Ex2340: Boltzmann gas confined in a capacitor

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The problem:

An ideal gas of N spin-less particles of mass m is inserted in between two parallel surfaces. To make sure that the particles won't "escape" a harmonic two dimensional potential is created in such a way that:

$$V(x,y,z) = \begin{cases} \frac{1}{2}m\omega^2(x^2+y^2) & z_1 < z < z_2 \\ \infty & \text{else} \end{cases}$$

Let us denote $L = z_1 + z_2$
This problem consist of two independent parts. Express your answers using $N, m, L, \omega, e, \mathcal{E}, T$

(I) (a) Calculate the classical partition function

$$\mathcal{Z}_1 = \int \frac{d^3p d^3x}{(2\pi)^3} e^{-\beta\mathcal{H}} \quad ; \quad \mathcal{Z}_N = \mathcal{Z}_1^N \tag{1}$$

find the heat capacity $C(T)$ of the gas.

(b) Calculate the quantum partition function in the limit where L is large. Find what L is large enough.
Guidance: What are the stationary states $|\phi\rangle$ of a single particle in a potential V? Calculate:

$$\mathcal{Z}_1 \equiv \sum_r e^{-\beta E_r} \quad ; \quad \mathcal{Z}_N \approx \frac{1}{N!}\mathcal{Z}_1^N \tag{2}$$

To calculate $\mathcal{Z}_1$ use factorization of the sum.

(c) Find the heat capacity $C(T)$ of the gas using the partition function you found in article (b). Check the behavior of the heat capacity in high temperature - define what is high temperature and see if you get the classical result from article (a).

(d) Calculate the forces F_1, F_2 that the particles apply on the upper and lower walls of the "box"

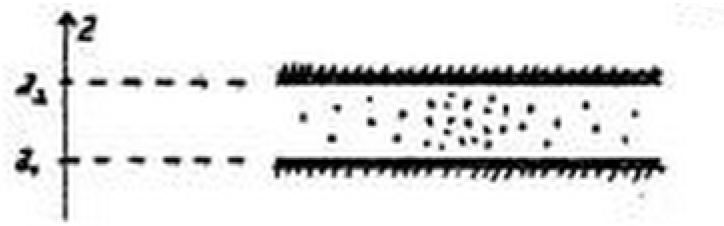
(II) We now add an electrical field $\vec{E} = \mathcal{E}\hat{z}$, assume that the particle are charged with e.

(e) Write down the one particle Hamiltonian and calculate the classical partition function. $\mathcal{Z}_1(\beta; z_1, z_2, \mathcal{E})$

(f) Calculate the forces F_1, F_2 that are acting on the upper and lower walls of the "box". What is the resultant force working on the system?

(g) Find the polarization $\tilde{\mathcal{P}}$ of the electron gas as a function of the electric field (The polarization $\tilde{\mathcal{P}}$ is defined by the formula $\bar{d}W = \tilde{\mathcal{P}}dE$)

(h) Write down $\mathcal{P}(\mathcal{E}) = \frac{1}{L}\tilde{\mathcal{P}}$ for a weak $\mathcal{E}$. Define what is a weak field. Bring the expression you receive to the following form $\mathcal{P}(\mathcal{E}) = \chi\mathcal{E} + O(\mathcal{E}^2)$ and find what is the susceptibility χ.



The Solution:

(a) The problem Hamiltonian is as follows:

$$\mathcal{H} = (\frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2) + (\frac{p_y^2}{2m} + \frac{1}{2}m\omega^2 y^2) + \frac{p_z^2}{2m} \tag{3}$$

All that is left for us to do is input the Hamiltonian into the Boltzmann exponent and solve a Gaussian integral which has a known solution.

$$\begin{aligned} \mathcal{Z}_1 &= \int \frac{d^3p d^3x}{(2\pi)^3} \mathrm{e}^{-\beta((\frac{p_x^2}{2m}+\frac{1}{2}m\omega^2x^2)+(\frac{p_y^2}{2m}+\frac{1}{2}m\omega^2y^2)+\frac{p_z^2}{2m})} & (4) \\ &= \iint_{-\infty}^{\infty} \frac{dp_x dx}{2\pi} \mathrm{e}^{-\beta(\frac{p_x^2}{2m}+\frac{1}{2}m\omega^2x^2)} \iint_{-\infty}^{\infty} \frac{dp_y dy}{2\pi} \mathrm{e}^{-\beta(\frac{p_y^2}{2m}+\frac{1}{2}m\omega^2y^2)} \int_{-\infty}^{\infty}\int_{z_1}^{z_2} \frac{dp_z dz}{2\pi} \mathrm{e}^{-\beta\frac{p_z^2}{2m}} & (5) \\ & & (6) \end{aligned}$$

