z_- \ll Z_+$, and we can expand Eq. (3.24) to find

$$\Delta = \frac{2}{\beta}\frac{Z_-}{Z_+}. \tag{3.25}$$

This expression has a nice interpretation. In this limit, Z_- is dominated by the sum of all paths which cross the origin exactly once (ie. single instantons), while Z_+ is dominated by those that never cross.

The single instanton events involve an avalanche which roughly takes a time of $1/\omega$. Thus there are roughly $\beta\omega$ independent times for the instanton to occur, and we can write

$$\frac{Z_-}{\sim}\beta\omega Z_0 \tag{3.26}$$

where Z_0 involves the sum of all paths which have the instanton at time $t = 0$. This can be caluclated by instead of using periodic boundary conditions in our action using zero boundary conditions.

Hence

$$\Delta \approx \beta\hbar\omega \frac{Z_{\text{zero boundary}}}{Z_{\text{periodic}}}. \tag{3.27}$$

Our task is now to calculate this ratio. One could use Monte-Carlo to do it, but we in the semiclassical limit we can analytically approximate the ratio. Getting the prefactor right is a bit of a pain, and its probably best to leave that to another day.

C.3. Saddle point approximation

We want to calculate

$$Z = \overline{\int \mathcal{D}x, e^{-\frac{}{\hbar}S_E[x]}}, \tag{3.28}$$

where $S_E(x) = \int_0^{\hbar\beta}[m\dot{x}^2/2 + V(x)]d\tau$ with some set boundary condition: periodic $x(0) = x(\beta)$ or vanishing $x(0) = x(\beta) = 0$. It should be clear that this integral will be dominated by the paths which make S_E stationary (and the nearby) paths.

We are most familiar with such minimization problems in the context of classical mechanics. Thus we often interpret S_E as an *action* – even though it is more like an energy. It is related to the "physical action" by the fact that the sign of the potential is reversed. Thus the paths which dominate the thermodynamics are those corresponding to motion in the *inverted* potential. This seems strange at first, but will be clear after an example.

Lets first do the crudest approximation

$$\overline{Z \approx e^{-\frac{}{\hbar}S_E[x^*]}}, \tag{3.29}$$

where x^* is the path which minimizes S_E. Equation (3.29) is pretty good, but it misses a multiplicative constant. Regardless, lets start there.

First for periodic boundary conditions a constant x^* is going to minimize $S_E(x)$. In our case where $V(x) = V_0x^2(x^2 - a^2)$, we can take

$$x_p^* = a/2. \tag{3.30}$$

One could just as well take $x^* = -a/2$. Each path contributes the same. For simplicity we will just do the $x > 0$ paths. The action for this constant path is

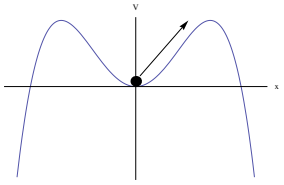
$$S_E[x_p^*] = \hbar\beta V(a/2) = \hbar\beta V_{\rm min}. \tag{3.31}$$

In this approximation $Z = 2e^{-\beta V}$. This is not so bad. It just misses the factor $e^{-\beta\hbar\omega/2}$ corresponding to the zero point energy. [Recall $\beta\Delta \ll 1$, so at this level we can neglect the spacing between the two levels.] We will show how to get this factor below.

For zero boundary conditions we need to do a bit more work. The constant path $x(\tau) = 0$ satisfies the boundary conditions, but has a high energy. The dominant path is the instanton that rolls from $x = 0$ to $x = a/2$ in time τ_i, stays there for a long time, then rolls back. Minimizing S_E with respect to x yields a differential equation:

$$m\frac{\partial^2 x}{\partial\tau^2} = V'(x) = -2V_0a^2x + 4V_0x^3. \tag{3.32}$$

This looks just like Newton's laws, but with a minus sign wrong! It looks like motion in the *inverted potential*. We want to calculate the "action" for the trajectory which starts in the "well" at $x = 0$, with just enough initial momentum to barely make it up the hill. It doesn't quite have the energy to reach the top, and just before $\tau = \hbar\beta$ it rolls back down.



For this cubic potential one can analytically solve Eq. 3.59, but you don't need to. Instead we will use our tricks from classical mechanics, noting that we have a conserved quantity, the "Euclidean Energy",

$$\mathcal{E} = \frac{1}{2}m\dot{x}^2 - V(x). \tag{3.33}$$

This quantity should be independent of time – allowing us to write a closed form expression for x, for any V.

