Computation of transition amplitude and partition functions

Let us compute $Z(t_f, \bar{\psi}_f ; t_i, \psi_i)$ & partition functions in both operator & path-integral.

Operator

We choose the symmetric ordering $\hat{H} = \frac{\omega}{2}[\hat{\psi}^\dagger, \hat{\psi}]$, $\hat{Q} = [\hat{\psi}^\dagger, \hat{\psi}]$.

The results for other orderings can be easily found after that and will be mentioned.

$$Z(t_f, \bar{\psi}_f ; t_i, \psi_i) = \langle \bar{\psi}_f | e^{-i\frac{t_f - t_i}{\hbar}\hat{H}} | \psi_i \rangle$$

$$= \langle 0 | \left(1 + \frac{1}{\hbar}\bar{\psi}_f \hat{\psi}\right) e^{-i\frac{t_f - t_i}{\hbar}\hat{H}} \left(1 + \frac{1}{\hbar}\hat{\psi}^\dagger \psi_i\right) | 0 \rangle$$

$$= \langle 0 | \left(1 + \frac{1}{\hbar}\bar{\psi}_f \hat{\psi}\right) \left(e^{i(t_f - t_i)\frac{\omega}{2}} + \frac{1}{\hbar} e^{-i(t_f - t_i)\frac{\omega}{2}} \hat{\psi}^\dagger \psi_i \right) | 0 \rangle$$

$$= e^{i(t_f - t_i)\frac{\omega}{2}} + \frac{1}{\hbar} e^{-i(t_f - t_i)\frac{\omega}{2}} \bar{\psi}_f \psi_i$$

$$= e^{i(t_f - t_i)\frac{\omega}{2}} \left(1 + \frac{1}{\hbar} e^{-i(t_f - t_i)\omega} \bar{\psi}_f \psi_i\right)$$

$$= e^{i(t_f - t_i)\frac{\omega}{2}} \, e^{\frac{1}{\hbar} e^{-i(t_f - t_i)\omega} \bar{\psi}_f \psi_i}$$

$$\mathrm{Tr}_{\mathcal{H}}\, e^{-\frac{T}{\hbar}\hat{H}} = e^{-\frac{T}{\hbar}\left(-\frac{\hbar\omega}{2}\right)} + e^{-\frac{T}{\hbar}\left(\frac{\hbar\omega}{2}\right)} = e^{\frac{\omega T}{2}} + e^{-\frac{\omega T}{2}}$$

$$\mathrm{Tr}_{\mathcal{H}}(-1)^F e^{-\frac{T}{\hbar}\hat{H}} = e^{-\frac{T}{\hbar}\left(-\frac{\hbar\omega}{2}\right)} - e^{-\frac{T}{\hbar}\left(\frac{\hbar\omega}{2}\right)} = e^{\frac{\omega T}{2}} - e^{-\frac{\omega T}{2}}$$

We may also compute symmetry-twisted partition function

$$\mathrm{Tr}_{\mathcal{H}}(\pm 1)^F e^{\frac{i\alpha}{\hbar}\hat{Q}}\, e^{-\frac{T}{\hbar}\hat{H}} = e^{\frac{\omega T}{2} - \frac{i\alpha}{2}} \pm e^{-\frac{\omega T}{2} + \frac{i\alpha}{2}}$$

A change of operator orderings

$$\hat{H} = (1-s)\,\omega\hat{\psi}^{\dagger}\hat{\psi} - s\,\omega\hat{\psi}\hat{\psi}^{\dagger} = \frac{\omega}{2}[\hat{\psi}^{\dagger},\hat{\psi}] - (s-\tfrac{1}{2})\hbar\omega,$$

$$\hat{Q} = (1-s')\hat{\psi}^{\dagger}\hat{\psi} - s'\hat{\psi}\hat{\psi}^{\dagger} = [\hat{\psi}^{\dagger},\hat{\psi}] - (s'-\tfrac{1}{2})\hbar$$

