2.3 Saddle point and instantons

Outline:

Various "semiclassical" approximations play an important role in quantum mechanics, and are associated with concepts like the Wentzel-Kramers-Brillouin (WKB) method, or eikonal method, or Gamow factor. Here we consider an expansion around a "saddle point", relevant for tunnelling.

In real time: (p. 33-35)

$\phi(t) = \phi_{cl}(t) + \delta\phi(t)$, ϕ_{cl} = solution of classical equations of motion $[\delta S_M/\delta\phi_{cl} = 0]$.

$$\Rightarrow K = e^{\frac{i}{\hbar}S_{cl}} \int_{\delta\phi(t_1)=0}^{\delta\phi(t_2)=0} \mathcal{D}\delta\phi(t)\, e^{\frac{i}{\hbar}\int_{t_1}^{t_2} dt \int_{t_1}^{t_2} dt' \frac{1}{2} \frac{\delta^2 S_M}{\delta\phi(t)\delta\phi(t')} \delta\phi(t)\delta\phi(t') + \ldots}.$$

In imaginary time: (p. 37-40)

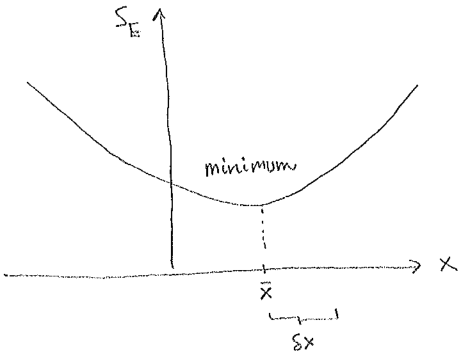
$\phi(\tau) = \bar\phi(\tau) + \delta\phi(\tau)$, $\bar\phi$ = solution of Euclidean equations of motion $[\delta S_E/\delta\bar\phi = 0]$, with boundary conditions $\bar\phi(\beta\hbar) = \bar\phi(0)$.

$$\Rightarrow Z = \int_{-\infty}^{\infty} d\bar\phi(0)\, e^{-\frac{1}{\hbar}\bar S_E} \int_{\delta\phi(0)=0}^{\delta\phi(\beta\hbar)=0} \mathcal{D}\delta\phi(\tau)\, e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau' \frac{1}{2}\frac{\delta^2 S_E}{\delta\phi(\tau)\delta\phi(\tau')}\delta\phi(\tau)\delta\phi(\tau') + \ldots}$$

Remarks:

* There can be more than one solution of the Euclidean equations of motion. A solution corresponding to a local maximum of S_E is called a saddle point.
* Importantly, the Euclidean solutions can describe phenomena that are not allowed classically, like tunnelling.

Example:



We consider a normal 1-dimensional integral:

$$Z \equiv \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{\hbar}S_E(x)}$$

$$= \int_{-\infty}^{\infty} d\delta x\, e^{-\frac{1}{\hbar}\left[S_E(\bar x) + \underbrace{S_E'(\bar x)\delta x}_{0} + \frac{1}{2}S_E''(\delta x)^2 + \frac{1}{3!}S_E'''(\delta x)^3 + \frac{1}{4!}S_E^{(4)}(\delta x)^4 + \ldots\right]}$$

$$= e^{-\frac{\bar S_E}{\hbar}}\sqrt{\hbar}\int_{-\infty}^{\infty} dy\, e^{-\frac{1}{2}S_E'' y^2 - \frac{\sqrt{\hbar}}{3!}S_E''' y^3 - \frac{\hbar}{4!}S_E^{(4)} y^4 + \ldots}$$

$\boxed{\delta x \equiv y\sqrt{\hbar}}$

$$= e^{-\frac{\bar S_E}{\hbar}}\sqrt{\frac{2\pi\hbar}{S_E''}}\left\{1 - \frac{\sqrt{\hbar}}{3!}S_E'''\langle y^3\rangle - \frac{\hbar}{4!}S_E^{(4)}\langle y^4\rangle + \frac{\hbar}{2(3!)^2}(S_E''')^2\langle y^6\rangle + \ldots\right\},$$

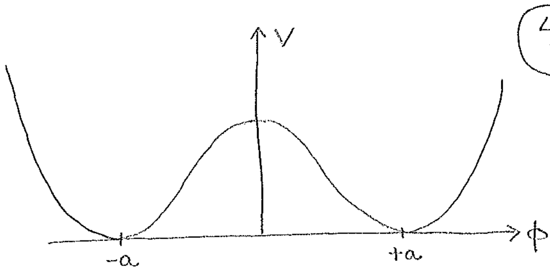
where $\langle y^n\rangle \equiv \dfrac{\int_{-\infty}^{\infty} dy\, y^n e^{-\frac{1}{2}S_E'' y^2}}{\int_{-\infty}^{\infty} dy\, e^{-\frac{1}{2}S_E'' y^2}}$. We can now employ Wick's theorem from p. 38, with $A^{-1} = \frac{1}{S_E''}$!

