Lecture 11 -12

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WKB in the path integral formalism.

First recall that in Lecture 3, we found the propagator of the simple harmonic oscillator:

$$\langle x''|e^{-\frac{i}{\hbar}HT}|x'\rangle =$$

$$\left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{1/2} e^{\frac{im\omega}{2\hbar\sin\omega T}\left((x'^2+x''^2)\cos\omega T-2x'x''\right)}$$

The exponential was the classical action to go from x' to x''. Let us now specialise to the case $x' = x'' = 0$. The classical path is then trivial: the particle just sits at the given point. (This is not true for $x'' = x' \neq 0$, because only 0 is a minimum of the potential). Hence the phase becomes 1. Also define $T = -i\tau$ (τ = "imaginary time"). Then

$$\langle 0|e^{-\frac{1}{\hbar}H\tau}|0\rangle = \sqrt{\frac{m\omega}{2\pi\hbar\sinh\omega\tau}}$$

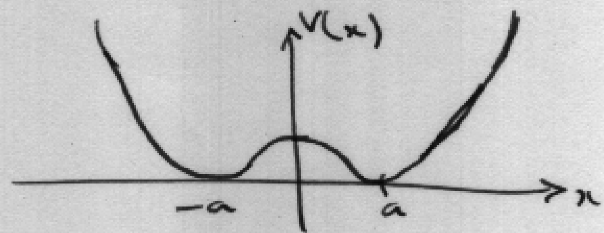
At large times, $\sinh\omega\tau \to \frac{1}{2}e^{\omega\tau}$ so

$$\langle 0|e^{-\frac{1}{\hbar}H\tau}|0\rangle \xrightarrow{\tau\to\infty} \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\omega\tau/2}.$$

As we emphasized before, the $e^{-\omega T/2}$ factor tells us that the ground state energy of the SHO is $E_0 = \hbar\omega/2$.

Now let us consider the double-well potential:

$V(x) = \frac{\lambda}{4!}(x^2-a^2)^2$ or any other function with a similar shape:



Now we cannot evaluate the path integral exactly, but will try to make an approximation which will turn out to be the WKB approx in functional integral language. What we would like to compute is:

$$\langle a|e^{-HT}|a\rangle = \langle -a|e^{-HT}|-a\rangle \quad \text{and}$$

$$\langle -a|e^{-HT}|a\rangle = \langle a|e^{-HT}|-a\rangle$$

We will use a semi-classical method to compute these. For this purpose, recall that

$$\langle x''|e^{-\frac{1}{\hbar}HT}|x'\rangle = \int [dx]\, e^{-\frac{S_E}{\hbar}}$$

where $$S_E = \int_{-T/2}^{T/2} d\tau' \left[\tfrac{1}{2}m\dot{x}^2 + V(x)\right]$$

Here we have chosen $t' = -T/2$, $t'' = +T/2$ to reflect the symmetry of the problem (instead of $t' = 0$, $t'' = T$)

The idea is now to expand $x(t)$ about classical solutions of the equations of motion following from the Euclidean action. So we write:

$$x(t) = x_{cl}(t) + \eta(t)$$

(t is always "Euclidean" time from now on).

where x_{cl} solves: $-m\ddot{x}_{cl} + V'(x_{cl}) = 0$

(The normal equation of motion is $m\ddot{x}_{cl} = -V'(x_{cl})$ but because ~~the~~ we are in imaginary time, V has gone to $-V$).

The boundary conditions are:

$$x_{cl}(-T/2) = x' \, , \quad x_{cl}(T/2) = x''$$

$$\eta(\pm T/2) = 0 \, .$$

Now we want to expand $\eta(t)$ over a complete set of orthonormal functions on the interval $(-T/2, T/2)$ that vanish ~~at~~ the end-points:

$$\eta(t) = \sum_n a_n y_n(t)$$

~~In principle we may choose~~

Then we will replace

$$[d\eta] \rightarrow \prod_n da_n$$

with an undetermined multiplicative constant in front.

