09.21.52 Safneðlisfræði
Tíma- og heimadæmi
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The problems have been borrowed from several different sources in equally many languages. Try to solve as many as possible. They are not ordered according to difficulty. Often similar examples are solved in our textbook.

1. Show that the following expressions for the entropy are equivalent in the thermodynamic limit
$$S = k_B \ln \omega(E, V, N)$$
$$S = k_B \ln \sigma(E, V, N)$$
where $\omega(E, V, N)$ is the volume of the phase space limited by the surface of constant energy $\mathcal{H}(p, q) = E$, and $\sigma(E, V, N)$ is the derivative with respect to E of the volume $\omega(E, V, N)$. The particles are considered to be free.

2. Consider a system of N free particles in which the energy of each particle can assume two and only two distinct values, 0 and E ($E > 0$). Denote by n_0 and n_1 the occupation numbers of the energy level 0 and E, respectively. The total energy of the system is U.
   (a) Find the entropy of such a system.
   (b) Find the most probable values of n_0 and n_1, and find the mean square fluctuation of these quantities.
   (c) Find the temperature as a function of U, and show that it can be negative.
   (d) What happens when a system of negative temperature is allowed to exchange heat with a system of positive temperature?
   (e) Show that the maximum (minimum) entropy corresponds to minimum (maximum) information on the system.
   (f) How many bits of information are lost if the system evolves from an initial state of zero temperature to a final state of infinite temperature?

3. Consider a classical system whose Hamiltonian can be expressed as $H = H_0 + \lambda H_1$, where $\lambda << 1$. Show that the expansion of the Helmholtz free energy in powers of λ has the form
$$F = F_0 + \lambda \langle H_1 \rangle_0 + \cdots,$$
where F_0 and $\langle \cdots \rangle_0$ denote the free energy and an expectation value calculated with $\lambda = 0$, and find the next term in this series. Within this expansion, find the internal energy $U = \langle H \rangle$ correct to the first order in λ.

4. Consider a classical system of N noninteracting diatomic molecules enclosed in a box of volume V at temperature T. The Hamiltonian for a single molecule is taken to be

$$\mathcal{H}(\mathbf{p}_1, \mathbf{p}_2, \mathbf{r}_1, \mathbf{r}_2) = \frac{1}{2m}(p_1^2 + p_2^2) + \frac{1}{2}K|r_1 - r_2|^2,$$

where $\mathbf{p}_1, \mathbf{p}_2, \mathbf{r}_1, \mathbf{r}_2$, are the momenta and coordinates of the two atoms in a molecule. Find

   (a) the Helmholtz free energy $F(T, V, N) = U - TS$ of the system;

   (b) the specific heat at constant volume;

   (c) the mean square molecule diameter $\langle |r_1 - r_2|^2 \rangle$.

5. Repeat the last problem, using the Hamiltonian

$$\mathcal{H}(\mathbf{p}_1, \mathbf{p}_2, \mathbf{r}_1, \mathbf{r}_2) = \frac{1}{2m}(p_1^2 + p_2^2) + \epsilon |r_{12} - r_0|$$

where ϵ and r_0 are given positive constants and $r_{12} \equiv |\mathbf{r}_1 - \mathbf{r}_2|$.

Answer:

$$\frac{C_V}{Nk} = 6 - \frac{x^2[2(x^2 - 2) + (x + 2)^2 \exp(-x)]}{(x^2 + 2 - \exp(-x))^2}$$

where $x \equiv \epsilon r_0 / kT$

6. Prove *Van Leeuwen's Theorem*: The phenomenon of diamagnetism does not exist in classical physics. The following hints may be helpful:

   (a) If $\mathcal{H}(\mathbf{p}_1, .., \mathbf{p}_N; \mathbf{q}_1, .., \mathbf{q}_N)$ is the Hamiltonian of a system of charged particles in the absence of an external magnetic field, then $\mathcal{H}[\mathbf{p}_1 - (e/c)\mathbf{A}_1, .., \mathbf{p}_N - (e/c)\mathbf{A}_N; \mathbf{q}_1, ..., \mathbf{q}_N]$ is the Hamiltonian of the same system in the presence of an external magnetic field $\mathbf{H} = \nabla \times \mathbf{A}$, where $\mathbf{A}_i$, is the value of $\mathbf{A}$ at the position $\mathbf{q}_i$.

