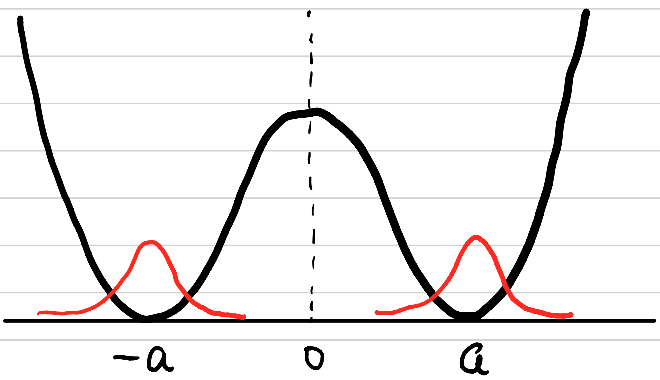
Instantons in quantum mechanics



$U(x)$ a double well potential

assume even, $U(x) = U(-x)$.

Classical $\exists$ 2 degenerate ground states : One at $x = a$
another at $x = -a$.

Quantum $\exists$ 2 approximate ground states of the same energy

$$E \approx \frac{\hbar\omega}{2} \; ; \quad \omega^2 = U''(\pm a).$$

But we know that the degeneracy is lifted by quantum tunneling effect. Only one state $\Psi_0(x)$, even $\Psi_0(x) = \Psi_0(-x)$, no zero point $\Psi_0(x) \neq 0 \;\forall x$, has the lowest energy.

$$\boxed{\text{Question : What is the energy splitting ?}}$$

Two methods :
- usual WKB
- instantons $\leftarrow$

$$Z_{\underbrace{E,}}{}_{T}(x_f ; x_i) := \int_{x(T/2)=x_f,\, x(-T/2)=x_i} \mathcal{D}x \; e^{-\frac{1}{\hbar}\int_{-T/2}^{T/2} d\tau \left(\frac{1}{2}\left(\frac{dx}{d\tau}\right)^2 + U(x)\right)}$$

omit below

$$= \sum_{n=0}^{\infty} \Psi_n(x_f)\, e^{-\frac{T}{\hbar}E_n}\, \Psi_n(x_i)^*$$

The low lying spectrum can be studied by looking at the behaviour as $T \to \infty$.

The measure $\mathcal{D}x$

Take any $\bar{x}(\tau)$ obeying B.C. $\bar{x}(T/2) = x_f$, $\bar{x}(-T/2) = x_i$

and write $x(\tau) = \bar{x}(\tau) + \xi(\tau)$; $\xi(\pm T/2) = 0$.

$\mathcal{F} :=$ space of such $\xi(\tau)$'s.

Inner product in $\mathcal{F}$: $(\xi_1, \xi_2) = \int_{-T/2}^{T/2} d\tau\, \xi_1(\tau)\xi_2(\tau)$.

Choose an orthonormal basis $\{x_n\} \subset \mathcal{F}$

$\forall \xi \in \mathcal{F}$ can be written uniquely as $\xi(\tau) = \sum_n \xi_n x_n(\tau)$

$$\boxed{\mathcal{D}x := N \cdot \prod_n \frac{d\xi_n}{\sqrt{2\pi\hbar}}}$$

$N =$ a fixed number to be determined.

Computation by saddle point approximation

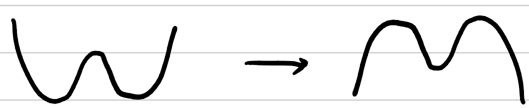
As $\hbar \searrow 0$, dominant contributions to the path-integral come from $x(\tau)$'s with smallest values of

$$S_E[x] = \int_{-T/2}^{T/2} d\tau \left[\frac{1}{2}\left(\frac{dx}{d\tau}\right)^2 + U(x) \right].$$

Suppose $\exists$.1. minimum $\bar{x}(\tau)$. It must obey the E-L eqn

$$-\frac{d^2}{d\tau^2}\bar{x}(\tau) + U'(\bar{x}(\tau)) = 0$$

[EOM for "upside down" potential


]

For $x(\tau) = \bar{x}(\tau) + \xi(\tau)$,

$$S_E[x] = S_E[\bar{x}] + \frac{1}{2}\int_{-T/2}^{T/2} d\tau\, \xi(\tau)\left[-\frac{d^2}{d\tau^2} + U''(\bar{x}(\tau))\right]\xi(\tau) + O(\xi^3)$$