$$\Rightarrow \langle y^3\rangle = 0, \quad \langle y^4\rangle = \frac{3}{(S_E'')^2}, \quad \langle y^6\rangle = \frac{5\cdot 3}{(S_E'')^3}$$

$$\Rightarrow Z = e^{-\frac{\bar S_E}{\hbar}}\sqrt{\frac{2\pi\hbar}{S_E''}}\left\{1 + \hbar\left[\frac{5}{24}\frac{(S_E''')^2}{(S_E'')^3} - \frac{1}{8}\frac{S_E^{(4)}}{(S_E'')^2}\right] + O(\hbar^2)\right\}.$$

"semiclassical" "fluctuation determinant" "⊖" "∞"

Tunnelling: $V(\phi) \equiv \lambda(\phi^2 - a^2)^2$



In the vicinity of $\phi = a$: $V(\phi) = \lambda(\phi+a)^2(\phi-a)^2 \approx 4\lambda a^2(\phi-a)^2$.
So it looks like a harmonic oscillator, with $m\omega^2 = 8\lambda a^2$.

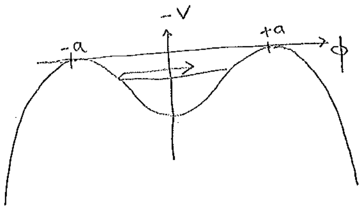
Q: Is there a twice degenerate (around $\pm a$) ground state with $E_0 \approx \frac{\hbar\omega}{2}$?

A: No, there are tunnellings which lift the degeneracy!

Saddle point: Consider "Z from close to $+a$" or, more precisely, $K \equiv \langle a | e^{-\beta\hat{H}} | a \rangle$:

$$Z = \underbrace{\int_{-\infty}^{\infty} d\phi_0}_{\text{"tr"}} \underbrace{\int_{\phi(0)=\phi_0}^{\phi(\beta\hbar)=\phi_0} \mathcal{D}\phi(\tau) \exp\left\{ -\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left[\frac{m}{2}\left(\frac{d\phi}{d\tau}\right)^2 + V(\phi) \right] \right\}}_{K(\phi_0, -i\beta\hbar; \phi_0, 0)}.$$

Extremum: $\frac{\delta S_E}{\delta \bar{\phi}} = 0 \iff m\frac{d^2\bar{\phi}}{d\tau^2} = V'(\bar{\phi})$.

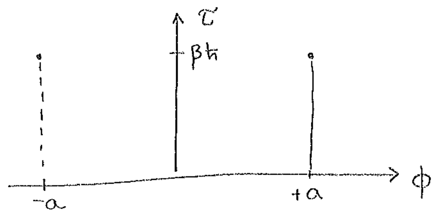


Compare with Newton: $m\frac{d^2\phi_{cl}}{dt^2} = -V'(\phi_{cl})$.

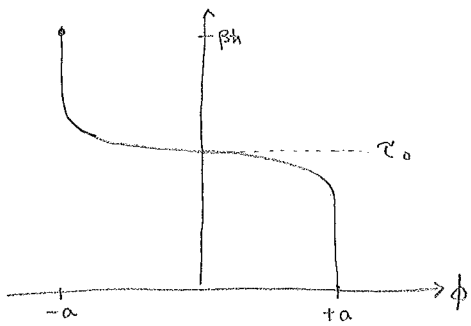
So effectively we consider classical motion, but in potential $-V$!
It follows that periodic paths do exist (cf. exercise 11.3).

Trajectories:

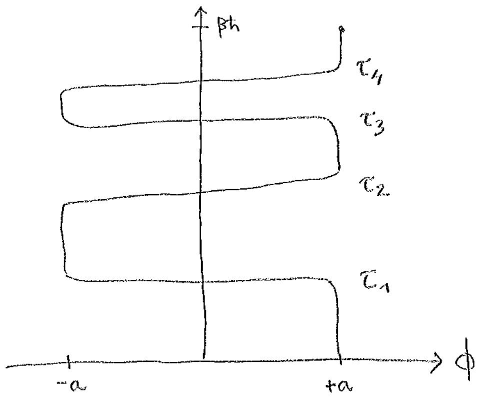
* minimal action:
  $\bar{\phi}(\tau) = +a \quad \forall \tau \in (0, \beta\hbar)$
  $\bar{\phi}(\tau) = -a \quad \forall \tau \in (0, \beta\hbar)$



* Instanton $\equiv$ non-trivial solution, saddle point:
  $\bar{\phi}(\tau) = a \tanh\left[\frac{\omega}{2}(\tau_0 - \tau)\right]$
  exercise 11.3
  (actually this requires $\beta\hbar \to \infty$!)



