14. Path Integrals in Quantum Statistics

(1)

a) The Partition Function

$$Z(\beta) := \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) \quad , \quad \beta = \frac{1}{k_B T}$$

↖ Boltzmann's constant

- Free Energy: $F := -\frac{1}{\beta} \ln Z$
- Mean Energy: $E := \frac{1}{Z} \mathrm{Tr}\left(\hat{H} e^{-\beta \hat{H}}\right) =$
- Entropy: $S := -\frac{\partial F}{\partial T} = k_B \ln Z + k_B \beta \frac{1}{Z} \mathrm{Tr}\left(\hat{H} e^{-\beta \hat{H}}\right) = \frac{E-F}{T}$

Take Trace in q-representation

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

with density matrix

$$\rho(x'', x') := \langle x'' | e^{-\beta \hat{H}} | x' \rangle$$

Use Lie-Trotter formula with $\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{Q})$ and V bounded below

$$e^{-\beta \hat{H}} = \lim_{N \to \infty} \left(e^{-\frac{\hat{P}^2}{2m}\frac{\beta}{N}} \, e^{-V(\hat{Q})\frac{\beta}{N}} \right)^N$$

and

$$\langle x_j | e^{-\frac{\hat{P}^2}{2m}\frac{\beta}{N}} | x_{j-1} \rangle = \int dp \, \underbrace{\langle x_j | p \rangle \langle p | x_{j-1} \rangle}_{= \frac{1}{2\pi\hbar} \exp\left\{\frac{i}{\hbar} p (x_j - x_{j-1})\right\}} \exp\left\{-\frac{p^2 \beta}{2mN}\right\}$$

$$= \sqrt{\frac{mN}{2\pi \hbar^2 \beta}} \exp\left\{ -\frac{m}{2\hbar^2} \frac{\Delta x_j^2}{\beta} N \right\}$$

Hence $$\rho(x'',x',\beta) = \int\cdots\int \prod_{j=1}^{N-1} dx_j \prod_{j=1}^{N} \left(\frac{mN}{2\pi\hbar^2\beta}\right)^{\frac{1}{2}} \exp\left\{-\frac{m}{2\hbar^2}\frac{\Delta x_j^2}{\beta}N - V(x_j)\frac{\beta}{N}\right\}$$

Let $t := \hbar\beta$ Euclidean time $\wedge$ $\varepsilon := \frac{t}{N} = \frac{\hbar\beta}{N}$,

- Euclidean propagator:

$$K_E(x'',x',t) := \rho(x'',x',t/\hbar)$$

$$= \int\int\int \prod_{j=1}^{N-1} dx_j \prod_{j=1}^{N} \sqrt{\frac{m}{2\pi\hbar\varepsilon}} \exp\left\{-\frac{m}{2\hbar}\frac{\Delta x_j^2}{\varepsilon} - \frac{1}{\hbar}V(x_j)\,\varepsilon\right\}$$

$$= \int_{x'=x(0)}^{x''=x(t)} \mathcal{D}[x(\tau)] \exp\left\{-\frac{1}{\hbar}\int_0^t d\tau \left(\frac{m}{2}\dot{x}^2 + V(x)\right)\right\}$$

- Euclidean action: $$S_E[x(\tau)] = \int_0^t d\tau \left[\frac{m}{2}\dot{x}^2 + V(x)\right]$$

cl. action for particle in inverted potential $U(x) = -V(x)$!

Formally $\frac{i}{\hbar}t \rightarrow \beta = t/\hbar$

quantum propagator $\rightarrow$ Euclidean propagator

- Path integral repr. of partition function

$$Z(\beta) = \int dx \; \rho(x, x, \beta)$$

$$= \oint_{x(0)=x(\hbar\beta)} \mathcal{D}[x(\tau)] \; e^{-\frac{1}{\hbar} S_E[x(\tau)]}$$

all periodic path with period $t = \hbar\beta$!