$Z_T(x_f, x_i)$

$$= e^{-\frac{1}{\hbar}S_E[\bar{x}]} \int N \cdot \prod_n \frac{d\xi_n}{\sqrt{2\pi\hbar}}\, e^{-\frac{1}{2\hbar}\int d\tau\, \xi\left[-\frac{d^2}{d\tau^2} + U''(\bar{x}(\tau))\right]\xi + \frac{1}{\hbar}O(\xi^3)}$$

$$\xi = \sqrt{\hbar}\,\tilde{\xi}$$

$$= e^{-\frac{1}{\hbar}S_E[\bar{x}]}\, N \cdot \underbrace{\left[\det\left(-\frac{d^2}{d\tau^2} + U''(\bar{x}(\tau))\right)\right]^{-\frac{1}{2}}}_{\text{fluctuation determinant}} \left(1 + O(\hbar)\right)$$

Suppose $S_E[x]$ is minimized by a family of configurations

$\{\bar{x}(s,\tau)\}_{s\in\mathcal{M}}$ ← an m-parameter space $s=(s^1,\cdots,s^m)$

Again $-\frac{\partial^2}{\partial\tau^2}\bar{x}(s,\tau)+U'(\bar{x}(s,\tau))=0 \quad \forall s$

$$\Rightarrow \left[-\frac{\partial^2}{\partial\tau^2}+U''(\bar{x}(s,\tau))\right]\frac{\partial\bar{x}(s,\tau)}{\partial s^a}=0 \qquad a=1,\cdots,m$$

$x_a(s,\tau)=\frac{\partial\bar{x}(s,\tau)}{\partial s^a}$ are zero modes of $-\frac{d^2}{d\tau^2}+U''(\bar{x}(s,\tau))$, (not necessarily orthonormal).

Write $x(\tau)=\bar{x}(s,\tau)+\sum_n{}' \xi_n x_n(s,\tau)$

$\{x_n\}$: orthonormal basis of $\{x_a(s,\ )\}^{\perp}\subset\mathcal{F}$.

Then $\mathcal{D}X = N\cdot\sqrt{\det(x_a,x_b)}\prod_{a=1}^{m}\frac{ds^a}{\sqrt{2\pi\hbar}}\prod_n{}'\frac{d\xi_n}{\sqrt{2\pi\hbar}}$ and

$Z_T(x_f;x_i)$

$$\simeq\int_{\mathcal{M}}\sqrt{\det(x_a,x_b)}\prod_{a=1}^{m}\frac{ds^a}{\sqrt{2\pi\hbar}}\,e^{-\frac{1}{\hbar}S_E[\bar{x}]}$$

$$\times N\cdot\left[\det{}'\left(-\frac{d^2}{d\tau^2}+U''(\bar{x}(s,\tau))\right)\right]^{-\frac{1}{2}}\left(1+O(\hbar)\right)$$

↑ determinant for non-zero modes only

<u>Example</u> $U(x) = \frac{\omega^2}{2} x^2$ Harmonic oscillator. $x_f = x_i = 0$.

3.1. minimum $\bar{x}(\tau) \equiv 0$.

$$Z_T(0,0) = N \cdot \Big[\det\Big(\underbrace{-\frac{d^2}{d\tau^2} + \omega^2}_{=:A}\Big)\Big]^{-\frac{1}{2}}$$ Exact. No $O(\hbar)$ correction.

$x_n(\tau) \propto \sin\left(\frac{\pi n}{T}\left(\tau + \frac{T}{2}\right)\right)$ diagonilizes A with eigenvalue $\left(\frac{\pi n}{T}\right)^2 + \omega^2$.

$$\therefore \det A = \prod_{n=1}^{\infty}\left[\left(\frac{\pi n}{T}\right)^2 + \omega^2\right] = \prod_{n=1}^{\infty}\left(\frac{\pi n}{T}\right)^2 \cdot \underbrace{\prod_{n=1}^{\infty}\left(1 + \left(\frac{\omega T}{\pi n}\right)^2\right)}_{\| \; \sinh(\omega T)/\omega T}$$

- zeroes at $\omega T = \pm \pi i n$, $n = 1, 2, 3, \ldots$
- $\to 1$ as $\omega T \to 0$

