Lecture 4

15 Statistical mechanics revisited

The partition function being the central object

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

- Free energy: $F := -\frac{1}{\beta}\ln Z$
- Mean energy: $E := \frac{1}{Z}\,\mathrm{Tr}\left(\hat{H}\mathrm{e}^{-\beta\hat{H}}\right)$
- Entropy: $S := -\frac{\partial F}{\partial T} = k_B \ln Z + \mathrm{Tr}\left(\hat{H}\mathrm{e}^{-\beta\hat{H}}\right) = \frac{1}{T}(E-F)$
- Euclidean propagator: $K_E(q'',q';\tau) := \langle q''|\mathrm{e}^{-\tau\hat{H}\hbar}|q'\rangle$
  is related to quantum propagator $K(q'',q';t) = \langle q''|\mathrm{e}^{-\mathrm{i}t\hat{H}\hbar}|q'\rangle$
  via Wick rotation $t \to -\mathrm{i}\tau$
  Euclidean time: $\tau = \mathrm{i}t$

  $$\Longrightarrow \qquad K_E(q'',q';\tau) = K(q'',q';-\mathrm{i}\tau)$$

- Partion function: $Z(\beta) = \int \mathrm{d}q\, K_E(q,q;\hbar\beta)\,, \qquad \tau = \hbar\beta$
- Density matrix: $\rho_\beta(q'',q') := \langle q''|\mathrm{e}^{-\beta\hat{H}\hbar}|q'\rangle = K_E(q'',q';\hbar\beta)$

16 Path integral representation of partition function

Remember Lie-Trotter formula for potentials bounded from below

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

We again insert $(N-1)$-times resolution of unity and observe that

$$\begin{aligned}
\langle x_j|\mathrm{e}^{-\frac{\hat{P}^2}{2m}\frac{\beta}{N}}|x_{j-1}\rangle &= \int \mathrm{d}p\,\langle x_j|p\rangle\langle p|x_{j-1}\rangle\,\mathrm{e}^{-\frac{p^2}{2m}\frac{\beta}{N}} \\
&= \frac{1}{2\pi\hbar}\int \mathrm{d}p\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x_j-x_{j-1})}\,\mathrm{e}^{-\frac{p^2}{2m}\frac{\beta}{N}} \\
&= \sqrt{\frac{mN}{2\pi\hbar^2\beta}}\,\exp\left\{-\frac{m}{2\hbar^2}\frac{(\Delta x_j)^2}{\beta}N\right\}
\end{aligned}$$

Hence we arrive at

$$\rho_\beta(x'',x') = \prod_{j=1}^{N-1}\int \mathrm{d}x_j \prod_{j=1}^{N}\left(\frac{mN}{2\pi\hbar^2\beta}\right)^{1/2}\exp\left\{-\frac{m}{2\hbar^2}\frac{(\Delta x_j)^2}{\beta}N - V(x_j)\frac{\beta}{N}\right\}$$

Taking the limit $N\to\infty$ provides us with a path integral representation of the density matrix / Euclidean propagator

- Euclidean propagator: $\beta = \tau/\hbar \qquad \varepsilon := \frac{\tau}{N} = \frac{\hbar\beta}{N}$

$$\begin{aligned} K_E(x'', x'; \tau) &= \rho_{\tau/\hbar}(x'', x') \\ &= \lim_{N\to\infty} \prod_{j=1}^{N-1} \int \mathrm{d}x_j \prod_{j=1}^{N} \left(\frac{m}{2\pi\hbar\varepsilon}\right)^{1/2} \exp\left\{-\frac{m}{2\hbar}\frac{(\Delta x_j)^2}{\varepsilon} - \frac{1}{\hbar}V(x_j)\varepsilon\right\} \\ &= \int_{x'=x(0)}^{x''=x(\tau)} \mathcal{D}[x(\tau)]\, \exp\left\{-\frac{1}{\hbar}\int_0^\tau \mathrm{d}\sigma\left(\frac{m}{2}\,\dot{x}^2 + V(x)\right)\right\} \end{aligned}$$

- Euclidean action

$$S_E[x(\tau)] := \int_0^\tau \mathrm{d}\sigma\left(\frac{m}{2}\,\dot{x}^2 + V(x)\right)$$

Is formally the classical action for a particle in inverted potential $U(x) = -V(x)$!!!