would result in a shift of the exponent in the overall factors

$$Z(t_f,\bar{\psi}_f; t_i,\psi_i) = e^{i(t_f-t_i)s\omega}\, e^{\frac{1}{\hbar}e^{-i(t_f-t_i)\omega}\bar{\psi}_f\psi_i}.$$

$$\mathrm{Tr}_{\mathcal{H}}(\pm 1)^F e^{\frac{i\alpha}{\hbar}\hat{Q}}\, e^{-\frac{T}{\hbar}\hat{H}} = e^{s\omega T - is'\alpha}\left(1 \pm e^{-\omega T + i\alpha}\right).$$

Path-integral

$$Z(t_f,\bar\psi_f;t_i,\psi_i)=\int_{\bar\psi(t_f)=\bar\psi_f,\ \psi(t_i)=\psi_i}\mathcal{D}\bar\psi\,\mathcal{D}\psi\ e^{\underbrace{\frac{1}{\hbar}\bar\psi\psi|_{t_f}+\frac{i}{\hbar}\int_{t_i}^{t_f}dt\,(i\bar\psi\dot\psi-\omega\bar\psi\psi)}_{\frac{i}{\hbar}\,@}}$$

Write $\psi=\psi_{cl}+\tilde\psi$, $\quad\tilde\psi(t_i)=0$,

$\bar\psi=\bar\psi_{cl}+\tilde{\bar\psi}$, $\quad\tilde{\bar\psi}(t_f)=0$,

where ψ_{cl} & $\bar\psi_{cl}$ are solution of EOM obeying boundary conditions,

$$\psi_{cl}(t)=\psi_i\,e^{-i\omega(t-t_i)},$$

$$\bar\psi_{cl}(t)=\bar\psi_f\,e^{i\omega(t-t_f)}.$$

Then,

$$@=-i\bar\psi_f\left(\psi_{cl}(t_f)+\tilde\psi(t_f)\right)$$

$$+\int_{t_i}^{t_f}dt\left(\underbrace{i(\bar\psi_{cl}+\tilde{\bar\psi})(\dot\psi_{cl}+\dot{\tilde\psi})-\omega(\bar\psi_{cl}+\tilde{\bar\psi})(\psi_{cl}+\tilde\psi)}\right)$$

$$(\bar\psi_{cl}+\tilde{\bar\psi})\underbrace{(i\dot\psi_{cl}-\omega\psi_{cl})}_{0}+\underbrace{(\bar\psi_{cl}+\tilde{\bar\psi})(i\dot{\tilde\psi}-\omega\tilde\psi)}$$

$$\frac{d}{dt}\left(i(\bar\psi_{cl}+\tilde{\bar\psi})\tilde\psi\right)\underbrace{-i\frac{d}{dt}(\bar\psi_{cl}+\tilde{\bar\psi})\tilde\psi-\omega(\bar\psi_{cl}+\tilde{\bar\psi})\tilde\psi}$$

$$(\underbrace{-i\dot{\bar\psi}_{cl}-\omega\bar\psi_{cl}}_{0}-i\dot{\tilde{\bar\psi}}-\omega\tilde{\bar\psi})\tilde\psi$$

$$= -i\bar{\psi}_f\left(\psi_i e^{-i\omega(t_f-t_i)} + \cancel{\tilde{\psi}(t_f)}\right)$$

$$+ i\Big(\underbrace{\bar{\psi}_{cl}(t_f)}_{\bar{\psi}_f} + \underbrace{\tilde{\bar{\psi}}(t_f)}_{0}\Big)\tilde{\psi}(t_f) - i\big(\bar{\psi}_{cl}(t_i) + \tilde{\bar{\psi}}(t_i)\big)\underbrace{\tilde{\psi}(t_i)}_{0}$$

$$+ \int_{t_i}^{t_f} dt\,\left(-i\dot{\tilde{\bar{\psi}}}\tilde{\psi} - \omega\tilde{\bar{\psi}}\tilde{\psi}\right)$$

$$= -i\bar{\psi}_f\psi_i e^{-i\omega(t_f-t_i)} + \int_{t_i}^{t_f} dt\,\left(-i\dot{\tilde{\bar{\psi}}}\tilde{\psi} - \omega\tilde{\bar{\psi}}\tilde{\psi}\right)$$