* "Liquid" of instantons and anti-instantons
  (but explicit construction difficult)



Fluctuations: Write now a general trajectory as

$$\phi(\tau) = \bar\phi(\tau) + \delta\phi(\tau)\,, \quad \delta\phi(\tau) = \sum_n c_n f_n(\tau)\,, \quad f_n(0) = f_n(\beta\hbar) = 0.$$

We choose f_n as eigenfunctions of $-m\frac{d^2}{d\tau^2} + V''(\bar\phi)$:

$$\left[-m\frac{d^2}{d\tau^2} + V''(\bar\phi(\tau))\right] f_n(\tau) = \lambda_n f_n(\tau)\,.$$

They can be orthonormalized as $\int_0^{\beta\hbar} d\tau\, f_n(\tau) f_m(\tau) = \delta_{nm}$.

The integration measure is expressed as $\int \mathcal{D}\delta\phi = J \int_{-\infty}^{\infty} \prod_n \frac{dc_n}{\sqrt{2\pi\hbar}}$, where the Jacobian J is fixed later. Then (cf. p.41)

$$\int \mathcal{D}\delta\phi \, \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\underbrace{\frac{m}{2}\left(\frac{d\bar\phi}{d\tau}\right)^2 + V(\bar\phi)}_{\bar S_E} + \underbrace{\frac{m}{2}\left(\frac{d\delta\phi}{d\tau}\right)^2 + \frac{1}{2}V''(\bar\phi)\,\delta\phi^2}_{} + \ldots\right]\right\}$$

after partial integration:
$$\frac{1}{2}\delta\phi\left[-m\frac{d^2}{d\tau^2} + V''(\bar\phi)\right]\delta\phi = \frac{1}{2}\sum_{n,n'} c_{n'} f_{n'}\, \lambda_n\, c_n f_n$$

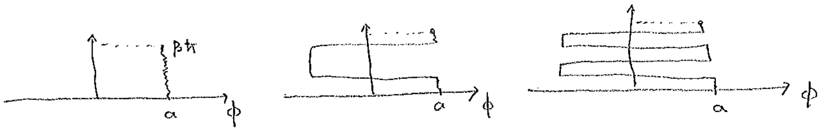
$$\approx e^{-\frac{\bar S_E}{\hbar}} J \int_{-\infty}^{\infty} \prod_n \frac{dc_n}{\sqrt{2\pi\hbar}} \exp\left\{-\frac{1}{2\hbar}\sum_n \lambda_n c_n^2\right\}$$

if $\lambda_n \neq 0$

$$= e^{-\frac{\bar S_E}{\hbar}} J \prod_n \frac{1}{\sqrt{\lambda_n}} \doteq e^{-\frac{\bar S_E}{\hbar}} J \left[\det\left(-m\frac{d^2}{d\tau^2} + V''(\bar\phi)\right)\right]^{-\frac{1}{2}}.$$

Instanton sum:

$$Z = Z_0 + Z_2 + Z_4 + \ldots$$



$$Z_0 \overset{*}{=} J\left[\det\left(-m\frac{d^2}{d\tau^2} + \underbrace{V''(a)}_{m\omega^2}\right)\right]^{-\frac{1}{2}} = Z_{HO} \underset{\text{p.38}}{\approx} \frac{1}{e^{\frac{\beta\hbar\omega}{2}} - e^{-\frac{\beta\hbar\omega}{2}}} \underset{\beta\hbar\to\infty}{\approx} e^{-\frac{\beta\hbar\omega}{2}}.$$

* From here we can solve for J, and substitute it above.