$\longrightarrow$ $\sinh(\omega T)/\omega T$

$$Z_T(0,0) = N \prod_{n=1}^{\infty} \frac{T}{\pi n} \cdot \boxed{\left(\frac{\omega T}{\sinh(\omega T)}\right)^{\frac{1}{2}}} \sim (2\omega T)^{\frac{1}{2}} e^{-\frac{\omega T}{2}} \quad \text{as } T \to \infty$$

Operator result:

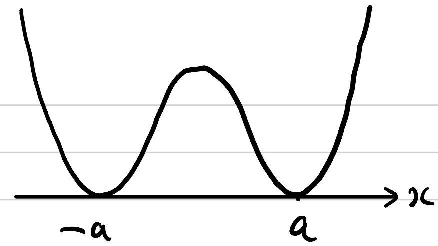
$$Z_T(0,0) = \sum_{n=0}^{\infty} |\Psi_n(0)|^2 e^{-\frac{T}{\hbar}E_n} \sim \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{\omega T}{2}} \quad \text{as } T \to \infty$$

$$\boxed{\Psi_0(x) = \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{\omega}{2\hbar}x^2}, \quad E_0 = \hbar\omega/2}$$

match (with $N \prod_{n=1}^{\infty} \frac{T}{\pi n} = 1/\sqrt{2\pi\hbar T}$) ✓

<u>Side</u> $\sum_{n=0}^{\infty} |\Psi_n(0)|^2 e^{-\frac{T}{\hbar}\hbar\omega(n+\frac{1}{2})} = \left(\frac{\omega/2\pi\hbar}{\sinh(\omega T)}\right)^{1/2}$ also holds.

The double well

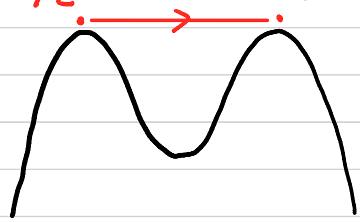


Compute $Z_T(\pm a; \pm a)$ & $Z_T(\pm a, \mp a)$.

- For $x_f = x_i = \pm a$, $\bar{x}(\tau) \equiv \pm a$ is the unique minimum

$$Z_T(\pm a, \pm a) \sim \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{\omega T}{2}} \quad \text{as } T \to \infty \quad \left(\omega^2 := U''(\pm a)\right)$$

- For $x_f = a$, $x_i = -a$, we look for trajectories like



As we are interested in $T \to \infty$, look for

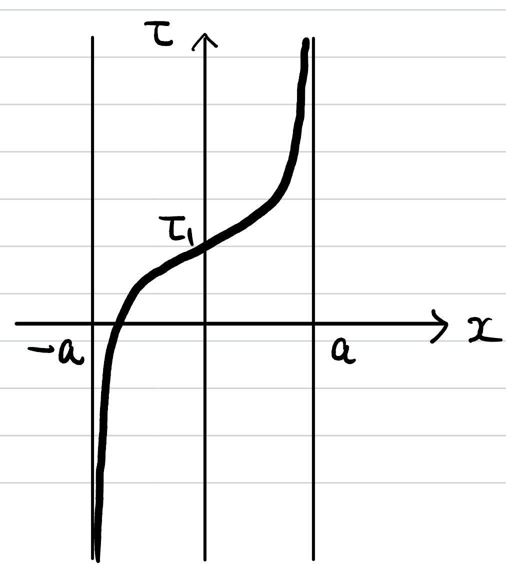
solutions $\bar{x}(\tau)$ s.t. $\bar{x}(\tau) \longrightarrow \begin{cases} a & \tau \to +\infty \\ -a & \tau \to -\infty \end{cases}$

Conservation of energy: $\frac{1}{2}\left(\frac{d\bar{x}}{d\tau}\right)^2 - U(\bar{x}) \equiv \text{const} \overset{\tau \to \pm\infty}{=} 0$