In principle we could choose any orthonormal set $y_n(t)$ but in general the integrand will become complicated. ~~[illegible]~~ But consider the integrand:

$$S_E[x] = S_E[x_{cl} + \eta]$$

$$= S_E[x_{cl}] + \frac{1}{2}\int \left.\frac{\delta^2 S_E}{\delta x^2}\right|_{x=x_{cl}} \eta^2 + \cdots$$

The second term is shorthand for

$$\frac{1}{2}\iint_{-T/2}^{+T/2} \frac{\delta^2 S_E}{\delta x(t)\,\delta x(t')}\,\eta(t)\,\eta(t')\,dt\,dt'$$

Now with $S_E = \int\left(\frac{1}{2}m\dot{x}^2 + V\right)dt$,

$$\frac{\delta^2 S_E}{\delta x(t)\,\delta x(t')} = -\frac{1}{2}\,\partial_t^2\,\delta(t-t') + V''\cdot\delta(t-t')$$

Therefore $\int \frac{\delta^2 S_E}{\delta x^2}\eta^2 =$

$$\int_{-T/2}^{+T/2} dt\;\eta(t)\left[-m\frac{d^2}{dt^2} + V''(x_{cl})\right]\eta(t)$$

There are higher-order terms in η that we neglect. Now the quadratic term above simplifies if we can find eigenfunctions $y_n(t)$ satisfying

$$-m\,y_n'' + V''(x_{cl})\,y_n = \lambda_n y_n$$

In that case the quadratic term in η becomes:

$$\int [d\eta]\, e^{-\frac{1}{\hbar}\cdot\frac{1}{2}\int \frac{\delta^2 S_E}{\delta x^2}\eta^2}$$

$$= \int \sum \prod da_n\, e^{-\frac{1}{2\hbar}\sum \lambda_n a_n^2}$$

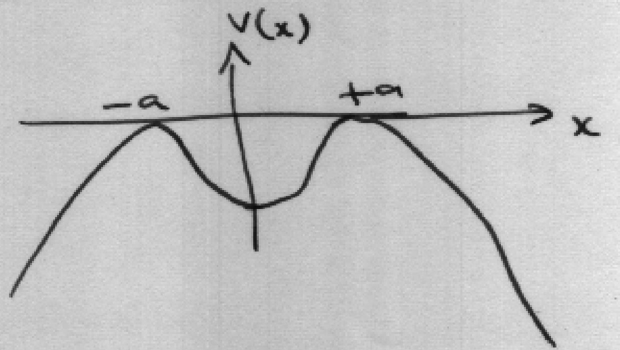
$$\simeq \prod_n \lambda_n^{-1/2}$$

Hence the path integral is approximated by:

$$\langle x''|e^{-\frac{1}{\hbar}H\tau}|x'\rangle = N\, e^{-\frac{S_E[x_{cl}]}{\hbar}} \prod_n \lambda_n^{-1/2}.$$

If there are many classical solutions, we sum over all of them.

Now for the double well, we note that the classical solutions between $-a$ and $-a$ are as follows:



i) Particle sits at $-a$ for all time.

(i) Particle rolls from $-a$ to $+a$ and back in time τ.

iii) Particle rolls from $-a$ to $+a$ and back <u>twice</u> in time τ, etc.

Similarly, if we consider classical solutions between $-a$ and $+a$, the particle can:

i) roll from $-a$ to a in time T

ii) roll from $-a$ to a to $-a$ to a in time T

--- etc.

We see that $\langle -a| e^{-\frac{1}{\hbar}HT} |a\rangle$, $\langle -a| e^{-\frac{1}{\hbar}HT} |-a\rangle$ involve an infinite sum over classical solutions!