Due to symmetry in p_x, p_y, p_z we can say that the solution over the kinetic parts of the Hamiltonian is the same as the cube of one of those integrals. The same can be done with the potential part of the Hamiltonian (excluding the z component), giving us

$$\mathcal{Z}_1 = \left(\int_{-\infty}^{\infty} \frac{dp}{2\pi} \mathrm{e}^{-\beta\frac{p^2}{2m}}\right)^3 \left(\int_{-\infty}^{\infty} \frac{dx}{2\pi} \mathrm{e}^{-\beta\frac{1}{2}m\omega^2x^2}\right)^2 \int_{z_1}^{z_2} dz = \frac{1}{(2\pi)^3}\left(\frac{2m\pi}{\beta}\right)^{\frac{3}{2}} \frac{2\pi}{\beta m\omega^2}(z_2 - z_1) \tag{7}$$

Giving us

$$\mathcal{Z}_1 = \left(\frac{m}{2\pi\beta}\right)^{\frac{1}{2}} \frac{1}{(\beta\omega)^2} L \tag{8}$$

Finally we get $\mathcal{Z}_N = \mathcal{Z}_1^N = \left(\left(\frac{m}{2\pi\beta}\right)^{\frac{1}{2}} \frac{1}{(\beta\omega)^2} L\right)^N$

We can now calculate the energy and from it the heat capacity.

$$\begin{aligned} \log(\mathcal{Z}_N) &= N\left(\log(\left(\frac{m}{2\pi\beta}\right)^{\frac{1}{2}}) + \log(\frac{1}{(\beta\omega)^2}) + \log(L)\right) & (9) \\ &= N\left(-\frac{1}{2}\log(\beta) - 2\log(\beta) + \text{const}\right) & (10) \end{aligned}$$

The energy and heat capacity:

$$E = -\frac{\partial \log(\mathcal{Z}_N)}{\partial \beta} = \frac{5}{2}NT \tag{11}$$

$$C(T) = \frac{dE}{dT} = \frac{5}{2}N \tag{12}$$

(b) The stationary state are $|p_z, n_y, n_x\rangle$; where $p_z = \frac{2\pi}{L}n_z$; $n_z = 0, 1, 2....$
So now the energy of the system is

$$E_{p_z,n_y,n_x} = \frac{p_z^2}{2m} + (\frac{1}{2} + n_y)\omega + (\frac{1}{2} + n_x)\omega \tag{13}$$

Calculating the partition function we get

$$\mathcal{Z}_1 = \int_{-\infty}^{\infty}\int_{z_1}^{z_2} dp_z dz \mathrm{e}^{-\beta\frac{p_z^2}{2m}} \sum_{n_x,n_y} \mathrm{e}^{-\beta(\frac{1}{2}+n_y)\omega+(\frac{1}{2}+n_x)\omega} \tag{14}$$

$$= L\left(\frac{2m\pi}{\beta}\right)^{\frac{1}{2}} \frac{\mathrm{e}^{-\frac{1}{2}\beta\omega}}{1-\mathrm{e}^{-\beta\omega}} \frac{\mathrm{e}^{-\frac{1}{2}\beta\omega}}{1-\mathrm{e}^{-\beta\omega}} \tag{15}$$

$$= L\left(\frac{2m\pi}{\beta}\right)^{\frac{1}{2}} \left(\frac{1}{2\sinh\frac{1}{2}\beta\omega}\right)^2 \tag{16}$$

$$\tag{17}$$

$$\mathcal{Z}_N = \left(L\left(\frac{2m\pi}{\beta}\right)^{\frac{1}{2}} \left(\frac{1}{2\sinh\frac{1}{2}\beta\omega}\right)^2\right)^N \tag{18}$$

We now ask ourselves when is L large enough for us to make the transition from sum on p_z to an integral. Let us write explicitly the sum on p_z:

$$\sum_{p_z} \mathrm{e}^{-\beta\frac{p_{n_z}^2}{2m}} = \sum_{n_z} \mathrm{e}^{-\frac{\beta}{2m}(\frac{2\pi}{L})^2 n_z^2} \to \int_{-\infty}^{\infty} dn\ \mathrm{e}^{-\frac{\beta}{2m}(\frac{2\pi}{L})^2 n_z^2} \tag{19}$$

