STATISTICAL PHYSICS 18/19

Quantum Statistical Mechanics **Tutorial Sheet 3**

The questions that follow on this and succeeding sheets are an integral part of this course. The code beside each question has the following significance:

- **K**: key question – explores core material
- **R**: review question – an invitation to consolidate
- **C**: challenge question – going beyond the basic framework of the course
- **S**: standard question – general fitness training!

3.1 **Particle Number Fluctuations for Fermions** [s]

(a) For a single fermion state in the grand canonical ensemble, show that

$$\langle (\Delta n_j)^2 \rangle = \bar{n}_j (1 - \bar{n}_j)$$

where $\bar{n}_j$ is the mean occupancy.

Hint: You only need to use the exclusion principle not the explict form of $\bar{n}_j$.

How is the fact that $\langle (\Delta n_j)^2 \rangle$ is not in general small compared to $\bar{n}_j$ to be reconciled with the sharp values of macroscopic observables?

(b) For a gas of noninteracting particles in the grand canonical ensemble, show that

$$\langle (\Delta N)^2 \rangle = \sum_j \langle (\Delta n_j)^2 \rangle$$

(you will need to invoke that n_j and n_k are *uncorrelated* in the GCE for $j \neq k$). Hence show that for noninteracting Fermions

$$\langle (\Delta N)^2 \rangle = \int g(\epsilon)\, f(1-f)\, d\epsilon$$

follows from (a) where $f(\epsilon, \mu)$ is the F-D distribution and $g(\epsilon)$ is the density of states.

(c) Show that for low temperatures $f(1-f)$ is sharply peaked at $\epsilon = \mu$, and hence that

$$\langle \Delta N^2 \rangle \simeq k_B T g(\epsilon_F) \qquad \text{where} \quad \epsilon_F = \mu(T=0)$$

[You may use without proof the result that $\int_{-\infty}^{\infty} \frac{e^x\, dx}{(e^x+1)^2} = 1$.]

3.2 **Entropy of the Ideal Fermi Gas** [C]

The Grand Potential for an ideal Fermi is given by

$$\Phi = -kT \sum_j \ln\left[1 + \exp \beta(\mu - \epsilon_j)\right]$$

Show that for Fermions

$$\Phi = kT \sum_j \ln(1 - p_j)\ ,$$

where $p_j = f(\epsilon_j)$ is the probability of occupation of the state j. Hence show that the entropy of a Fermi gas can be written in the form

$$S = -k \sum_j \left[p_j \ln p_j + (1 - p_j) \ln(1 - p_j)\right]$$

You will need to use $S = -\left(\frac{\partial \Phi}{\partial T}\right)_{\mu,V}$ and some patience to obtain the result!

Comment upon the result for the entropy from the standpoint of missing information.

3.3 **Geometric Series** [r] In problems we often make use of the geometric series in the form

$$\sum_{n=0}^{\infty} e^{-\alpha n} = \frac{1}{1 - e^{-\alpha}}, \qquad \text{for} \quad e^{-\alpha} < 1 \, .$$

Show that this form can be used to derive the results

$$\begin{aligned} \sum_{n=0}^{\infty} n \, e^{-\alpha n} &= \frac{e^{-\alpha}}{(1 - e^{-\alpha})^2} \\ \sum_{n=0}^{\infty} n^2 \, e^{-\alpha n} &= \frac{e^{-\alpha}}{(1 - e^{-\alpha})^2} + 2\frac{e^{-2\alpha}}{(1 - e^{-\alpha})^3} \, . \end{aligned}$$

3.4 **Particle Number Fluctuations for Bosons** [s] Use the results of the previous question to show that for Bosons in the Grand Canonical Ensemble the variance in occupancy for a given one-particle state j obeys

$$\langle \Delta n_j^2 \rangle = \bar{n}_j(\bar{n}_j + 1)$$

where $\bar{n}_j$ is the mean occupancy. Hence show that the existence of a Bose Condensate causes there to be macroscopic fluctuations in the particle number N of the system.

3.5 **Properties of the Density Matrix** [s] In lectures we introduced the idea of a density matrix. For the canonical ensemble the density matrix may be written in braket notation as

$$\rho = \sum_i p_i |i\rangle\langle i|$$

where p_i are classical probabilities for the energy eigenstates $\{|i\rangle\}$ are

a) Show that the components of the density matrix in the energy eigenbasis are given by

$$\rho_{ij} = p_i \delta_{ij}$$

b) Show that

$$\text{Tr}[\rho] = 1$$

and

$$\text{Tr}[\rho^2] \leq 1$$

When does $\text{Tr}[\rho^2] = 1$?

c) The von Neumann entropy is given by

$$S = -k \text{Tr}\left[\rho \ln \rho\right] \, .$$

Show that the von Neumann entropy reduces to the Gibbs-Shannon entropy. You will need to show

$$\rho^n = \sum_i p_i^n |i\rangle\langle i|$$

and use the expansion

$$\ln \rho = \ln[1 + (\rho - 1)] = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}(\rho - 1)^n}{n}$$

3.6 **Bosons in Harmonic Potentials [s/c]** Consider a gas of N weakly interacting bosons trapped in 3d harmonic potential (by a magnetic trap for example).

$$V_{\text{trap}} = \frac{1}{2} m w^2 (x^2 + y^2 + z^2)$$

a) Explain why the single particle quantum states have energies

$$\epsilon = \hbar w (n_x + n_y + n_z + 3/2)$$

b) Calculate the total number of quantum states with energies less that ϵ and from this deduce that the density of states $g(\epsilon)$ is

$$g(\epsilon) \simeq \frac{\epsilon^2}{2(\hbar w)^3} \qquad \text{for large} \quad \epsilon$$

Hint: This is the difficult bit since ϵ is a function of $\underline{n}$ rather than just the magnitude n. You need to convince yourself that a surface of constant energy is a plane in n-space and the number of states with energy less than ϵ is given by the volume of a tetrahedron.