Consider the single-transit solution:

$$x_{cl}(t=0) = -a, \qquad x_{cl}(t=T) = a,$$

$$-m\ddot{x}_{cl} + V'(x_{cl}) = 0$$

Multiplying by $\dot{x}_{cl}$ $\Rightarrow$

$$m\dot{x}_{cl}\ddot{x}_{cl} = V'\dot{x}_{cl} = \frac{dV}{dt}(x_{cl}) \Rightarrow \frac{1}{2}m\dot{x}^2 = V$$

So $\sqrt{m}\,\dot{x}_{cl} = \sqrt{2V(x_{cl})}$ and hence

$$t = \sqrt{m}\int_0^{x_{cl}} \frac{dx'}{\sqrt{2V(x')}}$$ where, by symmetry, $t = 0 \rightarrow x = 0$.

~~Suppose we find~~ Such a configuration is called an "instanton" or "pseudoparticle": a classical solution of the Euclidean action S_E that interpolates between minima of the original potential.

We can also find an "anti-instanton" by just considering $x_{cl}(-t)$.

What is the action of an instanton?

It is

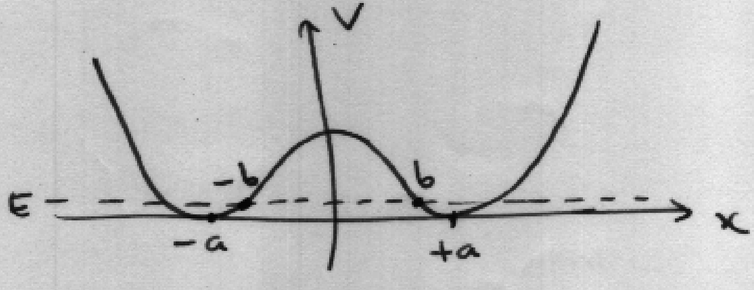
$$S_1 = \int_{-T/2}^{+T/2} dt \left(\tfrac{1}{2} m \dot{x}^2 + V(x) \right)$$

$$= \int_{-T/2}^{T/2} dt \, . \, 2V(x_{cl}(t))$$

Now $dt = \dfrac{\sqrt{m}\, dx}{\sqrt{2V}}$ so

$$S_1 = \sqrt{m} \int_{-a}^{+a} dx \sqrt{2V(x)}$$

Notice that this is related to the barrier penetration formula $\int |p| dx$! But the energy is $E = 0$ and correspondingly the turning points of the true motion are the stationary points of the potential:



As $E \to 0$, $-b \to -a$, $b \to a$ and $\sqrt{2m(V-E)}$
$\to \sqrt{2mV}$.

We can compute the instanton configuration for the potential $V(x) = \frac{\lambda}{4!}(x^2-a^2)^2$.

We have:

$$t = \sqrt{m}\sqrt{\frac{12}{\lambda}} \int_0^{x_{cl}} \frac{dx'}{a^2-x'^2}$$

$$= \sqrt{\frac{12m}{\lambda}} \frac{1}{2a} \log \frac{a+x_{cl}}{a-x_{cl}}$$

It follows that

$$x_{cl} = a \tanh \sqrt{\frac{\lambda a^2}{12m}}\, t = a \tanh \frac{\omega t}{2}$$

where $\omega = \sqrt{\frac{\lambda a^2}{3m}}$

Correspondingly the velocity is

$$\dot{x}_{cl} = \frac{\omega a}{2} \operatorname{sech}^2 \frac{\omega t}{2}$$

$$= \frac{\omega a}{2} \left(1 - \left(\frac{x_{cl}}{a}\right)^2\right)$$

$$= \frac{\omega}{2a}(a^2 - x_{cl}^2) \sim \omega(a - x_{cl})$$

Hence as $x_{cl} \to a$, $\dot{x}_{cl} \to 0$.

