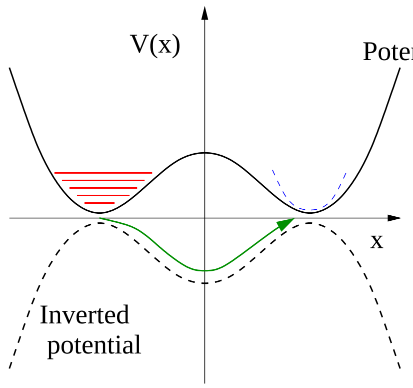
Lecture XIII: Double Well Potential: Tunneling and Instantons

How can phenomena of QM tunneling be described by Feynman path integral?

No semi-classical expansion!

▷ E.g QM transition probability of particle in double well: $G(a, -a; t) \equiv \langle a | e^{-i\hat{H}t/\hbar} | -a \rangle$



▷ Feynman Path Integral:

$$G(a, -a; t) = \int_{q(0)=-a}^{q(t)=a} Dq \exp\left[\frac{i}{\hbar}\int_0^t dt' \left(\frac{m}{2}\dot{q}^2 - V(q)\right)\right]$$

Stationary phase analysis: classical e.o.m. $m\ddot{q} = -\partial_q V$

$\mapsto$ only singular (high energy) solutions *Switch to alternative formulation...*

▷ Imaginary (Euclidean) time Path Integral: Wick rotation $t = -i\tau$

N.B. (relative) sign change! "$V \to -V$"

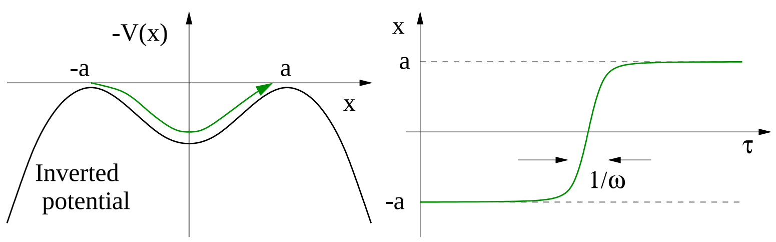
$$G(a, -a; \tau) = \int_{q(0)=-a}^{q(\tau)=a} Dq \exp\left[-\frac{1}{\hbar}\int_0^\tau d\tau' \left(\frac{m}{2}\dot{q}^2 + V(q)\right)\right]$$

Saddle-point analysis: classical e.o.m. $m\ddot{q} = +V'(q)$ in inverted potential!

solutions depend on b.c.

(1) $G(a, a; \tau) \rightsquigarrow q_{\text{cl}}(\tau) = a$
(2) $G(-a, -a; \tau) \rightsquigarrow q_{\text{cl}}(\tau) = -a$
(3) $G(a, -a; \tau) \rightsquigarrow q_{\text{cl}}$: rolls from $-a$ to a

Combined with small fluctuations, (1) and (2) recover propagator for single well



(3) accounts for QM tunneling and is known as an "instanton" (or "kink")

▷ Instanton: classically forbidden trajectory connecting two degenerate minima — i.e. topological, and therefore particle-like

For τ large, $\dot{q_{\rm cl}} \simeq 0$ (*evident*), i.e. "first integral" $m\dot{q_{\rm cl}}^2/2 - V(q_{\rm cl}) = \epsilon \stackrel{\tau\to\infty}{\to} 0$
precise value of ϵ fixed by b.c. (i.e. τ)

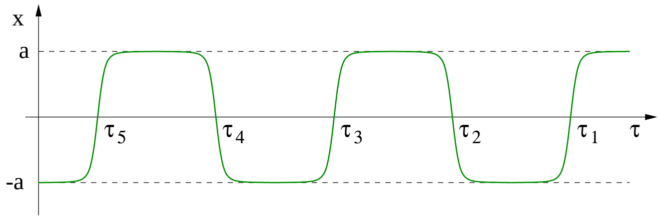
Saddle-point action *(cf. WKB $\int dq p(q)$)*

$$S_{\rm inst.} = \int_0^\tau d\tau' \left(\frac{m}{2}\dot{q}_{\rm cl}^2 + V(q_{\rm cl})\right) \simeq \int_0^\tau d\tau' m\dot{q}_{\rm cl}^2 = \int_{-a}^a dq_{\rm cl} m\dot{q}_{\rm cl} = \int_{-a}^a dq_{\rm cl}(2mV(q_{\rm cl}))^{1/2}$$

Structure of instanton: For $q \simeq a$, $V(q) = \frac{1}{2}m\omega^2(q-a)^2 + \cdots$, i.e. $\dot{q}_{\rm cl} \stackrel{\tau\to\infty}{\simeq} \omega(q_{\rm cl}-a)$

$q_{\rm cl}(\tau) \stackrel{\tau\to\infty}{=} a - e^{-\tau\omega}$, i.e. temporal extension set by $\omega^{-1} \ll \tau$

Imples existence of approximate saddle-point solutions involving many instantons (and anti-instantons): instanton gas



