HW1

1.1) let $I = \int_{-\infty}^{\infty} dx\, e^{-ax^2}$

$$I^2 = \left(\int_{-\infty}^{\infty} dx e^{-ax^2} \int_{-\infty}^{\infty} dy e^{-ay^2} \right)$$

$$= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\, e^{-a(x^2+y^2)} = \int_0^{\infty} dr \int_0^{2\pi} d\theta\, e^{-ar^2} \cdot r$$

let $r^2 = x^2 + y^2$ → polar coordinates

$$= 2\pi \int_0^{\infty} dr\, r e^{-ar^2} = \frac{\pi}{a} \int_0^{\infty} du\, e^{-u} = \frac{\pi}{a} \left[-e^{-u} \right]_0^{\infty} = \frac{\pi}{a}$$

$u = ar^2 \quad du = 2ar\, dr$

so $I^2 = \pi/a \Rightarrow I = \sqrt{\pi/a}$

or $$\int_{-\infty}^{\infty} e^{-ax^2}\,dx = \sqrt{\frac{\pi}{a}} \quad \checkmark$$

<u>1.2.i</u> $$\sqrt{\pi}\, a^{-1/2} = \int_{-\infty}^{\infty} e^{-ax^2}\,dx$$

deriv $\frac{d}{da}$

$$\sqrt{\pi} \cdot -\frac{1}{2} a^{-3/2} = \int_{-\infty}^{\infty} -x^2 e^{-ax^2}\,dx$$

$$\Rightarrow \int_{-\infty}^{\infty} x^2 e^{-ax^2}\,dx = \frac{\sqrt{\pi}}{2} a^{-3/2}$$

1.2.ii. $N(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \frac{x^2}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2} \, dx$$

let $u = x - \mu$ $\quad du = dx$

$$= \int_{-\infty}^{\infty} \frac{(u+\mu)^2}{\sqrt{2\pi\sigma^2}} e^{-u^2/2\sigma^2}$$

$$(u+\mu)^2 = u^2 + 2u + \mu^2$$

three pieces

a) $$\int_{-\infty}^{\infty} du \, \underbrace{\frac{\mu^2}{\sqrt{2\pi\sigma^2}}}_{\text{constant}} e^{-u^2/2\sigma^2} = \frac{\mu^2}{\sqrt{2\pi\sigma^2}} \cdot \underbrace{\sqrt{2\pi\sigma^2}}_{\text{eq }2} = \mu^2$$

"a" $= \frac{1}{2\sigma^2}$

b) $$\int_{-\infty}^{\infty} du \, \frac{2\mu}{\sqrt{2\pi\sigma^2}} \cdot u e^{-u^2/2\sigma^2} = 0$$

even function · odd function. can also do integral directly

c) $$\int_{-\infty}^{\infty} du \, \frac{u^2}{\sqrt{2\pi\sigma^2}} e^{-u^2/2\sigma^2} = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \frac{\sqrt{\pi}}{2} \cdot \left(\frac{1}{2\sigma^2}\right)^{-3/2} = \sigma^2$$

from 12.ii.

so $\langle x^2 \rangle = \mu^2 + \sigma^2$

if $\mu = 0$, $\langle x^2 \rangle = \sigma^2$ ✓ variance

[also $\langle (x-\mu)^2 \rangle = \langle x^2 \rangle - \underbrace{\langle 2x\mu \rangle}_{-2\mu^2} + \mu^2 = \sigma^2$

variance

$\Rightarrow \langle x^2 \rangle = \mu^2 + \sigma^2$ ✓]

1.2.iii $\int dx\, x^2 e^{-ax^2} = \frac{\sqrt{\pi}}{2} a^{-3/2}$ $\quad \frac{d}{da}$ again

$$\int dx\, x^4 e^{-ax^2} = \frac{3}{4}\sqrt{\pi}\, a^{-5/2}$$

$$\langle x^4 \rangle = \int_{-\infty}^{\infty} x^4 e^{-x^2/2\sigma^2} \cdot \frac{1}{\sqrt{2\pi\sigma^2}}$$

$$= \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \frac{3\sqrt{\pi}}{4} \cdot \left(\frac{1}{2\sigma^2}\right)^{-5/2} = 3\sigma^4$$

Note $\langle x^4 \rangle / \langle x^2 \rangle^2 = 3$ for gaussian

<u>1.3</u> $$Z = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp \; e^{-\beta\left[\frac{1}{2}kx^2 + p^2/2m\right]}$$

$$= \int_{-\infty}^{\infty} dx \; e^{-\beta/2 \, kx^2} \int_{-\infty}^{\infty} dp \; e^{-\frac{\beta}{2m}p^2} = \sqrt{\frac{\pi}{\left(\frac{\beta k}{2}\right)}} \sqrt{\frac{\pi}{\left(\frac{\beta}{2m}\right)}}$$

$$= 2\pi \cdot \sqrt{\frac{m}{k}} \cdot \frac{1}{\beta} = 2\pi \frac{k_B T}{\omega}$$

