Statistical Physics: Workshop Problems 1

(1) In a population of fifty million people, on average, two hundred people have the same DNA profile.

(a) What is the probability of two people with the same profile?

(b) What is the probability that the police, only knowing that a suspect from the population has a DNA profile that matches that found at the scene of crime, has found the guilty party?

(2) What is the probability that out of five people, none have the same birthday?

(3) Consider a system in which the allowed (non-degenerate) one-particle states have energies $0, \epsilon, 2\epsilon, 3\epsilon, \ldots$. The assembly has four distinguishable (localised) particles ($N = 4$) and a total energy of $U = 6\epsilon$. Identify the possible distributions, evaluate the number of microstates Ω, and statistical entropy S, and work out the average distribution (i.e., the average occupation $\langle n_i \rangle$ of each energy level) and the probability p_i that each one-particle energy level ϵ_i is occupied.

(4) A manufacturer knows that their resistors have values which are distributed as a Gaussian probability distribution with a mean resistance of 100 Ω and standard deviation of 5 Ω. What percentage of resistors have resistances between 95 and 105 Ω? What is the probability of selecting a resistor with resistance less than 80 Ω?

Reminder: For a continuous probability distribution, the probability $p(a \le x \le b) = \int_a^b dx\, f(x)$. For the Gaussian probability distribution,

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$$

You may use:

$$\frac{1}{\sqrt{2\pi}} \int_{-1}^{1} dx \, \exp\left(-\frac{x^2}{2}\right) = 0.68269\,, \quad \frac{1}{\sqrt{2\pi}} \int_{-2}^{2} dx \, \exp\left(-\frac{x^2}{2}\right) = 0.95450$$

$$\frac{1}{\sqrt{2\pi}} \int_{-3}^{3} dx \, \exp\left(-\frac{x^2}{2}\right) = 0.99730\,, \quad \frac{1}{\sqrt{2\pi}} \int_{-4}^{4} dx \, \exp\left(-\frac{x^2}{2}\right) = 0.99994$$

Statistical Physics: Workshop Problems 2

(1) A particle can be in one of six degenerate states, $i = 1, 2, \ldots, 6$. The probability that the particle is in state i is p_i and the probabilities are normalised, $\sum_{i=1}^{6} p_i = 1$. The Gibbs statistical entropy of the particle for the probability distribution $\{p_1, p_2, \ldots, p_6\}$ is

$$S(\{p_i\}) = -k_{\mathrm{B}} \sum_{i=1}^{6} p_i \ln p_i.$$

Show that the set of probabilities that maximise the entropy under the constraint of normalisation (use a Lagrange multiplier), satisfy $p_i = 1/6$. Comment on the principle of equal *a priori* probabilities for a microcanonical ensemble.

(2) In a non-degenerate system the partition function Z is given by a sum over the single-particle states

$$Z = \sum_{\text{s.p. state } j} e^{-\beta\epsilon_j} = \underbrace{e^{-\beta\epsilon_1}}_{\text{s.p. state 1}} + \underbrace{e^{-\beta\epsilon_2}}_{\text{s.p. state 2}} + \ldots$$

where ϵ_j is the energy of the non-degenerate single-particle state j.

(a) What is the expression for Z when each energy level has degeneracy two?

(b) Given the (hopefully simple) result in (a) state the partition function for the case where energy levels have degeneracy $g(j)$?

(3) (a) Consider a three-dimensional (3D) simple harmonic oscillator (SHO). The energy levels are

$$\epsilon_n = (n + 3/2)h\nu.$$

The degeneracy of the n-th level is

$$g(\epsilon_n) = (n+1)(n+2)/2.$$

Show that the partition function Z_{3D} for the 3D SHO is given by

$$\log Z_{3D} = 3 \log Z_{1D}$$

where Z_{1D} is the partition function of the equivalent 1D SHO.