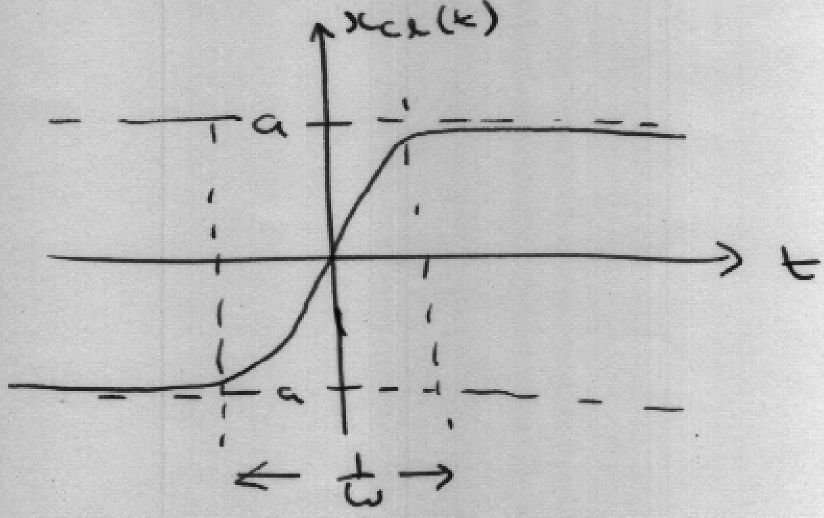
Also, as $t \to \infty$,

$$x_{cl} \sim a\frac{(1-e^{-\omega t})}{1+e^{-\omega t}} \sim a(1-2e^{-\omega t})$$

or $a - x_{cl} \sim 2ae^{-\omega t}$, so $\dot{x} \sim 2a\omega e^{-\omega t}$ as $t \to \infty$.

This is vanishingly small for $t > \frac{1}{\omega}$

So the instanton has a shape:



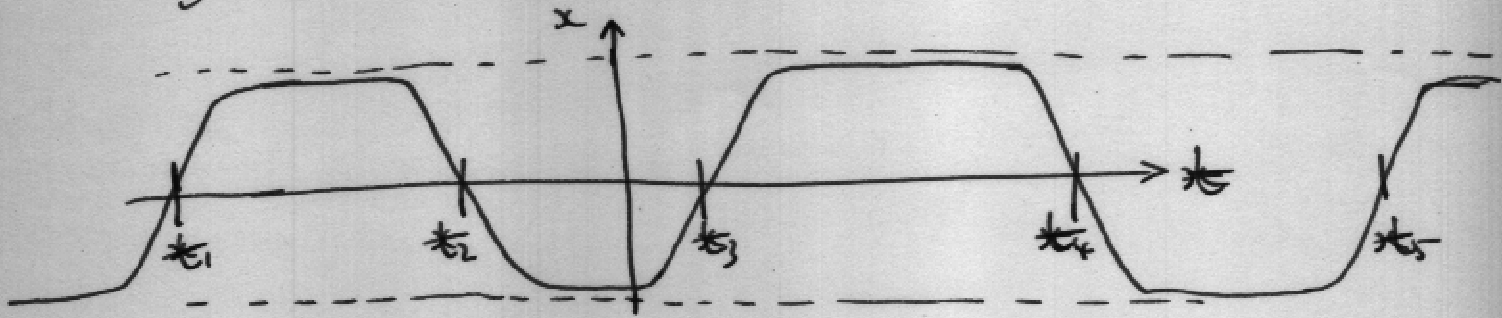
If one thinks of the instanton as a particle extended in (imaginary) time, rather than space, then its size would be $\sim \frac{1}{\omega}$, where $\omega = \sqrt{\frac{\lambda a^2}{3m}}$.

In this example, the action of the one-instanton solution is

$$S_1 = \sqrt{m} \int_{-a}^{+a} dx \, \sqrt{2V(x)} \qquad \text{with } V(x) = \frac{\lambda}{4!}(x^2-a^2)^2$$

$$= \sqrt{\frac{\lambda m}{12}} \int_{-a}^{+a} dx \, (a^2 - x^2) = \frac{2}{3}\sqrt{\frac{\lambda m}{3}}\, a^3$$

So far we have only found one classical solution that interpolates from $-a$ to $+a$. However since the total time T is very large, we can build up "multi-instantons" by joining solutions together:



This solution has three instantons with two anti-instantons in between. It is not obvious that this represents an exact classical solution - rather, as long as ~~[illegible]~~ $t_i - t_{i+1} \gg \frac{1}{\omega}$, one expects it to be a good approximate solution.