$$\Rightarrow \quad \frac{d\bar{x}}{d\tau} = \sqrt{2U(\bar{x})}$$

i.e. $\tau = \tau_1 + \int_0^{\bar{x}(\tau)} \frac{dx}{\sqrt{2U(x)}}$

integration constant $\bar{x}(\tau_1) = 0$

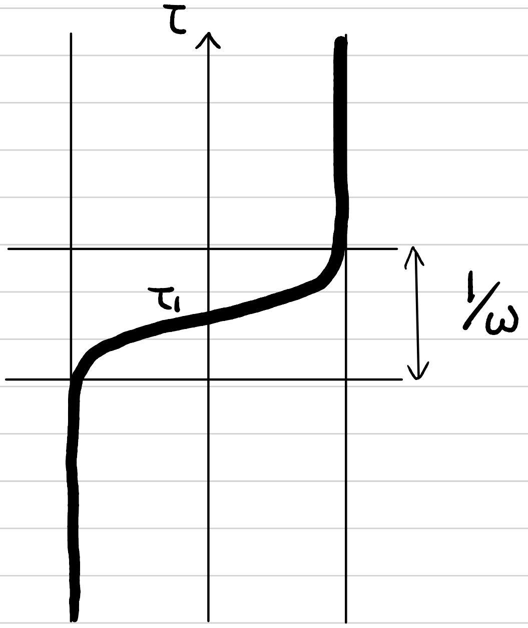


Remarks

- $\bar{x}(\tau)$ is monotone as $\sqrt{2U(x)} > 0$ for $-a < x < a$.

- $$S_E[\bar{x}] = \int_{-\infty}^{\infty} d\tau \left[\frac{1}{2}\left(\frac{d\bar{x}}{d\tau}\right)^2 + U(\bar{x}) \right] = \int_{-\infty}^{\infty} d\tau \left(\frac{d\bar{x}}{d\tau}\right)^2$$
$$= \int_{-\infty}^{\infty} d\tau\, \frac{d\bar{x}}{d\tau}\sqrt{2U(\bar{x})} = \int_{-a}^{a} dx \sqrt{2U(x)} =: S_0$$

- Near $x = \pm a$, $U(x) \approx \frac{1}{2}\omega^2 (x \mp a)^2$
$$\Rightarrow \frac{d\bar{x}}{d\tau} \approx \omega|\bar{x} \mp a| \Rightarrow |\bar{x} \mp a| \propto e^{-\omega|\tau|} \quad \text{as } \tau \to \pm\infty$$



instantaneous jump

$\longrightarrow$ "instanton"

e.g. $U(x) = \dfrac{\omega^2}{2}\left(\dfrac{x^2 - a^2}{2a}\right)^2$

$$\bar{x}(\tau) = a \tanh\left(\frac{\omega}{2}(\tau - \tau_1)\right) = \pm a \frac{1 - e^{-\omega|\tau-\tau_1|}}{1 + e^{-\omega|\tau-\tau_1|}} \quad \text{for } \tau \gtrless \tau_1 .$$

- τ_1 is a parameter of the solution.

The zero mode associated with τ_1 shift is

$$x_1(\tau) = \frac{\partial}{\partial \tau_1} \bar{x}(\tau_1, \tau) = -\frac{d\bar{x}}{d\tau}(\tau)$$

$$(x_1, x_1) = \int_{-\infty}^{\infty} d\tau \left(-\frac{d\bar{x}}{d\tau}\right)^2 = S_0$$

All other modes have $-\frac{d^2}{d\tau^2} + U''(\bar{x}(\tau)) > 0$

Regard it as a Schrödinger operator. The $E=0$ mode $x_1(\tau)$ has no zero point (as $\bar{x}(\tau)$ is monotone).
$\therefore$ It is the ground state. All other state has $E > 0$.

This makes sure that τ_1 is the only parameter.

End of Remarks

Thus, the contribution to $Z_\infty(a, -a)$ is

$$\int_{-\infty}^{\infty} \sqrt{S_0} \frac{d\tau_1}{\sqrt{2\pi\hbar}} e^{-\frac{1}{\hbar}S_0} N \cdot \left[\det{}'\left(-\frac{d^2}{d\tau^2} + U''(\bar{x})\right)\right]^{-\frac{1}{2}} (1 + O(\hbar))$$

The integrand is τ_1-independent $\Rightarrow$ The integral diverges.

But for finite (and large) T, $\int d\tau_1 \to T$.