   (b) The induced magnetization of the system along the direction of $\mathbf{H}$ is given by

$$M = \langle -\frac{\partial \mathcal{H}}{\partial H} \rangle = kT \frac{\partial}{\partial H} \log Z(T, H, N)$$

   where $\mathcal{H}$ is the Hamiltonian in the presence of $\mathbf{H}$, $H = |\mathbf{H}|$, and $Z(T, H, N)$ is the partition function of the system in the presence of the external magnetic field $\mathbf{H}$.

7. Compute the average energy and the heat capacity of a classical system of N non-identical particles in d spatial dimensions, that has a Hamiltonian of the form

$$H = \sum_{i=1}^{N} A_i |\mathbf{p}_i|^s + B_i |\mathbf{q}_i|^t.$$

The parameters A_i and B_i characterize individual particles, while s and t are positive integers, and the system is maintained at a fixed temperature T. As a special case, obtain the average energy and heat capacity for N three-dimensional harmonic oscillators.

8. A simple model of the DNA molecule describes it as two strings with N connecting links. The links can be opened like teeth in a zipper, first the link at one end is opened and then the links closest to the end in a sliding action. To open one link the energy $\epsilon > 0$ is needed. Calculate the mean number of open links as a function of T, if $\epsilon >> k_B T$.

9. A 'lattice gas' consists of a lattice of N sites, each of which be empty, in which case the energy is zero, or occupied by one particle, in which case its energy is ϵ. Each particle has a magnetic moment of magnitude μ which, in the presence of an applied magnetic field B, can adopt two orientations (parallel or antiparallel to the field).

   (a) Find the canonical partition function for this system.

   (b) Evaluate the average energy and the magnetization of the system.

10. A system of three-level particles has a Hamiltonian of the form

$$H = -h \sum_{i=1}^{N} S_i, \quad S_i = -1, 0, +1,$$

   where h is a positive constant. If n_S is the average number of particles in the state S, use the microcanonical ensemble to find the ratio n_{-1}/n_{+1} in terms of the temperature in the limit $N \to \infty$. Hence find the Helmholtz free energy $F(T, N)$ by using the canonical ensemble (which is much easier). Identify the limits in which the information on the state of the system is maximum and minimum and find the entropy in these cases.

11. A molecule consisting of two different atoms has the moment of inertia I. We shall here only consider the rotational degree of freedom. The molecule is in contact with a heat bath with temperature T. The rotational states of the molecule have the energy

$$E_j = \frac{j(j+1)\hbar^2}{2I}$$

   with the degeneracy $(2j + 1)$.

   (a) Find the average energy of the molecule.

   (b) Use approximations to calculate the heat capacity of the molecule for a low temperature, and a high temperature. Give arguments in which interval the approximation is good.

(c) The classical energy of the molecule is $E = I\omega^2/2$. Evaluate the classical heat capacity. How does it compare to the quantum mechanical one?

12. The particles in an ideal gas have a magnetic moment μ. In a magnetic field the magnetic moment can assume two directions. A homogeneous magnetic field of strength B is in one half of the gas container and none in the other half. Find the ratio between the number of particles in each half of the container.

13. Show that in a 3D dilute quantum gas the thermal equation of state is

$$\frac{p}{kT} = n \pm n\left(\frac{1}{2^{5/2}}\right)(n\lambda^3) + O\left((n\lambda^3)^3\right),$$

where $+$ stands for fermions and $-$ for bosons.

14. Red blood cells can bind both oxygen, O_2 and carbon monoxide, CO. Consider the cells as a lattice with N_0 sites which can either be empty or occupied by oxygen or carbon monoxide. The binding energy for an oxygen molecule is $-\epsilon_A$ and for carbon monoxide $-\epsilon_B$. Find how the ratio of bound molecules of either type depends on the energy difference $\epsilon_B - \epsilon_A$ and the relative quantity of carbon monoxide in the atmosphere. The ratio of monoxide in the atmosphere is 10^{-3} at $T = 37°$ C. How large can the energy difference be in eV without carbon monoxide binding easier than oxygen?

