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Solution to the exam in TFY4230 STATISTICAL PHYSICS

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This solution consists of 6 pages.

Problem 1. Particles in a spherical volume

A system of N classical non-relativistic particles is confined to a spherical (3-dimensional) volume with "soft" walls, described by the Hamiltonian

$$H = \sum_{i=1}^{N} \frac{1}{2m}\boldsymbol{p}_i^2 + \varepsilon_0 \left(\frac{\boldsymbol{x}_i^2}{r_0^2}\right)^n, \tag{1}$$

where ε_0 is a positive constant, r_0 is a length characterizing the radius of the sphere, and n is a positive integer.

a) Write down the canonical partition function Z for this system at temperature T.

Since all particles have the same finite mass m it is *very likely* that they are identical. Hence

$$Z = \frac{1}{N!}\int \prod_i \frac{\mathrm{d}^3p_i\,\mathrm{d}^3x_i}{h^3}\,\mathrm{e}^{-\beta H} = \frac{1}{h^{3N}\,N!}\left[\int \mathrm{d}^3p\,\mathrm{e}^{-\beta\boldsymbol{p}^2/2m}\int \mathrm{d}^3x\,\mathrm{e}^{-\beta\varepsilon_0\left(\boldsymbol{x}^2/r_0^2\right)^n}\right]^N. \tag{2}$$

b) Calculate the internal energy $U = \langle H\rangle$ and heat capacity C for this system.

Since we have

$$\langle H\rangle = -\frac{1}{Z}\frac{\partial}{\partial\beta}Z = -\frac{\partial}{\partial\beta}\ln Z,$$

we only need to factor out the β-dependence of the integrals. As simple way to do this is by introducting new integration variables, $\boldsymbol{\pi} = \beta^{1/2}\boldsymbol{p}$ and $\boldsymbol{\xi} = \beta^{1/2n}\boldsymbol{x}$. Since $\mathrm{d}^3p = \beta^{-3/2}\mathrm{d}^3\pi$ and $\mathrm{d}^3x = \beta^{-3/2n}\mathrm{d}^3\xi$ this gives

$$Z = \beta^{-3N/2-3N/(2n)}\,\bar{Z},$$

where $\bar{Z}$ does not depend on β. It follows that

$$\langle H\rangle = \frac{3}{2}\left(1+\frac{1}{n}\right)N\frac{\partial}{\partial\beta}\ln\beta = \frac{3}{2}\left(1+\frac{1}{n}\right)Nk_BT, \tag{3}$$

$$C = \frac{\partial}{\partial T}\langle H\rangle = \frac{3}{2}\left(1+\frac{1}{n}\right)Nk_B. \tag{4}$$

c) Does your result for C agree with the equipartition theorem when $n = 1$ or $n = \infty$?

The case $n = 1$ corresponds to N three-dimensional oscillators, each contributing $3k_B$ to the heat capacity according to the equipartition theorem. The case $n = \infty$ corresponds to N particles in a volume with hard walls, each contributing $\frac{3}{2}k_B$ to the heat capacity according to the equipartition theorem. The result (4) agrees with these statements.

d) Calculate the mean particle density, defined as

$$\rho(\boldsymbol{x}) = \left\langle \sum_{i=1}^{N} \delta(\boldsymbol{x} - \boldsymbol{x}_i) \right\rangle. \tag{5}$$

We have

$$\rho(\boldsymbol{x}) = \frac{1}{Z} \sum_{i=1}^{N} \frac{1}{N!} \int \prod_{j=1}^{N} \frac{\mathrm{d}^3 p_j\, \mathrm{d}^3 x_j}{h^3}\, \delta(\boldsymbol{x} - \boldsymbol{x}_i) \mathrm{e}^{-\beta H}.$$

Due to the factorized form of the integrand most factors of the integral cancels against identical factors in Z, leaving N identical contributions,

$$\rho(\boldsymbol{x}) = \frac{N}{\mathcal{Z}} \int \mathrm{d}^3 x_1\, \delta(\boldsymbol{x} - \boldsymbol{x}_1)\, \mathrm{e}^{-\beta\varepsilon_0 \left(\boldsymbol{x}_1^2/r_0^2\right)^n} = \frac{N}{\mathcal{Z}}\, \mathrm{e}^{-\beta\varepsilon_0 \left(\boldsymbol{x}^2/r_0^2\right)^n}. \tag{6}$$