with $\quad S_E[x(\tau)] = \int_0^{\hbar\beta} d\tau \left(\frac{m}{2} \dot{x}^2 + V(x) \right)$

$$Z(\beta) = \lim_{N\to\infty} \int \cdots \int \prod_{j=1}^{N} dx_j \prod_{j=1}^{N} \sqrt{\frac{m}{2\pi\hbar\varepsilon}} \exp\left\{ -\frac{m}{2\hbar} \frac{\Delta x_j^2}{\varepsilon} - \frac{1}{\hbar} V(x_j)\varepsilon \right\}$$

with $\beta = \frac{N\varepsilon}{\hbar}$

- Free Particle: $\hat{H} = \frac{\hat{p}^2}{2m}$

$$K_E(x'', x', t) = \langle x'' | e^{-\frac{t}{\hbar}\hat{H}} | x' \rangle = \sqrt{\frac{m}{2\pi\hbar t}} \exp\left\{ -\frac{m}{2\hbar} \frac{(x''-x')^2}{t} \right\}$$

Partition function of particle in a box of volume V $(d=3)$

$$Z(\beta) = \int_V d^3\vec{x}'' \; K_E(\vec{x}'', \vec{x}'', t) = \left(\frac{m}{2\pi\hbar t} \right)^{3/2} \int_V d^3\vec{x} \; 1$$

$$= V \left(\frac{m}{2\pi\hbar t} \right)^{3/2} = V \left(\frac{m}{2\pi\hbar^2\beta} \right)^{3/2}$$

- Harmonic Oscillator: $\hat{H} = \frac{\hat{P}^2}{2m} + \frac{m}{2}\omega^2 \hat{Q}^2$

We know
$$\langle x''| e^{-\frac{i}{\hbar}\hat{H}t} |x'\rangle = \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega t}} \exp\left\{\frac{i}{\hbar}\frac{m\omega}{2\sin\omega t}\left[(x''^2+x'^2)\cos\omega t - 2x''x'\right]\right\}$$

Wick rotation: $it \to t \leadsto i\sin\omega t \to i\sin(-i\omega t) = \sinh\omega t$
$\cos\omega t \to \cosh\omega t$

$$\rho(x'',x',\beta) = \sqrt{\frac{m\omega}{2\pi\hbar\sinh\omega t}} \exp\left\{-\frac{m\omega}{2\hbar\sinh\omega t}\left[(x''^2+x'^2)\cosh\omega t - 2x''x'\right]\right\}$$

Partition function:

$$Z(\beta) = \int dx\, \rho(x,x,\beta)$$

$$= \int dx \sqrt{\frac{m\omega}{2\pi\hbar\sinh\omega t}} \exp\left\{-\frac{m\omega}{\hbar\sinh\omega t} x^2 \underbrace{(\cosh\omega t - 1)}_{=2\sinh^2\frac{\omega t}{2}}\right\}$$

$$= \sqrt{\frac{m\omega}{2\pi\hbar\sinh\omega t}} \sqrt{\frac{\pi\hbar\sinh\omega t}{m\omega\, 2\sinh^2\frac{\omega t}{2}}} = \frac{1}{2\sinh\frac{\omega t}{2}} = \frac{1}{2\sinh(\frac{\hbar\omega}{2}\beta)}$$

$$= \frac{e^{-\frac{\omega t}{2}}}{1-e^{-\omega t}}$$

Note: $\sum_{n=0}^{\infty} e^{-n\omega t} = \frac{1}{1-e^{-\omega t}}$

$$\leadsto \quad Z(\beta) = e^{-\frac{\omega t}{2}} \sum_{n=0}^{\infty} e^{-n\omega t} = \sum_{n=0}^{\infty} e^{-(n+\frac{1}{2})\omega t} = \sum_{n=0}^{\infty} e^{-\hbar\omega(n+\frac{1}{2})t}$$

b) Classical Limit

$$Z(\beta) = \oint\limits_{x(0)=x(\hbar\beta)} \mathcal{D}[x(\tau)]\, e^{-\frac{1}{\hbar} S_E[x(\tau)]}$$

For small $\hbar$ major contribution from paths minimising S_E

$$S_E = \int_0^{\hbar\beta} d\tau \left[\frac{m}{2}\dot{x}^2 + V(x) \right] \qquad \text{with } t = \hbar\beta \text{ very small}$$

