Harmonic oscillator – statistical mechanics – path integral

easy way:

$\hat{H}|n\rangle = \hbar\omega(n+1/2)|n\rangle \qquad n=0,1,2,\ldots$

$$Z = \sum_{n=0}^{\infty} \langle n| e^{-\beta\hat{H}} |n\rangle = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+1/2)} = \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}} =$$

$$= \boxed{\frac{1}{2\sinh\left(\frac{\hbar\omega}{2k_BT}\right)}}$$

Path integral

$x(\tau)$ arbitrary function on $(0, \beta\hbar)$ and periodic $\quad x((\beta\hbar)^-) = x(0^+)$

Fourier sum

$$\boxed{x(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} x_n e^{i\omega_n \tau}}$$

Due to periodicity

$$e^{i\omega_n \beta\hbar} = 1 = e^{i2\pi n} \rightarrow \boxed{\omega_n = \frac{2\pi n}{\beta\hbar}}$$

Matsubara frequencies $\qquad n \in \mathbb{Z}$

x_n – matsubara modes

From reality of $x(\tau) \in \mathbb{R}$

$$x^*(\tau) = x(\tau) \Longrightarrow \boxed{x_n^* = x_{-n}}$$

writing $x_n = a_n + i b_n$

$$x_n^* = a_n - i b_n = x_{-n} = a_{-n} + i b_{-n} \Rightarrow \boxed{\begin{cases} a_n = a_{-n} \\ b_n = -b_{-n} \end{cases} \quad b_0 = 0}$$

also $\boxed{x_{-n}\, x_n = a_n^2 + b_n^2}$

$$\Rightarrow \quad x(\tau) = \frac{1}{\beta}\Big[\underset{\substack{\uparrow \\ \text{amplitude of} \\ \text{Matsubara zero mode}}}{a_0} + \sum_{n=1}^{\infty} (a_n + i b_n) e^{i\omega_n \tau} + (a_n - i b_n) e^{-i\omega_n \tau} \Big] \quad (\circ)$$

In general we have

$$\boxed{\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, x(\tau)\, y(\tau)} = \frac{1}{\beta^2}\sum_{mn} x_n y_m \underbrace{\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, e^{i(\omega_n+\omega_m)\tau}}_{\beta\,\delta_{n,-m}} =$$

$$= \frac{1}{\beta^2}\sum_{mn} x_n y_m\, \beta\,\delta_{n,-m} =$$

$$= \boxed{\frac{1}{\beta}\sum_{n} x_n\, y_{-n}} \quad (*)$$

For our problem, $\qquad V(x) = \frac{1}{2} m \omega^2 x^2$

$$-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, \frac{m}{2}\Big[\frac{dx(\tau)}{d\tau}\frac{dx(\tau)}{d\tau} + \omega^2 x(\tau)\, x(\tau) \Big] =$$

$$\overset{(*)}{=} -\frac{m}{2\beta}\sum_{n=-\infty}^{\infty} x_n \big[i\omega_n\, i\omega_{-n} + \omega^2 \big] x_{-n} \overset{(\omega_{-n} = -\omega_n)}{=}$$

$$= -\frac{m}{2\beta}\sum_{n=-\infty}^{\infty} (\omega_n^2 + \omega^2)(a_n^2 + b_n^2) \overset{(\circ)}{=}$$

$$= -\frac{m}{2\beta}\,\omega^2 a_0^2 - \frac{m}{\beta}\sum_{n=1}^{\infty} (\omega_n^2 + \omega^2)(a_n^2 + b_n^2)$$

Integration measure

$x(\tau) \to a_0, a_n, b_n, \; n \geq 1$

$$\mathcal{D}[x(\tau)] = \underbrace{\left| \det\left[\frac{\delta x(\tau)}{\delta x_n}\right]\right|}_{\text{Jacobian}} da_0 \prod_{n\geq 1} da_n\, db_n$$