Here the normalization factor $\mathcal{Z}$ is the single uncancelled factor of Z,

$$\mathcal{Z} = \int \mathrm{d}^3 x_1\, \mathrm{e}^{-\beta\varepsilon_0 \left(\boldsymbol{x}_1^2/r_0^2\right)^n} = \left(\frac{1}{\beta\varepsilon_0}\right)^{1/2n} \frac{4\pi}{2n} r_0^3 \int_0^\infty \frac{\mathrm{d}t}{t}\, t^{3/2n}\, \mathrm{e}^{-t} = \left(\frac{1}{\beta\varepsilon_0}\right)^{1/2n} \frac{4\pi}{2n} r_0^3\, \Gamma\left(\frac{3}{2n}\right). \tag{7}$$

Note that $(\beta\varepsilon_0)^{1/2n} \to 1$, $\frac{1}{2n}\Gamma\left(\frac{3}{2n}\right) \to \frac{1}{3}$, and $\mathcal{Z} \to \frac{4\pi}{3} r_0^3$ when $n \to \infty$.

Next assume the particles to have charge Q measured in units of the positron charge e, and that the system is exposed to a magnetic field $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$. This implies that we must make the substitution

$$\boldsymbol{p}_i \to \boldsymbol{p}_i + Qe\boldsymbol{A}(\boldsymbol{x}_i) \tag{8}$$

in the Hamiltonian (1).

e) What is the effect of this magnetic field on the classical partition function Z?

There is *no effect* of a magnetic field in classical statistical mechanics. This is known as the *Bohr–van Leuween theorem* (pointed out by Niels Bohr in his doctoral dissertation of 1911 — before the advent of quantum mechanics). A simple proof is that we may introduce new momentum integration variables, $\boldsymbol{\pi}_i = \boldsymbol{p}_i + Qe\boldsymbol{A}(\boldsymbol{x}_i)$ in the partition function integrals, thereby removing every trace of the magnetic field from the integrand.

The Gamma function:

$$\Gamma(\nu) = \int_0^\infty \frac{\mathrm{d}t}{t}\, t^\nu\, \mathrm{e}^{-t}, \quad \Gamma(1+\nu) = \nu\, \Gamma(\nu), \tag{9}$$

$$\Gamma(1) = 1, \quad \Gamma(\frac{1}{2}) = \sqrt{\pi}, \quad \Gamma(\nu) = \nu^{-1} + \cdots \text{ when } \nu \to 0. \tag{10}$$

Problem 2. Monte-Carlo simulation of a thermal system

Here you should to prepare for a numerical simulation of the system discussed in the previous problem, for the case of $N = 1$ and $n = 2$. We further simplify the system to be one-dimensional.

a) Write down the classical equations of motion dictated by the Hamiltonian (1).

After reduction to one space dimension one obtains

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}, \tag{11}$$

$$\dot{p} = -\frac{\partial H}{\partial x} = -\frac{2n\varepsilon_0}{r_0} \left(\frac{x^2}{r_0^2}\right)^{n-1} x. \tag{12}$$

Remark: The three-dimensional version of these equations is not much different,

$$\dot{\boldsymbol{x}} = \frac{\boldsymbol{p}}{m}, \tag{13}$$

$$\dot{\boldsymbol{p}} = -\frac{2n\varepsilon_0}{r_0} \left(\frac{\boldsymbol{x}^2}{r_0^2}\right)^{n-1} \boldsymbol{x}. \tag{14}$$

b) Find suitable units for time and length so that the equations of motion can be written in terms of dimensionless variables.