$\rightsquigarrow$ use short time approximation ($N=1$ in Lie-Trotter sufficient)

$$\rho(x'', x', \beta) \approx \sqrt{\frac{m}{2\pi\hbar^2\beta}} \exp\left\{ -\frac{m}{2\hbar^2\beta}(x''-x')^2 \right\} \exp\left\{ -V(x'')\beta \right\}$$

$$Z_{cl}(\beta) = \int dx\, \rho(x, x, \beta) \simeq \sqrt{\frac{m}{2\pi\hbar^2\beta}} \int dx\, \exp\left\{ -\beta V(x) \right\}$$

classical approach:

$$Z_{cl}(\beta) = \iint \frac{dp\,dq}{2\pi\hbar}\, e^{-\beta\left(\frac{p^2}{2m} + V(q)\right)}$$

cl. Hamiltonian

$$= \frac{1}{2\pi\hbar} \sqrt{\frac{\pi\, 2m}{\beta}} \int dx\, e^{-\beta V(x)}$$

$$= \sqrt{\frac{m}{2\pi\hbar^2\beta}} \int dx\, e^{-\beta V(x)}$$

c) Wigner – Kirkwood Expansion (higher-order corrections in ħ)

$$\rho(x,x,\beta) = \int_x^x \mathcal{D}[x(\tau)] \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{m}{2}\dot{x}^2 + V(x)\right]\right\}$$

Let $x(\tau) = x + q(\tau)$ with $q(0) = 0 = q(\hbar\beta)$

$$\rightsquigarrow V(x+q(\tau)) = V(x) + q V'(x) + \frac{1}{2} q^2 V''(x) + O(q^3)$$

$$= V - \frac{V'^2}{2V''} + \frac{1}{2} V'' \left(q + \frac{V'}{V''}\right)^2 + O(q^3)$$

shift in paths: $\eta(\tau) := q(\tau) + \frac{V'(x)}{V''(x)}$ $\rightsquigarrow$ $\eta(0) = \frac{V'}{V''} = \eta(\beta\hbar)$

$$\rho(x,x,\beta) \approx e^{-\beta\left(V - \frac{V'^2}{2V''}\right)} \int_{V'/V''}^{V'/V''} \mathcal{D}[\eta(\tau)] \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{m}{2}\dot{\eta}^2 + \frac{1}{2}V''\eta^2\right]\right\}$$

harmonic oscillator with $\omega^2 = \frac{1}{m}V''(x)$

$$\rho_{\omega^2}(\tilde{x},\tilde{x},\beta) = \sqrt{\frac{m\omega}{2\pi\hbar\sinh\omega t}} \exp\left\{-\frac{m\omega}{\hbar\sinh\omega t}\tilde{x}^2(\cosh\omega t - 1)\right\} \text{ with } \tilde{x} = \frac{V'(x)}{V''(x)}$$

and $\rho(x,x,\beta) \approx e^{-\beta\left(V - \frac{V'^2}{2V''}\right)} \rho_{\omega^2}(\tilde{x},\tilde{x},\beta)$

Homework: Problem 13 β small

$$\rightsquigarrow \rho(x,x,\beta) \approx \sqrt{\frac{m}{2\pi\hbar^2\beta}}\, e^{-\beta V(x)} \left(1 + \frac{\hbar^2\beta^2}{24m}\left(\beta V'^2(x) - 2V''(x)\right)\right)$$

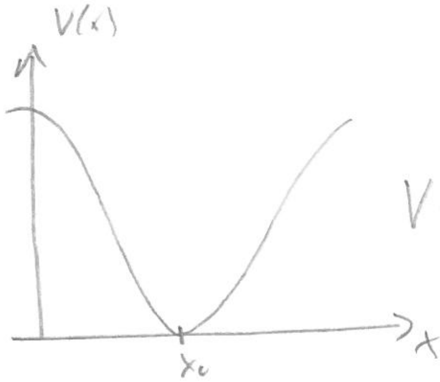
$$\rightsquigarrow \boxed{Z(\beta) = \int dx\, \rho(x,x,\beta) \approx \sqrt{\frac{m}{2\pi\hbar^2\beta}} \int dx\, e^{-\beta V_{eff}(x)}}$$ like cl. result

eff. classical potential:

$$\boxed{V_{eff}(x) = V(x) - \frac{\hbar^2\beta}{24m}V''(x) \approx V(x) - \frac{\hbar^2\beta^2}{24m}V'^2(x)}$$