1.4

$$\left\langle \frac{1}{2}kx^2 \right\rangle = \frac{\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp \; \frac{1}{2}kx^2 \, e^{-\beta\left[p^2/2m + \frac{1}{2}kx^2\right]}}{Z}$$

do p integral

$$= \frac{\sqrt{\frac{\pi}{(\beta/2m)}}}{2\pi \frac{k_B T}{\omega}} \cdot \frac{1}{2}k \underbrace{\int_{-\infty}^{\infty} dx \; x^2 e^{-\beta \cdot \frac{1}{2}kx^2}}_{\frac{\sqrt{\pi}}{2}\left(\frac{\beta k}{2}\right)^{-3/2}}$$

$$= \frac{1}{8}\frac{\omega k}{k_B T} \cdot \sqrt{2mk_BT} \cdot \left(\frac{2k_BT}{k}\right)^{3/2} = \frac{1}{8}\left(\frac{\omega k}{k_BT}\right)\left(\frac{2k_BT}{\omega}\right)\left(\frac{2k_BT}{k}\right)$$

$$= \frac{1}{2}k_BT \; !$$

$$\left\langle \frac{p^2}{2m} \right\rangle = \frac{1}{Z} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp \, e^{-\beta\left(\frac{1}{2}kx^2 + p^2/2m\right)} \cdot \frac{p^2}{2m}$$

$$= \frac{\omega}{4\pi m k_B T} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp \, p^2 e^{-\beta\left(\frac{kx^2}{2} + p^2/2m\right)}$$

do x integral ...

$$= \frac{\omega}{4\pi m k_B T} \cdot \sqrt{\frac{2\pi}{\beta k}} \int_{-\infty}^{\infty} dp \, p^2 e^{-\beta p^2/2m}$$

$$= \frac{\omega}{4\pi m k_B T} \sqrt{\frac{2\pi}{\beta k}} \cdot \frac{\sqrt{\pi}}{2} \cdot \left(\frac{\beta}{2m}\right)^{-3/2} = \frac{\omega}{8 m k_B T} \cdot \sqrt{\frac{2\pi k_B T}{k}} \cdot \sqrt{2 m k_B T} \cdot (2 m k_B T)$$

$$= k_B T/2 \checkmark$$

... so $\langle KE \rangle = k_B T/2$

$\langle PE \rangle = k_B T/2$

$\langle \varepsilon \rangle = \langle KE + PE \rangle = k_B T$, makes sense!

[in fact, any quadratic energy term in the Hamiltonian contributes $\frac{k_B T}{2}$ to avg ε]

2 N-harmonic oscillators

a) $$Z = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_N \int_{-\infty}^{\infty} dp_1 \int_{-\infty}^{\infty} dp_2 \cdots \int_{-\infty}^{\infty} dp_N \cdots$$

$$e^{-\beta\left[\sum_{i=1}^{N} \frac{k_i x^2}{2} + p_i^2/2m_i\right]}$$

b) $$e^{A+B} = e^a e^b \quad \text{so} \quad = \prod_{i=1}^{N} e^{-\frac{\beta k_i x^2}{2}} \prod_{j=1}^{N} e^{-\beta p_j^2/2m}$$

integrals separate

$$= \left(\prod_{i=1}^{N} \int dx_i e^{-\frac{\beta k_i x^2}{2}}\right)\left(\prod_{j=1}^{N} \int dp_j e^{-\beta p_j^2/2m}\right)$$

$$\text{so } Z = \prod_{i=1}^{N} \left(\sqrt{\frac{2\pi k_B T}{k_i}} \right) \prod_{j=1}^{N} \sqrt{2\pi k_B T\, m_i}$$

$$= \prod_{i=1}^{N} \left[2\pi k_B T \cdot \frac{1}{\omega_i} \right] \quad \text{where} \quad \omega_i = \sqrt{k_i/m_i}$$

$$= \left(\frac{2\pi}{\beta} \right)^N \cdot \prod_{i=1}^{N} \omega_i^{-1}$$

$$\langle \varepsilon \rangle = -\frac{\partial \log Z}{\partial \beta} = +\frac{\partial}{\partial \beta} \left[N \log \beta + \text{const} \right]$$

$$= N/\beta = \underline{\underline{N k_B T}} = N \cdot \text{single oscillator!}$$

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

$$= e^{-\frac{\beta\hbar\omega}{2}} \sum_{n=0}^{\infty} \left(e^{-\beta\hbar\omega}\right)^n$$

