Week 8 - Instantons and the double well potential

I. IMAGINARY TIME EULER LAGRANGE EQUATIONS

The Harmonic oscillator example showed that it is easy to integrate over harmonic fluctuations, and also thought us the importance of Matsubara frequencies, and how to handle them.

Typically, the path integral will not consist of just Gaussian fluctuations, because, for instance, the potential will be non-quadratic. For such difficult cases we can carry out a steepest descent approximation: first find the extremal action, and then expand to quadratic order around it.

The 'action' is the argument in the exponent of the path integral:

$$S = \int_0^\beta d\tau \left(E_k + V\right) = \int_0^\beta d\tau \overline{L}(\dot{x}, x) \tag{1}$$

The $\overline{L}$ function plays the role of a Lagrangian, but a funny one at that - it is the kinetic energy *plus* the potential energy. The Euler-Lagrange equation will still give us the extremum condition for the action:

$$\frac{d}{d\tau}\frac{\partial \overline{L}}{\partial \dot{x}} = \frac{\partial \overline{L}}{\partial x} \tag{2}$$

Which, for the imaginary time second law of motion gives:

$$m\ddot{x} = \frac{\partial V}{\partial x} \tag{3}$$

which is like $ma = -F\ldots$ This is what life is in imaginary time.

Let's see how this funny rule applies to the harmonic oscillator:

$$m\ddot{x} = kx \tag{4}$$

and:

$$x = Ae^{\pm\omega_0\tau} \tag{5}$$

This tends to diverge - either at $\tau = \infty$, or the opposite. But the trajectory must be continuus and periodic. So the only continuus and *periodic* orbit in this case is $A = 0$, which is essentially what we expanded around before.

II. INSTANTONS AND THE DOUBLE WELL POTENTIAL

But the situation is starkly different when we consider a double-well potential:

$$V(x) = V_0(x-a)^2(x+a)^2. \tag{6}$$

A. Double well quantum mechanics

To keep you in the game, I feel obliged to explain a bit how to analyze the quantum mechanical problem of the double well, at least at low temperatures. The Hamiltonian is:

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V_0(x-a)^2(x+a)^2. \tag{7}$$

Don't even start thinking about solving the differential equation... Instead, let's think of the problem; we have two wells - centered at $x = a$ and $x = -a$. Near the $x = a$ well we can approximate the potential as quadratic:

$$V(x) \approx V_0(a+a)^2(x-a)^2 = 4V_0a^2(x-a)^2 \tag{8}$$

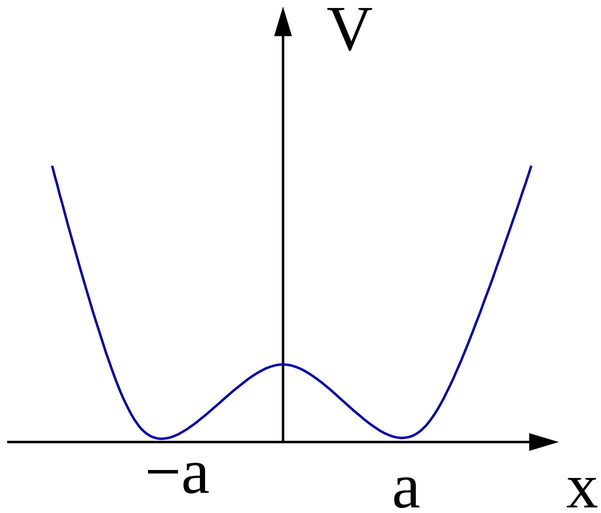

FIG. 1: The double well potential. In imaginary time, the E-L equations describe the motion of a particle in the potential $-V$, with instantons connecting the maxima of $-V$ at a and $-a$.

similarly near $x = -a$ we have:

$$V(x) \approx V_0(a+a)^2(x-a)^2 = 4V_0a^2(x+a)^2 \tag{9}$$

Just two harmonic oscillators. Let us therefore define k as:

$$V_0 = \frac{1}{8a^2}k. \tag{10}$$

This gives:

$$V(x) \approx \frac{1}{2}k(x \mp a)^2 \tag{11}$$

for the two wells. If the two wells would not talk to eachother, he spectrum of the particle would correspond to, first, choosing which well it is in, and then, having the spectrum of an harmonic oscillator. So the states are $E_n = (n+\frac{1}{2})\hbar\omega_0$, each with degeneracy 2 for the two wells.

But actually, the two wells are not independent; the particle can tunnel between the two wells. When the particle tunnels, however, it must conserve energy, and therefore it can only tunnel between the level $|n, -a\rangle$ to $|n, a\rangle$ and vice versa. Concentrating just on the subspace for the n'th levels, we can write the wave function as a two-tuple vector, $(u,\, v)$. If the tunneling strength is Δ, we can write the Hamiltonian as:

$$\hat{\mathcal{H}} = \begin{pmatrix} (\frac{1}{2}+n)\hbar\omega_0 & \Delta \\ \Delta & (\frac{1}{2}+n)\hbar\omega_0 \end{pmatrix} \tag{12}$$

If $\Delta = 0$ we get the doubly degenerate E_n, but with a nonzero Δ we get that the eigenvalues are:

$$E_{n,\pm} = (\frac{1}{2}+n)\hbar\omega_0 \pm \Delta \tag{13}$$

Corresponding to the symmetric an antisymmetric superpositions.