$\therefore Z(t_f, \bar{\psi}_f ; t_i, \psi_i)$

$$= e^{\frac{1}{\hbar}\bar{\psi}_f\psi_i e^{-i\omega(t_f-t_i)}} \underbrace{\int_{\tilde{\bar{\psi}}(t_f)=0,\ \tilde{\psi}(t_i)=0} \mathcal{D}\tilde{\bar{\psi}}\,\mathcal{D}\tilde{\psi}\, e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\left(-i\dot{\tilde{\bar{\psi}}}\tilde{\psi} - \omega\tilde{\bar{\psi}}\tilde{\psi}\right)}}_{=:\ F(t_f-t_i)}$$

$$= F(t_f-t_i)\, e^{\frac{1}{\hbar}\bar{\psi}_f\psi_i e^{-i\omega(t_f-t_i)}}$$

Constraint on $F(t)$:

$$\hat{Z}_{t_f,t_i} : \Psi(\bar{\psi}) \longmapsto \int \hbar\, d\bar{\psi}'\, d\psi'\, Z(t_f, \bar{\psi} ; t_i, \psi')\, e^{\frac{1}{\hbar}\psi'\bar{\psi}'}\, \Psi(\bar{\psi}')$$

is (i) unitary and

obeys (ii) $\hat{Z}_{t_3,t_2} \circ \hat{Z}_{t_2,t_1} = \hat{Z}_{t_3,t_1}$.

Recall $\langle \Psi_1 | \Psi_2 \rangle = \int \hbar\, d\bar{\psi}\, d\psi\ \Psi_1(\psi)^* e^{\frac{1}{\hbar}\psi\bar{\psi}}\ \Psi_2(\bar{\psi})$.

Then ⓘ $\Longleftrightarrow$ $|F(t)|^2 = 1$

ⓘⓘ $\Longleftrightarrow$ $F(t_3-t_2)F(t_2-t_1) = F(t_3-t_1)$

These require

$$F(t) = e^{iAt} \quad \text{for a real } A.$$

$$\therefore\ Z(t_f, \bar{\psi}_f ; t_i, \psi_i) = e^{iA(t_f-t_i)}\, e^{\frac{1}{\hbar}\bar{\psi}_f \psi_i e^{-i\omega(t_f-t_i)}} \qquad (\#)$$

This A can be regarded as an ambiguity in the definition of $\mathcal{D}\bar{\psi}\mathcal{D}\psi$. It can also be absorbed by a shift of L by a constant which result in overall shift of energy.

The result $(\#)$ match with the Operator result where the ambiguity in the definition of $\mathcal{D}\bar{\psi}\mathcal{D}\psi$ corresponds to operator ordering ambiguity.

For partition function, first do Wick rotation:

$$L = i\bar{\psi}\dot{\psi} - \omega\bar{\psi}\psi$$

$$\rightsquigarrow \quad L_E = -\left(i\bar{\psi}\, i\frac{d\psi}{d\tau} - \omega\bar{\psi}\psi\right) = \bar{\psi}\left(\frac{d}{d\tau} + \omega\right)\psi$$