Returning to our formula

$$\langle a | e^{-\frac{1}{\hbar} H T} | -a \rangle = N e^{-\frac{S_E[x_{cl}]}{\hbar}} \prod_n \lambda_n^{-1/2}$$

we note that λ_n are eigenvalues of the differential operator

$$-\frac{d^2}{dt^2} + V''(x_{cl}).$$

Now we have seen that near $x = a$,

$$\dot{x}_{cl} \sim \omega(a - x_{cl})$$

Such a region is far away from any instanton. In this region,

$$\ddot{x}_{cl} = -\omega \dot{x}_{cl} = -\omega^2(a - x_{cl}) = \frac{V'}{m}$$

So $\quad V' = -m\omega^2(a - x_{cl})$

and $\quad V''\big|_{x=a} = m\omega^2$

For such a V'', the problem reduces to a harmonic oscillator. The path integral over fluctuations would then evaluate to

$$\sim \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\omega T/2} .$$

The presence of an instanton corrects this by multiplying with

$$K e^{-\frac{S_1}{\hbar}} T$$

where K is roughly the ratio:

$$\left| \frac{\det\left(-\frac{d^2}{dt^2} + \omega^2\right)}{\det\left(-\frac{d^2}{dt^2} + V''(x_{cl})\right)} \right|^{1/2}$$

which we calculate later on.

The factor $e^{-S/\hbar}$ is the classical action of the instanton:

$$S_1 = \sqrt{m} \int_{-a}^{+a} dx \sqrt{2V(x)}$$

and T comes from integrating over all locations of the instanton "centre" between $-T/2$ and $T/2$.

To get from $-a$ to a we need $1, 3, 5 \ldots$ alternating instantons of anti-instantons. We now make the "dilute gas" approximation and sum independently over the location of each one, ie

$$\int_{-T/2}^{T/2} dt_n \int_{-T/2}^{t_n} dt_{n-1} \;\cdots\; \int_{-T/2}^{t_2} dt_1$$

$$= \frac{1}{n!} \int_{-T/2}^{T/2} dt_n \;\cdots\; \int_{-T/2}^{T/2} dt_1$$

- Hence

$$\langle a | e^{-\frac{1}{\hbar} H T} | -a \rangle \simeq \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} e^{-\omega T/2}$$

$$\sum_{\substack{n \text{ odd} \\ =1,3,5\ldots}} \frac{\left(K e^{-S_1/\hbar} T \right)^n}{n!}$$

The sum gives sine-hyperbolic:

$$\langle a | e^{-\frac{1}{\hbar} H T} | -a \rangle \simeq \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} e^{-\omega T/2} \, \sinh\left(K e^{-S_1/\hbar} T \right)$$

$$\simeq \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} e^{-\omega T/2} \cdot \frac{1}{2} \left[e^{K e^{-S_1/\hbar} T} - e^{-K e^{-S_1/\hbar} T} \right]$$

Similarly

$$\langle a | e^{-\frac{1}{\hbar} H T} | a \rangle \simeq \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} e^{-\omega T/2} \cosh\left(K e^{-S_1/\hbar} T \right)$$

We can now extract the ground-state energy of the system in the ~~[illegible]~~ dilute-instanton approximation:

$$\langle a | e^{-\frac{1}{\hbar} H T} | -a \rangle \simeq (\quad) e^{-\omega T/2 + K e^{-S_1/\hbar} T}$$

$$+ (\quad) e^{-\omega T/2 - K e^{-S_1/\hbar} T}$$

It follows that

$$E_{\pm} = \tfrac{1}{2}\hbar\omega \pm \hbar K e^{-S_1/\hbar}$$

and the splitting

$$\Delta E = 2\hbar K e^{-S_1/\hbar}$$

with $S_1 = \int_{-a}^{+a} \sqrt{2V(x)}\, dx$

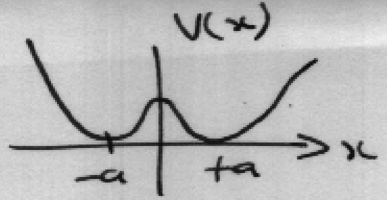
which is the standard WKB expression $\int |p|\, dx$ for ~~[illegible]~~ classical energies close to 0.