The Partition function is then:

$$Z = \frac{e^{-\beta\hbar\omega_0/2}}{1-e^{-\beta\hbar\omega_0}} \cdot 2\cosh(\Delta\beta) \tag{14}$$

Note, however, that we don't really know what Δ is.

B. Double well in imaginary time

Let's now see what the imaginary path integral says. If we write the E-L equations for this potential we get:

$$m\ddot{x} = \frac{\partial}{\partial x}\left(\frac{1}{8a^2}k(x^2-a^2)^2\right) \tag{15}$$

Which perhaps should be looked at in their integrated form:

$$\frac{1}{2}m\dot{x}^2 = \frac{1}{8a^2}k(x^2-a^2)^2 + \overline{E} \tag{16}$$

With $\overline{E}$ an integration constant.

There are two simple solutions for the E-L equations:

$$x = \pm a \tag{17}$$

These immediately satisfy the EOM's. Integrating over fluctuation then gives the partition function of just the two decoupled harmonic osscillators, since the potential near these solutions is just $V(x) \approx \frac{1}{2}k(x \pm a)^2$. This will result in:

$$Z = 2\frac{e^{-\beta\hbar\omega_0/2}}{1-e^{-\beta\hbar\omega_0}}. \tag{18}$$

But what about other solutions? As an equation of motion, this one is quite funny. Again, there are trajectories with $|x| > a$ which seem to accelerate - gaining imaginary kinetic energy as imaginary time progresses. Well - this is what happens when we turn the potential upside down. When we look at a motion in an upside-down double well potentials, we see that bound states exist with $\overline{E} < 0$ - but they are oscillating near $x = 0$ with the frequency $\frac{1}{\sqrt{2}}\omega_0$ in imaginary time. They are quite high energy, and we will ignore them. Also, one would need a very carefully tuned temperature to have an integer number of periods of these oscillations in the imaginary-time line $0 \leq \tau < \beta$.

Instanton solution

A special solution, though, exists when $\overline{E} = 0$. Try:

$$x_S = a\tanh(t/T_0) \tag{19}$$

Plugging this into the E-L equation gives:

$$\frac{1}{2}m\frac{a^2}{T_0^2}\frac{1}{\cosh^4(t/T_0)} = \frac{1}{2}\frac{k}{4a^2}a^4(\tanh^2(t/T_0)-1)^2 \tag{20}$$

This simplifies to:

$$\frac{1}{2}m\frac{a^2}{T_0^2} = \frac{1}{8}ka^2 \tag{21}$$

and:

$$T_0 = \sqrt{\frac{4m}{k}}. \tag{22}$$

Instanton gas

The instanton solution, Eq. (19) tells us how the particle can, with minimum action, move from one well to the other. This is a quantum process though - it can't appear with the two-slice path integral. What is this process? Tunnneling.

If the particle has enough imaginary time to carry out tunneling:

$$\hbar\beta > T_0 \tag{23}$$

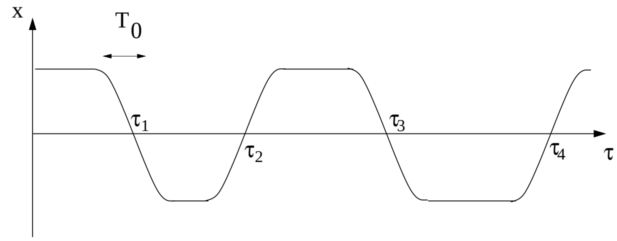

FIG. 2: The instantonic path in a polot of x vs. τ. The width of each instanton is T_0, and instantons must appear in alternating order.

we need to consider these processes. This gives a rather interesting correspondence between the *imaginary time* of an instanton, and the temperature in which tunneling phenomena appears. Naively, we would expect that the tunneling processes are important only in temperatures lower than the tunneling strength - but here we have a different condition, which is a bit less stringent, we'll see.

A particle carrying out this unique imaginary time trajectories, must still obey the periodicity condition - it must return to where it started after β time. So it must carry out at least two tunneling events. If they are separated by more than T_0, then we can treat these two events independently. By the same token, we can have many pairs of instantons. This allows us to write a $2n$ instanton trajectory, which is nearly a solution for the E-L equation:

$$x = \overbrace{\pm a \prod_{i=1}^{2n} \tanh \frac{\tau - \tau_i}{T_0}}^{x_I} + \Delta x \tag{24}$$

The first part is the instantonic contribution, and the second is a small fluctuation about the instanton solution of the E-L equations, which we will assume is small, and neglect $\Delta x^3 \to 0$.