The difference between the action for the path with zero boundaries, and the action for the periodic path is

$$S_I = \int_0^{\beta\hbar} d\tau \left[\frac{1}{2}m\dot{x}^2 + V(x) - V(a/2)\right] \tag{3.34}$$

$$= \int_0^{\beta\hbar} d\tau \left[\mathcal{E} - V(a/2) + m\dot{x}^2\right]. \tag{3.35}$$

The energy of the path we are interested in is essentially $\mathcal{E} = V(a/2)$. We then change variables to get

$$S_I = 2\int_0^{a/2} dx m\dot{x} = 2\int_0^{a/2} dx\sqrt{2m(V(a/2) - V(x))}. \tag{3.36}$$

Putting this result together with Eq. (3.27), we have

$$\Delta \approx \hbar\omega e^{\int_{-a/}^{a/} \sqrt{2m(V(a/2)-V(x))}dx}. \tag{3.37}$$

It is clear that this argument generalizes nicely to higher dimensions, and one just replaces in Eq. (3.37) the integral with a line integral through the higher dimensional space, chosen to minimize the argument of the exponent.

Prefactor

Although it is largely irrelevant to us, it makes us feel smart if we can calculate the prefactors and not just the exponent. The standard approach is to not just include the saddle point path, but quadratic fluctuations about it. In fact any time you do a saddle point approximation, you get the prefactor wrong if you don't include points away from the very top. A simple example is a Gaussian:

$$I = \int dx\, e^{A - B(x-x_0)^2} = \sqrt{\frac{\pi}{B}} e^A. \tag{3.38}$$

The naive approximation we used was just $I = e^A$.

As with the standard saddle point approximation, to get the prefactor we just need to do a Gaussian integral. In practice it is a bit of a pain here since it is a very high dimensional Gaussian integral. There are a number of very formal approaches to calculating it. Here is a reasonably physical one. We start with the most general path integral,

$$Z = \int \frac{dx_1}{\lambda}\cdots\frac{dx_N}{\lambda} e^{-\frac{\delta\tau}{\hbar}\left[\sum_{j=1}^{N}\frac{m}{2}\left(\frac{x_j - x_{j-1}}{\delta\tau}\right)^2 + \sum_{j=1}^{N} V(x_j) + \alpha x_0^2 - 2\beta x_0 x_N + \gamma x_N^2\right]}. \tag{3.39}$$

For periodic boundary conditions $\alpha = \beta = \gamma = m/2\delta\tau^2$, while for the zero boundary conditions $\alpha = \beta = \gamma = 0$. We expand about the saddle point solution: $x_j = x_j^* + y_j$. Keeping terms only to second order in the y's, we have

$$\begin{aligned}\frac{Z}{Z_0} &= \int \frac{dy_1}{\lambda}\cdots\frac{dy_N}{\lambda} \\ &\quad \times e^{-\frac{\delta\tau}{\hbar}\left[\sum_{j=1}^{N}\frac{m}{2}\left(\frac{y_j - y_{j-1}}{\delta\tau}\right)^2 + \sum_{j=1}^{N}\frac{m\omega_j^2}{2}y_j^2 + \left(\frac{2}{\delta\tau}\right)(A\, y_0 - 2B\, y_N + C\, y_N)\right]}, \\ &= \int \frac{dy_1}{\sqrt{\pi}}\cdots\frac{dy_N}{\sqrt{\pi}} e^{-\left[\sum_{j,k=1}^{N}(y_j - y_{j-1})\Omega_{jk}(y_k - y_{k-1}) + \sum_{j,k=1}^{N} y_j\Omega_{jk}y_k + \left(\frac{2}{\delta\tau}\right)(A\, y_0 - 2B\, y_N + C\, y_N)\right]},\end{aligned} \tag{3.40}$$

where $Z_0 = e^{-\beta S}$ is the partition function contribution just from the saddle point path. This looks like the path integral for a particle in a "time dependent" harmonic oscillator potential, with $m\omega_j^2/2 = V''(x_j^*)$. Of course ω_j^2 is negative near the top of the barrier. For periodic boundary conditions, as $\delta\tau \to 0$ we can approximate $A_1 = (2\delta\tau^2/m)\alpha = 1$, $B_1 = (2\delta\tau^2/m)\beta = 1$, and $C_1 = (2\delta\tau^2/m)\gamma = 1$, and for zero boundary conditions these are all 0. In the second line we have rescaled y and defined

$$\Omega_j = \omega_j^2 \delta\tau^2 \ll 1. \tag{3.41}$$

We will now integrate out y_1. After performing the Gaussian integral, the expression should look like

$$\frac{Z}{Z_0} = Z_2 \int \frac{dy_2}{\sqrt{\pi}} \cdots \frac{dy_N}{\sqrt{\pi}} e^{-\sum_{j=2}^{N} (y_j - y_j)^2 + \sum_{j=2}^{N} \Omega_j y_j^2 (A_j y_j - 2B_j y_j y_N + C\ y_N)^2]}.$$

Group Activity: What are the constants A_2, B_2, C_2, and Z_2 in terms of A_1, B_1, C_1?