It seems obvious that r_0 must be a suitable unit of time. I.e., we write $x = r_0\xi$ with ξ dimensionless. It follows from equation (1) that ε_0 has dimension energy, i.e. that $\left(\varepsilon/mr_0^2\right)^{-1/2}$ has dimension time and could serve as a suitable unit of time. However, it seems that

$$t_0 = \sqrt{\frac{mr_0}{2n\varepsilon_0}} \tag{15}$$

is a slightly better choice. We write $t = t_0\tau$ with τ dimensionless, so that $\frac{\mathrm{d}}{\mathrm{d}t} = \frac{1}{t_0}\frac{\mathrm{d}}{\mathrm{d}\tau}$. A natural unit of momentum then is $p_0 = \frac{mr_0}{t_0}$. Hence we write $p = p_0\eta$ with η dimensionless. This leads to the dimensionless equations

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\xi = \eta, \tag{16}$$

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\eta = -\xi^{2n-1}. \tag{17}$$

Remark: The fastest way to solve this problem, completely acceptable (in fact the recommended one when time is scarce), is to say that we may choose units for length so that $r_0 = 1$, for mass so that $m = 1$, and for energy so that $2n\varepsilon_0 = 1$.

c) How would you discretize the differential equations for a numerical solution of the problem?

We sample the function at discrete times $\tau_k = k\Delta\tau$, and approximate the time derivative with the discrete difference,

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\xi(\tau)\right|_{\tau=k\Delta\tau} = \frac{\xi_{k+1}-\xi_k}{\Delta\tau}, \quad \text{with } \xi_k \equiv \xi(k\Delta\tau), \tag{18}$$

and similar for $\eta(\tau)$. This leads to the difference equations

$$\xi_{k+1} = \xi_k + \Delta\tau\,\eta_k, \tag{19}$$

$$\eta_{k+1} = \eta_k - \Delta\tau\,\xi_k^{2n-1}. \tag{20}$$

which can be solved iteratively.

d) To simulate temperature one has to introduce additional fluctuating and a damping forces. Indicate how this should be done.

In addition to the force $-\frac{\partial H}{\partial x}$ we should add a dissipative (damping) force $\Gamma\,p$ and a completely random (fluctuating) force F. In dimensionless form this changes the difference equations to

$$\xi_{k+1} = \xi_k + \Delta\tau\,\eta_k, \tag{21}$$

$$\eta_{k+1} = \eta_k - \Delta\tau\,\xi_k^{2n-1} - \gamma\Delta\tau\,\eta_k + \sqrt{\Delta\tau}f_k, \tag{22}$$

where the f_k's are random numbers generated independently for each k, and γ is a dimensionless parameter.

Hamilton's equations:

$$\dot{\boldsymbol{x}}_\alpha = \frac{\partial H}{\partial \boldsymbol{p}_\alpha}, \qquad \dot{\boldsymbol{p}}_\alpha = -\frac{\partial H}{\partial \boldsymbol{x}_\alpha}. \tag{23}$$

Problem 3. Quantum statistics of thermal radiation

The eigen-energies for the free radiation field can be written

$$E = \sum_{\boldsymbol{k},r} \hbar\omega_{\boldsymbol{k}}\, N(\boldsymbol{k},r) \tag{24}$$

where $\omega_{\boldsymbol{k}} = c\,|\boldsymbol{k}|$, and where $N(\boldsymbol{k},r) = 0,1,\ldots$ is the *occupation number* of the state with wavevector $\boldsymbol{k}$ and polarization r. We have subtracted the zero-point energy. With av volume V and periodic boundary conditions the allowed values for $\boldsymbol{k}$ lie on a lattice,

$$\boldsymbol{k} = \frac{2\pi}{V^{1/3}}\,(n_x, n_y, n_z) \quad \text{with all } n\text{'s integer.} \tag{25}$$

a) Show that the partition function for this system can be written

$$\ln Z = -\sum_{\boldsymbol{k},r} \ln\left(1 - \mathrm{e}^{-\beta\hbar\omega_{\boldsymbol{k}}}\right). \tag{26}$$

Background: The following general background was not expected as part of the solution; it is included as a review of the concepts involved.