- Partition function

$$\begin{aligned} Z(\beta) &= \int \mathrm{d}x\, \rho_\beta(x, x) \\ &= \oint_{x(0)=x(\tau)} \mathcal{D}[x(\tau)]\, \mathrm{e}^{-\frac{1}{\hbar}S_E[x(\tau)]} \end{aligned}$$

Here integrate over all periodic paths with period $\tau = \hbar\beta$

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

Recall $\quad \beta = N\varepsilon/\hbar$
Note: Here we have N integrations due to the trace !!!

17 The free particle partition function

The Euclidean propagator trivially follows from the quantum propagator through Wick rotation

$$K_E(x'', x'; \tau) = \langle x''|\mathrm{e}^{-\tau\hat{H}/\hbar}|x'\rangle = \sqrt{\frac{m}{2\pi\hbar\tau}}\exp\left\{-\frac{m}{2\hbar}\frac{(x''-x')^2}{\tau}\right\}$$

For partition function confine to a finite volume V in $\mathbb{R}^3$

$$Z_0(\beta) = \int_V \mathrm{d}^3\vec{x}\, K_E(\vec{x}, \vec{x}; \hbar\beta) = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2} \int_V \mathrm{d}^3\vec{x} = V\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2}$$

18 The harmonic oscillator

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{m}{2}\omega^2\hat{Q}^2\,, \qquad \omega > 0\,.$$

Recall quantum result for $0 < \omega t < \pi$

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

Wick rotation: $t = -\mathrm{i}\tau \quad \Longrightarrow \quad \mathrm{i}\sin(\omega t) = \mathrm{i}\sin(-\mathrm{i}\omega\tau) = \sinh(\omega\tau)\,, \quad \cos(\omega t) = \cosh(\omega\tau)\,.$

$$\rho_\beta(x'', x') = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega\tau)}}\exp\left\{-\frac{m\omega}{2\hbar\sinh(\omega\tau)}\left[(x''^2 + x'^2)\cosh(\omega\tau) - 2x''x'\right]\right\}$$

Partition function:

$$\begin{aligned}
Z_\omega(\beta) &= \int_{-\infty}^{\infty} \mathrm{d}x\, \rho_\beta(x,x) \\
&= \int_{-\infty}^{\infty} \mathrm{d}x \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega\tau)}} \exp\left\{ -\frac{m\omega x^2}{\hbar\sinh(\omega\tau)} \underbrace{[\cosh(\omega\tau)-1]}_{2\sinh^2\frac{\omega\tau}{2}} \right\} \\
&= \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega\tau)}} \left(\frac{\pi\hbar\sinh(\omega\tau)}{2m\omega\sinh^2\frac{\omega\tau}{2}} \right)^{1/2} = \frac{1}{2\sinh\frac{\omega\tau}{2}} \\
&= \frac{1}{2\sinh\frac{\hbar\omega}{2}\beta} = \frac{\mathrm{e}^{-\frac{\omega\tau}{2}}}{1-\mathrm{e}^{-\omega\tau}}
\end{aligned}$$

Remember: $\displaystyle\sum_{n=0}^{\infty} \mathrm{e}^{-n\omega\tau} = \frac{1}{1-\mathrm{e}^{-\omega\tau}}$

$$Z_\omega(\beta) = \mathrm{e}^{-\frac{\omega\tau}{2}} \sum_{n=0}^{\infty} \mathrm{e}^{-n\omega\tau} = \sum_{n=0}^{\infty} \mathrm{e}^{-(n+\frac{1}{2})\omega\tau} = \sum_{n=0}^{\infty} \mathrm{e}^{-(n+\frac{1}{2})\hbar\omega\beta} = \mathrm{Tr}\,\mathrm{e}^{-\beta\hat{H}}$$

19 The Wigner-Kirkwood expansion

Consider the quasi-classical limit $\hbar \to 0$ of partition function

$$\begin{aligned}
Z(\beta) &= \oint \mathcal{D}[x(\sigma)] \exp\left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} \mathrm{d}\sigma \left(\frac{m}{2}\dot{x}^2(\sigma) + V(x(\sigma)) \right) \right\} \\
&\quad \text{let} \qquad \sigma = \hbar s \\
&= \oint \mathcal{D}[x(\sigma)] \exp\left\{ -\frac{1}{\hbar} \int_0^{\beta} \mathrm{d}s\, \hbar \left(\frac{m}{2\hbar^2}\mathring{x}^2 + V(x) \right) \right\} \\
&= \oint \mathcal{D}[x(s)] \exp\left\{ -\int_0^{\beta} \mathrm{d}s \left(\frac{m}{2\hbar^2}\dot{x}^2(s) + V(x(s)) \right) \right\}
\end{aligned}$$