This transition to integral is only justified if $L >> (\frac{1}{mT})^{\frac{1}{2}}$

(c) In the exact same manner as in article (a) we can calculate the energy and the heat capacity for the quantum partition function.

$$\log \mathcal{Z}_n = N\log\left(L\left(\frac{2m\pi}{\beta}\right)^{\frac{1}{2}} \left(\frac{1}{2\sinh\frac{1}{2}\beta\omega}\right)^2\right) \tag{20}$$

$$= -\frac{1}{2}N\log\beta - 2N\log 2\sinh\left(\frac{1}{2}\beta\omega\right) + \text{const} \tag{21}$$

$$E = -\frac{\partial \log \mathcal{Z}_N}{\partial \beta} = \frac{1}{2}NT + N\omega\coth(\frac{1}{2}\beta\omega) \tag{22}$$

$$C(T) = \frac{dE}{dT} = \frac{1}{2}N + N\omega\frac{d\coth\frac{1}{2}\beta\omega}{dT} = \{\frac{d}{dT} = -\frac{1}{T^2}\frac{d}{d\beta}\} = \tag{23}$$

$$= \frac{1}{2}N - \frac{N\omega}{T^2}\frac{d\coth\frac{1}{2}\beta\omega}{d\beta} = \frac{1}{2}N + \frac{1}{2}N(\frac{\omega}{T})^2\frac{1}{\sinh^2\frac{1}{2}\beta\omega} \tag{24}$$

Finally giving us

$$C(T) = \frac{1}{2}N + 2N(\frac{\omega}{T})^2 \frac{e^{\frac{\omega}{T}}}{(e^{\frac{\omega}{T}} - 1)^2} \tag{25}$$

Taking high temperature - meaning $T >> \omega$ - we receive:

$$C(T) = \frac{1}{2}N + 2N(\frac{\omega}{T})^2 \frac{1}{(1 + \frac{\omega}{T} - 1)^2} = \frac{5}{2}N \tag{26}$$

Which is the exact same result as in the classical case.

(d) The force is giving by $F = T\frac{\partial \log \mathcal{Z}_N}{\partial X}$, in our case we are looking for the forces on the upper and lower walls.
We notice that in both classical and quantum cases we have $\log \mathcal{Z}_N = N \log L + f(T)$ finally giving us the forces on both walls,

$$F_1 = T\frac{\partial \log \mathcal{Z}_N}{\partial z_1} = -\frac{NT}{L} \tag{27}$$

$$F_2 = T\frac{\partial \log \mathcal{Z}_N}{\partial z_2} = \frac{NT}{L} \tag{28}$$

(e) The new Hamiltonian will be constructed by the previous Hamiltonian and an addition of the electric field

$$H = H_{class} - e\mathcal{E}z \tag{29}$$

The partition function will be calculated in the same way as article (a) only with the addition of the field, giving us

$$\mathcal{Z}_1 = \int \frac{d^3p d^3x}{(2\pi)^3} e^{-\beta((\frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2) + (\frac{p_y^2}{2m} + \frac{1}{2}m\omega^2 y^2) + \frac{p_z^2}{2m} - e\mathcal{E}z)} \tag{30}$$

$$= \iint\limits_{-\infty}^{\infty} \frac{dp_x dx}{2\pi} e^{-\beta(\frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2)} \iint\limits_{-\infty}^{\infty} \frac{dp_y dy}{2\pi} e^{-\beta(\frac{p_y^2}{2m} + \frac{1}{2}m\omega^2 y^2)} \int\limits_{-\infty}^{\infty} \int\limits_{z_1}^{z_2} \frac{dp_z dz}{2\pi} e^{-\beta(\frac{p_z^2}{2m} - e\mathcal{E}z)} \tag{31}$$

Due to the same reason we listed in article (a) this integral is equal to

$$\mathcal{Z}_1 = \left(\int\limits_{-\infty}^{\infty} \frac{dp}{2\pi} e^{-\beta\frac{p^2}{2m}} \right)^3 \left(\int\limits_{-\infty}^{\infty} \frac{dx}{2\pi} e^{-\beta\frac{1}{2}m\omega^2 x^2} \right)^2 \int\limits_{z_1}^{z_2} dz e^{\beta e\mathcal{E}z} \tag{32}$$

$$= \frac{1}{(2\pi)^3} \left(\frac{2m\pi}{\beta} \right)^{\frac{3}{2}} \frac{2\pi}{\beta m\omega^2} \frac{e^{e\beta\mathcal{E}z_2} - e^{e\beta\mathcal{E}z_1}}{e\beta\mathcal{E}} \tag{33}$$