15) Large t Behaviour of Euclidean Propagator (Quasi-cl. Approximation)

a) Single-well Potential



$V(x_0) = 0$

Consider $x'' = x_0 = x'$

that is $\langle x_0 | e^{-tH/\hbar} | x_0 \rangle \sim \int Dx \, e^{-\frac{S[x]}{\hbar}}$

• classical path: $\bar{x}(\tau)$ Newton's equation for $-V(\bar{x})$

$$m\ddot{\bar{x}} = V'(\bar{x}) \quad \text{with} \quad \bar{x}(\pm t/2) = x_0$$

$$\rightsquigarrow \quad S[\bar{x}] \equiv S_0 = 0$$

• Quasi-classical approximation:

$$\langle x_0 | e^{-tH/\hbar} | x_0 \rangle \approx F_{\omega^2}(t) \, e^{-S_0/\hbar} \qquad \text{where } \omega^2 = \frac{V''(x_0)}{m} = \text{const.}$$

$$= \sqrt{\frac{m\omega}{2\pi\hbar \sinh \omega t}} = \sqrt{\frac{m\omega}{\pi\hbar}} \left(e^{\omega t} - e^{-\omega t}\right)^{-1/2} = \sqrt{\frac{m\omega}{\pi\hbar}} \, e^{-\frac{\omega}{2}t} \left(1 - e^{-2\omega t}\right)^{-1/2}$$

$$\overset{\omega t \gg 1}{\approx} \sqrt{\frac{m\omega}{\pi\hbar}} \, e^{-\frac{\omega}{2}t} \left(1 + \tfrac{1}{2} e^{-2\omega t} + O(e^{-4\omega t})\right)$$

• Spectral representation: $H = \sum_n e^{-E_n t/\hbar} |n\rangle\langle n|$

$$\rightsquigarrow \langle x_0 | e^{-tH/\hbar} | x_0 \rangle \overset{t\to\infty}{\approx} |\langle x_0 | \varphi_0 \rangle|^2 e^{-E_0 t/\hbar} \left[1 + e^{-t(E_1 - E_0)/\hbar} \left| \frac{\langle x_0 | \varphi_1 \rangle}{\langle x_0 | \varphi_0 \rangle} \right|^2 + \dots \right]$$

vanishes for $V(x_0+x) = V(x_0-x)$ as φ_1 is antisymmetric, so not in quasi-cl. approx.

Hence: $E_0 \approx \frac{\hbar\omega}{2}$ $\quad |\langle x_0 | \varphi_0 \rangle|^2 \approx \sqrt{\frac{m\omega}{\pi\hbar}}$

$E_2 - E_0 \approx 2\hbar\omega$ $\quad |\langle x_0 | \varphi_2 \rangle|^2 \approx \frac{1}{2} \sqrt{\frac{m\omega}{\pi\hbar}}$

↗ H.O. where $x_0 = 0$

Remarks:
- Zero order approximation for anharmonic oscillator
- With $x'' = x_c = x'$ (cl. Ground state) no info on 1. excited state

  Way out: use different x'' and x' $\rightsquigarrow$ difficult

  higher order beyond quad. approximation
- No non-perturbative effects considered as $S_0 = 0$

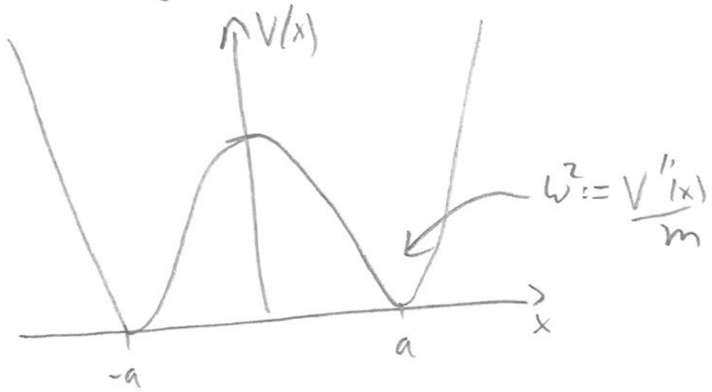
  There may be local minima of cl action with $0 < S_0 < \infty$