As only $\hbar^2$ shows up we expect

$$Z(\beta) = Z_{\mathrm{cl}}(\beta) + O(\hbar^2)$$

• Classical partition function

Let $h(p,q) := \frac{p^2}{2m} + V(q)$ be the classical Hamilton function representing Hamiltonian $\hat{H}$

$$\begin{aligned}
Z_{\mathrm{cl}}(\beta) &= \int \frac{\mathrm{d}p\mathrm{d}q}{2\pi\hbar} \exp\{-\beta h(p,q)\} \\
&= \frac{1}{2\pi\hbar} \int \mathrm{d}p\, \mathrm{e}^{-\beta p^2/2m} \int \mathrm{d}q\, \mathrm{e}^{-\beta V(q)} \\
&= \sqrt{\frac{m}{2\pi\hbar^2\beta}} \int \mathrm{d}x\, \mathrm{e}^{-\beta V(x)}
\end{aligned}$$

Classical parts contributing to path integral appear to come from constant paths $x(s) = x$.

Suggests expansion: $\quad x(s) = x + \hbar q(s)$

Euclidean action: $\quad S_E = \displaystyle\int_0^\beta \left(\frac{m}{2}\dot{q}^2 + V(x+\hbar q) \right)$

Partition function:

$$Z(\beta) = \int \mathrm{d}x \oint_{q'=0}^{q''=0} \mathcal{D}[q(s)] \exp\left\{ -\int_0^\beta \mathrm{d}s \left(\frac{m}{2}\dot{q}^2 + V(x+\hbar q) \right) \right\}$$

Expansion of potential:

$$\begin{aligned} V(x+\hbar q) &= V(x) + \hbar q V'(x) + \tfrac{1}{2}\hbar^2 q^2 V''(x) + O(\hbar^3) \\ &= V(x) - \frac{1}{2}\frac{V'^2(x)}{V''(x)} + \frac{1}{2}V''(x)\left(\hbar q + \frac{V'(x)}{V''(x)}\right)^2 + O(\hbar^3) \qquad (*) \end{aligned}$$

• The lowest order: $\quad V(x+\hbar q) \approx V(x)$

$$Z_{\mathrm{cl}}(\beta) = \int \mathrm{d}x\, \mathrm{e}^{-\beta V(x)} \underbrace{\oint_{q'=0}^{q''=0} \mathcal{D}[q(s)] \exp\left\{-\int_0^\beta \mathrm{d}s\, \frac{m}{2}\dot{q}^2\right\}}_{\text{free particle } = \sqrt{\frac{m}{2\pi\hbar^2\beta}}}$$

$\Longrightarrow$ expected and known result

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

• Next order: Set $\eta := \hbar q + \dfrac{V'}{V''}$ as suggested by $(*)$
All V's are now taken at x

$$Z(\beta) = \int \mathrm{d}x\, \mathrm{e}^{-\beta\left(V - \frac{1}{2}\frac{V'^2}{V''}\right)} \underbrace{\oint_{\eta'=\frac{V'}{V''}}^{\eta''=\frac{V'}{V''}} \mathcal{D}[\eta(s)] \exp\left\{-\int_0^\beta \mathrm{d}s\, \frac{m}{2\hbar^2}\dot{\eta}^2 + \frac{1}{2}V''\eta^2\right\}}_{\text{harmonic oscillator with } \omega^2 = \frac{V''}{m}}$$

$$Z(\beta) = \int \mathrm{d}x\, \mathrm{e}^{-\beta\left(V - \frac{1}{2}\frac{V'^2}{V''}\right)} \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega\tau)}} \exp\left\{-\frac{m\omega\tilde{x}^2}{\hbar\sinh(\omega\tau)}\left(\cosh(\omega\tau) - 1\right)\right\}$$

where $\tilde{x} := \frac{V'}{V''}$ and $\omega\tau = \hbar\omega\beta$.

Homework problem 13:

$$\rho_\beta(x,x) = \frac{m}{2\pi\hbar^2\beta}\mathrm{e}^{-\beta V(x)}\left[1 + \frac{\hbar^2\beta^2}{24m}\left(\beta V'^2(x) - 2V''(x)\right) + O(\hbar^4)\right]$$

and

$$Z(\beta) = \int \mathrm{d}x\, \rho_\beta(x,x) \approx \sqrt{\frac{m}{2\pi\hbar^2\beta}} \int \mathrm{d}x\, \mathrm{e}^{-\beta V_{\mathrm{eff}}(x)}$$

with effective potential

$$\boxed{V_{\mathrm{eff}}(x) = V(x) - \frac{\hbar^2\beta}{24m}V''(x) + O(\hbar^4) = V(x) - \frac{\hbar^2\beta^2}{24m}V'^2(x) + O(\hbar^4)}$$

Similar in form to classical result but potential receives a quantum correction.

