

HW1

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

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

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

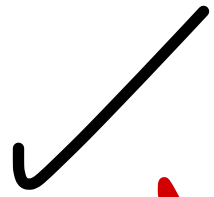
let $r^2 = x^2 + y^2$ \rightarrow polar coordinates

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

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

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

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



deriv
d
da

$$\underline{1.2.i} \quad \sqrt{\pi} a^{-1/2} = \int_{-\infty}^{\infty} e^{-ax^2} dx$$

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

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

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

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

$$\text{let } u = x - \mu \quad du = dx$$

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

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

three pieces

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

↑
"a" = $\frac{1}{2\sigma^2}$

b)
$$\int_{-\infty}^{\infty} du \underbrace{\frac{2\mu}{\sqrt{2\pi\sigma^2}}}_{\text{even function}} \cdot u e^{-u^2/2\sigma^2} = 0$$

odd function · odd function. can also do integral directly

c)
$$\int_{-\infty}^{\infty} du \underbrace{\frac{u^2}{\sqrt{2\pi\sigma^2}}}_{\text{even function}} e^{-u^2/2\sigma^2} = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \frac{\sqrt{\pi}}{2} \cdot \left(\frac{1}{2\sigma^2}\right)^{1/2} = \sigma^2$$

from 12.i.

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

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

[also $\langle (x - \mu)^2 \rangle = \langle x^2 \rangle - \langle 2x\mu \rangle + \mu^2 = \sigma^2$ ✓ variance
variance $\Rightarrow \langle x^2 \rangle = \mu^2 + \sigma^2$ ✓]

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

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

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

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

1.4 $\langle \frac{1}{2} k x^2 \rangle = \frac{\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp \frac{1}{2} k x^2 e^{-\beta [\frac{p^2}{2m} + \frac{1}{2} k x^2]}}{Z}$

do p
integral

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

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

$$= \frac{1}{2} k_B T !$$

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

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

do x integral ...

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

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

$$= k_B T/2 \quad \checkmark$$

... so $\langle K\varepsilon \rangle = k_B T / 2$
 $\langle P\varepsilon \rangle = k_B T / 2$

$$\langle \varepsilon \rangle = \langle K\varepsilon + P\varepsilon \rangle = k_B T, \text{ makes sense!}$$

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

2 N -harmonic oscillators

$$a) \quad Z = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \dots \int_{-\infty}^{\infty} dx_N \int_{-\infty}^{\infty} dp_1 \int_{-\infty}^{\infty} dp_2 \dots \int_{-\infty}^{\infty} dp_N \dots$$
$$e^{-\beta \left[\sum_{i=1}^N \frac{k_i x_i^2}{2} + \frac{p_i^2}{2m_i} \right]}$$

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

integrals separate

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

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

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

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

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

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

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

$$= e^{-\beta \hbar \omega \frac{1}{2}} \sum_{n=0}^{\infty} \left(e^{-\beta \hbar \omega} \right)^n$$

↪ "r"

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

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

formula valid when $\hbar \omega / k_B T > 0$

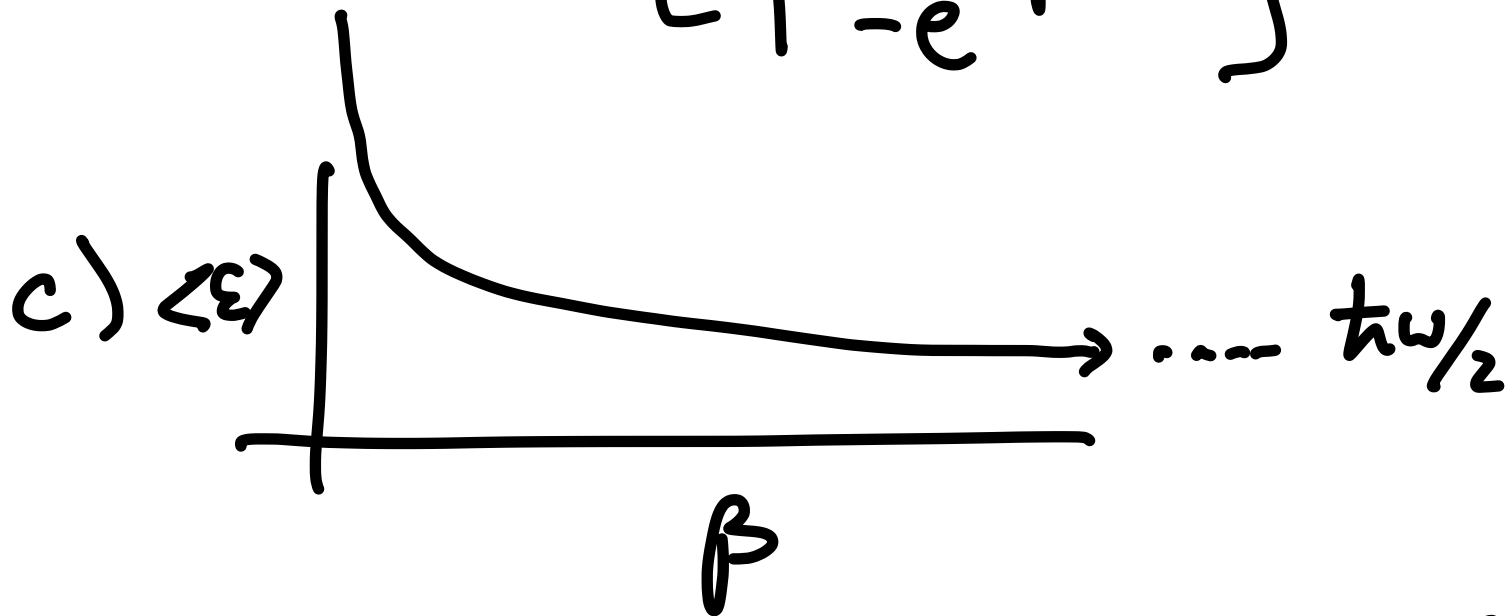
$\frac{\hbar\omega}{k_B T} > 0$ except if $\omega = 0$ $\int k = 0$ or $m \rightarrow \infty$
 or $T = \infty$ so generally fine

$$b) \quad z = \frac{1}{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}}$$

$$\begin{aligned}
 -\frac{\partial \log z}{\partial \beta} &= \frac{\partial}{\partial \beta} \log [e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}] \\
 &= \frac{1}{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}} \cdot \left[\frac{\hbar\omega}{2} e^{\beta\hbar\omega/2} + \frac{\hbar\omega}{2} e^{-\beta\hbar\omega/2} \right]
 \end{aligned}$$

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

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



@ low T , large β , $\mathcal{E} = \frac{\hbar\omega}{2}$, 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 $\beta \rightarrow 0$, can Taylor expand

$\beta \hbar \omega$ small

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

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

$= k_B T!$ classical limit!