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PHYS 403: HOMEWORK ASSIGNMENT No. 2: CANONICAL ENSEMBLE

(Feb. 8th, 2022)

HOMEWORK DUE: MONDAY, Feb 21st, 2022

To be uploaded by 11.59 pm, Monday Feb 21st - Late Homework will not be accepted

QUESTION (1) SET of 2-LEVEL SYSTEMS: Consider a set of N non-interacting 2-level systems (TLS), with level energies E_1 and E_2 for each of the TLS.

1(a) At temperature T, find the average energy $U(T)$ and the specific heat $C_V(T)$ for the system.

1(b) Find expressions for $U(T)$ and $C_V(T)$ when $kT \gg |E_1 - E_2|$. You should find the $T = \infty$ result, and also the first correction to this result, for finite (but very large) T.

1(c) Now let's consider an approximate result for a set of weakly interacting spin-1/2 spins. Suppose this is found to have an entropy $S(U)$ as a function of energy U which looks roughly like $S(U) = S_o - \alpha U^2$, for $U^2 < \alpha$, and zero for $U^2 > \alpha$, as a function of the total energy U. Find U in terms of T, and sketch a graph of it.

1(d) What is the specific heat of the system in 1(c), system, in the temperature range $-\infty < T < \infty$? How do you interpret this result for $T < 0$?

QUESTION (2) DIATOMIC GAS: A symmetric diatomic molecule has 7 degrees of freedom, viz., 3 translational modes of the molecular centre of mass, 3 rotational modes abut the centre of mass, and the distance between the 2 atoms. We will suppose these degrees of freedom to be independent, ie., with no coupling between them. The diatom is made from 2 atoms, each with mass m, and mean separation a_o. The moment of inertia of the rotating diatom is $I = 1/2ma_o^2$. We also suppose that the frequency of small harmonic oscillation of the distance x around the mean a_o between the atoms is ω_o.

2(a): Show that we can write the total canonical partition function $\mathcal{Z}$ for a gas of N such diatoms as $\mathcal{Z} = Z_{tr} Z_{rot} Z_{vib}$, where Z_{tr} comes from the translational degrees of freedom, $Z_{rot} = z_I^N$ is for rotational motion,and $Z_{vib} = z_{\omega_o}^N$ is for vibrational motion; and then show that

$$z_I = \sum_{j=0}^{\infty} (2j+1) \exp[-\beta \hbar^2 j(j+1)/2I] \; ; \qquad\qquad z_{\omega_o} = \sum_{n=o}^{\infty} \exp[-\beta\hbar(n + \tfrac{1}{2})\omega_o]$$

There is no need to evaluate the translational term Z_{tr}.

2(b) Evaluate the vibrational partition function $z_{\omega_o}(\beta)$, and show that the vibrational contribution to the energy of the system is $U_{vib}(\beta) = \frac{1}{2} N\hbar\omega_o \coth(\beta\hbar\omega_o/2)$. From this find also the contribution $C_V^{vib}(\beta)$ to the specific heat, and then sketch the behaviour of both $U_{vib}(\beta)$ and $C_V^{vib}(\beta)$ as functions of the temperature T.

2(c) Now consider Z_{rot}. Find the low T behaviour by taking just the first 2 terms in the sum. From this find expressions for $U_{rot}(T)$ and $C_V^{rot}(T)$ for the N diatoms in the low T regime.

For the high-T behaviour one can approximate the sum as an integral. Show that when $kT \gg \hbar^2/2I$, one gets a simple result $\propto kT$. From this result, find the energy U_{rot} and $C_V^{rot}(T)$ for the N diatoms in this high T regime.

Finally, plot sketches for U_{rot} and $C_V^{rot}(T)$ for the N diatoms as a function of T.

2(d) The "third" contribution to the specific heat coming from the translational degrees of freedom is just that from a 3-d classical gas, for which $C_V = 3Nk_B/2$. Typically, the vibrational zero point energy $\hbar\omega_o/2 \gg \hbar E_o$, where $E_o = \hbar^2/2I$ is the rotational zero point energy. Using the results you have derived above for $C_V^{rot}(T)$ and $C_V^{vib}(T)$, sketch the result you expect for the TOTAL specific heat $C_V(T)$ for a gas of N diatoms, as a function of T. Explain the limiting behaviour you find for $C_V(T)$ for (i) high T (ie., for $T \gg \hbar\omega_o/2$) and for low T (ie., for $kT \ll \hbar^2/2I$)?

END of 2ND HOMEWORK ASSIGNMENT