$$Z_2 \approx Z_0 \cdot \int_0^{\beta\hbar} d\tau_2 \int_0^{\tau_2} d\tau_1 \,\{w_{inst}\}^2\,,$$

w_{inst} = contribution of a single instanton (p.44)

$$Z_4 \approx Z_0 \int_0^{\beta\hbar} d\tau_4 \int_0^{\tau_4} d\tau_3 \int_0^{\tau_3} d\tau_2 \int_0^{\tau_2} d\tau_1 \,\{w_{inst}\}^4.$$

$$\Rightarrow \quad Z \approx Z_0 \sum_{n=0}^{\infty} \frac{1}{(2n)!}(\beta\hbar)^{2n}(w_{inst})^{2n}$$

$$= Z_0 \cosh(\beta\hbar w_{inst}) \underset{\beta\hbar\to\infty}{\approx} e^{-\frac{\beta\hbar\omega}{2}} \frac{e^{\beta\hbar w_{inst}} + e^{-\beta\hbar w_{inst}}}{2}$$

because we were around $\phi = +a$

From here we see that $E_0 \approx \frac{\hbar\omega}{2} \pm \hbar w_{inst}$, i.e. that the degeneracy has been lifted!

Single instanton: We still need to finalize the single instanton computation, producing w_{inst}. On p.43 we computed the fluctuation determinant, assuming $\lambda_n \neq 0$. But actually there is a "zero mode"! For, taking a derivative of $m \frac{d^2\bar{\phi}}{d\tau^2} = V'(\bar{\phi})$ (cf. p.42), yields

$$\Big[\underbrace{-m \frac{d^2}{d\tau^2} + V''(\bar{\phi}) \Big] \frac{d\bar{\phi}}{d\tau}}_{f_0 \propto \frac{d\bar{\phi}}{d\tau}} = 0 = \underbrace{0}_{\lambda_0 = 0} \cdot \frac{d\bar{\phi}}{d\tau} .$$

The zero eigenvalue cannot appear inside the determinant, so the zero mode needs to be handled separately*.

* Could there also be negative modes? Exercise 11.3
$\Rightarrow$ $\bar{\phi}$ is monotonic
$\Rightarrow$ $\frac{d\bar{\phi}}{d\tau}$ has no zeros (nodes)
$\Rightarrow$ $\frac{d\bar{\phi}}{d\tau}$ is ground state
$\Rightarrow$ no!

Zero mode: (i) Normalization: we want (p.43) $\int_0^{\beta\hbar} d\tau\, f_0(\tau) f_0(\tau) = 1$.

For a single instanton ("half" of exercise 11.3): $\int_0^{\beta\hbar} d\tau\, m \left(\frac{d\bar{\phi}}{d\tau}\right)^2 = \bar{S}_E$.

$$\Rightarrow f_0(\tau) = \sqrt{\frac{m}{\bar{S}_E}} \frac{d\bar{\phi}}{d\tau} .$$

(ii) Integration domain: we may note that

$$\bar{\phi}(\tau) + c_0 f_0(\tau) = \bar{\phi}(\tau) + c_0 \sqrt{\frac{m}{\bar{S}_E}} \frac{d\bar{\phi}(\tau)}{d\tau} \approx \bar{\phi}\Big(\tau + c_0\sqrt{\frac{m}{\bar{S}_E}}\Big) .$$

So the zero mode corresponds to translations of an instanton. As the domain is periodic, we should restrict translations as

$$0 \leq \underbrace{c_0 \sqrt{\frac{m}{\bar{S}_E}}}_{\equiv \tau_0} \leq \beta\hbar$$

So, $\int \frac{dc_0}{\sqrt{2\pi\hbar}} = \sqrt{\frac{\bar{S}_E}{2\pi\hbar m}} \int_0^{\beta\hbar} d\tau_0$, where $\int_0^{\beta\hbar} d\tau_0$ corresponds to the translation integrals that we had on p.43.

Final result: Writing a single-instanton partition function as $Z_1 \approx Z_0 \int_0^{\beta\hbar} d\tau_0 \{w_{inst}\}$, we now deduce from pages 43 and 44 that

$$w_{inst} = \left(\frac{\bar{S}_E}{2\pi\hbar m}\right)^{\frac{1}{2}} \left(\frac{\det[-m\frac{d^2}{d\tau^2} + V''(a)]}{\det'[-m\frac{d^2}{d\tau^2} + V''(\bar{\phi})]} \right)^{\frac{1}{2}} e^{-\frac{\bar{S}_E}{\hbar}} ,$$

where det' means that the zero mode is excluded, as it now appears explicitly in the prefactor. The single-instanton action corresponds to the "Gamow factor" of tunnelling, $\bar{S}_E = \underbrace{\int_{-a}^{a}}_{\text{exerice 11.3 with } E\to 0^+} d\bar{\phi} \sqrt{2mV(\bar{\phi})}$.

Summary: Semiclassical instanton computations involve a lot of "argumentation", e.g. it is unclear how to improve on their accuracy. Nevertheless they have been very influential in many branches of physics.