  Instantons?

b) Instanton Method for Double-Well Potentials

Consider sym. double-well

Example: $V(x) = \frac{\omega^2 m}{8a^2}\left(x^2 - a^2\right)^2$

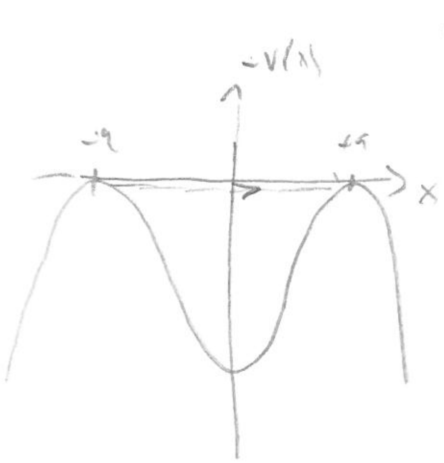


Idea: Consider Euclidean propagator in quasi-classical approximation and extract info on ground and 1. excited state from long t behaviour with $x'' = a$, $x' = -a$

- classical paths: $\bar{x}(\pm t/2) = \pm a$

  Energy: $E = \frac{m}{2}\dot{x}^2 - V(\bar{x})$ for $t \to \infty$ $\bar{x}(\pm t/2) = \pm a$

  $\rightsquigarrow$ $\dot{x} \to 0$ for $t \to \infty$

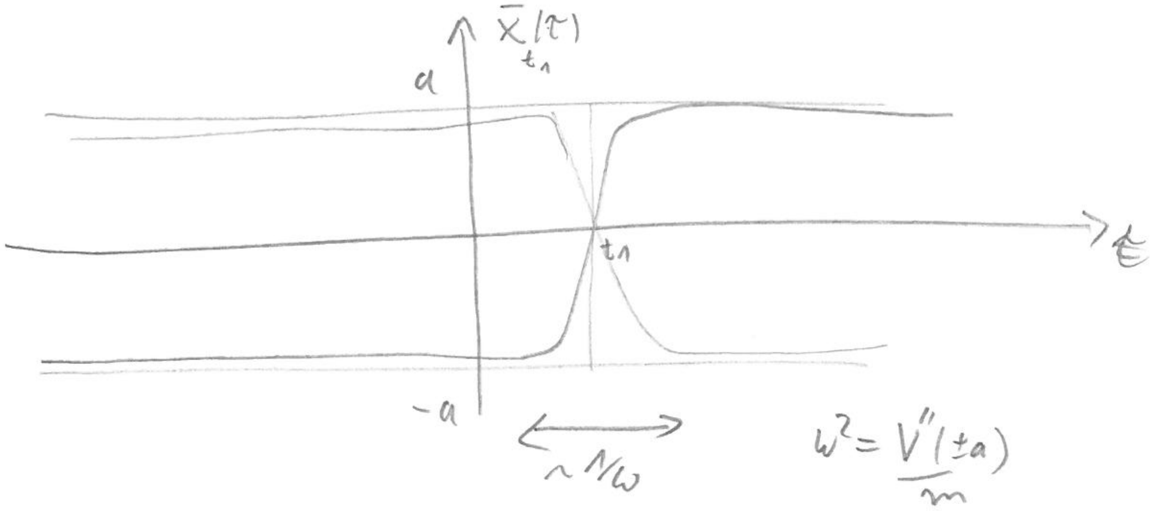


$\rightsquigarrow$ $E = 0$

$$\dot{x} = \pm\sqrt{\frac{2V(\bar{x})}{m}}$$

Instanton

Anti-Instanton



Our example:

$$\dot{x} = \pm \frac{\omega}{2a}(x^2 - a^2) \quad \rightsquigarrow \quad \bar{x}_{t_1}(\tau) = \pm a \tanh\left[\frac{\omega}{2}(\tau - t_1)\right]$$

$$\bar{x}_{t_1}(\tau) = a \tanh\left(\frac{\omega}{2}\left(\pm(\tau - t_1)\right)\right) = \bar{x}_0(\pm(\tau - t_1))$$ translation invariant!