▷ Accounting for fluctuations around n-instanton configuration

$$G(a,\pm a;\tau) \simeq \sum_{n\ \text{even / odd}} K^n \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n \overbrace{A_n(\tau_1,\ldots,\tau_n)}^{A_{n,\rm cl.}A_{n,\rm qu.}},$$

constant K set by normalisation

$A_{n,\rm cl.} = e^{-nS_{\rm inst.}/\hbar}$ — 'classical' contribution

$A_{n,\rm qu.}$ — quantum fluctuations (imported from single well): $G_{\rm s.w.}(0,0;t) \sim \frac{1}{\sqrt{\sin\omega t}}$

$$A_{n,\rm qu.} \sim \prod_i^n \frac{1}{\sqrt{\sin(-i\omega(\tau_{i+1}-\tau_i))}} \sim \prod_i^n e^{-\omega(\tau_{i+1}-\tau_i)/2} \sim e^{-\omega\tau/2}$$

$$G(a,\pm a;\tau) \simeq \sum_{n\ \text{even / odd}} K^n e^{-nS_{\rm inst.}/\hbar} e^{-\omega\tau/2} \overbrace{\int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n}^{\tau^n/n!}$$
$$= \sum_{n\ \text{even / odd}} e^{-\omega\tau/2}\frac{1}{n!}\left(\tau K e^{-S_{\rm inst.}/\hbar}\right)^n$$

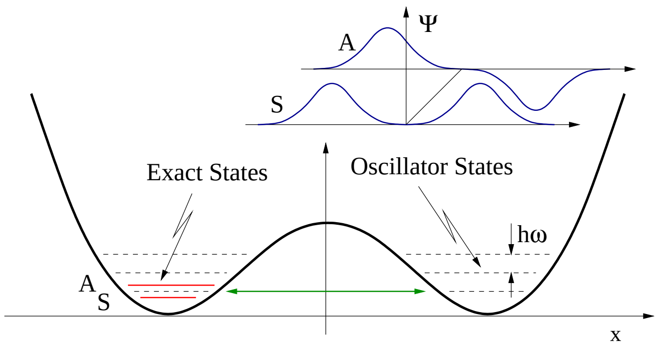
Using $e^x = \sum_{n=0}^\infty x^n/n!$, N.B. non-perturbative in $\hbar$!

$$\begin{aligned} G(a,a;\tau) &\simeq Ce^{-\omega\tau/2}\cosh\left(\tau K e^{-S_{\rm inst.}/\hbar}\right) \\ G(a,-a;\tau) &\simeq Ce^{-\omega\tau/2}\sinh\left(\tau K e^{-S_{\rm inst.}/\hbar}\right) \end{aligned}$$

Consistency check: main contribution from

$$\bar{n} = \langle n \rangle \equiv \frac{\sum_n n X^n/n!}{\sum_n X^n/n!} = X = \tau K e^{-S_{\text{inst.}}/\hbar}$$

no. per unit time, $\bar{n}/\tau$ exponentially small, and indep. of τ, i.e. dilute gas



▷ Physical interpretation: For infinite barrier — two independent oscillators, coupling splits degeneracy — symmetric/antisymmetric

$$G(a, \pm a; \tau) \simeq \langle a|S\rangle e^{-\epsilon_S \tau/\hbar}\langle S| \pm a\rangle + \langle a|A\rangle e^{-\epsilon_A \tau/\hbar}\langle A| \pm a\rangle$$

$$|\langle a|S\rangle|^2 = \langle a|S\rangle\langle S| - a\rangle = \frac{C}{2}, \qquad |\langle a|A\rangle|^2 = -\langle a|A\rangle\langle A| - a\rangle = \frac{C}{2}$$

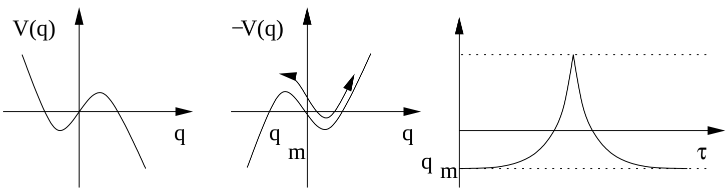
Setting: $\epsilon_{A/S} = \hbar\omega/2 \pm \Delta\epsilon/2$

$$G(a, \pm a; \tau) \simeq \frac{C}{2}\left(e^{-(\hbar\omega - \Delta\epsilon)\tau/2\hbar} \pm e^{-(\hbar\omega+\Delta\epsilon)\tau/2\hbar}\right) = Ce^{-\omega\tau/2}\begin{cases} \cosh(\Delta\epsilon\tau/\hbar) \\ \sinh(\Delta\epsilon\tau/\hbar)\end{cases}.$$

▷ Remarks:

(i) Legitimacy? How do (neglected) terms $O(\hbar^2)$ compare to $\Delta\epsilon$?

In fact, such corrections are bigger but act equally on $|S\rangle$ and $|A\rangle$
i.e. $\Delta\epsilon = \hbar K e^{-S_{\text{inst.}}/\hbar}$ is dominant contribution to splitting



(ii) Unstable States and Bounces: survival probability: $G(0, 0; t)$? No even/odd effect:

$$G(0, 0; \tau) = Ce^{-\omega\tau/2}\exp\left[\tau K e^{-S_{\text{inst}}/\hbar}\right] \overset{\tau=it}{=} Ce^{-i\omega t/2}\exp\left[-\frac{\Gamma}{2}t\right]$$

Decay rate: $\Gamma \sim |K|e^{-S_{\text{inst}}/\hbar}$ (i.e. K imaginary) *N.B. factor of* 2