Hint 1: One can evaluate the infinite sum in the definition of the partition function for Z_{3D} and compare to Z_{1D}. However a simpler method is to note that the single-particle state n of a 3D SHO is given by specifying the states j, k, l of three 1D SHOs in the directions x, y, z: $n = j + k + l$, with $j, k, l = 0, 1, \ldots$. The energy ϵ_n is given by $\epsilon_n = \epsilon_j + \epsilon_k + \epsilon_l = (j + 1/2)h\nu + (k + 1/2)h\nu + (l + 1/2)h\nu$. Note that the single-particle energy levels of the 3D oscillator are degenerate but the single-particle energy levels of the 1D oscillators are not degenerate.

Hint 2: If you want to ignore Hint 1 then note that

$$\sum_{n=0}^{\infty} (n+1)(n+2)e^{-nx} = \frac{2e^{3x}}{(e^x - 1)^3}.$$

(b) From the partition function find the internal energy U, free energy F and the entropy S for a system of N distinguishable 3D SHOs.

(4) What is the heat capacity, C_V, for a system of N 3D SHOs? (This is the Einstein heat capacity of a solid.) Show that it gives a constant heat capacity for high temperatures. Using this result, explain the Dulong and Petit law, that the molar heat capacity of any solid is approximately ~ 25 J/(mol K).

Statistical Physics: Workshop Problems 3

(1) (a) Find the entropy of rolling an octahedral dice and a dodecahedral dice.

(b) How does the phase space density of a microcanonical ensemble in equilibrium change with time?

(c) What are the units of each the micro-canonical, the canonical and the grand-canonical partition functions?

(d) Which quantities are constant in the micro-canonical ensemble, the canonical ensemble and the grand-canonical ensemble?

(2) A molecule has 3 non-degenerate vibrational modes with frequencies ω, 2ω and 3ω.

(a) Calculate the vibrational partition function of the molecule and hence obtain the probability of each of the modes being excited when the molecule is in contact with a heat bath at temperature T.

(b) Determine the high and low temperature limits of the probabilities and sketch a graph showing the probabilities as a function of temperature.

(c) What is the internal energy and free energy of the molecule at temperature T. What the difference is between internal energy and free energy?

(3) A system contains non-degenerate states with energies 0, ϵ, 2ϵ, 3ϵ,... . 3 particles are distributed amongst these states such that the internal energy, U, of the system is 3ϵ. By tabulating the number of microstates in the possible distributions work out what is the probability of finding the most likely distribution of particles in the states if the particles are (a) classical, (b) Fermions and (c) Bosons?

(4) A system of classical particles occupying single-particle levels is in thermal contact with a heat reservoir at a temperature T. The population distribution in the three lowest non-degenerate energy levels is given below. What is the mean temperature of the system?

State	Energy (meV)	Population
3	21.5	8.5%
2	12.9	23.0%
1	4.3	63.0%

Statistical Physics: Workshop Problems 4

(1) Consider a particle in a box. Derive the density of states in k space, $g(k)$, and in energy space, $g(\epsilon)$, in (a) two and in (b) three dimensions.

(2) The single-particle partition function for a particle in a 3D box is

$$Z_1 = \int_0^\infty d\epsilon\, g(\epsilon)\, e^{-\beta\epsilon} = V\left(\frac{2\pi M}{\beta h^2}\right)^{3/2}.$$

- (a) What is the partition function Z_N for a gas of N such particles in volume V, classically?
- (b) Obtain the internal energy U, the free energy F and entropy S of the gas of particles.
- (c) Are the internal energy, the free energy and the entropy of the gas extensive quantities? [Hint: in order to check, double the number of particles and the volume and check if U, F also double.]
- (d) When the particles in the gas are indistinguishable, how can one correct the N particle partition function in order to obtain extensive quantities? What is the extensive expression for the entropy?
- (e) A container with a gas of identical particles is divided by a partition in two compartments of equal volume ($V/2$) and equal number ($N/2$) of particles.
  - (i) The two compartments contain the same kind of indistinguishable particles and hence the removal of the partition is a reversible process that does not involve the exchange of heat or work. What is the change in entropy when the partition is removed? Is this result expected? (Use the expression for the entropy where the indistinguishability of particles is taken into account).
  - (ii) Each of the two compartments contains a different kind of indistinguishable particles. What is the change in entropy when the partition is removed? (Entropy of mixing.)