- classical action:

$$S_0 := \int_{-t/2}^{t/2} d\tau \left(\frac{m\dot{\bar{x}}^2}{2} + V(\bar{x})\right) = \int_{-t/2}^{+t/2} d\tau\, m\dot{\bar{x}}^2 = \int_{-a}^{+a} d\bar{x}\, m\dot{\bar{x}}$$

$$S_0 = \int_{-a}^{a} dx \sqrt{2mV(x)}$$ potential barrier strength is independent of t_1!

- Further approximate solutions for large t

1) Single (Anti-) Instanton solution is approximate solution for large t (becomes exact only for $t \to \infty$)

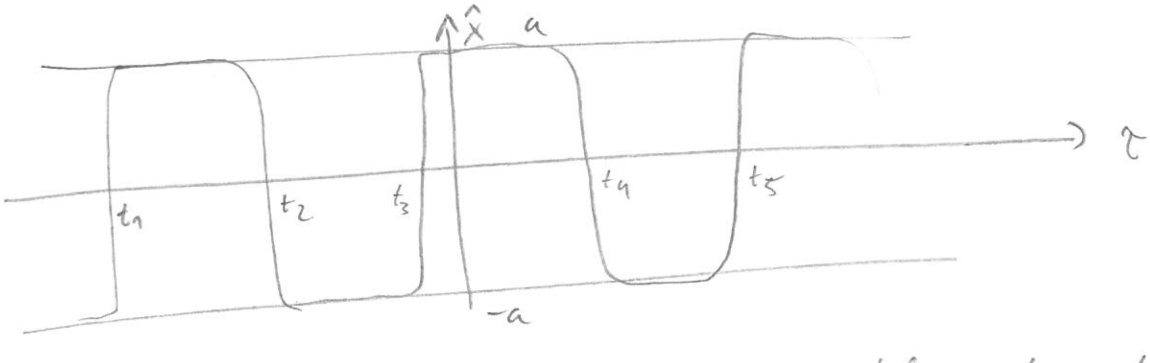
2) Further approximate solution consist of multi-Instantons

$\rightsquigarrow$ local minima of action

n-Instanton solution:

$$\hat{X}_{t_1,t_2,\dots t_n}(\tau) := \bar{x}_0(t-t_1) + \underset{\text{anti-Instanton}}{\bar{x}_0(t_2-t)} + \bar{x}_0(\tau-t_3) \dots + \bar{x}_0(\tau-t_n)$$

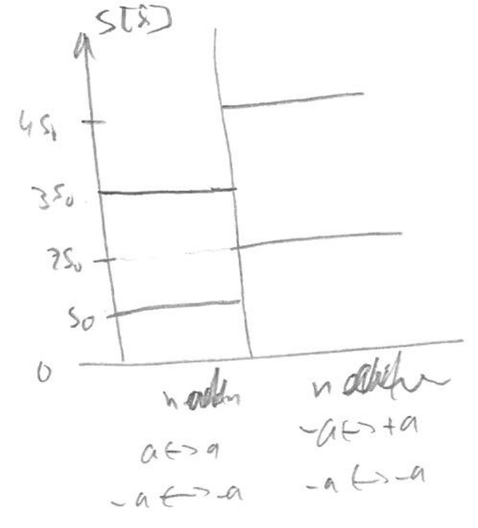
$$-\tfrac{T}{2} < t_1 < t_2 \dots < t_n < \tfrac{T}{2}$$



n-Instanton action: $S[\hat{x}] = n S_0 +$ exponentially small corrections

- Quasi-cl. evaluation for all multi-Instanton solutions

n-Instanton Contribution $e^{-nS_0/\hbar}$ so exponentially small but we have so of them!