You should find

$$Z_2 = (1 + A_1)^{-1/2} \tag{3.42}$$

$$A_2 = \Omega_2 + \frac{A_1}{1 + A_1} \tag{3.43}$$

$$B_2 = \frac{B_1}{1 + A_1} \tag{3.44}$$

$$C_2 = C_1 - \frac{B_1^2}{1 + A_1}. \tag{3.45}$$

Repeating the procedure m times produces

$$\frac{Z}{Z_0} = Z_m \int \frac{dy_2}{\sqrt{\pi}} \cdots \frac{dy_N}{\sqrt{\pi}} e^{-\sum_{j=m}^{N} (y_j - y_j)^2 + \sum_{m}^{N} \Omega_j y_j^2 (A_m y_m - 2B_m y_m y_N + C\ y_N)^2]} \tag{3.46}$$

with

$$Z_m = Z_{m-1}(1 + A_m)^{-1/2} \tag{3.47}$$

$$A_m = \Omega_m + \frac{A_{m-1}}{1 + A_{m-1}} \tag{3.48}$$

$$B_m = \frac{B_{m-1}}{1 + A_{m-1}} \tag{3.49}$$

$$C_m = C_{m-1} - \frac{B_{m-1}^2}{1 + A_{m-1}}. \tag{3.50}$$

If we can solve these recursion relations we can calculate Z.

A good starting point is to consider the case of periodic boundary conditions, where $\Omega_m = (\omega\delta\tau)^2$ is a constant, independent of m. Under those circumstances, one would expect that A_m, B_m, and C_m will reach some sort of steady state. The equation for the steady state A is

$$A = \Omega + \frac{A}{1+A} \tag{3.51}$$

which is a quadratic equation. For $\Omega \ll 1$, the solution is

$$A = \sqrt{\Omega} \ll 1. \tag{3.52}$$

Thus A drops from its initial value of 1 to $\sqrt{\Omega}$. For large N the integral is going to be dominated by the steady state contribution, rather than the boundaries, and we can approximate

$$Z_N \approx (1+A)^{-N/2} \approx e^{-AN/2} = e^{-\beta\hbar\omega/2}, \tag{3.53}$$

which is the correct contribution of the zero point energy to the partition function.

The more general case needs more thought. One approach is to try to write the recursion relationships as a differential equation. For example:

$$A_{m+1} - A_m = \frac{dA}{d\tau}\delta\tau = \Omega(\tau) - \frac{A^2}{1+A}. \tag{3.54}$$

In the context of our steady state result this makes sense. Initially A is large ($A \approx 1$), and you can neglect the first term. Then A rapidly drops until $A \sim \sqrt{\Omega} \sim \delta\tau$. The timescale for this drop is of order $1/\omega$. However, the timescale for A to be small compared to 1 is of order $\delta\tau$. Since the initial decay is so fast, it is reasonable (at least at first) to throw away the A in the denominator, writing

$$\delta\tau\partial_\tau A = \Omega(\tau) - A^2. \tag{3.55}$$

We have seen this equation before: this is the eikonal equation from the WKB approximation. In particular, if I define a new function X sattisfying

$$\partial_\tau X = A \tag{3.56}$$

and introduce a function

$$\psi = e^{X/\delta\tau} \tag{3.57}$$

then

$$\partial_\tau^2\psi = \frac{1}{\delta\tau}\left[\partial_\tau A + \frac{A^2}{\delta\tau}\right]\psi \tag{3.58}$$

$$= \frac{\Omega}{\delta\tau^2}\psi, \tag{3.59}$$

with boundary condition

$$\psi(0) = 1 \tag{3.60}$$

$$\psi'(0) = \frac{A(0)}{\delta\tau}. \tag{3.61}$$

This is just the time independent Schrodinger equation. One can also identify $Z_N = \sqrt{1/\psi(N\delta\tau)}$. [For those who are experts in path integrals, this is more-or-less the Gelfund-Yaglom formula for the functional determinant.] One has to be a bit cautious about what we mean by Eq. (3.61), as we don't want $A(0)$ there, what we really want is A at some small time where we can neglect the 1 in Eq. (3.54). For the zero boundary conditions $A(0) = 0$, and things are simple.

Once again we can reproduce the periodic boundary condition result. Clearly for large τ we have $\psi = e^{\sqrt{\Omega}\tau/\delta\tau}$ up to some multiplicative constant. Since $\Omega = \omega^2\delta\tau^2$ this reproduces our last result.

For the instanton solution, there are some neat tricks to solving Eq. (3.59). What one does is find two linearly independent solutions, then take the appropriate combination to match the boundary condition. For example, one solution is $\psi(\tau) = \partial_\tau x$, where $x(\tau)$ is the classical trajectory of the instanton. Another solution can be written in closed form as an integral of this function.