The change of variables is purely kinematical and independent of $V(x)$ therefore we write

$$c' \equiv c \left| \det\left[\frac{\delta x(\tau)}{\delta x_n}\right]\right|$$

Gaussian integration

$$\left[\int dx\, e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}, \; \alpha > 0 \right.$$

$$Z = c' \int_{-\infty}^{\infty} da_0 \int_{-\infty}^{\infty} \prod_{n\geq 1} da_n\, db_n\, e^{-\frac{1}{2\beta} m \omega^2 a_0^2 - \frac{m}{\beta} \sum_{n\geq 1} (\omega_n^2 + \omega^2)(a_n^2 + b_n^2)} =$$

$$(\bullet) = c' \underbrace{\sqrt{\frac{2\pi\beta}{m\omega^2}}}_{} \prod_{n=1}^{\infty} \frac{\pi\beta}{m(\omega_n^2 + \omega^2)}, \qquad \omega_n = \frac{2\pi n}{\beta\hbar}$$

diverges in $\omega \to 0$ limit

How to get c'

1) c' does not depend on $V(x)$, we find it for $\omega = 0$

2) however, $\int da_0$ is divergent (infrared) in $\omega \to 0$ limit

zero mode is the lowest energy mode

3) we can get $\omega \to 0$ limit if we regulate $\int da_0$ interval

From $(\bullet)$ $\quad \frac{1}{\beta\hbar} \int_0^{\beta\hbar} d\tau\, x(\tau) = \frac{a_0}{\beta}$ ← average value of $x(\tau)$ over the τ-interval

We regulate the $\int da_0$ integral by limiting it to $\Delta x \sqrt{\beta}$ periodic box

$$\lim_{\omega\to 0} Z_{rep} = c' \int_{\beta\Delta x} da_0 \int_{-\infty}^{\infty} \prod_{n\geq 1} da_n\, db_n\, e^{-\frac{m}{\beta}\sum_{n\geq 1}\omega_n^2 (a_n^2+b_n^2)} =$$

$$= c' \,\beta\Delta x \prod_{n=1}^{\infty} \frac{\pi\beta}{m\,\omega_n^2}$$

On the other hand, for free particle ($V(x)=0$)

$$\lim_{\omega\to 0} Z_{rep} = \int_{\Delta x} dx \langle x | e^{-\beta\frac{\hat{p}^2}{2m}} | x\rangle =$$

$$= \int_{\Delta x} dx \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \langle x | e^{-\frac{\hat{p}^2}{2m}\beta} | p\rangle\langle p | x\rangle =$$

$$= \int_{\Delta x} dx \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, e^{-\frac{p^2}{2m}\beta} \underbrace{\langle x | p\rangle\langle p | x\rangle}_{1 = e^{ipx/\hbar} e^{-ipx/\hbar}} =$$

$$= \frac{\Delta x}{2\pi\hbar}\sqrt{\frac{2\pi m}{\beta}}$$

Comparing these two results

$$\boxed{c' = \frac{1}{2\pi\beta\hbar}\sqrt{\frac{2\pi m}{\beta}} \prod_{n\geq 1} \frac{m\,\omega_n^2}{\pi\beta}}$$

Therefore,

$$Z = \frac{1}{\beta \hbar \omega} \prod_{n=1}^{\infty} \frac{\omega_n^2}{\omega_n^2 + \omega^2} = \frac{1}{\beta \hbar \omega} \frac{1}{\prod_{n \geq 1} \left(1 + \left(\frac{\hbar \omega \beta}{2 \pi n} \right)^2 \right)}$$

Using the identity

$$\frac{\sinh(\pi x)}{\pi x} = \prod_{n=1}^{\infty} \left(1 + \frac{x^2}{n^2} \right)$$

$$\boxed{Z = \frac{1}{2 \sinh\left(\frac{\hbar \omega}{2 k_B T} \right)}}$$

In case of many physically relevant observables the C' drops out and the derivation is simpler.