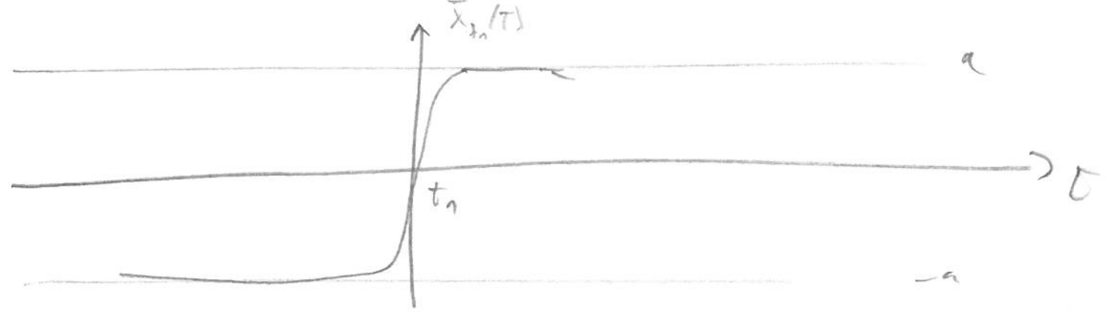
- Contribution of one Instanton

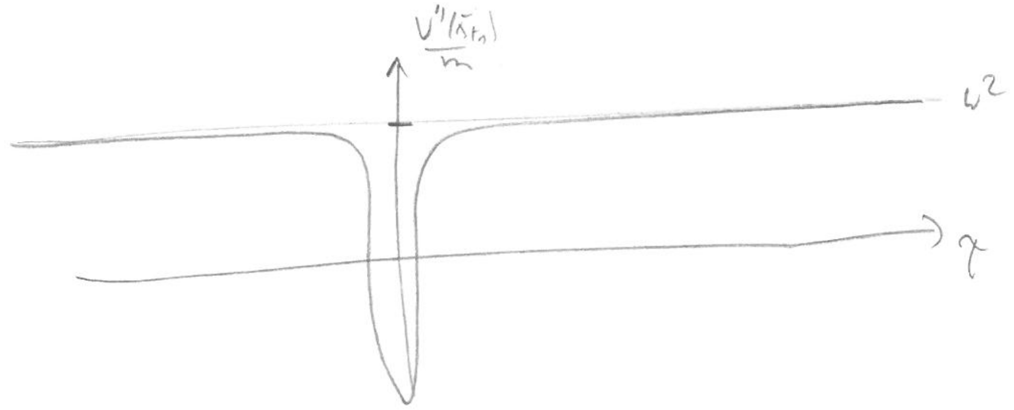
$$\langle a| e^{-tH/\hbar} |-a\rangle \approx F_{V''(x)/m}(t)\, e^{-S_0/\hbar} = F_{\omega^2}(t)\, K(t)\, e^{-S_0/\hbar}$$

where
$$K(t) := \frac{F_{V''(x)/m}(t)}{F_{\omega^2}(t)} = \left[\frac{\det(-\partial_t^2+\omega^2)}{\det\left(-\partial_t^2+\frac{V''(\bar{x})}{m}\right)}\right]^{1/2} \quad \text{Calculation?}$$

classical dynamics:

- $-\frac{t}{2} < \tau < t_1$: Particle oscillates in left/right well with ω
- $\tau \approx t_1$: Particle jumps to other well (tunneling)
- $t_1 < \tau < \frac{t}{2}$: Particle oscillates in right/left well with ω





Lemma:

$K_0 := \lim_{t\to\infty} K(t)$ is independent of t_1 Proof via Coleman?