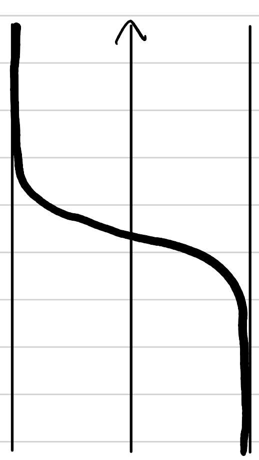
This would give

$$Z_T(a,-a)\Big|_{\text{instanton}}$$

$$= T\sqrt{\frac{S_0}{2\pi\hbar}}\, e^{-\frac{1}{\hbar}S_0}\, N\cdot\left[\det{}'\left(-\frac{d^2}{d\tau^2}+U''(\bar{x})\right)\right]^{-\frac{1}{2}}\left(1+O(\hbar)\right).$$

Note that the $\bar{x}(\tau)$'s solving $\frac{d\bar{x}}{d\tau}=\sqrt{2U(\bar{x})}$ does not satisfy the B.C. for finite T, and the above formula for $Z_T(a,-a)\big|_{\text{instanton}}$ is only an approximation. But we expect that the approximation is better and better as T is larger and larger.

- For $x_f=-a$, $x_i=a$, anti-instantons contribute.



$$Z_T(-a,a)\Big|_{\text{anti-instanton}}$$

= the same as above but

$\bar{x}_{\text{instanton}} \to \bar{x}_{\text{anti-instanton}}$

(same value).

There are other approximate saddle points :

Chain of instantons & anti-instantons

- action $\sim n S_0$
- Fluctuation determinant

$$\sim \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{\omega T}{2}} \cdot K^n$$

- Integration of parameters

$$\int_{\frac{T}{2} \geq \tau_n \geq \cdots \geq \tau_2 \geq \tau_1 \geq -\frac{T}{2}} d\tau_n \cdots d\tau_2 d\tau_1 \cdot 1 = \frac{T^n}{n!}$$

$$\rightsquigarrow \quad \frac{T^n}{n!} e^{-\frac{n}{\hbar} S_0} \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{\omega T}{2}} \cdot K^n \left(1 + O(\hbar)\right) =: Z_n$$

$$\left.\begin{aligned} Z_0 &= N \cdot \left[\det\left(-\frac{d^2}{d\tau^2} + \omega^2\right)\right]^{-\frac{1}{2}} \left(1 + O(\hbar)\right) \\ Z_1 &= T \sqrt{\frac{S_0}{2\pi\hbar}}\, e^{-\frac{1}{\hbar} S_0} N \cdot \left[\det{}'\left(-\frac{d^2}{d\tau^2} + U''(\bar{x})\right)\right]^{-\frac{1}{2}} \left(1 + O(\hbar)\right) \end{aligned}\right\}$$

$$\Rightarrow \quad K = \left[\frac{S_0}{2\pi\hbar} \cdot \det\left(-\frac{d^2}{d\tau^2} + \omega^2\right) \Big/ \det{}'\left(-\frac{d^2}{d\tau^2} + U''(\bar{x}(\tau))\right)\right]^{\frac{1}{2}} \left(1 + O(\hbar)\right)$$

$$Z_n = \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{\omega T}{2}} \frac{1}{n!}\left(KT e^{-\frac{1}{\hbar}S_0}\right)^n (1+O(\hbar))$$

$$Z_T(\pm a, \pm a) = \sum_{n:\,\text{even}}^{\infty} Z_n$$

$$= \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{\omega T}{2}} \frac{1}{2}\left[e^{KTe^{-\frac{1}{\hbar}S_0}} + e^{-KTe^{-\frac{1}{\hbar}S_0}}\right](1+O(\hbar))$$

$$Z_T(\pm a, \mp a) = \sum_{n:\,\text{odd}}^{\infty} Z_n$$

$$= \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{\omega T}{2}} \frac{1}{2}\left[e^{KTe^{-\frac{1}{\hbar}S_0}} - e^{-KTe^{-\frac{1}{\hbar}S_0}}\right](1+O(\hbar))$$

∴ The ground state :

$$E_0 = \left(\frac{\hbar\omega}{2} - \hbar K e^{-\frac{1}{\hbar}S_0}\right)(1+O(\hbar))$$

$$\Psi_0(a) = \Psi_0(-a) = \left(\frac{1}{2}\left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}}\right)^{\frac{1}{2}}(1+O(\hbar)) \quad \text{even}$$

1st excited state :