15. Investigate the statistical thermodynamics of an ideal Bose gas in a uniform gravitational field (of acceleration g). Show, in particular, that the phenomenon of Bose-Einstein condensation sets in at a temperature T, given by

$$T_c \approx T_c^0\left[1 + \frac{8}{9}\frac{1}{\zeta(3/2)}\left(\frac{\pi mgL}{kT_c^0}\right)^{1/2}\right]$$

where L is the hight of the container and $(mgL) << (kT_c^0)$. Also show that the condensation is accompanied by a discontinuity in the specific heat of the gas:

$$(\Delta C_V)_{T=T_c} \approx -\frac{9}{8\pi}\zeta\left(\frac{3}{2}\right)Nk\left(\frac{\pi mgL}{kT_c^0}\right)^{1/2}$$

16. Consider an ideal Bose gas composed of molecules with internal degrees of freedom. Assuming that, besides the ground state $\epsilon = 0$, it is only the first excited state ϵ_1 of the *internal* spectrum that needs to be taken into account, determine the condensation temperature of the gas as a function of ϵ_1. Show in particular that, for $(\epsilon_1/(kT_c^0)) >> 1$,

$$\frac{T_c}{T_c^0} \approx 1 - \frac{\frac{2}{3}}{\zeta\left(\frac{3}{2}\right)} \exp\left(-\frac{\epsilon_1}{kT_c^0}\right)$$

and for $(\epsilon_1/(kT_c^0)) << 1$,

$$\frac{T_c}{T_c^0} \approx \left(\frac{1}{2}\right)^{2/3} \left[1 + \frac{2^{4/3}}{3\zeta(3/2)} \left(\frac{\pi\epsilon_1}{kT_c^0}\right)\right]^{1/2}.$$

17. Evaluate the grand partition function of a two-dimensional ideal Bose gas and derive an expression for the (equilibrium) number of particles *per unit area* of the system as a function of the parameters z and T. Show that this system does not exhibit the phenomenon of Bose-Einstein condensation.

18. Show that, in *two* dimensions, the specific heat $C_V(N, T)$ of an ideal gas of fermions is identical with the specific heat of a corresponding gas of bosons, for all values of N and T. Further show that in the extreme relativistic case the same result holds in *one* dimension.

19. Evaluate the entropy, S, the internal energy, U, and the heat capacity, C, of the one-dimensional Ising model in the case of no external magnetic field B.

20. Write down the transfer matrix for the one-dimensional spin-1 Ising model in zero field which is described by

$$H = -I \sum_i \sigma_i \sigma_{i+1}, \quad \sigma_i = \pm 1, 0. \tag{1}$$

Hence calculate the free energy per spin of this model and show that it has the expected behavior in the the limits $T \to 0$ and $T \to \infty$.

Answer:

$$F = -k_B T \ln \left[\frac{1 + 2\cosh\beta I + \sqrt{(2\cosh\beta I - 1)^2 + 8}}{2}\right]. \tag{2}$$

21. Consider an interface in the one-dimensional Ising model,

$$\sigma_i = -1, i < 0; \quad \sigma_i = 1, i \geq 0. \tag{3}$$

By writing down the energy and the entropy associated with such an excitation argue that the one-dimensional Ising model cannot sustain long-range order for any non-zero temperature.

22. Calculate the correlation function

$$\Gamma_R = (\langle \sigma_0 \sigma_R \rangle - \langle \sigma_0 \rangle \langle \sigma_R \rangle), \tag{4}$$

and the correlation length

$$\xi^{-1} = \lim_{R \to \infty} \left\{ -\frac{1}{R} \ln |\langle \sigma_0 \sigma_R \rangle - \langle \sigma_0 \rangle \langle \sigma_R \rangle| \right\}, \tag{5}$$

of the one-dimensional Ising model using the technique of transfer matrices.