$\rightsquigarrow$ Instanton/anti-Instanton have <u>same</u> contribution

Contribution of one (anti)-Instanton:

$$F_{\omega^2}(t)\, K_0\, e^{-S_0/\hbar} \approx \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{\omega t}{2}}\, K_0\, e^{-S_0/\hbar} \quad \text{for large } t$$

⑥

- Contribution of n Instantons:

$$\sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{\omega t}{2}} \left(K_0\, e^{-S_0/\hbar} \right)^n \qquad \text{(semi-group property of Euclidean propagator)}$$

- Contribution of all n Instantons:

$$\int_{-t/2}^{t/2} dt_n \int_{-t/2}^{t_n} dt_{n-1} \cdots \int_{-t/2}^{t_2} dt_1 = \frac{1}{n!} \int_{-t/2}^{t/2} dt_n \int_{-t/2}^{t/2} dt_{n-1} \cdots \int_{-t/2}^{t/2} dt_1 = \frac{t^n}{n!}$$

- Total contribution of all Instantons:

$$\langle \pm a | e^{-tH/\hbar} | \mp a \rangle = \sum_{n=1,3,5} \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{\omega t}{2}} \frac{1}{n!} \left(t K_0\, e^{-S_0/\hbar} \right)^n$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{\omega t}{2}} \sinh\left(t K_0\, e^{-S_0/\hbar} \right)$$

$$\langle \pm a | e^{-tH/\hbar} | \pm a \rangle = \sum_{n=0,2,4,} \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{\omega t}{2}} \frac{1}{n!} \left(t K_0\, e^{-S_0/\hbar} \right)^n$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{\omega t}{2}} \cosh\left(t K_0\, e^{-S_0/\hbar} \right)$$

c) The Tunneling Splitting

Consider

$$\langle a| e^{-tH/\hbar} |\mp a\rangle \approx \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\omega t/2}\, \frac{1}{2}\left(e^{tK_0 e^{-S_0/\hbar}} \mp e^{-tK_0 e^{-S_0/\hbar}}\right)$$

$$= \frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}}\, \exp\left\{-\frac{\omega t}{2} + tK_0 e^{-S_0/\hbar}\right\}\left(1 \mp e^{-2tK_0 e^{-S_0/\hbar}}\right)$$

Spectral rep s:

$$\langle a|e^{-tH/\hbar}|\mp a\rangle = \langle a|\varphi_0\rangle\langle\varphi_0|\mp a\rangle\, e^{-tE_0/\hbar}\left(1+\frac{\langle a|\varphi_1\rangle\langle\varphi_1|\mp a\rangle}{\langle a|\varphi_0\rangle\langle\varphi_0|\mp a\rangle}\, e^{-\frac{t}{\hbar}(E_1-E_0)} + \dots\right)$$

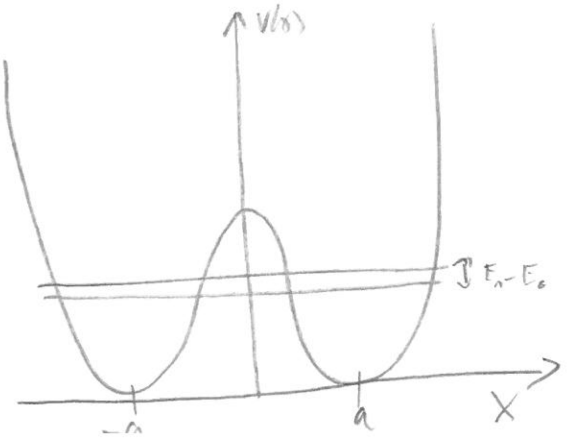
$\Rightarrow$

- $|\langle a|\varphi_0\rangle|^2 = |\langle -a|\varphi_0\rangle|^2 = \frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}}$ half amplitude of single-well ground state
  symmetric in $\pm a$

- $E_0 = \frac{\hbar\omega}{2} - \hbar K_0 e^{-S_0/\hbar}$ non-perturbative correction to ground state energy
  Note: Perturbative contributions $O(\hbar^2)$ are larger
  but no tunneling-effect!

- $\langle a|\varphi_1\rangle\langle\varphi_1|\mp a\rangle = \mp\frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}}$ as for ground-state but anti-symmetric

- $\boxed{E_1 - E_0 \simeq 2\hbar K_0 e^{-S_0/\hbar}}$ Tunneling splitting (non-perturbative)
  perturbative correction to E_0 and E_1 cancel each other



$$\boxed{\varphi_{0/1}(x) \approx \left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\left(e^{-\frac{m\omega}{2\hbar}(x-a)^2} \pm e^{-\frac{m\omega}{2\hbar}(x+a)^2}\right)}$$