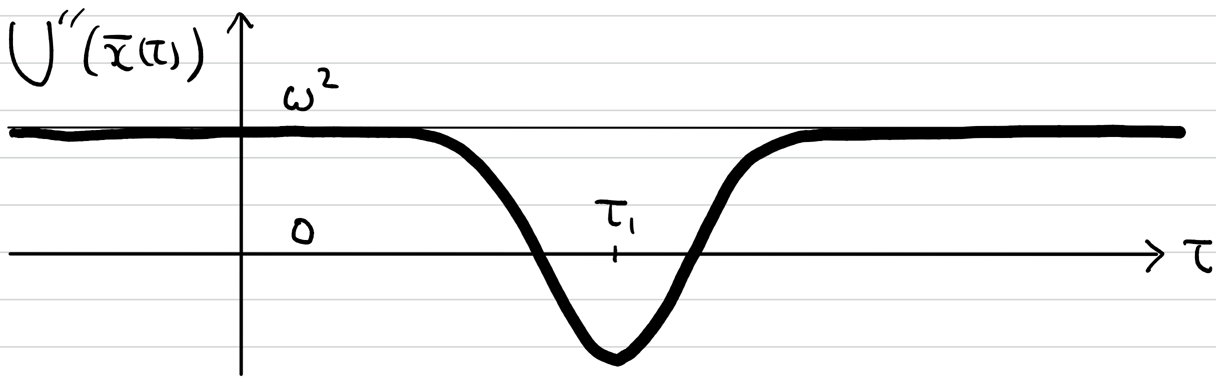
$$E_1 = \left(\frac{\hbar\omega}{2} + \hbar K e^{-\frac{1}{\hbar}S_0}\right)(1+O(\hbar))$$

$$\Psi_1(a) = -\Psi_1(-a) = \left(\frac{1}{2}\left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}}\right)^{\frac{1}{2}}(1+O(\hbar)) \quad \text{odd}$$

$$\therefore \boxed{E_1 - E_0 = 2\hbar K e^{-\frac{1}{\hbar}S_0}(1+O(\hbar))}$$

$$K = \left[\frac{S_0}{2\pi\hbar} \cdot \det\left(-\frac{d^2}{d\tau^2} + \omega^2\right) \Big/ \det{}'\left(-\frac{d^2}{d\tau^2} + U''(\bar{x}(\tau))\right) \right]^{\frac{1}{2}}$$

can be computed.



The spectra of $-\frac{d^2}{d\tau^2} + \omega^2$ & $-\frac{d^2}{d\tau^2} + U''(\bar{x}(\tau))$ are close

at large eigenvalues ($\gg \omega^2$)

$\rightsquigarrow$ The ratio of the determinants is well-defined.

It can be computed and is $2\omega A^2$ with

$$S_0^{\frac{1}{2}} A := \omega \lim_{x_* \to a} |x_* - a| \exp\left(\int_0^{x_*} \frac{\omega\, dx}{\sqrt{2U(x)}} \right).$$

[see the additional note]

$$\therefore K = \sqrt{\frac{\omega}{\pi\hbar}}\, S_0^{\frac{1}{2}} A \quad \Rightarrow$$

$$\boxed{E_1 - E_0 = 2\hbar\omega \sqrt{\frac{\omega}{\pi\hbar}}\, e^{-S_0/\hbar} \lim_{x_* \to a} |x_* - a|\, e^{\int_0^{x_*} \frac{\omega\, dx}{\sqrt{2U(x)}}} \left(1 + O(\hbar)\right)}$$

<u>Exercise</u> Derive this using standard WKB.

<u>Exercise</u> $U(x) = \frac{\omega^2}{2}\left(\frac{x^2-a^2}{2a}\right)^2$

$$\Rightarrow E_1 - E_0 = 4\hbar\omega\sqrt{\frac{\omega a^2}{\pi\hbar}}\, e^{-\frac{1}{\hbar}\frac{2}{3}\omega a^2}$$

The above is called the dilute gas approximation.

It is valid when the dominant contribution comes from the configurations where instantons/anti-instantons are well-separated.