(3) Consider a gas of N free fermions of spin 1/2 enclosed either in a box of side a and volume V (in 3D), or enclosed in a square of side a and area A (in 2D). At $T = 0$, the N fermions occupy the single-particle states in k-space, from $k = 0$ up to the Fermi wave vector $k = k_F$. The Fermi energy (ϵ_F) is

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2M}$$

where M is the mass of the free fermions.

- (a) What is the density of states (in energy) of the fermion gas in the two cases?
- (b) Calculate the Fermi wave vector k_F and the Fermi energy ϵ_F at $T = 0$ for the two cases. Note that the Fermi energy is when $n(k_F) = N$.

Statistical Physics: Workshop Problems 5

(1) A gas of N classical weakly-interacting particles is in contact with a heat bath at temperature T. The gas has a number of independent degrees of freedom.

(a) Using the Boltzmann distribution the average energy for a degree of freedom x with energy $\epsilon(x)$ is

$$\langle \epsilon(x) \rangle = \frac{\int_{-\infty}^{\infty} \epsilon(x) \exp[-\beta\epsilon(x)]dx}{\int_{-\infty}^{\infty} \exp[-\beta\epsilon(x)]dx}.$$

If $\epsilon(x) = ax^2$, where $a > 0$ and the variable x takes values in the range $-\infty < x < \infty$, obtain the average energy of a particle in this system. Note that

$$\int_{-\infty}^{\infty} \exp(-b\,x^2)dx = \sqrt{\frac{\pi}{b}}.$$

(b) Show that the internal energy U of this system of N particles, when there are η such degrees of freedom (each associated with a quadratic energy term) is

$$U = \eta\,\frac{N k_{\mathrm{B}} T}{2}.$$

This result is known as the *Equipartition Theorem.*

(2) The heat capacity at constant volume is defined as $C_V = [dU/dT]_V$. Use the Equipartition Theorem to obtain C_V in each of the following cases (ignoring electron excitations).

(a) A gas of N monoatomic neon atoms (translational motion only).

(b) A gas of N diatomic molecules of oxygen (O_2) at room temperature, due to the translational and rotational motion only (at room temperature, these are excited mainly).

(c) A gas of N diatomic molecules of oxygen (O_2) at higher temperatures, due to the contribution of vibrations only.

(d) A gas of N diatomic molecules of oxygen (O_2) at higher temperatures, due to translations, rotations and vibrations.

(3) The vibrations of a diatomic molecule can be approximated as one dimensional harmonic oscillations with energies $\epsilon_n^{\mathrm{vibr}} = (n + 1/2)\hbar\omega$, with $n = 0, 1, 2, \ldots$ and ω is the frequency of the oscillation.

(a) Derive the single-particle partition function Z_1^{vibr} for the vibrations of a diatomic molecule.

[Hint: $1 + r + r^2 + \ldots = (1 - r)^{-1}$, for $|r| < 1$.]

(b) Derive the vibrational energy, U^{vibr}, and heat capacity at constant volume, C_V^{vibr}, for a gas of N molecules of O_2. Compare your answer with that of question (2).

(c) The characteristic temperature for the excitation of vibrations, T^{vibr}, in a diatomic molecule is defined as $k_{\mathrm{B}} T^{\mathrm{vibr}} = \hbar\omega$. Write the vibrational heat capacity in terms of the ratio T^{vibr}/T.