The quantum partition function can in general be written

$$Z = \sum_E \mathrm{e}^{-\beta E},$$

where the sum runs over all possible eigenenergies E. You should be familiar with the fact that the eigenstates are usually labeled by several quantum numbers, like n (the principal quantum number), ℓ (the total angular momentum quantum number) and m (the magnetic quantum number — labels the z-component of the angular momentum vector) in atomic physics. Likewise the states of a 3-dimensional harmonic oscillator may be labelled by non-negative integer quantum numbers N_x, N_y, and N_z describing excitations of the oscillator in respectively the x-, y-, and z-directions. In the latter case the eigen-energies of the system is

$$\begin{aligned} E = E_{N_x,N_y,N_z} &= \hbar\left(\omega_x N_x + \omega_y N_y + \omega_z N_z\right) + E_0 \\ &= \sum_{\alpha=x,y,x} \hbar\omega_\alpha N_\alpha + E_0 \end{aligned}$$

where the second term of each line is the *zero-point energy* $E_0 = \frac{1}{2}\hbar\sum_{\alpha=x,y,x}\omega_\alpha$. Ignoring the zero-point energy, the partition function can be written

$$\begin{aligned} Z &= \sum_{N_x,N_y,N_z} \mathrm{e}^{-\beta E_{N_x,N_y,N_z}} = \sum_{N_x,N_y,N_z} \mathrm{e}^{-\beta\hbar(\omega_x N_x + \omega_y N_y + \omega_z N_z)} \\ &= \sum_{N_x=0}^{\infty} \mathrm{e}^{-\beta\hbar\omega_x N_x} \sum_{N_y=0}^{\infty} \mathrm{e}^{-\beta\hbar\omega_y N_y} \sum_{N_z=0}^{\infty} \mathrm{e}^{-\beta\hbar\omega_z N_z} \\ &= \prod_{\alpha=x,y,z} \sum_{N_\alpha=0}^{\infty} \mathrm{e}^{-\beta\hbar\omega_\alpha N_\alpha} = \prod_{\alpha=x,y,z} \frac{1}{\left(1 - \mathrm{e}^{-\beta\hbar\omega_\alpha}\right)}. \end{aligned}$$

I.e., since the logarithm of a product is the sum of logarithms of its factors,

$$\ln Z = -\sum_{\alpha=x,y,z} \ln\left(1 - \mathrm{e}^{-\beta\hbar\omega_\alpha}\right).$$

The eigenstates of the radiation field is like those of the 3-dimensional oscillator, except that we don't have 3 but infinitely many "directions" — each "direction" labeled by a wavenumber $\boldsymbol{k}$ and a polarization r (which together specifies a possible propagation mode of the electromagnetic field). The occupation number $N(\boldsymbol{k},r)$ then specifies the excitation of that mode.

Solution: We have

$$Z = \prod_{\boldsymbol{k},r} \sum_{N(\boldsymbol{k},r)=0}^{\infty} \mathrm{e}^{-\beta\hbar\omega_{\boldsymbol{k}}} = \prod_{\boldsymbol{k},r} \frac{1}{(1-\mathrm{e}^{-\beta\hbar\omega_{\boldsymbol{k}}})}, \tag{27}$$

so that

$$\ln Z = -\sum_{\boldsymbol{k},r} \ln\left(1-\mathrm{e}^{-\beta\hbar\omega_{\boldsymbol{k}}}\right). \tag{28}$$

b) Explain why the the average occupations numbers can be written as

$$\langle N(\boldsymbol{k},r)\rangle = -\frac{1}{2}\frac{1}{\beta\hbar}\frac{\partial}{\partial\omega_{\boldsymbol{k}}} \ln Z. \tag{29}$$

Since the occupation probabilities of differents modes are independent we have

$$\langle N(\boldsymbol{k},r)\rangle = \frac{1}{Z(\boldsymbol{k},r)} \sum_{N(\boldsymbol{k},r)=0}^{\infty} N(\boldsymbol{k},r)\,\mathrm{e}^{-\beta\hbar\omega_{\boldsymbol{k}}N(\boldsymbol{k},r)}, \quad \text{with}$$

$$Z(\boldsymbol{k},r) = \sum_{N(\boldsymbol{k},r)=0}^{\infty} \mathrm{e}^{-\beta\hbar\omega_{\boldsymbol{k}}N(\boldsymbol{k},r)}.$$