Let us compute

$$Z_\alpha(S^1_T) := \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \; e^{-\frac{1}{\hbar}\int_0^T d\tau\, L_E}$$

$$\bar{\psi}(\tau+T) = e^{i\alpha}\bar{\psi}(\tau), \quad \psi(\tau+T) = e^{-i\alpha}\psi(\tau).$$

mode expansion
$$\begin{cases} \bar{\psi} = \sum_{n\in\mathbb{Z}} \bar{\psi}_n \frac{1}{\sqrt{T}} e^{i(2\pi n+\alpha)\tau/T} \\ \psi = \sum_{n\in\mathbb{Z}} \psi_n \frac{1}{\sqrt{T}} e^{i(2\pi n-\alpha)\tau/T} \end{cases},$$

$$S_E = \int_0^T d\tau \sum_{n,m} \bar{\psi}_m \frac{1}{\sqrt{T}} e^{i(2\pi m+\alpha)\tau/T} \left(i\frac{2\pi n-\alpha}{T} + \omega\right)\psi_n \frac{1}{\sqrt{T}} e^{i(2\pi n-\alpha)\tau/T}$$

$$= \sum_{n\in\mathbb{Z}} \bar{\psi}_{-n}\left(i\frac{2\pi n-\alpha}{T} + \omega\right)\psi_n$$

Let us put $\mathcal{D}\bar{\psi}\mathcal{D}\psi := \prod_{n\in\mathbb{Z}} d\bar{\psi}_{-n}\, d\psi_n$ and use ζ-fcn reg.

$$Z_\alpha(S^1_T) = \int \prod_{n\in\mathbb{Z}} d\bar\psi_{-n}\, d\psi_n \; e^{-\frac{1}{\hbar}\sum_{n\in\mathbb{Z}} \bar\psi_{-n}\left(i\frac{2\pi n-\alpha}{T}+\omega\right)\psi_n}$$

$$= \prod_{n\in\mathbb{Z}} \frac{1}{\hbar}\left(i\cdot\frac{2\pi n-\alpha}{T}+\omega\right)$$

$$= \underbrace{\prod_{n\in\mathbb{Z}} \frac{i(2\pi n-\alpha)}{\hbar T}}_{\text{Ⓐ}} \cdot \underbrace{\prod_{n\in\mathbb{Z}}\left(1-\frac{i\omega T}{2\pi n-\alpha}\right)}_{\text{Ⓑ}}$$

$$\text{Ⓐ} = \frac{\alpha}{\hbar T i}\cdot\prod_{n=1}^{\infty}\frac{n-\alpha/2\pi}{\hbar T/2\pi i}\cdot\frac{n+\alpha/2\pi}{-\hbar T/2\pi i}$$

[ζ-function regularization (see * below):

$$\prod_{n=1}^{\infty}\frac{n+y}{x} = \sqrt{2\pi x}/\Gamma(1+y)$$

$$= \frac{\alpha}{\hbar T i}\;\frac{\sqrt{\hbar T/i}}{\Gamma(1-\frac{\alpha}{2\pi})}\;\frac{\sqrt{\hbar T i}}{\Gamma(1+\frac{\alpha}{2\pi})} = \frac{\alpha}{i}\left(\Gamma\left(1-\frac{\alpha}{2\pi}\right)\Gamma\left(1+\frac{\alpha}{2\pi}\right)\right)^{-1}$$

[$\Gamma(1-z)\Gamma(1+z) = z\Gamma(1-z)\Gamma(z) = \dfrac{\pi z}{\sin\pi z}$

$$= \frac{\alpha}{i}\;\frac{\sin(\pi\frac{\alpha}{2\pi})}{\pi\frac{\alpha}{2\pi}} = -2i\sin\left(\frac{\alpha}{2}\right)$$

* ζ-function regularization

Generalized zeta function $\zeta(s,a) = \sum_{n=0}^{\infty} (n+a)^{-s}$

is absolutely convergent for $\mathrm{Re}(s) > 1$ and has analytic continuation which is regular at $s=0$, with

$$\zeta(0,a) = \frac{1}{2} - a, \quad \zeta'(0,a) = \log\Gamma(a) - \frac{1}{2}\log 2\pi.$$

Here $\Gamma(a)$ is Gamma function.

(A convenient property : $\Gamma(a+1) = a\Gamma(a)$, $\Gamma(a)\Gamma(1-a) = \frac{\pi}{\sin\pi a}$.)

