Set #3

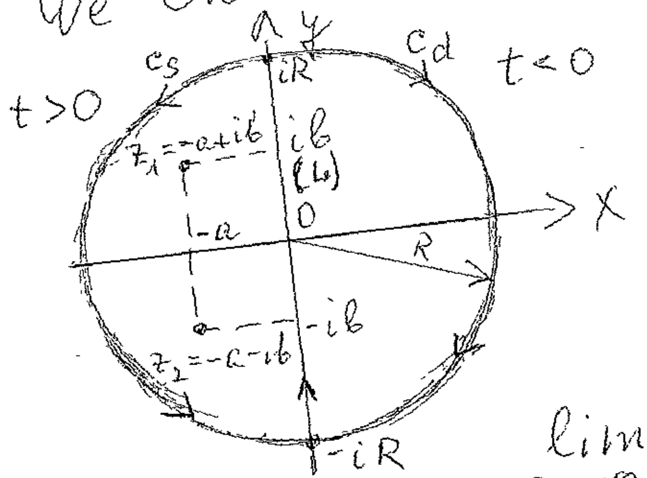
① Define $\varphi(z) \equiv \frac{e^{tz}(z+a)}{(z+a)^2+b^2}$.

The function $\varphi(z)$ has two poles: $z_1=-a+ib$ and $z_2=-a-ib$ with residuals:

$$\operatorname{Res}\varphi(z_1)=\frac{1}{2}e^{(-a+ib)t}$$

$$\operatorname{Res}\varphi(z_2)=\frac{1}{2}e^{(-a-ib)t}$$

We choose the contours of integration:



Applying the integral theorem of Cauchy and Jordan's lemma:

$$\lim_{R\to\infty}\int_{c_d'}\frac{e^{zt}(z+a)}{(z+a)^2+b^2}dz=\int_{-i\infty}^{+i\infty}\frac{e^{zt}(z+a)}{(z+a)^2+b^2}dz=0 \quad (t<0)$$

and $$\lim_{R\to\infty}\int_{c_s'}\frac{e^{zt}(z+a)}{(z+a)^2+b^2}dz=\int_{-i\infty}^{+i\infty}\frac{e^{zt}(z+a)}{(z+a)^2+b^2}dz=2\pi i\, e^{-at}\cos bt, \quad (t>0)$$

where c_d' and c_s' - closed contours formed from L (on imaginary axis) from $(-iR)$ to (iR), and c_d and c_s - found to the right and left of the imaginary axis.

Hence, $$f(t)=\begin{cases}0 & \text{for } t<0;\\ e^{-at}\cos bt & \text{for } t>0.\end{cases}$$

(2) (a). Since the oscillators are now distinguishable there is no $N!$ factor in the partition function, which is now

$$Z = \left(\frac{2\pi}{\beta \hbar \omega}\right)^N$$

The specific heat is

$$c_v = \beta^2 \frac{\partial^2}{\partial \beta^2} \ln Z = N \qquad (k_B = 1)$$

(b). To obtain the expressions to $O(\alpha)$, it is sufficient to approximate

$$e^{-\beta \alpha x^4} \approx 1 - \beta \alpha x^4.$$

Using $\int dx\, e^{-ax^2} x^4 = \sqrt{\pi}\, \frac{3}{4}\, a^{-5/2}$, the partition function for a single oscillator easily becomes $Z(\alpha) = Z(0)\left(1 - \frac{3\alpha}{\beta m^2 \omega^4}\right)$

Since the total $Z_{tot} = z(\alpha)^N$, the specific heat is

$$c_v = \beta^2 \frac{\partial^2}{\partial \beta^2} \ln Z_{tot} = N - \frac{6\alpha N}{\beta m^2 \omega^4}.$$

