Homework HW 5

due *2017-04-11*

Exams	final: **Monday, May 8, 2017**, *12:00-13:59* (tentative)

XVI. HARMONIC OSCILLATOR *[(9+9) PTS]*

A harmonic oscillator has the energy eigenvalues

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots .$$

a) Calculate the partition function $Z^{(c)} = \sum_n e^{-\beta E_n}$, the internal energy $E = \langle\mathcal{H}\rangle = -\frac{\partial}{\partial\beta}\ln Z^{(c)}$, the entropy $S = k_B\left(\beta E + \ln Z^{(c)}\right)$, and the heat capacity $C = \frac{\partial E}{\partial T}$ depending on temperature. Use the dimensionless variable $x \equiv \frac{1}{2}\beta\hbar\omega > 0$.

b) Write the entropy as a function of the dimensionless energy $\eta \equiv 2E/(\hbar\omega)$. Recalculate the entropy using the definition of the Boltzmann entropy. To this end consider $N \gg 1$ equal (indistinguishable) oscillators and their possible distributions on the microstates given a total energy E, which defines the macrostate.

XVII. CONTINUUM LIMIT *[10 PTS]*

For the calculation of particle fluctuations, we usually replace the summation over particle numbers by integrals, e.g.

$$\left\langle(\Delta N)^2\right\rangle = \frac{\sum_N (\Delta N)^2 e^{\Delta S(N)/k_B}}{\sum_N e^{\Delta S(N)/k_B}} \approx \frac{\int dN\,(\Delta N)^2 e^{\Delta S(N)/k_B}}{\int dN\, e^{\Delta S(N)/k_B}}$$

with $\Delta S(N) \approx -k_B\frac{c}{2}(\Delta N)^2$. Determine under which condition this continuum approximation is valid. Approximate the error by using the Poisson summation formula

$$\sum_{N=-\infty}^{\infty} f(N) = \sum_{k=-\infty}^{\infty}\int_{-\infty}^{\infty} dN\, f(N) e^{2\pi\imath kN}\,.$$

XVIII. QUANTUM LIOUVILLE EQUATION *[6 PTS]*

Show that the microscopic density

$$\hat{\rho} = \frac{1}{N}\sum_\nu n_\nu \left|x_\nu\right\rangle\left\langle x_\nu\right|$$

satisfies the Quantum Liouville equation

$$\frac{\partial\hat{\rho}}{\partial t} = -\frac{\imath}{\hbar}\left[\hat{H},\hat{\rho}\right]\,.$$

XIX. N-LEVEL SYSTEM, NEGATIVE TEMPERATURES *[(2+3+4+4+5) PTS]*

The eigen-energies of the system we consider here are equidistant and their number is finite, f, i.e.,

$$E_\nu = (\nu - 1)\epsilon\,; \;\; \nu = 1, 2, \ldots, f\,; \;\; \epsilon > 0\,.$$

a) Calculate the canonical partition function $Z^{(c)} = \sum_\nu e^{-\beta E_\nu}$.
   Remark: Since the spectrum is limited from above, $Z^{(c)}$ exists for all real values of β - in particular also for negative temperatures. It is useful to introduce the dimensionless variable $x \equiv e^{-\beta\epsilon}$ with $0 < x < \infty$.

b) Using $Z^{(c)}$, calculate the internal energy $E = -\frac{\partial}{\partial\beta}\ln Z^{(c)} = \epsilon x \frac{d}{dx}\ln Z^{(c)}$. At which temperature does E take its minimum, maximum, or value exactly between those?

c) What are the 'occupation numbers' n_ν, which allow to write the internal energy as $E = \sum_{\nu=1}^{f} n_\nu E_\nu$? Show and interpret that $n_\nu(x^{-1}) = n_{f-\nu+1}(x)$ ("inversion of the occupation numbers"). Justify why $\beta = -\infty$ (or $T = 0^-$) should be the highest accessible temperature. What is the occupation number of the highest or lowest level at high or low temperatures, respectively?

d) Calculate the entropy, $S = k_B(\ln Z^{(c)} + \beta E)$ as function of x and find an expression for S, which only depends on the occupation numbers. Calculate the heat capacity $C = \frac{\partial E}{\partial T}$.

e) Simplify the expressions for $Z^{(c)}$, E, S, and C for the case of a two-level system, $f = 2$, which already shows all the relevant properties of the more general case. Sketch and discuss the qualitative graph of $S(E)$.

XX. GRAND CANONICAL ENSEMBLE *[(3+5) PTS]*

The canonical partition function of a Boltzmann gas is given by (see lecture)

$$Z^{(c)}(\beta, V, N) = \frac{1}{N!}\left(\frac{V}{\lambda_\beta^3}\right)^N ,$$

where $\lambda_\beta = h/\sqrt{2\pi m T}$ is the thermal de Broglie wave length.

a) Calculate the grand canonical partition function using $Z^{(c)}$ from above.

b) Calculate the squared deviations of the particle number $\Delta N^2 = \left\langle (N - \langle N \rangle)^2 \right\rangle$ in the grand canonical ensemble and show that the relative deviation $\Delta N / \langle N \rangle$ vanishes in the thermodynamic limit.

XXI. THERMODYNAMIC RELATIONS *[(3+6) PTS]*

Here we consider a system of N identical particles. E, T, V, and μ are the energy, the temperature, the volume, and the chemical potential, respectively.

a) Prove the following relations:

$$\left(\frac{\partial E}{\partial N}\right)_{T,V} = \mu - T\left(\frac{\partial \mu}{\partial T}\right)_{V,N} ,$$

$$\left(\frac{\partial E}{\partial V}\right)_{T,N} = T\left(\frac{\partial S}{\partial V}\right)_{T,N} - p\,, \;\; \left(\frac{\partial S}{\partial p}\right)_{T,N} = -\left(\frac{\partial V}{\partial T}\right)_{p,N} .$$

b) Prove the following relation for a system with fixed number of particles:

$$K_T - K_S = V\frac{T\alpha_p^2}{C_p}\,, \;\; \frac{C_p}{C_V} = \frac{K_T}{K_S}\,,$$

where

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = T\left(\frac{\partial S}{\partial T}\right)_V \,, \;\; C_p = \left(\frac{\partial H}{\partial T}\right)_p = T\left(\frac{\partial S}{\partial T}\right)_p \,,$$

$$\alpha_p = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p \,, \;\; K_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T \,, \;\; K_S = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_S \,.$$

Hint: Use the relation derived in the lecture:

$$C_p - C_V = VT\frac{\alpha_p^2}{K_T} \,.$$