Note : $\zeta'(s,a) := \frac{\partial}{\partial s}\zeta(s,a) = \sum_{n=0}^{\infty} -\log(n+a)(n+a)^{-s}$.

Using these we find

$$\prod_{n=1}^{\infty} \frac{n+y}{X} = \exp\left(\sum_{n=1}^{\infty}\left(\log(n+y) - \log X\right)\right)$$

$$= \exp\left(-\zeta'(0,1+y) - \log X \cdot \zeta(0,1)\right)$$

$$= \exp\left(-\Gamma(1+y) + \frac{1}{2}\log 2\pi + \frac{1}{2}\log X\right)$$

$$= \frac{\sqrt{2\pi X}}{\Gamma(1+y)}.$$

$$(B) = \prod_{n \in \mathbb{Z}} \left(1 - \frac{i\omega T}{2\pi n - \alpha}\right)$$

- 1 at $i\omega T = 0$
- simple zero at $i\omega T = 2\pi n - \alpha \quad (n \in \mathbb{Z})$

$$= \frac{\sin\left(\frac{i\omega T + \alpha}{2}\right)}{\sin\left(\frac{\alpha}{2}\right)}$$

$$= \left(e^{i\frac{i\omega T + \alpha}{2}} - e^{-i\frac{i\omega T + \alpha}{2}}\right) \Big/ 2i\sin\left(\frac{\alpha}{2}\right)$$

$$= \left(e^{-\frac{\omega T}{2} + i\frac{\alpha}{2}} - e^{\frac{\omega T}{2} - i\frac{\alpha}{2}}\right) \Big/ 2i\sin\left(\frac{\alpha}{2}\right)$$

$$\therefore Z_\alpha(S^1_T) = (A) \cdot (B) = e^{\frac{\omega T}{2} - i\frac{\alpha}{2}} - e^{-\frac{\omega T}{2} + i\frac{\alpha}{2}}$$

This match with the operator result for

$$\mathrm{Tr}_{\mathcal{H}} (-1)^F e^{i\frac{\alpha}{\hbar}\hat{Q}} e^{-\frac{T}{\hbar}\hat{H}}$$ with the symmetric ordering

$$\hat{H} = \frac{\omega}{2}[\hat{\psi}^\dagger, \hat{\psi}], \quad \hat{Q} = \frac{1}{2}[\hat{\psi}^\dagger, \hat{\psi}].$$

$\therefore$ ζ-function regularization

corresponds to the symmetric ordering.

<u>Remark</u> (O_p) The two cases "$\pm$" of the operator result

$$\mathrm{Tr}_{\mathcal{H}} (\pm 1)^F e^{\frac{i\alpha}{\hbar}\hat{Q}} e^{-\frac{T}{\hbar}\hat{H}} = e^{s\omega T - is'\alpha}\left(1 \pm e^{-\omega T + i\alpha}\right).$$

is consistent with each other. Indeed, for $s'=0$,

$$\hat{Q} = \begin{cases} 0 \\ \hbar \end{cases} \quad \text{and} \quad e^{\frac{i\alpha}{\hbar}\hat{Q}} = \begin{cases} 1 \\ e^{i\alpha} \end{cases} \quad \text{on} \begin{cases} |0\rangle \\ \hat{\psi}^\dagger|0\rangle, \end{cases}$$

and in particular $e^{\frac{i\alpha}{\hbar}\hat{Q}} = (-1)^F$ for $\alpha \equiv \pi \mod 2\pi$.

Thus, $\alpha \to \alpha + \pi$ does

- $e^{\frac{i\alpha}{\hbar}\hat{Q}} \longrightarrow (-1)^F e^{\frac{i\alpha}{\hbar}\hat{Q}}$
- $1 + e^{-\omega T + i\alpha} \longrightarrow 1 - e^{-\omega T + i\alpha}$

That is, the two cases $+$ & $-$ are swapped by $\alpha \to \alpha + \pi$ for $s'=0$ in which $e^{i\frac{\pi}{\hbar}\hat{Q}} = (-1)^F$.