Relevant terms in the sum are those n with

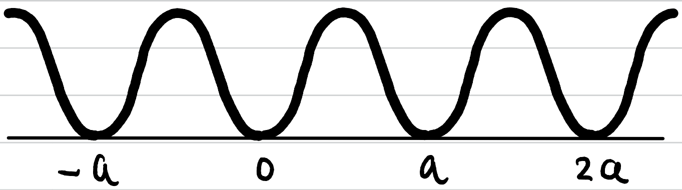
$$n \lesssim KTe^{-S_0/\hbar}.$$

The density of instantons/anti-instantons is

$$\frac{n}{T} \lesssim Ke^{-S_0/\hbar}.$$

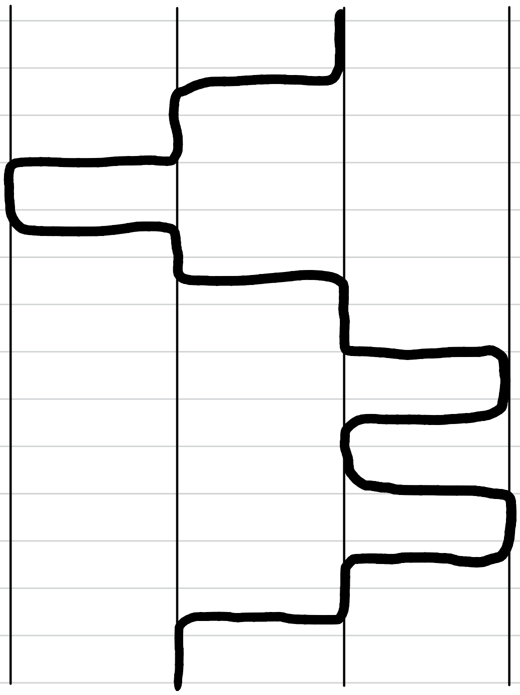
As long as $S_0 \gg \hbar$, it is vanishingly small, and the dilute gas approximation is valid.

Periodic potential



infinitely many classical vacua

at $x = ja \quad (j \in \mathbb{Z})$



$$Z_T(j_f a, j_i a)\Big|_{\substack{n \text{ instantons} \\ \bar{n} \text{ anti-instantons}}} \qquad (n - \bar{n} = j_f - j_i)$$

$$= \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\omega T/2} K^{n+\bar{n}} e^{-(n+\bar{n})S_0/\hbar}$$

$$\left.\begin{aligned} &\cdot \int d\tau_n \cdots d\tau_1 \, d\bar{\tau}_{\bar{n}} \cdots d\bar{\tau}_1 \\ &T/2 \geq \tau_n \geq \cdots \geq \tau_1 \geq -T/2 \\ &T/2 \geq \bar{\tau}_{\bar{n}} \geq \cdots \geq \bar{\tau}_1 \geq -T/2 \end{aligned}\right\} \frac{T^n}{n!} \frac{T^{\bar{n}}}{\bar{n}!}$$

$$Z_T(j_f a, j_i a) = \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\omega T/2} \sum_{n,\bar{n}}^{\infty} \underbrace{\delta_{n-\bar{n}, j_f - j_i}}_{\int_0^{2\pi} \frac{d\theta}{2\pi} e^{i\theta(n-\bar{n}-j_f+j_i)}} \frac{\left(KTe^{-S_0/\hbar}\right)^{n+\bar{n}}}{n!\,\bar{n}!}$$