(d) The characteristic temperature for vibrations in O_2 is $T^{\mathrm{vibr}} = 2200$ K. At room temperature (293 K) what is the vibrational heat capacity C_V^{vibr} and the percentage contribution of the vibrations to the total heat capacity of O_2 gas at constant volume?

Statistical Physics: Workshop Problems 6

(1) (a) Explain in what circumstances Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics are appropriate making reference to the number of particles that can occupy energy states and their degeneracies.

(b) Give a physical discussion on why differences in the three statistics become unimportant at high temperatures.

(c) At what temperature (order of magnitude) will quantum statistics have to be used for a system containing $10^{18}/\mathrm{cm}^3$ of neutrons?

(2) Consider a material where each of the constituent atoms may occupy one of two sites. For each atom the sites have energy ϵ_i and $-\epsilon_i$, where i labels the atom.

(a) If the energy levels are the same two values for all of the atoms (ϵ and $-\epsilon$ say) calculate the contribution of the atoms to the heat capacity of the material.

(b) Now return to the case where the energies are atom dependent (ϵ_i and $-\epsilon_i$). Find the behaviour of the low temperature heat capacity (i.e. $k_B T \ll \epsilon$). Express the result as both a sum and an integral (do not attempt to evaluate either).

(3) The quantum energy levels of a rigid rotor of mass m and length a are

$$\epsilon_j \quad = \quad j(j+1)\frac{h^2}{8\pi^2 m a^2}$$

where $j = 0, 1, 2, ...$ The degeneracy of each level is $g_j = 2j + 1$.

(a) Find the general expression for the partition function and show that at high temperatures it can be approximated by an integral (and evaluate the integral).

(b) Evaluate the high temperature energy and heat capacity.

(c) Find a low temperature approximation for the partition function and hence the low temperature internal energy and heat capacity.

(4) The electronic energy levels of a hydrogen atom are given by $E_n = -E_0/n^2$ where E_0 is a constant and $n = 1, 2, 3...$ and the degeneracy of the states are $g_n = 2n^2$.

(a) Write down the expression for the electronic partition function for a single isolated hydrogen atom at temperature T (do not try to evaluate the sum). Does the expression diverge for $T = 0$ and what about for $T \neq 0$?

(b) Is this divergence caused by the chosen zero of energy? [Add some constant E' onto the expressions for energy levels].

(c) Calculate average thermal energy,

$$\langle E \rangle \quad = \quad \frac{\sum_i E_i e^{-E_i/k_B T}}{Z},$$

of the system.

(d) We seem to have non-physical results. Can you explain what is going on? Consider what happens when an atom is confined to a large finite volume L^3 in a quantum calculation of the full partition function (you don't need this full calculation, just think degeneracies and energy levels).

Statistical Physics: Workshop Problems 7

(1) (a) The density of states in k-space for weakly interacting particles moving at relativistic speeds is the same as the non-relativistic case,

$$g(k)dk = \frac{V}{2\pi^2}k^2 dk,$$

however the energy-wavevector (momentum) relation differs; it is $\epsilon = c\hbar k$. Calculate the density of states with respect to energy, $g(\epsilon)d\epsilon$.

(b) What is the partition function for the relativistic particles? Compare the temperature dependence of the partition function to that of the non-relativistic case.

(2) (a) The density of states of non-relativistic particles is

$$g(\epsilon)d\epsilon = \frac{2\pi V}{h^3}(2M)^{3/2}\sqrt{\epsilon}d\epsilon.$$

If a system contains N particles the Fermi energy, E_F, can be defined via

$$N = \int_0^{E_F} g(\epsilon)f(\epsilon)d\epsilon$$

where $f(\epsilon)$ is a statistical distribution function. Find an expression for the Fermi energy and also the Fermi temperature of Fermions at $T = 0$.

(b) Similarly, calculate the Fermi energy for a system of N relativistic Fermions.