Because the instanton contribution is roughly the solution of the E-L equation, we can write:

$$\begin{aligned} Z &= \int D[x] \exp\left(-\int_0^\beta d\tau \left(\tfrac{1}{2} m \dot{x}^2 + \tfrac{1}{8a^2} k (x^2 - a^2)^2 \right) \right) \\ &\approx \int D[\Delta x] \exp\left(-\int_0^\beta d\tau \left(\tfrac{1}{2} m \dot{\Delta x}^2 + \tfrac{1}{2} k \Delta x^2 \right) \right) \cdot \tfrac{1}{(2n)!} \int \prod_{i=1}^{2n} (\Lambda d\tau_i) \exp\left(-\int_0^\beta d\tau \left(\tfrac{1}{2} m \dot{x_I}^2 + \tfrac{1}{8a^2} k (x_I^2 - a^2)^2 \right) \right) \end{aligned} \tag{25}$$

The first piece is just the deviation from one of the harmonic oscillator valleys; we assume that the instanton gas is dilute, and therefore most of the time the particle is close to one of the minima. This will give the partition function of an harmonic oscillator,

$$Z_{\Delta x} = \frac{e^{-\omega_0 \beta / 2}}{1 - e^{-\beta \omega_0}}. \tag{26}$$

The second piece is just the sum over all instanton trajectories, assuming a discretization of imaginary time for the gas which is $1/Lambda$. An instanton in an imaginary time stretch β has $\beta\Lambda$ opportunities to occur, and hence the normalization. We don't know a-priori what Λ is, but we can guess - it should be a number times the resonant frequency of the oscillator - that is the only time scale we have for the problem. Λ is called the attempt frequency. Also, notice that the instanton gas must be an alternating gas - right then left then right, etc. Hence we need $1/(2n)!$ to eliminate over counting of the time integrals.

The instantons are far away from each other, and only interact with eachother with an exponentially decaying strength. Therefore, we can approximate the second part in teh product as:

$$Z_I \approx \sum_{n=0}^{\infty} 2 \frac{1}{(2n)!} (\beta\Lambda)^{2n} \left[\exp\left(-\int_{-\infty}^{\infty} d\tau \left(\frac{1}{2} m \dot{x}_S^2 + V(x_S) \right) \right) \right]^{2n} \tag{27}$$

where x_S is the single-instanton solution, Eq. (19). the 2 is added in front to mark the two possibilities: starting at $x = a$ or at $x = -a$, which is the reason also for the $\pm$ in Eq. (24).

The single instanton action can be easily evaluated:

$$\begin{aligned}\int_{-\infty}^{\infty} d\tau \left(\tfrac{1}{2}m\dot{x}_S^2 + V(x_S)\right) = 2\int_{-\infty}^{\infty} \tfrac{1}{2}m\dot{x}_S^2 = \tfrac{ma^2}{T_0}\int_{-\infty}^{\infty} du \tfrac{1}{\cosh^4 u} \\ = \tfrac{ma^2}{T_0}\int_{-1}^{1} d\tanh(u)(1-\tanh^2 u) = \tfrac{ma^2}{T_0}(2-\tfrac{2}{3}) = \tfrac{4}{3}\tfrac{ma^2}{T_0} \\ = \tfrac{2}{3}a^2\sqrt{mk}\end{aligned} \tag{28}$$

Now comes the big simplification:

$$\begin{aligned}Z_I = 2\sum_{n=0}^{\infty}\tfrac{1}{(2n)!}\left(\beta\Lambda e^{-\frac{2}{3}a^2\sqrt{mk}}\right)^{2n} \\ = 2\cosh\left[\beta\cdot\left(\Lambda e^{-\frac{2}{3}a^2\sqrt{mk}}\right)\right]\end{aligned} \tag{29}$$

Putting together

$$Z = Z_{\Delta x}\cdot Z_I = 2\frac{e^{-\omega_0\beta/2}}{1-e^{-\beta\omega_0}}\cosh\left[\beta\cdot\left(\Lambda e^{-\frac{2}{3}a^2\sqrt{mk}}\right)\right] \tag{30}$$

By comparing with the QM analysis we recognize immediately the energy splitting:

$$\Delta = \Lambda e^{-\frac{2}{3}a^2\sqrt{mk}} \tag{31}$$

The first term is the attempt frequency - how often can try to tunnel from side to side. The exponent, is the action, which suppresses the tunneling process.

Now, what is really the attempt frequency? As it turns out, it is a rather complicated question to answer. You could guess that it is just the frequency of the oscillations in each well. This can not be too far from the truth, since we can vies the exponent as the probablity to go across the tunneling barrier every time the particle approaches it:

$$\Lambda = B\sqrt{\frac{k}{m}}. \tag{32}$$

And we would expect B to be of order 1. Actually, here there is a surprise. While there is only one frequency, there are several ways of constructing dimensionless numbers. One is:

$$S_I/\hbar \tag{33}$$

It turns out that the number B contains one of these numbers. In the end:

$$\Lambda = b\sqrt{\frac{S_I}{\hbar}}\sqrt{\frac{k}{m}} \tag{34}$$

with the exact determination of b, which is really a number of order 1, being quite a difficult algebraic problem. In this case it turns out to be:

$$b = \sqrt{\frac{12}{2\pi}}. \tag{35}$$

What we did here, essentially, is a WKB analysis of the tunneling between the two minima. We could have done it by solving Schrödinger's equation. But this was so much more satisfying.