It is easy to see that when $\mathcal{E} \to 0$ we can expand the exponents and receive the original classical partition function.
In the same way as throughout this entire exercise, $\mathcal{Z}_N = \mathcal{Z}_1^N$

(f) Calculating the forces on each wall we use the formula $F = T\frac{\partial \log \mathcal{Z}_N}{\partial X}$ resulting in the following

$$F_1 = T\frac{\partial \log \mathcal{Z}_N}{\partial z_1} = NT\frac{-e\beta\mathcal{E}\mathrm{e}^{e\beta\mathcal{E}z_1}}{(\mathrm{e}^{e\beta\mathcal{E}z_2} - \mathrm{e}^{e\beta\mathcal{E}z_1})} \tag{34}$$

$$F_2 = T\frac{\partial \log \mathcal{Z}_N}{\partial z_2} = NT\frac{e\beta\mathcal{E}\mathrm{e}^{e\beta\mathcal{E}z_2}}{(\mathrm{e}^{e\beta\mathcal{E}z_2} - \mathrm{e}^{e\beta\mathcal{E}z_1})} \tag{35}$$

Using only the allowed parameters we finally get the forces

$$F_1 = -Ne\mathcal{E}\frac{1}{(\mathrm{e}^{e\beta\mathcal{E}L} - 1)} \tag{36}$$

$$F_2 = T\frac{\partial \log \mathcal{Z}_N}{\partial z_2} = Ne\mathcal{E}\frac{1}{(1 - \mathrm{e}^{-e\beta\mathcal{E}L})} \tag{37}$$

And the resultant force working the system: $F_{tot} = F_1 + F_2 = Ne\mathcal{E}$ as expected.

(g) The polarization is giving by: $\tilde{\mathcal{P}} = T\frac{\partial \log \mathcal{Z}_N}{\partial \mathcal{E}}$. Using the properties of log we get

$$\tilde{\mathcal{P}} = Ne\frac{\partial(\log \frac{\mathrm{e}^{e\beta\mathcal{E}z_2} - \mathrm{e}^{e\beta\mathcal{E}z_1}}{e\beta\mathcal{E}})}{\partial \mathcal{E}} + \frac{\partial}{\partial \mathcal{E}}(\text{const}) \tag{38}$$

$$= Ne\left(-\frac{1}{e\beta\mathcal{E}} + \frac{z_2\mathrm{e}^{e\beta\mathcal{E}z_2} - z_1\mathrm{e}^{e\beta\mathcal{E}z_1}}{\mathrm{e}^{e\beta\mathcal{E}z_2} - \mathrm{e}^{e\beta\mathcal{E}z_1}}\right) \tag{39}$$

Unless we want an un-physical constant in our equation we will need to choose the middle of the system as our zero. Thus making $z_2 = \frac{L}{2}$ and $z_1 = -\frac{L}{2}$ and giving us

$$\tilde{\mathcal{P}} = Ne\left(-\frac{1}{e\beta\mathcal{E}} + \frac{1}{2}L\coth\frac{1}{2}e\beta\mathcal{E}L\right) \tag{40}$$

(h) In order to expand $\tilde{\mathcal{P}}$ we must first demand

$$e\beta\mathcal{E}L << 1 \;\rightarrow\; L << \frac{T}{e\mathcal{E}} \tag{41}$$

we can now expand the coth up to first order and receive

$$\mathcal{P} = \frac{Ne}{L}\left(-\frac{1}{e\beta\mathcal{E}} + \frac{1}{2}L\coth\frac{1}{2}e\beta\mathcal{E}L\right) = \{\coth x \approx \frac{1}{x} + \frac{x}{3} + O(x^3)\} = \tag{42}$$

$$= \left(-\frac{Ne}{e\beta\mathcal{E}L} + \frac{1}{2}\frac{NeL}{\frac{1}{2}e\beta\mathcal{E}L^2} + \frac{\frac{1}{4}e\beta\mathcal{E}L^2Ne}{3L} + O(\mathcal{E}^3)\right) = \tag{43}$$

$$= \frac{Ne^2\beta\mathcal{E}L}{12} + O(\mathcal{E}^3) \tag{44}$$

We can now easily identify $\chi = \frac{Ne^2\beta L}{12}$