(c) Show that the internal energy, U, of the relativistic Fermion gas is $3NE_F/4$. Similarly show that the internal energy in the non-relativistic case is $3NE_F/5$.

(d) Calculate the Fermi energy (in eV) and Fermi temperature of

(i) liquid ^{3}He with density 0.0823 g cm^{-3},

(ii) electrons in aluminium which has valence 3 and a density of 2.7 g cm^{-3},

(iii) neutrons in the nucleus of ^{16}O given that the radius r of an atomic nucleus is $r \approx 1.2A^{1/3}$ fm where A is the atomic mass number.

(3) (a) This question uses results from (2) and (3). The electrons, protons and neutrons in a white dwarf star obey quantum statistics as the system is very dense, in fact so dense that $T = 0$ is a reasonable approximation (compare Fermi temperature of an atomic nucleus). Assume the star has radius R, mass M and contains equal numbers of protons, neutrons and electrons, and that the electrons can be treated non-relativistically. Show that the internal energy of the electrons is given by

$$U_{\text{elec}} = 0.0088\frac{h^2 M^{5/3}}{m_e m_p^{5/3} R^2}$$

where m_e is the electron mass and m_p is the proton or neutron mass.

(b) The gravitational potential energy of a star is

$$U_{\text{grav}} = -\frac{3}{5}\frac{GM^2}{R}.$$

Let $U_{\text{total}} = U_{\text{elec}} + U_{\text{grav}}$, then the white dwarf's radius, R, will be the value that minimises U_{total}. Derive an expression for the equilibrium radius, $R(M)$, of a white dwarf star as a function of the star's mass, M.

(c) Show that the radius of a white dwarf star that is the mass of our sun is approximately the radius of the Earth.

(d) Calculate the Fermi energy of the electrons in a white dwarf star of one solar mass. Do you think the non-relativistic treatment of the electrons was reasonable?

(e) If the electrons were treated relativistically show that $U_{\text{elec}} \sim R^{-1}$ rather than R^{-2}.

(f) Use (e) to explain why a white dwarf star will not be stable over a certain mass and will collapse further.

Statistical Physics: Workshop Problems 8

(1) Take a system with N free electrons in a metal with volume V. Calculate to within a reasonable approximation the following.

(a) The specific heat C_V.

(b) The magnetic susceptibility which can defined as

$$\chi = \mu_B^2 g(E_F)$$

where μ_B is the Bohr magneton and E_F is the Fermi energy.

(c) The average kinetic energy of the (non-interacting) electrons.

(d) The electron pressure (remembering how pressure is related to kinetic energy will be useful).

(2) In a Fermi gas model of atomic nuclei, except for the Pauli exclusion principle, the nucleons can be assumed to be a completely degenerate Fermi gas in a sphere of volume V. Let N be the number of neutrons and Z be the number of protons (and for simplicity let $N = Z$). If $A = N + Z$ then compute the kinetic energy per nucleon in this model if the volume of the atomic nucleus is $V = 4\pi R_0^3 A/3$ where $R_0 = 1.4 \times 10^{-13}$ cm.

(3) Non-relativistically, at what particle density does a gas of free electrons at $T = 0$ have enough kinetic energy (i.e. Fermi energy) to allow the reaction

$$\text{electron} + \text{proton} + 0.8\text{MeV} \quad \rightarrow \quad \text{neutron}.$$

Use this to estimate the minimum density of a neutron star. Look up the minimum density of a neutron star and decide whether this non-relativistic result is valid.

(4) Consider a $T = 0$ gas of N non-interacting electrons in a volume V.

(a) Find an equations that relates the volume, energy and pressure of the gas in the extreme relativistic case ($\epsilon = cp$).

(b) Estimate when the result in (a) is approximately valid.

(5) In the very early universe $k_B T$ is large and so we can assume an extreme relativistic limit where particle masses and chemical potentials are approximately zero. Calculate the average number density and energy density of a gas of Fermions in these conditions.