Exam TFY4230 Statistical Physics kl 09.00 - 13.00 Wednesday 01. June 2016

Problem 1. Ising ring (Points: 10+10+10=30)

A system of Ising spins $\sigma_i = \pm 1$ on a ring with periodic boundary conditions is defined by the Hamiltonian

$$H = -J\sum_{i=1}^{N} \sigma_i \sigma_{i+1} - h\sum_{i=1}^{N} \sigma_i$$

where i denotes a lattice site, and $\sigma_{N+1} = \sigma_1$. J is the strength of the nearest neighbor interaction between spins, and h is a uniform external magnetic field. The partition function for this system is given by

$$Z = \sum_{\{\sigma_i\}} e^{-\beta H} = e^{-\beta G},$$

where G is the Gibbs energy of the system. An explicit calculation yields $Z = \lambda_+^N + \lambda_-^N$, where

$$\lambda_{\pm} = e^K \left[\cosh(\omega) \pm \sqrt{\sinh^2(\omega) + e^{-4K}} \right],$$

where $K \equiv \beta J$ and $\omega \equiv \beta h$. Here, $\beta \equiv 1/k_B T$, k_B is Boltzmann's constant, and T is temperature.

<u>a</u>.

Write out the sum in the partition function explicitly for N=3, collecting all terms of equal Boltzmann weight $e^{-\beta H}$.

Show that the magnetization $m \equiv \lim_{N \to \infty} (M/N) = \lim_{N \to \infty} (1/N) \sum_{i=1}^{N} \langle \sigma_i \rangle$ of this system is given by the expression

$$m = \frac{\sinh(\omega)}{\sqrt{\sinh^2(\omega) + e^{-4K}}}.$$

b.

Explain on physical grounds the difference in the results for J > 0 and J < 0.

Consider now a slightly different model of Ising-spins on a ring with the following Hamiltonian

$$H = -\sum_{i=1}^{N} [J_1 \ \sigma_i \sigma_{i+1} + J_2 \ \sigma_i \sigma_{i+2}]$$

where $J_1 > 0$ is the interaction strength between nearest neighbor spins, and $J_2 > 0$ is the interaction strength between next-nearest neighbor spins. There is no external magnetic field. Compute the Gibbs energy G for this system for $N \to \infty$. From this, find the limiting values of G for low temperatures $\beta J_1 \gg 1$, $\beta J_2 \gg 1$. Give a physical explanation of the result.

(Hint: Introduce the new spin variable $\tau_i = \sigma_i \sigma_{i+1}$ and use periodic boundary conditions on the τ_i .)

<u>Problem 2.</u> Ideal gas in a 3D anharmonic trap (Points: 10+10+10=30)

The canonical partition function Z for a system of N classical non-relativistic particles of equal mass m which are in thermal equilibrium with their surroundings and moving in three spatial dimension 3D in an anharmonic trap potential, is given by

$$Z = \frac{1}{N!h^{3N}} \int d\mathbf{r}_1..d\mathbf{r}_N \int d\mathbf{p}_1..d\mathbf{p}_N \ e^{-\beta H} = e^{-\beta F}$$

where $\beta = 1/k_BT$, k_B is Boltzmann's constant, T is temperature, h is Plank's constant, F = U - TS is the Helmholz free energy, and the Hamiltonian H of the system is given by

$$H = \sum_{i=1}^{N} H_i$$

$$H_i = \frac{\mathbf{p}_i^2}{2m} + \alpha |\mathbf{r}_i|^3.$$

Here, α is a dimensionful constant which gives the strength of the anharmonic trap-potential $\alpha |\mathbf{r}_i|^3$. The 3D volume of the system to which the particles are confined is defined by a sphere of radius R, with volume $V = 4\pi R^3/3$. The coordinates $\{\mathbf{r}_i\}$ are all measured from the center of this sphere.

a.

Show that the partition function of the system is given by

$$Z = \frac{1}{N!} \frac{V^N}{\Lambda^{3N}} \left[\frac{1 - e^{-x}}{x} \right]^N$$

$$x \equiv \frac{3\beta\alpha V}{4\pi}$$

$$\Lambda \equiv \frac{h}{\sqrt{2\pi m k_B T}}.$$

<u>b</u>

Compute the internal energy $U=\langle H\rangle$ of the system for the limits $3\beta\alpha V/4\pi\ll 1$ and $3\beta\alpha V/4\pi\gg 1$. Explain your results on physical grounds in each case.