E. Wigner, *On the Quantum Correction For Thermodynamic Equilibrium*, Phys. Rev. 40 (1932) 749.

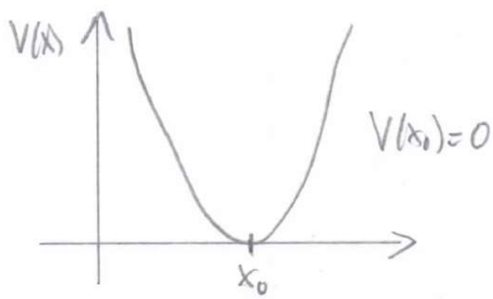
J.G. Kirkwood, *Quantum Statistics of Almost Classical Assemblies*, Phys. Rev. 44 (1933) 31.

20 The large τ behaviour

Or the low temperature limit $\qquad \beta = \tau/\hbar \to \infty$

20.1 Single-well potential

Let us assume a single well potential V with minimum at x_0, $V(x_0) = 0$ for convenience



We consider the diagonal element of the Euclidean propagator

$$K_E(x_0, x_0, \tau) = \int_{x_0}^{x_0} \mathcal{D}[x] \mathrm{e}^{-\frac{1}{\hbar} S_E[x]}$$

$$S_E[x] = \int_{-\tau/2}^{\tau/2} \mathrm{d}\sigma \, \left[\frac{m}{2}\dot{x}^2 + V(x)\right]$$

- Classical path: $\qquad \overline{x}(\sigma)$ obeys Newton's equation for $U(x) = -V(x)$

$$m\ddot{\overline{x}} = V'(x) \qquad \text{with} \qquad \overline{x}(\pm\tfrac{\tau}{2}) = x_0\,, \qquad \tau \quad \text{large}$$

Hence it stays at x_0 forever at unstable balance $\overline{x}(\sigma) = x_0$ and $S[\overline{x}] \equiv S_0 = 0$.

- Quasi-classical approximation: $\qquad \omega^2 = \frac{1}{m}V''(x_0)$

$$\begin{aligned}
\langle x_0|\mathrm{e}^{-\tau\hat{H}/\hbar}|x_0\rangle \quad &\approx F_{\omega^2}\,\mathrm{e}^{-S_0/\hbar} = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega\tau)}} = \sqrt{\frac{m\omega}{\pi\hbar}}\left(\mathrm{e}^{\omega\tau} - \mathrm{e}^{-\omega\tau}\right)^{-1/2} \\
&= \sqrt{\frac{m\omega}{\pi\hbar}}\mathrm{e}^{-\frac{\omega}{2}\tau}\left(1 - \mathrm{e}^{-2\omega\tau}\right)^{-1/2} \\
&\overset{\omega\tau \gg 1}{\approx} \sqrt{\frac{m\omega}{\pi\hbar}}\mathrm{e}^{-\frac{\omega}{2}\tau}\left(1 + \frac{1}{2}\mathrm{e}^{-2\omega\tau} + O(\mathrm{e}^{-4\omega\tau})\right)
\end{aligned}$$

- Spectral representation: $\qquad \hat{H} = \sum_n E_n\,|\varphi_n\rangle\langle\varphi_n|$

$$\begin{aligned}
\langle x_0|\mathrm{e}^{-\tau\hat{H}/\hbar}|x_0\rangle \quad &\overset{\omega\tau \gg 1}{\approx} \mathrm{e}^{-E_0\tau/\hbar}|\langle x_0|\varphi_0\rangle|^2 \\
&\times\left(1 + \mathrm{e}^{-(E_1-E_0)\tau/\hbar}\frac{|\langle x_0|\varphi_1\rangle|^2}{|\langle x_0|\varphi_0\rangle|^2} + \mathrm{e}^{-(E_2-E_0)\tau/\hbar}\frac{|\langle x_0|\varphi_2\rangle|^2}{|\langle x_0|\varphi_0\rangle|^2} + \cdots\right)
\end{aligned}$$

Note: In harmonic approximation $V(x_0 + x) = V(x_0 - x)$ and hence φ_1 is antisymmetric
$\Longrightarrow \qquad \varphi_1(x_0) = 0 \qquad$ first correction term above vanishes

