Example questions for Particles part of PHY293 Final Exam – SOLUTIONS

Examples of Short Answer Part (typically worth 4 points each):

Please answer the following questions showing your reasoning as well as your final answer. To receive full marks for your answer, both your reasoning and your answer must be correct.

1. At low temperatures, the temperature dependence of the heat capacity of a metal can be described by: $C_v = aT + bT^3$.

Briefly describe the origin of each of the terms in this equation and the model system we used to derive each term.

aT term – is from the conduction electrons in the metal we derived it using the degenerate Fermi gas for electrons model bT³ term – is from the lattice vibrations in the metal crystal we derived it using the Debye model of a solid

2. You have a 1000 cm³ container of 10²⁶ neon atoms in thermal equilibrium at room temperature and pressure. The mass of an atom of neon is 3.2x10⁻²⁶ kg. Calculate the temperature range over which quantum statistics would apply to this system.

Quantum statistics apply when the volume per molecule is of the same order of magnitude as the quantum volume or smaller. So first we solve T as if these are of the same order of magnitude.

$$\frac{V}{N} \approx v_Q = \left(\frac{h^2}{2\pi m kT}\right)^{3/2} \therefore T = \frac{h^2}{2\pi m kT} \left(\frac{N}{V}\right)^{2/3}$$

The density of the neon atoms in the container is:

$$\frac{N}{V} = \frac{10^{26} \text{ atoms}}{0.001 \text{ m}^3} = 10^{29} \text{ m}^{-3}.$$

Substituting into the expression above, we get:

$$T = \frac{\left(6.626 \times 10^{-34} \text{ Js}\right)^2}{2\pi \cdot 3.2 \times 10^{-26} \text{ kg} \cdot 1.38 \times 10^{-23} \text{ J/K}} \left(10^{29}\right)^{2/3} \text{m}^{-2}$$

$$T \approx 3.4 \text{ K or lower.}$$

Now we have brought the inequality back into the answer. Since the volume per atom has to be smaller than or of the same order of magnitude as the quantum volume, the temperature range where this is valid is equal to or less than 3.4 K.

3. A Boltzmann factor $(e^{-E(s)/kT})$ is proportional to the probability of finding the system in a state, s, with a specific energy, E(s). The figure below shows a bar graph of the Boltzmann factors versus energy for a hypothetical system at temperature, T. Based on the information presented in this plot, what are the energy, E(s), and the Boltzmann factor for the system in its lowest energy (or ground state)? Using two labelled sketches, show how the distribution of Boltzmann factors will change when the temperature of this system is increased (T₁ >T) and when it is decreased (T₂ < T).

4. (cont.)



E(s) for the lowest energy state or ground state, E(0), is equal to zero (as shown on the graph, at E(s) = 0kT). Therefore, the Boltzmann factor is 1.

For the system at T_1 , the curve describing the Boltzmann distribution would fall off more gradually (gentler slope to curve connecting Boltzmann factors). For the system at T_2 , the curve describing the Boltzmann distribution would fall off more suddenly (sharper slope to curve). [Labelled sketches would include the axis labels and a clear indication which sketch corresponded to which temperature.]

5. The Sackur-Tetrode Equation describes how the entropy of an ideal monatomic gas depends on its volume, total energy and number of particles. From this equation, write down an expression for the change in entropy, ΔS, when only the volume changes from V_i to V_f. For an ideal monatomic gas freely expanding into a vacuum, such that V_f=2 V_i, calculate the change in entropy, ΔS, for this process. What is the change in total energy for this process? Briefly explain this result.

$$S = Nk \left[\ln \left(\frac{V}{N v_{Q}} \right) + \frac{5}{2} \right]$$

If only the volume changes, the expression for the change in entropy is:

$$\Delta S = S_f - S_i = Nk \ln \frac{V_f}{V_i}.$$

Note: if question says to "derive" rather than "write down", more detail is needed to get full marks.

The change in entropy for this free expansion process is:

$$\Delta S = Nk \ln \frac{2V_i}{V_i} = Nk \ln 2.$$

In this free expansion process, no heat has entered or left the system and no work is done. Therefore $\Delta U=Q+W=0$.

Examples of Derivation Part (typically worth 20 points each):

Please answer the following questions showing all the mathematical steps that led to your final answer providing sufficient explanations to justify your answer.

- 6. For a diatomic molecule consisting of distinguishable atoms (such as CO or HCI), the energy for a particular rotational level is given by: $E(J) = J(J+1)\varepsilon$. The degeneracy of this energy level is given by: (2J+1). Consider a single molecule for this question.
 - a. Write down an expression for the rotational partition function of a diatomic molecule as a function of *J*.

For a single molecule, the rotational partition function is:

$$Z_1 = \sum_{J} (2J+1) e^{-\beta \varepsilon J(J+1)}.$$

b. In the low-temperature limit, each term in the rotational partition function is much smaller than the one before it. By truncating the sum after the second term, determine the rotational partition function in the low-temperature limit.