$\underline{\mathbf{c}}.$

Compute the pressure of the system for general values of $3\beta\alpha V/4\pi$. Consider then the limits $3\beta\alpha V/4\pi \ll 1$ and $3\beta\alpha V/4\pi \gg 1$ and compute the equation of state in these limits. Explain your results on physical grounds in each case. (Hint: Use F = U - TS and TdS = dU + pdV to express pressure p in terms of Z.) Useful formulae:

$$U = \frac{1}{Z} \frac{1}{N! h^{3N}} \int d\mathbf{r}_1 ... d\mathbf{r}_N \int d\mathbf{p}_1 ... d\mathbf{p}_N \ H \ e^{-\beta H}$$

$$\int d^{\nu} \mathbf{r} \ F(|\mathbf{r}|) = \Omega_{\nu} \int dr \ r^{\nu-1} \ F(r); \quad \Omega_{\nu} = \frac{2\pi^{d/2}}{\Gamma(d/2)}; \quad \Gamma(z+1) = z \ \Gamma(z)$$

$$\int_0^a dx \ x^{\nu-1} \ e^{-x^{\nu}} = \frac{1}{\nu} \int_0^{a^{\nu}} du \ e^{-u}$$

<u>Problem 3.</u> d-dimensional Bose system (Points: 10+10+10=30)

Ultra-relativistic non-interacting bosons moving in d dimensions have a Hamiltonian given by

$$\begin{split} H &=& \sum_{\mathbf{k}} \, \varepsilon_{\mathbf{k}} \; n_{\mathbf{k}}; \quad n_{\mathbf{k}} = 0, 1, 2, \dots \\ \varepsilon_{\mathbf{k}} &=& \hbar c |\mathbf{k}| \end{split}$$

where c is the speed of light, $\hbar = h/2\pi$ with h Planck's constant, and **k** is a wavenumber uniquely determining the single-particle bosonic states.

The grand canonical partition function Z_q for a system of non-interacting bosons is given by

$$\ln Z_g = -\sum_{\mathbf{k}} \ln \left[1 - e^{-\beta(\varepsilon_{\mathbf{k}} - \mu)} \right] = \beta p V$$

Here, $\beta = 1/k_BT$, k_B is Boltzmann's constant, T is temperature, p is pressure and V is the volume of the system. It can be shown (need not be shown!) that the density of states g(e) for this system is given by

$$g(e) = \frac{V}{(2\pi\hbar c)^d} \; \frac{2\pi^{d/2}}{\Gamma(d/2)} \; e^{d-1}\Theta(e)$$

where $\Theta(e) = 1, e \ge 0; \Theta(e) = 0, e < 0.$

 $\underline{\mathbf{a}}$.

The average number of particles in the system is given by $\langle N \rangle = \partial \ln Z_g / \partial(\beta \mu) = \sum_{\mathbf{k}} n_{\mathbf{k}}$ where $n_{\mathbf{k}}$ is the average number of particles with wavenumber \mathbf{k} . The internal energy U is given by $U = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} n_{\mathbf{k}}$. Show that

$$\begin{array}{rcl} \langle N \rangle & = & \displaystyle \sum_{\mathbf{k}} \frac{1}{e^{\beta(\varepsilon_{\mathbf{k}} - \mu)} - 1} \\ U & = & \displaystyle \sum_{\mathbf{k}} \frac{\varepsilon_{\mathbf{k}}}{e^{\beta(\varepsilon_{\mathbf{k}} - \mu)} - 1} \end{array}$$

b

Introduce the density of states g(e) and the fugacity $z = e^{\beta \mu}$. Show that

$$\langle N \rangle = V \sum_{l=1}^{\infty} l b_l z^l$$

$$\frac{\beta U}{d} = V \sum_{l=1}^{\infty} b_l z^l$$

and thereby determine b_l . Compute the ratio U/pV.

c.

Compute the first and second virial coefficients $E_1(T)$ and $E_2(T)$ in the virial expansion for the internal energy, $U = E_1(T)\rho + E_2(T)\rho^2 + \dots$ Show that $E_2(T) \neq 0$ is a quantum effect, and give a physical explanation for the sign of $E_2(T)$.

TFY4230 01. June 2016 Useful formulae:

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$$\sum_{\mathbf{k}} F(\varepsilon_{\mathbf{k}}) = \int_{-\infty}^{\infty} de \ g(e) \ F(e)$$

$$g(e) \equiv \sum_{\mathbf{k}} \delta(e - \varepsilon_{\mathbf{k}})$$

$$\Gamma(z) = \int_{0}^{\infty} dx \ x^{z-1} e^{-x}$$

$$\Gamma(z+1) = z \ \Gamma(z)$$