Conclusion:

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

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

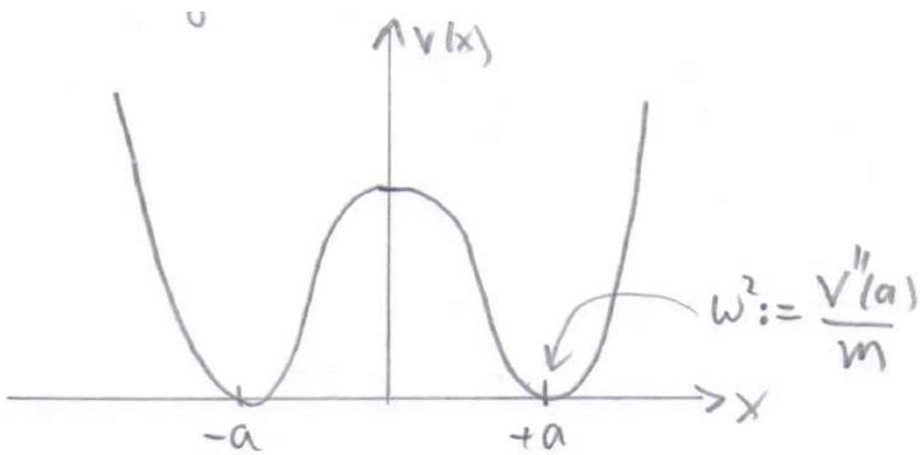
Remarks:

- Zero order approximation for anharmonic oscillator is harmonic

- For $x'' = x_0 = x'$, i.e. the classical ground state, no info is obtained on 1. exited state. One may consider $x'' \neq x'$ but that is difficult to handle
- No non-perturbative effects are considered in this approach as $S_0 = 0$. There may be local minima of action with $0 < S_0 < \infty$ being of order $e^{-S_0/\hbar}$ (Instantons !!!)

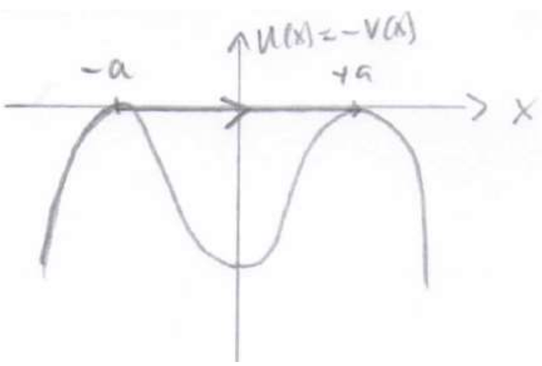
20.2 Double-well potential

Now we assume a symmetric double-well potential of the typical form like
$V(x) = \frac{\omega^2 m}{8a^2}(x^2 - a^2)^2$ with two local minima $V(\pm a) = 0$.



Idea: Consider Euclidean propagator in quasi-classical approximation and extract info on ground state and first excited state from the asymptotic behaviour for large τ with $x' = -a$ and $x'' = a$.

- **Classical paths**: $\bar{x}(\pm\frac{\tau}{2}) = \pm a$ for $\tau \to \infty$

