Exercise #4

due date: December 14th 2020

- a) Consider a classical perfect gas and calculate the entropy in the canonical ensemble. Compare the result with that given, in the microcanonical ensemble, by the Sakur-Tetrode formula and show the ensemble equivalence in the thermodynamic limit.
- b) Consider the following Hamiltonian for N independent spin $\sigma=\pm 1$

$$H = -gB\sum_{i}\sigma_{i}$$

Where *B* is the external magnetic field along *z*, *g* a coupling constant and σ_i the Pauli matrix σ_z at a given site *i*. Spin operators at different sites commute.

Perform the calculation in the microcanonical ensemble at fixed total **energy**, calculate the entropy. Plot the dimensionless entropy per spin (S/k_BN) as a function of a suitably defined dimensionless energy.

Perform the calculation of the entropy in the canonical ensemble at fixed total **temperature**.

Compare the results of the previous two points by expressing the canonical entropy as a function of the internal energy.

Comment the result.

c) In the grandcanonical ensemble calculate the dimensionless ratio $\beta P/\rho$ where $\rho = N/V$ is the number density by performing a fugacity expansion in $z = \exp(\beta \mu)$ up to second order in z.

Perform the calculation in the case of an interacting classical gas with pair interactions.

Perform the calculation in the case of a quantum perfect gas in the case of Fermi-Dirac and Bose-Einstein statistics.

Express the result in term of the number density in both cases. Comment the two results.

d) Consider two one particle states made by one-dimensional gaussians

$$g_1\left(x\right) = A\left(\exp\left(-\frac{(x-x_0)}{2\sigma^2}\right)\right)^{1/2}$$

$$g_2\left(x\right) = A\left(\exp\left(-\frac{(x+x_0)}{2\sigma^2}\right)\right)^{1/2}$$

with *A* being a normalisation constant. Using these states write a possible state for 2 fermions and 2 bosons in state 1 or 2 neglecting the spin component. Calculate the average distance $\langle x_1 - x_2 \rangle$ as a function of x_0 (you can choose $\sigma^2 = 1$). Comment the results.