The role of K is to correct for the fact that this is not "standard" WKB! Instead of a linear behaviour near the turning point (valid for $E \gg \hbar\omega$) we have a <u>quadratic</u> behaviour of V at the turning point $x \sim \pm a$.

Later we will see how to compute K, known as the "instanton determinant".

Let us summarise what we have done so far.

i) Pick a double-well potential:



ii) Write $\langle a | e^{-\frac{1}{\hbar} H T} | -a \rangle = (\ ) \int [dx] \, e^{-\frac{1}{\hbar} \int_{-T/2}^{+T/2} L_E \, dt}$

where $L_E = \frac{1}{2} m \dot{x}^2 + V(x)$

iii) Approximate the path integral by finding classical solutions that interpolate between $-a$ and $+a$ in the potential $-V(x)$ and expanding about these. We must sum over classical solutions, with the corresponding determinant about each soln:

$$\langle a | e^{-\frac{1}{\hbar} H T} | -a \rangle = (\ ) \sum_{\text{cl. solns}} \left\{ e^{-\frac{1}{\hbar} S_{cl}} \cdot \det{}^{-\frac{1}{2}} \left(-m \frac{d^2}{dt^2} + V''(x_{cl}) \right) \right\}$$

iv) Use the dilute-gas approximation: each classical soln is a multi-instanton consisting of 1, 3, 5 .. alternating instantons and anti-instantons. The action is just the sum of instanton actions:

$$S_{cl}^{(n)} = n S_1$$

where S_1 is the 1-instanton action.

v) In the dilute-gas approximation, the determinant which is:

$$\det\left(-m\frac{d^2}{dt^2} + V''(x_{cl})\right)$$

is re-written:

$$\det{}^{-1/2}\left(-m\frac{d^2}{dt^2} + m\omega^2\right) \left[\frac{\det\left(-m\frac{d^2}{dt^2} + V''(x_{cl}^1)\right)}{\det\left(-m\frac{d^2}{dt^2} + m\omega^2\right)}\right]^{-n/2}$$

The first factor has already been calculated to be

$$\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\omega T/2}$$

while the second factor is the n-th power of the 1-instanton contribution

$$K = \left[\frac{\det\left(-m\frac{d^2}{dt^2} + V''(x_{cl}^1)\right)}{\det\left(-m\frac{d^2}{dt^2} + m\omega^2\right)}\right]^{-1/2}$$

Even without knowing K, we have performed the sum over instantons to get:

$$\langle a| e^{-\frac{1}{\hbar}HT} |a\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\omega T/2} \sinh\left(K e^{-S_1/\hbar}\, T\right)$$

(Recall that $\omega^2 = \frac{V''}{m}\Big|_{x=\pm a}$.)

In a separate note we discuss the evaluation of the "instanton determinant" K.

We will show that

$$K = \frac{\alpha}{\sqrt{\pi\hbar}}$$

where α is the coefficient in

$$\dot{x}_{cl} = \alpha\, e^{-\omega|t|} \quad \text{as} \quad |t| \to \infty .$$

We have previously shown that $\alpha = 2a\omega$

where $\omega^2 = \left.\frac{V''}{m}\right|_{x=\pm a}$

In our example with $V(x) = \frac{\lambda}{4!}(x^2-a^2)^2$,

we find:

$$\omega = \sqrt{\frac{\lambda a^2}{3m}} \qquad \text{so} \qquad \alpha = 2\sqrt{\frac{\lambda}{3m}}\, a^2$$