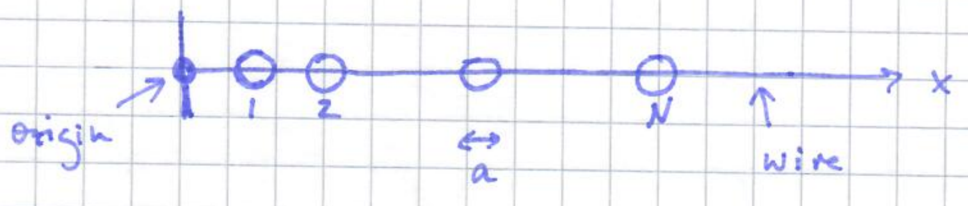
E3a

Problem:

Consider N impenetrable beads of diameter a on a frictionless 1D wire. The rightmost bead is subjected to a constant force that is directed toward the origin (let the strength of the force be F).



Since the beads cannot pass through each other, they should be considered distinguishable and the $N!$ should be omitted in the definition of the partition function.

(a) Calculate the partition function of the system as a function of N, β, and F.

(b) Calculate the specific heat of the system and the average position of the rightmost particle as a function of T.

(c) Show that the equation of state is $P = \frac{nkT}{1-na}$, where P is the pressure and n the density, $n = \frac{N}{\langle x_N \rangle}$.

Note: The pressure for this 1D system is equal to F.

(a) Each bead has a kinetic energy: $\frac{p_n^2}{2m}$

Only the N^{th} bead feels a potential:

$U = F x_N$

$$\Rightarrow \mathcal{H} = \sum_{n=1}^{N} \frac{p_n^2}{2m} + F x_N$$

We know: $x_1 < x_2 < \ldots < x_N$

Moreover: $\frac{a}{2} \leq x_1$; $x_1 + a \leq x_2$; $x_2 + a \leq x_3$; ... $x_{N-1} + a \leq x_N$

$$Q = \frac{1}{h^N} \underbrace{\left(\int_{-\infty}^{\infty} e^{-\beta p^2/2m} \, dp \right)^N}_{\left(\frac{2\pi m}{\beta}\right)^{N/2}} \underbrace{\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \int \ldots \int dx_N \, e^{-\beta F x_N}}_{\text{we know something about the limits ...}}$$

$$\int_{-\infty}^{\infty} dx_1 \int_{x_1+a}^{\infty} dx_2 \int_{x_2+a}^{\infty} dx_3 \ldots \int_{x_{N-1}+a}^{\infty} dx_N \, e^{-\beta F x_N}$$

the limit for x_2 depends on where the first particle is

Let's perform a variable transformation:

$$(x_1, x_2, x_3, \ldots, x_N) \rightarrow (u_1, u_2, u_3, \ldots, u_N)$$

where
$$u_1 = x_1 - \frac{a}{2}$$
$$u_2 = x_2 - (x_1 + a)$$
$$\vdots$$
$$u_N = x_N - (x_{N-1} + a)$$

It can be seen: $u_1 + u_2 + \ldots + u_N = x_N - (N-1)a - \frac{a}{2}$
$$= x_N - (N - \tfrac{1}{2})a$$

E.g.: For $x_2 = x_1 + a$, we have $u_2 = 0$

$$\Rightarrow \quad Q = \left(\frac{2\pi m}{\beta h^2}\right)^{N/2} \int_0^\infty du_1 \int_0^\infty du_2 \ldots \int_0^\infty du_N \, e^{-\beta F(u_1 + \ldots + u_N + (N-\frac{1}{2})a)}$$

$$= \left(\frac{2\pi m}{\beta h^2}\right)^{N/2} e^{-\beta F (N-1)a} \Bigg(\underbrace{\int_0^\infty e^{-\beta F u} du}_{\frac{1}{\beta F}}\Bigg)^N$$

$$\boxed{Q = \left(\frac{2\pi m}{\beta^3 h^2 F^2}\right)^{N/2} e^{-\beta F (N-\frac{1}{2})a}}$$

E3d

(b) Specific heat $C_v = \frac{\partial U}{\partial T}$

Want to calculate U:

$$U = -\frac{\partial}{\partial \beta} \log Q$$

$$= -\frac{\partial}{\partial \beta}\left(\underbrace{\log \left[\left(\frac{2\pi m}{\beta^3 h^2 F^2} \right)^{N/2} e^{-\beta F (N-\frac{1}{2}) a} \right]}_{\frac{N}{2}\log(2\pi m) - \underbrace{\frac{N}{2}\log(\beta^3 h^2 F^2)}_{-\frac{3N}{2}\log\beta - \frac{N}{2}\log(h^2F^2)} - \beta F (N-\frac{1}{2}) a} \right)$$

$$= \frac{3N}{2\beta} + F(N-\tfrac{1}{2})a$$

$$\boxed{U = \frac{3N}{2} kT + F(N-\tfrac{1}{2})a}$$

$$\frac{\partial U}{\partial T} = \frac{3N}{2} k \quad \Rightarrow \quad \boxed{C_v = \frac{3N}{2} k}$$

Average $\langle x_N \rangle$?

$$\langle x_N \rangle = -\frac{1}{\beta}\left(\frac{\partial}{\partial F} Q \right) \frac{1}{Q}$$

$$= -\frac{1}{\beta} \frac{\partial}{\partial F}\left(\log Q \right)$$

$$-\frac{\partial}{\partial F}\log Q = N F^{-1} + \beta(N-\tfrac{1}{2})a$$

$$\Rightarrow \boxed{\langle X_N\rangle = +\underbrace{kTN\frac{1}{F}}_{N\frac{kT}{aF}\cdot a} + (N-\tfrac{1}{2})a}$$

for $F\to\infty$: $\langle X_N\rangle = (N-\frac{1}{2})a$

for $F\to 0$: $\langle X_N\rangle\to\infty$

more precisely, look at $\frac{kT}{aF} \ll 1$ and $\gg 1$

(c)

Solve the last eq. for F:

$$F\left(\langle X_N\rangle - (N-\tfrac{1}{2})a\right) = kTN$$

$$\Rightarrow F = \frac{kTN}{\langle X_N\rangle - (N-\frac{1}{2})a}$$

$$= \frac{kT\frac{N}{\langle X_N\rangle}}{1 - a\frac{N-\frac{1}{2}}{\langle X_N\rangle}}$$

$$\xrightarrow{N\text{ large}} \frac{kTn}{1-an}$$

where $n = \frac{N}{\langle X_N\rangle}$

Thus: $p = \frac{kTn}{1-an}$

pressure is positive!

$\langle X_N\rangle > (N-\frac{1}{2})a$

$\Rightarrow n < \frac{N}{(N-\frac{1}{2})a}$

$\Rightarrow an < \frac{N}{N-\frac{1}{2}} < 1$

assuming $N-\frac{1}{2}\cong N$