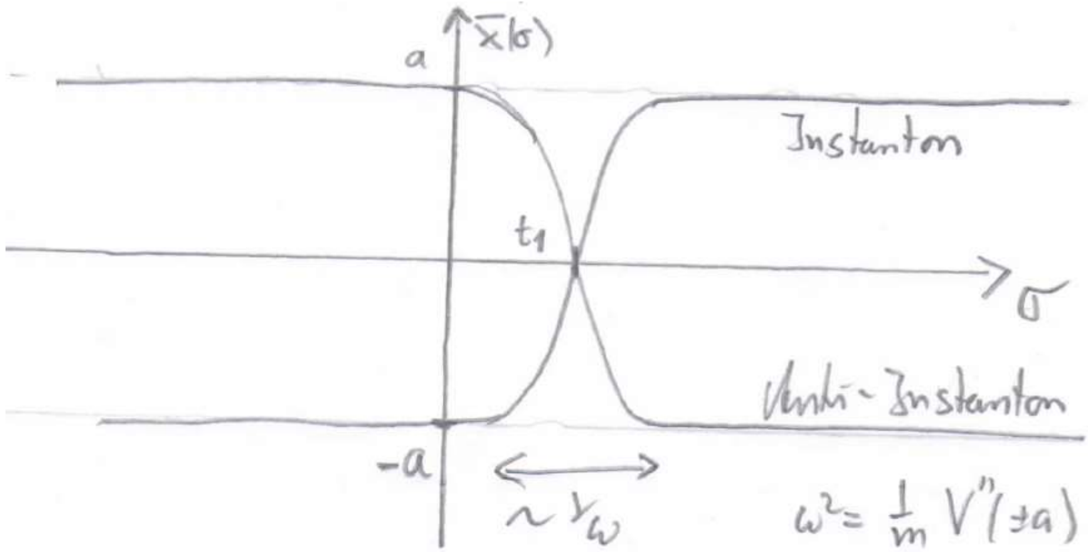


To move from $-a$ to $+a$ in a very long time $\tau \to \infty$ particle must have an energy $E \approx 0$

$$E = \frac{m}{2}\dot{\bar{x}}^2 + U(\bar{x}) = \frac{m}{2}\dot{\bar{x}}^2 - V(\bar{x}) = 0 \qquad \Longrightarrow \qquad \dot{\bar{x}} = \pm\sqrt{\frac{2V(\bar{x})}{m}}$$

Instanton (+) moves from left to right
Anti-Instanton (-) moves from right to left

- **Instanton**: For most of the time particle sits at $-a$, at some instants t_1 it rolls from $-a$ to $+a$ and stays there for rest of time



In our example:

$$\dot{\overline{x}} = \pm\frac{\omega}{2a}(x^2 - a^2) \qquad \Longrightarrow \qquad \overline{x}_{t_1}(\sigma) = \pm a \tanh\left[\frac{\omega}{2}(\sigma - t_1)\right]$$

Translation invariance in time

$$\overline{x}_{t_1}(\sigma) = a \tanh\left[\pm\frac{\omega}{2}(\sigma - t_1)\right] = \overline{x}_0(\pm(\sigma - t_1))$$

• **Classical action**:

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

$\Longrightarrow$

$$S_0 = \int_{-a}^{a} \mathrm{d}x\, \sqrt{2mV(x)}$$

Potential barrier strength is independent of t_1!

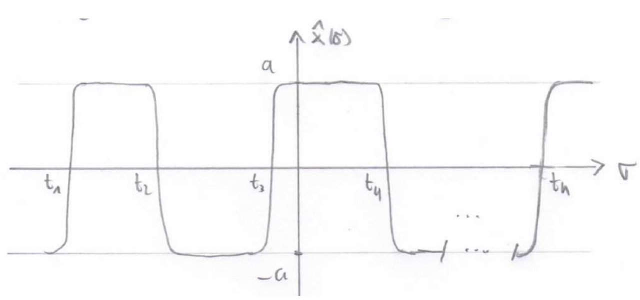
• **Multi instantons**:
Single (anti-) instanton solution is approximate solution for large τ becoming exact only in the limit $\tau \to \infty$.

Further approximate solutions exist and consist of several instantons and anti-instantons. These are local minima of action.

• **The n-instanton solution**:
Let

$$-\frac{\tau}{2} < t_1 < t_2 < \cdots < t_n < \frac{\tau}{2}$$

then the n-instanton solution is given by



$$\hat{x}_{t_1,t_2,\ldots,t_n} := \overline{x}_0(\sigma - t_1) + \overline{x}_0(t_2 - \sigma) + \overline{x}_0(\sigma - t_3) + \cdots + \overline{x}_0(\sigma - t_n)$$

n-Instanton action:

$$S[\hat{x}] = nS_0 + \text{exponentially small corrections}$$

Contributes factor $\mathrm{e}^{-nS_0/\hbar}$ to Euclidean propagator.
Is exponentially small but there is an infinite number of them as $n \to \infty$.

• **Contribution of one instanton**:

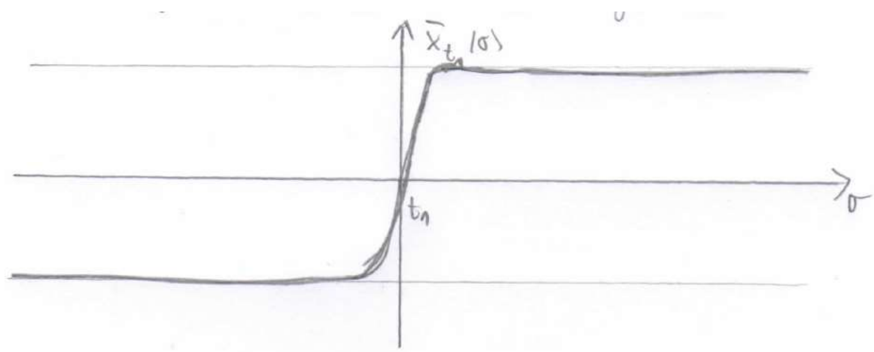
$$\langle a|\mathrm{e}^{-\tau\hat{H}/\hbar}|-a\rangle \approx F_{\frac{V''(\overline{x})}{m}}(\tau)\,\mathrm{e}^{-S_0/\hbar} = K(\tau)F_{\omega^2}(\tau)\,\mathrm{e}^{-S_0/\hbar}$$