In the low temperature limit, this rotational partition function is: $Z_1 = 1 + 3e^{-2\beta\epsilon}$. (with truncation as indicated in question).

c. Calculate the average energy in the low-temperature limit. Simplify your answer by keeping only the leading order term.

Calculate the average energy using the partition function.

$$\overline{E} = -\frac{1}{Z_1} \frac{\partial Z_1}{\partial \beta}$$
$$= -\frac{1}{1+3e^{-2\beta\varepsilon}} \frac{\partial}{\partial \beta} \left(1+3e^{-2\beta\varepsilon}\right)$$
$$= -\frac{1}{1+3e^{-2\beta\varepsilon}} \left[\left(-2\varepsilon\right) 3e^{-2\beta\varepsilon} \right]$$
$$\overline{E} = \frac{6e^{-2\beta\varepsilon}}{1+3e^{-2\beta\varepsilon}}.$$

This is simplified by keeping only the leading terms in the numerator and the denominator, $\overline{E} \approx 6\varepsilon e^{-2\beta\varepsilon}$.

d. Using your simplified answer from part (c), calculate the heat capacity in the low-temperature limit.

First, calculate the total energy, $U = N\overline{E} = N \cdot 6\varepsilon e^{-2\beta\varepsilon} = 6\varepsilon e^{-2\beta\varepsilon}$ (since N=1). Then, calculate the heat capacity using:

$$C_{V} = \left(\frac{\partial U}{\partial T}\right)_{V} = \frac{\partial}{\partial T} \left(6\varepsilon e^{-2\varepsilon/kT}\right) = \left(6\varepsilon\right) \left(-\frac{2\varepsilon}{k}\right) \left(-\frac{1}{T^{2}}\right) \left(e^{-2\varepsilon/kT}\right) = \frac{12\varepsilon^{2}}{kT^{2}} e^{-2\varepsilon/kT}.$$

- 7. Consider a particular crystalline solid consisting of *N* non-interacting atoms. The atoms are located at fixed locations in the crystal lattice and the nuclei of the atoms have spin one. Therefore each nucleus has three allowed independent spin states labelled by the quantum number *m*, where m = +1, 0, or -1. The energies of these states are equal to zero in the *m* = 0 state and equal to $\mu_{N}\epsilon$ in the m = +1 and m = -1 states, where μ_{N} is the nuclear magneton and ϵ is the field strength.
 - a. Calculate the partition function for this system.

The partition function for one atom in this three state system is: $Z_{1}=e^{-0\beta}+e^{-\mu_{N}\epsilon\beta}+e^{-\mu_{N}\epsilon\beta}=1+2e^{-\mu_{N}\epsilon\beta}.$

For the crystal of N atoms, the partition function is:

$$Z = \left(Z_1\right)^N = \left(1 + 2e^{-\mu_N \varepsilon\beta}\right)^N,$$

since all of the particles are distinguishable. They are at fixed locations in the lattice.

b. Determine the Helmholtz free energy, F.

The Helmholtz free energy can be calculated from the partition function.

$$F = -kT \ln Z$$

$$= -kTN \ln \left[1 + 2e^{-\mu_N \epsilon \beta}\right].$$

c. Calculate the total energy for the crystal. Simplify your answer to obtain the most compact expression.

Here start with the expression for the average energy per atom.

$$\overline{E} = \frac{1}{Z} \sum_{s} E(s) e^{-E(s)/kT}$$
$$= \frac{1}{Z} \Big[\mu_N \varepsilon e^{-\mu_N \varepsilon \beta} + \mu_N \varepsilon e^{-\mu_N \varepsilon \beta} + 0 \Big]$$
$$\overline{E} = \frac{2\mu_N \varepsilon e^{-\mu_N \varepsilon \beta}}{1 + 2e^{-\mu_N \varepsilon \beta}}.$$

Then calculate U using $U = N \cdot \overline{E} = \frac{2N\mu_N \varepsilon e^{-\mu_N \varepsilon \beta}}{1 + 2e^{-\mu_N \varepsilon \beta}}.$

d. Show explicitly how your answers to parts (a) and (b) would change if the energies of the m = +1 and m = -1 states of the atomic nucleus were $+\mu_N \epsilon$ and $-\mu_N \epsilon$, respectively.

Single atom partition function would be: $Z_1 = e^{-0\beta} + e^{-\mu_N \epsilon \beta} + e^{+\mu_N \epsilon \beta} = 1 + 2 \cosh(\mu_N \epsilon \beta)$. Partition function for N-atom solid would be: $Z = (1 + 2 \cosh(\mu_N \epsilon \beta))^N$. The Helmholtz free energy would be: $F = -kTN \ln[1 + 2 \cosh(\mu_N \epsilon \beta)]$.