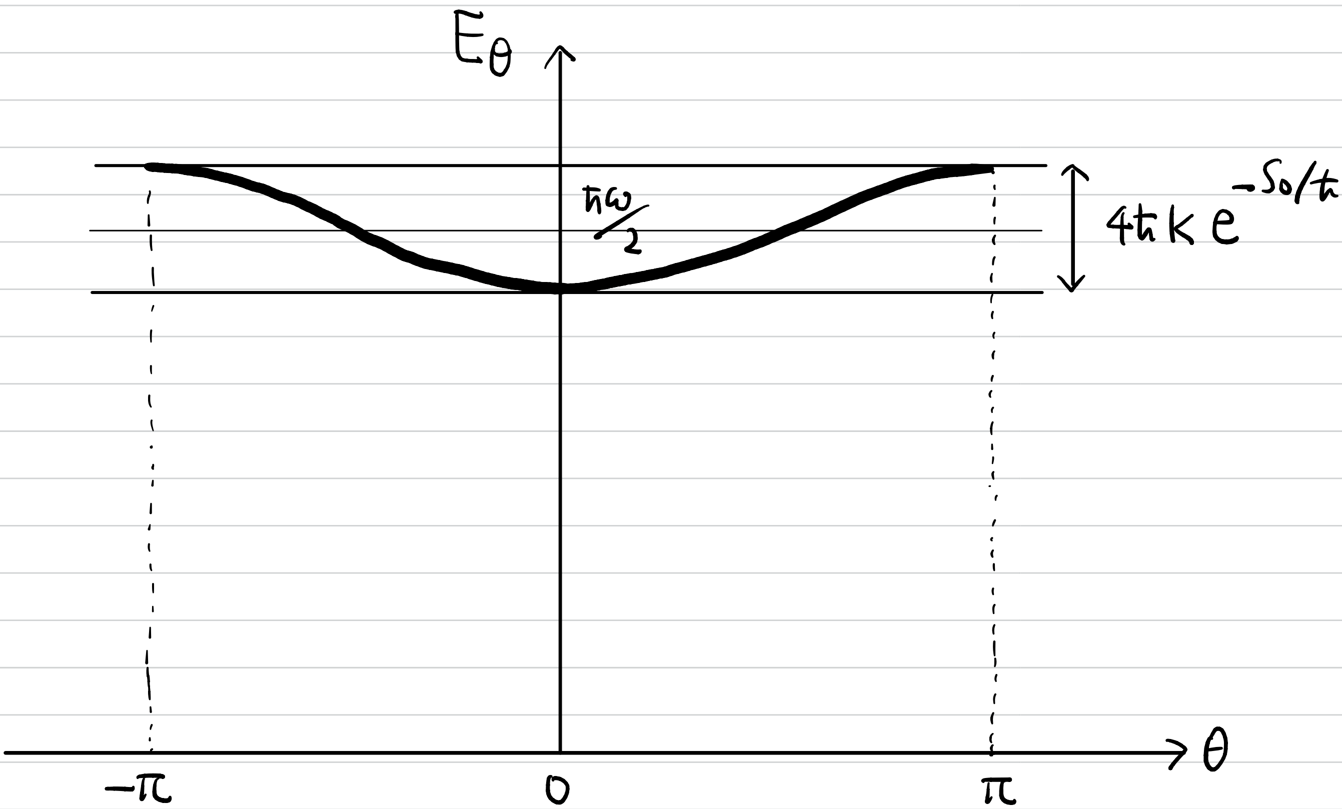
$$= \left(\frac{\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\omega T/2} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i\theta(j_f - j_i)} \exp\Big[\underbrace{\underbrace{KTe^{-\frac{1}{\hbar}S_0 + i\theta}}_{\text{instantons}} + \underbrace{KTe^{-\frac{1}{\hbar}S_0 - i\theta}}_{\text{anti-instantons}}}_{2KT\cos\theta \, e^{-S_0/\hbar}}\Big]$$

$\Rightarrow$ Continuum of energy eigenstates Ψ_θ

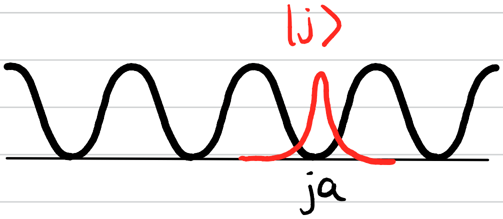
labelled by $\theta \in \mathbb{R}/2\pi\mathbb{Z}$.

$$E_\theta = \left[\frac{\hbar\omega}{2} - 2\hbar K \cos\theta \, e^{-S_0/\hbar} \right] (1 + O(\hbar))$$

$$\Psi_\theta(ja) = \left(\frac{\omega}{\pi\hbar} \right)^{\frac{1}{4}} e^{-ij\theta} \, (1 + O(\hbar))$$



⋯⋯ matches with well-known result in Q.M.



Suppose $\exists$ states $\{|j\rangle\}_{j\in\mathbb{Z}}$ localized at $x=ja$, $\langle x|j\rangle = f(x-ja)$,

s.t.

$$\langle j'|H|j\rangle = \begin{cases} E_0 & j'=j \\ -\Delta & j'-j=\pm 1 \\ 0 & |j'-j|\geq 2 \end{cases}$$

"tight binding approximation"

Then,

$$\Psi_\theta := \sum_{j\in\mathbb{Z}} e^{-ij\theta}|j\rangle$$ are energy eigenstates :

$$E_\theta = E_0 - 2\Delta\cos\theta$$

$$\Psi_\theta(x) = \underbrace{e^{-i\frac{\theta}{a}x}}_{\text{plain wave}} \underbrace{u_\theta(x)}_{\text{periodic: } u_\theta(x+a)=u_\theta(x)}$$ (Bloch's theorem)

$k=\frac{\theta}{a} \in \mathbb{R}/2\pi a\mathbb{Z}$ (Brioullin zone)

$$\rightsquigarrow \Psi_\theta(ja) = e^{-ij\theta}\underbrace{u_\theta(ja)}_{j\text{- independent}}$$