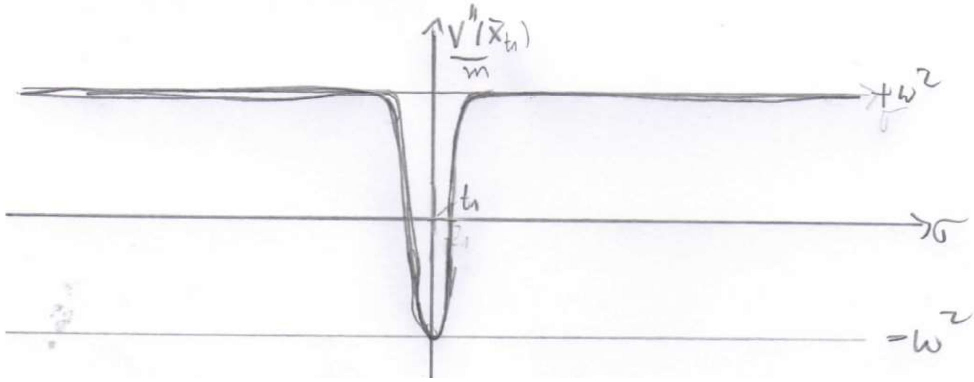
where

$$K(\tau) := \frac{F_{\frac{V''(\overline{x})}{m}}(\tau)}{F_{\omega^2}(\tau)} = \sqrt{\frac{\det\left(-\partial_\sigma^2 + \omega^2\right)}{\det\left(-\partial_\sigma^2 + \frac{V''(\overline{x})}{m}\right)}}$$

Classical dynamics:

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





Lemma: (see tutorial)

$$K_0 := \lim_{\tau\to\infty} K(\tau) \qquad \text{does not dependent on } t_1$$

In addition, instanton and anti-instanton have same contribution.
For large τ the contribution of one (anti-) instanton is given by

$$F_{\omega^2}(\tau)K_0\mathrm{e}^{-S_0/\hbar} \approx \sqrt{\frac{m\omega}{\pi\hbar}}\,\mathrm{e}^{-\frac{\omega\tau}{2}}K_0\,\mathrm{e}^{-S_0/\hbar}$$

• **Contributions of n instantons**
at fixed t_n'

$$\sqrt{\frac{m\omega}{\pi\hbar}}\,\mathrm{e}^{-\frac{\omega\tau}{2}}\left(K_0\,\mathrm{e}^{-S_0/\hbar}\right)^n$$

• **Dilute instanton gas approximation**

We assume that $\omega|t_i - t_j| \gg 1$. That is, instantons are well separated.
We give up the ordering of the t_i's by permuting them and correct by the factor $1/n!$.
So now $t_i \in [-\frac{\tau}{2}, \frac{\tau}{2}]$
Integration over all instances then provides the factor

$$\frac{1}{n!}\int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} \mathrm{d}t_1 \cdots \int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} \mathrm{d}t_n = \frac{\tau^n}{n!}$$

• **Collecting the result:**

To $\langle \pm a|\mathrm{e}^{-\tau\hat{H}\hbar}| \mp a\rangle$ contribute all odd n's.

To $\langle \pm a|\mathrm{e}^{-\tau\hat{H}\hbar}| \pm a\rangle$ contribute all even n's.

Explicitly

$$\begin{aligned}\langle \pm a|\mathrm{e}^{-\tau\hat{H}\hbar}| \mp a\rangle &= \sum_{n=1,3,5,\ldots}^{\infty} \sqrt{\frac{m\omega}{\pi\hbar}}\,\mathrm{e}^{-\frac{\omega\tau}{2}}\,\frac{1}{n!}\left(\tau K_0\,\mathrm{e}^{-S_0/\hbar}\right)^n \\ &= \sqrt{\frac{m\omega}{\pi\hbar}}\,\mathrm{e}^{-\frac{\omega\tau}{2}}\,\sinh\left(\tau K_0\,\mathrm{e}^{-S_0/\hbar}\right)\end{aligned}$$