"r"

$$= e^{-\beta\hbar\omega/2} \cdot \frac{1}{1-e^{-\beta\hbar\omega}}$$

$$= \frac{1}{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}} = \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

formula valid when $\hbar\omega/k_BT > 0$

$\frac{\hbar\omega}{k_B T} > 0$ except if $\omega = 0$ $\left[\begin{array}{l} k = 0 \\ \text{or } m \to \infty \end{array}\right.$

or $T = \infty$ so generally fine

b) $Z = \dfrac{1}{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}}$

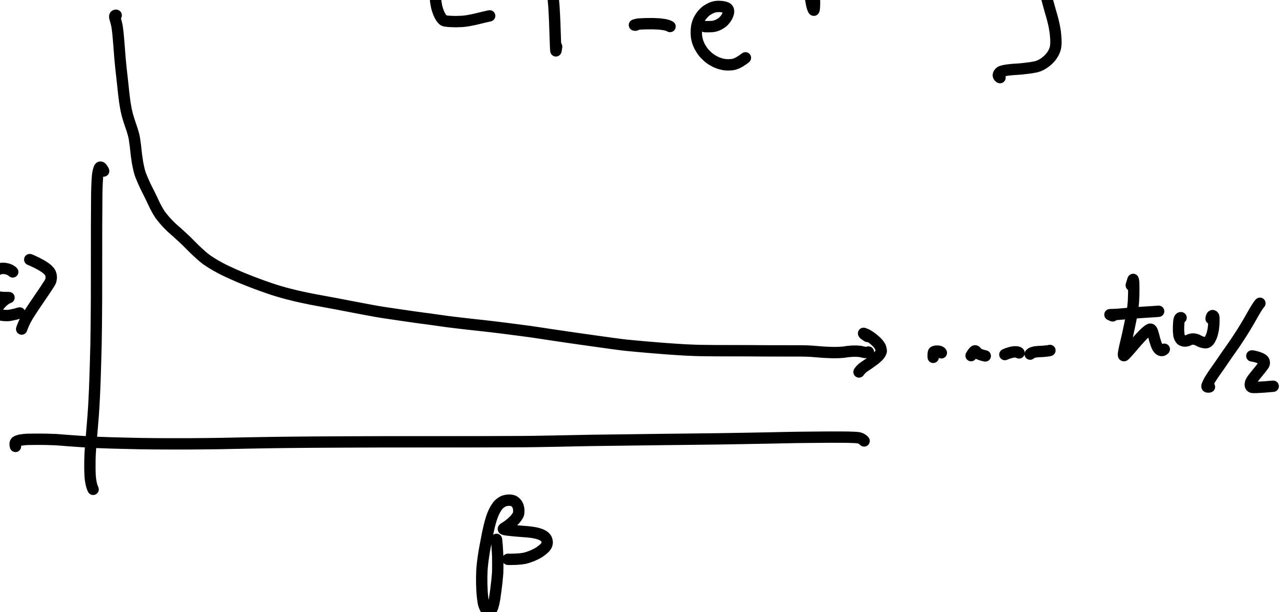
$$-\frac{\partial \log Z}{\partial \beta} = \frac{\partial}{\partial \beta} \log\left[e^{\beta\frac{\hbar\omega}{2}} - e^{-\beta\hbar\omega/2}\right]$$

$$= \frac{1}{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}} \cdot \left[\frac{\hbar\omega}{2} e^{\beta\hbar\omega/2} + \frac{\hbar\omega}{2} e^{-\beta\hbar\omega/2}\right]$$

$$\ldots Z = \frac{\hbar\omega}{2} \frac{e^{\frac{\beta\hbar\omega}{2}} + e^{-\beta\hbar\omega/2}}{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}} = \frac{\hbar\omega}{2}\coth\frac{\beta\hbar\omega}{2}$$

$$= \frac{\hbar\omega}{2}\cdot\left[\frac{1+e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}\right] = \langle\varepsilon\rangle$$

c) $\langle\varepsilon\rangle$



@ low T, large β, $\varepsilon = \frac{\hbar\omega}{2}$, zero point

@ high T, energy diverges ... but also ...

$$\langle E\rangle = \frac{\hbar\omega}{2}\cdot\left[\frac{1+e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}\right]$$

as $\beta \to 0$, can taylor expand

$\beta\hbar\omega$ small

$$e^{-\beta\hbar\omega} \approx 1-\beta\hbar\omega + \frac{(\beta\hbar\omega)^2}{2} + \cdots$$

$$\langle E\rangle \approx \frac{\hbar\omega}{2}\left[\frac{1+1-\beta\hbar\omega+\cdots}{\beta\hbar\omega+\cdots}\right] \approx \frac{\hbar\omega}{2}\cdot\frac{2}{\beta\hbar\omega}$$

$= k_B T$! classical limit!

d)

$$Z = \frac{1}{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}}$$

$$\lim_{\beta \to 0} Z = \frac{1}{0 - 0} \to \infty$$, many states as $T \to \infty$

actually, for small β $e^{\beta\hbar\omega/2} \approx 1 + \frac{\beta\hbar\omega}{2}$

$e^{-\beta\hbar\omega/2} \approx 1 - \beta\hbar\omega/2$

$Z \to \frac{1}{\beta\hbar\omega}$ = classical limit

$$\lim_{\beta\to\infty} Z = \frac{1}{\infty \sim 0} = 0,$$ number of accessible states gets small as $T \to 0$

Even though $Z \to 0$, the case is that only one state is accessible

Prob of state 0 =

$$P_0 = e^{-\beta\varepsilon_0}/Z = \frac{e^{-\beta\hbar\omega/2}}{\sum_n e^{-\beta\hbar\omega(n+1/2)}} \xrightarrow{\lim_{\beta\to\infty}} 1$$