This is also the case when s' is an even integer.

For a general s', $e^{i\frac{\pi}{\hbar}\hat{Q}} = (-1)^F e^{-i\pi s'}$, and the two cases are also swapped by $\alpha \to \alpha + \pi$.

(P.I.) On the other hand, the path-integral result

$$Z_\alpha(S^1_T) := \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \, e^{-\frac{1}{\hbar}\int_0^T d\tau \, L_E}$$

$$\bar{\psi}(\tau+T) = e^{i\alpha}\bar{\psi}(\tau), \quad \psi(\tau+T) = e^{-i\alpha}\psi(\tau)$$

$$= e^{\frac{\omega T}{2} - i\frac{\alpha}{2}} - e^{-\frac{\omega T}{2} + i\frac{\alpha}{2}}$$

is a bit strange. The definition appears to be periodic under $\alpha \to \alpha + 2\pi$, but the result is periodic only under $\alpha \to \alpha + 4\pi$.

Related problem: $Z_\alpha(S^1_T)$ for $\alpha = \pm\pi$ is the path-integral over $\psi(\tau)$, $\bar{\psi}(\tau)$ which is antiperiodic under $\tau \to \tau + T$, and this is supposed to be equal to $\mathrm{Tr}_{\mathcal{H}}(e^{-\frac{T}{\hbar}\hat{H}})$.

However the results

$$Z_{\pm\pi}(S^1_T) = \mp i\left(e^{\omega T/2} + e^{-\omega T/2}\right) \quad \text{and}$$

$$\mathrm{Tr}_{\mathcal{H}}(e^{-\frac{T}{\hbar}\hat{H}}) = e^{\omega T/2} + e^{-\omega T/2}$$

differ by phases.

At first sight, it appears that the problem is in the ζ-function regularization

$$\textcircled{A} := \prod_{n\in\mathbb{Z}} \frac{i(2\pi n-\alpha)}{\hbar T} \overset{\downarrow}{=} -2i\sin\left(\frac{\alpha}{2}\right)$$

LHS appears to be periodic under $\alpha \to \alpha + 2\pi$, but RHS changes its sign under $\alpha \to \alpha + 2\pi$.

However, whatever regularization you use, the ∞-product $\prod_{n\in\mathbb{Z}} \frac{i(2\pi n-\alpha)}{\hbar T}$ must change its sign under $\alpha \to \alpha + 2\pi$:

As $\alpha \to \alpha + 2\pi$, one particular $2\pi n - \alpha$ changes its sign and the set of other $(2\pi n - \alpha)$'s goes back to itself.

Nothing is particularly wrong about ζ-function regularization.

A way-out of the problem is to modify the definition of the path-integral measure as

$$\mathcal{D}\bar{\psi}\,\mathcal{D}\psi = e^{i(m+\frac{1}{2})\alpha} \prod_{n\in\mathbb{Z}} d\bar{\psi}_{-n}\, d\psi_n \quad \text{with } m \in \mathbb{Z},$$

which results in

$$Z_\alpha(S^1_T) = e^{\frac{\omega T}{2} + im\alpha} - e^{-\frac{\omega T}{2} + i(m+1)\alpha}.$$

This is the same as the operator result for $S = \frac{1}{2}$, $S' = -m$.

It is periodic under $\alpha \to \alpha + 2\pi$, and indeed

$$Z_0(S^1_T) = \mathrm{Tr}_{\mathcal{H}} (-1)^F e^{-\frac{T}{\hbar}\hat{H}}$$
$$Z_\pi(S^1_T) = \mathrm{Tr}_{\mathcal{H}} e^{-\frac{T}{\hbar}\hat{H}}.$$

This looks like a "cheap trick" and it looks strange that it depends on an additional parameter $m \in \mathbb{Z}$.

However, it turns out to be a "reasonable solution" in a certain sense. We will see that when we systematically study anomaly.