

Thermal and Statistical Physics Fall 2020

Midterm Exam

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You must show your work. No credits will be given if you don't show how you get your answers.

You may use the following formula:

- Let p_j be the probability of a system being at the j -th state, the dimensionless information entropy σ of the system is defined as $\sigma = -\sum_j p_j \ln p_j$.
- The thermodynamic entropy S is related to the information entropy as $S = k_B \sigma$, where k_B is the Boltzmann constant.
- The internal energy U is defined as $U = \sum_j p_j E_j$, where E_j is the energy of the j -th state.
- The temperature T and pressure P can be defined as

$$\frac{1}{T} \equiv \left(\frac{\partial S}{\partial U} \right)_{V,N}, \quad \frac{P}{T} \equiv \left(\frac{\partial S}{\partial V} \right)_{U,N},$$

where N, V are the number of particles and the volume of the system.

- From the above definition and the first law the thermal dynamics, one can identify the heat transfer $dQ = TdS$, and thus the first law can be written as $TdS = dU + PdV$.
- The heat capacity at fixed volume is $C_v = \left(\frac{T \partial S}{\partial T} \right)_V$.
- Given the constraints $U = \sum_j p_j E_j$ and probability conservation, the probability distribution which maximizes σ is the Boltzmann distribution $p_j = \frac{e^{-\beta E_j}}{Z}$, where $\beta = (k_B T)^{-1}$, and Z is the partition function $Z = \sum_j e^{-\beta E_j}$.
- The Helmholtz free energy $F = U - TS$. It tends to be minimized during

a process at constant T and V .

- Useful relations:

$$U = -\frac{\partial}{\partial \beta} \ln Z,$$

$$\sigma = \beta U + \ln Z,$$

$$F = -k_B T \ln Z.$$

- Sackur-Tetrode equation for monoatomic ideal gas

$$\sigma = N \left[\ln \left(\frac{n_Q}{n} \right) + \frac{5}{2} \right], \quad \left(\ln \left(\frac{n_Q}{n} \right) + \frac{5}{2} \right) + N \left(\frac{N}{n_Q V} - \frac{n_Q V}{N} \right)$$

where $n_Q = \left(\frac{mk_T}{2\pi\hbar^2} \right)^{3/2}$ is the quantum concentration, and $n = N/V$.

- For a system at thermal equilibrium with temperature T and diffusive equilibrium, the chemical potential μ is defined as

$$-\frac{\mu}{T} \equiv \left(\frac{\partial S}{\partial N} \right)_{V,U},$$

and the grand partition function is

$$\mathcal{Z} = \sum_i e^{\beta(\mu N_i - E_i)},$$

where N_i and E_i are all possible number of particles and energies of the system. The probability of the system having N_j particles with (total) energy E_j is

$$p_j = \frac{e^{\beta(\mu N_j - E_j)}}{\mathcal{Z}}.$$

- The first law the thermal dynamics, taking into account the change in particle numbers, can be written as

$$dU = TdS - PdV + \mu dN.$$

$$F = U - TS. \quad dF = dU - TdS - SdT$$

- The Stirling's formula $\ln N! \approx N \ln N - N$.

dS

$$\ln \cdot \frac{n_Q V}{N}$$

$$k_B T \cdot \ln \frac{1}{n_Q V} + k_B T \ln N.$$

$\frac{na}{N}$

1. Consider a three-state system with energy levels $E = -\Delta, 0, +\Delta$ ($\Delta > 0$). The system has N distinguishable particles and it is at thermal equilibrium of temperature T :

$U = Td$
 $TdS = dU = TdS - PdV$

- (a) What is the internal energy U of this system? (2 points)
 (b) The splitting among energy levels Δ usually changes when you compress or expand the system. Suppose Δ changes with respect to volume V as $\frac{\partial \Delta}{\partial V} = -\gamma \frac{\Delta}{V}$, show that the pressure P is related to U and V as

(2 points) $P = \gamma \frac{U}{V}$. $\frac{P}{T} = \left(\frac{\partial S}{\partial V} \right)_U$

- (c) Write down an expression for the entropy S of the system. How does S behave at low and high temperatures? (4 points)
 [Note: Please explain what you mean by "low" and "high" temperatures. If you have problem solving the math, partial credits may be given if you can explain the limiting behaviors in physics.]
 (d) Explain in physics the behaviors of the heat capacity C_v at low and high temperatures. No need to carry out the exact calculations. (2 points)

2. For a monoatomic ideal gas molecule with mass m , temperature T , and occupying a volume V , the one-particle partition function Z_1 is $n_Q V$, where $n_Q = \left(\frac{mk_B T}{2\pi \hbar^2} \right)^{3/2}$.

- (a) What is the partition function of N molecules? Please explain your reasoning. (1 point)
 (b) [Bonus] Derive the Sackur-Tetrode equation using your result from part (a). (2 points)
 [Hint: Use the Stirling's formula.]
 (c) Derive the chemical potential μ for the ideal gas from (i) the entropy and (ii) the Helmholtz free energy. Do you get the same result from approach (i) and approach (ii)? If not, can you explain the reason and choose the "correct" one? (4 points)

$\beta = \frac{1}{k_B T}$

[Note: You should get the same result if you perform the calculations correctly for both ways. However, in case you found one method seems to give you the wrong answer, if you can explain what went wrong in your derivation, full credits will be given if you get the right answer from the other method.]

- (d) If the density of the ideal gas is doubled, does μ increase or decrease? By how much? (2 points)

[Note: Even if you don't know how to derive μ , partial credit may be given if you can explain the behavior of μ in physics.]

3. Consider a material which can absorb a certain type of gas molecule. A surface made of such material is surrounded by this gas. Suppose the surface has N absorption sites. If a gas molecule is absorbed, it is attached to one of the absorption sites with energy $-\epsilon$ ($\epsilon > 0$). Each site can only absorb one molecule. The surface and the gas is at equilibrium with temperature T . The chemical potential of the gas is μ .

- (a) For one site, what is the probability of absorption (the probability that the site is occupied by a gas molecule)? (2 points)
- (b) What is the expected number of occupied sites at high temperature? Explain your reasoning. (2 points)
- (c) What is the expected number of occupied sites at low temperature? Can you see why $\mu + \epsilon > 0$ is called "strong binding" while $\mu + \epsilon < 0$ is "weak binding"? (4 points)

