Statistical Physics: Tutorial 3

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A: Core problems: An exercise in generalised black-body radiation

1. **Chemical potential** A box of volume V has walls at temperature T that can emit and absorb particles of mass m, which occupy the box without interacting amongst themselves. The equilibrium population of particles inside the box will adjust the numbers of particles so as to minimise the free energy, F. Hence deduce that the chemical potential, μ, vanishes in equilibrium, so that there is no distinction between the partition function, Z, and the grand partition function, Z_G.

2. **Momentum-space integrals** Hence show that the number density and energy density of quanta can be written as

$$\mathcal{N} \equiv \frac{N}{V} = \frac{4\pi g}{h^3} \int n(p)\, p^2\, dp; \quad U \equiv \frac{E}{V} = \frac{4\pi g}{h^3} \int n(p)\, \epsilon(p)\, p^2\, dp,$$

where $n(p)$ is the occupation number and $\epsilon(p)$ is the energy of a single-particle state of momentum p. What is the general form of $\epsilon(p)$ according to special relativity? Show that it has the limits $\epsilon = mc^2 + p^2/2m$ when the momentum is small ($pc \ll mc^2$), and $\epsilon = pc$ in the opposite limit.

3. **Partition function** Because $Z = \sum_{n_1} \sum_{n_2} \cdots \exp[-(n_1\epsilon_1 + n_2\epsilon_2 + \cdots)/kT]$, show that the partition function is a product over states: $Z = \prod_j Z_j$, where $Z_j = \sum_{n_j} \exp[-n_j\epsilon)_j/kT]$ is a single-state-partition function. Evaluate this single-state function for fermions and bosons. For the latter, you will need a geometric series:

$$\sum_{n=0}^{\infty} e^{-\alpha n} = \frac{1}{1-e^{-\alpha}} \quad \Rightarrow \quad \sum_{n=0}^{\infty} n\, e^{-\alpha n} = \frac{e^{-\alpha}}{(1-e^{-\alpha})^2}.$$

Prove these results, and thus obtain $\langle n \rangle$ for bosons and for fermions. Hence show that at high temperatures, $kT \gg mc^2$, we have $\mathcal{N} \propto T^3$ and $U \propto T^4$.

4. **Pressure** The partition function gives the free energy, via $F = -kT \ln Z$. Hence show that

$$P = -\frac{F}{V} = \frac{4\pi g kT}{h^3} \int \ln\left[(1 \pm \exp[-\epsilon(p)/kT])^{\pm 1} \right] p^2\, dp.$$

Integrate by parts to convert this to

$$P = \frac{4\pi g}{h^3} \int n(p)\, \frac{p^2c^2}{3\epsilon(p)}\, p^2\, dp.$$

Hence show that $P = U/3$ in the high-temperature ultrarelativistic limit ($kT \gg mc^2$). In the opposite low-temperature limit, show that this recovers the classical expressions for a perfect gas: $P = \mathcal{N}kT$ and $P = \mathcal{N}m\langle v^2 \rangle/3$.

5. **Entropy** Show that the alternative expressions $S = (E - F)/T$ and $S = -\left.\partial F/\partial T\right|_V$ give the same result in this case. In the ultrarelativistic limit, show that this is $S = 4E/3T$, and that this is proportional to the total number of particles.

B: Further problems

1. **Particle number fluctuations for fermions**

   (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 explicit 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

   $$\langle\Delta N^2\rangle \simeq kTg(\epsilon_{\mathrm{F}}) \qquad \text{where} \quad \epsilon_{\mathrm{F}} = \mu(T=0)$$

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

2. **Particle number fluctuations for Bosons** 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. **Entropy of the ideal Fermi gas**

   The Grand Potential for an ideal Fermi gas 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 $S = -\left(\dfrac{\partial\Phi}{\partial T}\right)_{\mu,V}$ and some patience to obtain the result.

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

4. **Bosons in Harmonic Potentials** Consider a gas of N weakly interacting bosons trapped in a 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 pyramid.

5. **Properties of the Density Matrix** In lectures we introduced the idea of a density matrix. For the canonical ensemble the density matrix may be written in bra-ket notation as

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

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

(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

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