(3) The Gibbs formula for S: $S = -k_B \sum_i p_i \ln p_i$

Using Boltzmann probability in the canonical ensemble, $p_i = e^{-\beta E_i}/Z$, we have

$$S = -k_B \sum_i p_i \left(\frac{-E_i}{k_B T} - \ln Z\right) = \frac{U}{T} + k_B \ln Z$$

$$\Rightarrow \quad U - TS = -k_B T \ln Z, \quad \text{where } \sum_i p_i = 1;\ U = \sum_i p_i E_i$$

4 (a). Available phase space for N particles:

$$\Omega = \frac{1}{N!\,h^{3N}} \int_{H=E} d^3\vec{q}_1 \dots d^3\vec{q}_N \, d^3\vec{p}_1 \dots d^3 p_N ,$$

where $E = \sum_{i=1}^{N} P_i^2/2m \implies \sum_i P_i = 2mE$

Performing momentum integrals:

$$\Omega = \frac{(2mE)^{3N/2-1}}{N!\,h^{3N}} \frac{2\pi^{3N}}{(3N/2-1)!} \int d^3\vec{q}_1 \dots d^3\vec{q}_N$$

Performing the second integral:

1st particle explores a volume V

2nd " — " — " — " $V - \omega$

cont. (4):

the 3rd " — " — " — " $V - 2\omega$,

So,

$$\int d^3\vec{q}_1 \dots d^3\vec{q}_N = V(V-\omega)(V-2\omega)\dots[V-(N-1)\omega]$$

Approximating, $(V-\omega)\times[V-(N-a)\omega] \approx$

$$\approx (V - N\omega/2)^2,$$

we obtain

$$\int d^3\vec{q}_1 \dots d^3\vec{q}_N \simeq \left(V - \frac{N\omega}{2}\right)^N.$$

So, $S = k_B \ln\Omega \simeq N k_B \ln\left[\frac{e}{N}\left(V - \frac{N\omega}{2}\right)\left(\frac{4\pi m E e}{3Nh^2}\right)^{3/2}\right]$

(b). $\frac{P}{T} = \left(\frac{\partial S}{\partial V}\right)_{E,N} \simeq \frac{N k_B}{V - N\omega/2}$

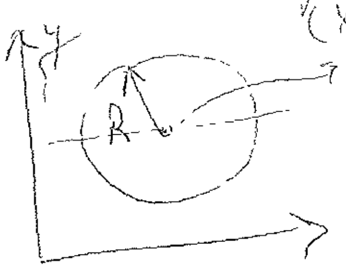
$$\Rightarrow P\left(V - \frac{N\omega}{2}\right) = N k_B T \qquad (EOS)$$

(c). $K_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T$

$$\Rightarrow K_T = \frac{N k_B T}{P^2 V} > 0 \Rightarrow \text{always positive.}$$

(5) (a) Legendre transform of a circle

(x_0, y_0)



concave part of a circle

$$y = y_0 + \sqrt{R^2 - (x - x_0)^2}$$

convex part of a circle

$$y = y_0 - \sqrt{R^2 - (x - x_0)^2}$$

$$f(x) = \begin{cases} y_0 + \sqrt{R^2 - (x - x_0)^2} & \text{concave part} \\ y_0 - \sqrt{R^2 - (x - x_0)^2} & \text{convex part} \end{cases}$$

$$F(p) = \begin{cases} y_0 - x_0 p + R\sqrt{p^2+1} & \text{concave part} \\ -y_0 + x_0 p + R\sqrt{p^2+1} & \text{convex part} \end{cases}$$

circle $\longrightarrow$ hyperbola

(b) $f(x) = ax^2$

$$p = \frac{df}{dx} = 2ax \longrightarrow x = \frac{p}{2a}$$

$$F(p) = px - ax^2 = \frac{p^2}{2a} - a\frac{p^2}{4a^2} = \frac{p^2}{4a^2}$$

$$\Longrightarrow \quad ax^2 \longrightarrow \frac{p^2}{4a^2}$$

parabola $\longrightarrow$ parabola