I.e.,

$$\langle N(\boldsymbol{k},r)\rangle = -\frac{1}{Z(\boldsymbol{k},r)}\frac{\partial}{\beta\hbar\partial\omega_{\boldsymbol{k}}} Z(\boldsymbol{k},r) = -\frac{\partial}{\beta\hbar\partial\omega_{\boldsymbol{k}}} \ln Z(\boldsymbol{k},r) = -\frac{1}{2}\frac{1}{\beta\hbar}\frac{\partial}{\partial\omega_{\boldsymbol{k}}} \ln Z. \tag{30}$$

There are two terms in $\ln Z$ which depends on $\omega_{\boldsymbol{k}}$, one for each value of r. The factor $\frac{1}{2}$ compensates for this.

c) Find an explicit expression for $\langle N(\boldsymbol{k},r)\rangle$.

We find

$$\langle N(\boldsymbol{k},r)\rangle = \frac{\partial}{\beta\hbar\partial\omega_{\boldsymbol{k}}} \ln\left(1-\mathrm{e}^{-\beta\hbar\omega_{\boldsymbol{k}}}\right) = \frac{1}{(\mathrm{e}^{\beta\hbar\omega_{\boldsymbol{k}}}-1)}. \tag{31}$$

d) To evaluate many physical quantities explicitly in the limit $V\to\infty$ one makes the substitution

$$\sum_{\boldsymbol{k},r} F(\boldsymbol{k},r) \to V\mathcal{N}\sum_r \int \mathrm{d}^3k\, F(\boldsymbol{k},r), \tag{32}$$

valid for continuous functions $F(\boldsymbol{k},r)$.

Explain the origin of this substitution. What is the dimensionless number $\mathcal{N}$?

The vector $\boldsymbol{k}$ runs over the points of a cubic lattice, with volume

$$\Delta v = \frac{(2\pi)^3}{V} \tag{33}$$

of each elementary cell. As V becomes large the points becomes very close together, and we may approximate the sum by an integral,

$$\sum_{\boldsymbol{k},r} F(\boldsymbol{k},r) = \frac{V}{(2\pi)^3}\sum_r\sum_{\boldsymbol{k}} \Delta v\, F(\boldsymbol{k},r) \approx \frac{V}{(2\pi)^3}\sum_r \int \mathrm{d}^3k\, F(\boldsymbol{k},r), \tag{34}$$

where we in the last step have interpreted the sum over $\boldsymbol{k}$ as a Riemann approximation to the integral. As V becomes very large this approximation becomes very good.

We have found that

$$\mathcal{N} = \frac{1}{(2\pi)^3}. \tag{35}$$

e) In most of the universe the photons have a temperature $T = 2.725$ K.

How many photons $N = \sum_{\boldsymbol{k},r} \langle N(\boldsymbol{k}, r) \rangle$ are there on average per m^3?

We find

$$N = 2\,\frac{V}{(2\pi)^3} \int \frac{\mathrm{d}^3k}{\mathrm{e}^{\beta\hbar\omega_{\boldsymbol{k}}} - 1} = 2\,\frac{V}{(2\pi)^3} \times 4\pi \int_0^\infty \frac{k^2\mathrm{d}k}{\mathrm{e}^{\beta\hbar ck} - 1}$$
$$= \frac{1}{\pi^2}\,V \left(\frac{k_BT}{\hbar c}\right)^3 \int_0^\infty \frac{x^2\mathrm{d}x}{\mathrm{e}^x - 1} = \frac{2}{\pi^2}\,\zeta(3)\,V \left(\frac{k_BT}{\hbar c}\right)^3 = 4.105 \times 10^8. \tag{36}$$

Some physical constants, and an integral:

$$\hbar = 1.054\,571\,628 \times 10^{-34}\ \mathrm{Js}, \quad k_B = 1.380\,6503 \times 10^{-23}\ \mathrm{J/K}, \quad c = 299\,792\,458\mathrm{m/s} \tag{37}$$

$$\int_0^\infty \frac{x^2\mathrm{d}x}{\mathrm{e}^x - 1} = 2\zeta(3) \approx 2.404\ldots \tag{38}$$