

Problem Sheet 9

I. CUMULANT EXPANSION

In statistical physics it occurs very often that one has to average expression like

$$\int dx P(x) e^{A(x)}. \quad (1.1)$$

We have seen examples in the lecture, e.g.,

$$\int dx P(x) [\dots] \rightarrow \int \frac{d^3 p d^3 q}{(2\pi\hbar)^3} e^{-\beta H_{\text{cl}}(p, q)} [\dots] \quad (1.2)$$

$$A(x) \rightarrow -\beta \delta H(p, q) \quad (1.3)$$

where δH is a classical potential perturbation, or a quantum perturbation of the classical Hamiltonian, for example.

If $A(x)$ can be considered small, it makes sense to expand $e^{A(x)}$ in powers of A and to re-exponentiate the average in a systematic series in powers of A and its moments:

$$\langle e^{A(x)} \rangle := \int dx P(x) e^{A(x)} = \left\langle \sum_{k=0}^{\infty} \frac{A^k(x)}{k!} \right\rangle = \exp \left[\sum_{k=1}^{\infty} \frac{C_k(A)}{k!} \right]. \quad (1.4)$$

$C_1(A) = \langle A(x) \rangle$, $C_2(A) = (\langle A^2(x) \rangle - \langle A(x) \rangle^2)/2$, etc. The terms $C_k(A)$ is called the k 'th cumulant of A .

a) Show that it can be defined formally as

$$C_k(A) = \frac{d^k}{d\lambda^k} (\log [\langle e^{\lambda A(x)} \rangle]) |_{\lambda=0} \quad (1.5)$$

b) Find the first 4 cumulants $C_k(A)$ in terms of the moments of A , $M_k(A) := \langle A^k \rangle$. In turn, express the 3rd and 4th moments as functions of the cumulants, e.g.,

$$M_1(A) = C_1(A) \quad (1.6)$$

$$M_2(A) = C_2(A) + C_1(A)^2 \quad (1.7)$$

$$M_3(A) = ? \quad (1.8)$$

c) Try to generalize the pattern you find by guessing the connection between the coefficients and the number of partitions of k objects into subgroups with a given number of objects in the subgroups. **Challenge: Prove your guess!**

A. Corrections in the ideal gas equation due to exchange and interactions

In the lecture we have seen that several corrections lead to deviations from non-interacting classical systems. In the classical limit we saw that the partition function can be written as

$$Z_N = \frac{1}{N!} \left(\frac{V}{\lambda^3} \right)^N \int \frac{d^{3N}q}{V^N} \exp \left(-\beta \left[\sum_{i<j} V_{\text{cl}}(q_i - q_j) + V_s(q_i - q_j) + V_q(q_i - q_j) \right] \right) \quad (1.9)$$

where the quantum corrections of the potential are given by $V_q(q_i - q_j) \frac{\lambda^2}{48} \partial_{q_i}^2 V_{\text{cl}}(q_i - q_j)$ to lowest order \hbar . For simplicity we neglect the three body term

$$V_3 \sim \sum_{i \neq j \neq k} \lambda^2 \partial_{q_i} V_{\text{cl}}(q_i - q_j) \partial_{q_i} V_{\text{cl}}(q_i - q_k) \quad (1.10)$$

which is of the same order as the two-body quantum correction.

In the above V_{cl} is the (classical) interaction potential, which we assume to be of Lenard-Jones type:

$$V_{LJ}(r) = 4\epsilon \left[\left(\frac{r_0}{r} \right)^{12} - \left(\frac{r_0}{r} \right)^6 \right] \quad (1.11)$$

and V_s is the "statistical interaction" (which is not a true interaction of course)

$$V_s(q_i - q_j) = -T \log(1 \pm e^{-2\pi(q_i - q_j)^2/\lambda^2}). \quad (1.12)$$

i) Calculate the second virial coefficient due to V_s

$$B_2 = \frac{1}{2} \int d^3q (1 - \exp(-\beta V_s(q))). \quad (1.13)$$

and discuss its effect on the equation of state!

ii) Estimate the contribution to B_2 from the other two terms as well. At which temperature and density does the quantum correction to the potential become as important as the potential itself?

Discuss which of the three terms becomes important first (at fixed density) when coming from high temperature! Show that the answer depends on the ratio of the typical interaction potential at the given density and the quantum degeneracy temperature!

In fermionic systems with Coulomb interactions this ratio is known as the parameter r_s which is defined as the ratio between Coulomb energy and Fermi energy, $r_s = E_{\text{Cb}}/E_F$. When $r_s \ll 1$ the system can form a so-called Wigner crystal, which is an insulator as opposed to the conducting, metallic Fermi sea. (The critical value of r_s depends on the dimension, but it is rather large.)

iii) Show that up to a factor of order $O(1)$, r_s is also the ratio between interparticle distance at density n and the Bohr radius a_B !

iv) Note that you have 4 typical length's in your problem: r_0 , λ , a_B and $n^{-1/3}$. Assume you are in a liquid phase where $n^{-1/3} \approx r_0$. Rephrase the conditions for the importance of the two quantum corrections in terms of these length scales!

II. PERTURBATION THEORY FOR INTERACTING BOSONS AT LOW T

In boson systems at low enough density ($n \ll 1/a^3$ where a is the so-called scattering length of the two-boson potential) the Hamiltonian can be approximated by the "s-wave pseudopotential"

$$H = H_0 + H_1 = \sum_{i=1}^N \frac{p_i^2}{2m} + \frac{4\pi a \hbar^2}{m} \sum_{i < j} \delta(\vec{q}_i - \vec{q}_j) \quad (2.1)$$

i) Determine the normalized, symmetrized eigenfunctions of H_0 ! Pay attention to the case when several momentum states are multiply occupied!

ii) Before calculating: What is the order of magnitude that you expect for your result? (There is only one dimensionless result which makes sense!)

iii) Calculate to first order in perturbation the effect of the interactions H_1 on the ground state of H_0 .

iv) **Challenge:** Calculate to first order in perturbation the effect of the interactions H_1 on the eigenstates of H_0 ! Show that the ground state receives the smallest shift upward in energy!

v) What happens in the attractive case? Argue that the Hamiltonian above has an instability: The energy can be lowered indefinitely by concentrating the particles on an arbitrarily small volume. In practice this will not really happen because of short range repulsions, but one must nevertheless be careful with calculations in this case.