$$\begin{aligned}\langle \pm a|\mathrm{e}^{-\tau\hat{H}\hbar}| \pm a\rangle &= \sum_{n=0,2,4,\ldots}^{\infty} \sqrt{\frac{m\omega}{\pi\hbar}}\,\mathrm{e}^{-\frac{\omega\tau}{2}}\,\frac{1}{n!}\left(\tau K_0\,\mathrm{e}^{-S_0/\hbar}\right)^n \\ &= \sqrt{\frac{m\omega}{\pi\hbar}}\,\mathrm{e}^{-\frac{\omega\tau}{2}}\,\cosh\left(\tau K_0\,\mathrm{e}^{-S_0/\hbar}\right)\end{aligned}$$

20.3 The tunneling splitting

Let us consider

$$\begin{aligned}\langle a|\mathrm{e}^{-\tau\hat{H}\hbar}| \mp a\rangle &= \sqrt{\frac{m\omega}{\pi\hbar}}\,\mathrm{e}^{-\frac{\omega\tau}{2}}\,\frac{1}{2}\left(\mathrm{e}^{\tau K_0\,\mathrm{e}^{-S_0/\hbar}} \mp \mathrm{e}^{-\tau K_0\,\mathrm{e}^{-S_0/\hbar}}\right) \\ &= \frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}}\,\exp\left\{-\frac{\omega\tau}{2} + \tau K_0\,\mathrm{e}^{-S_0/\hbar}\right\}\left(1 \mp \mathrm{e}^{-2\tau K_0\,\mathrm{e}^{-S_0/\hbar}}\right)\end{aligned}$$

Compare with spectral representation

$$\langle a|\mathrm{e}^{-\tau\hat{H}\hbar}| \mp a\rangle \quad = \langle a|\varphi_0\rangle\langle\varphi_0| \mp a\rangle\mathrm{e}^{-\tau E_0/\hbar}\left(1 + \frac{\langle a|\varphi_1\rangle\langle\varphi_1| \mp a\rangle}{\langle a|\varphi_0\rangle\langle\varphi_0| \mp a\rangle}\mathrm{e}^{-\tau(E_1-E_0/\hbar} + \cdots\right)$$

• Ground state:

$$|\langle a|\varphi_0\rangle|^2 = |\langle -a|\varphi_0\rangle|^2 \approx \frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}}$$

Half of the probability of the single well ground state as expected, symmetric in $\pm a$

• Ground state energy:

$$E_0 \approx \frac{\hbar\omega}{2} - \hbar K_0\mathrm{e}^{-S_0/\hbar}$$

Non-perturbative correction to ground-state energy of single well!
There are perturbative corrections of $O(\hbar^2)$ being larger but they cannot characterize the tunneling splitting

- First exited state:

$$\langle a|\varphi_1\rangle\langle\varphi_1|\mp a\rangle \approx \mp\frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}}$$

Similar to ground state but anti-symmetric in a

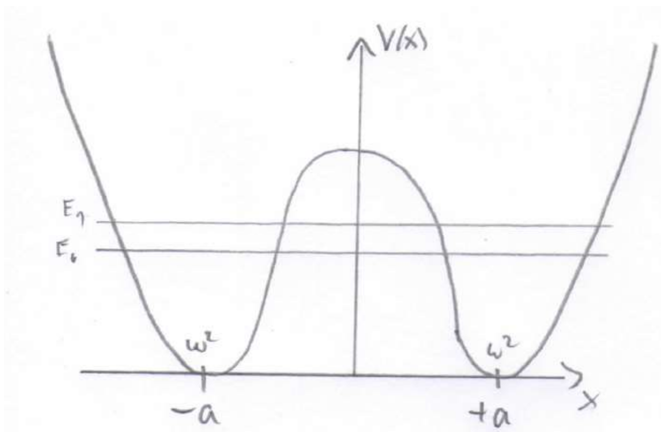
- The tunneling splitting:

$$\boxed{E_1 - E_0 = 2\hbar K_0 \mathrm{e}^{-S_0/\hbar}}$$

Recall: $S_0 = \int_{-a}^{a} \mathrm{d}x\,\sqrt{2mV(x)}$

Tutorial: $K_0 = \sqrt{\frac{m\omega}{\pi\hbar}} \lim_{\tau\to\infty} \mathrm{e}^{\omega\tau}\dot{x}_0(\tau)$

Obviously non-perturbative (in $\hbar$) correction to energy splitting.
Any perturbative corrections would cancel each other in this difference



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