**PHYS20352: Thermal and Statistical Physics**

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**Example Sheet 11**

1. (Exam question 1995) The diatomic molecules of certain gas (each with moment of inertia $I$) have rotational energy levels given by

$$\epsilon_l = \frac{\hbar^2 l(l+1)}{2I}, \quad l = 0, 1, 2, \ldots,$$

with degeneracy $g_l = (2l+1)$.
(a) Show that the one-body rotational partition function, $Z_1$, is given by

$$Z_1 = 1 + 3e^{-\hbar^2/Ik_BT}$$

in the low-temperature limit ($T \ll \hbar^2/k_BI$), and by

$$Z_1 = \frac{2Ik_BT}{\hbar^2}$$

in the high-temperature limit ($T \gg \hbar^2/k_BI$).

[In the latter case the summation over $l$ may be replaced by an integral (why?), which may then be evaluated by the substitution $x = l(l+1)$.]

(b) Calculate the rotational contribution to the internal energy of one mole of $N_2$ at 20 °C, given that $I = 1.42 \times 10^{-46}$ kg m$^2$.

2. The partition function of a classical ideal gas of $N$ identical monatomic molecules was obtained in class as

$$Z_N = \frac{1}{N!} Z_1^N, \quad Z_1 = V\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2}.$$

(a) Calculate its Helmholtz free energy $F$ and then entropy $S$. Compare your entropy result with the following thermodynamic result of Q2(a) of Example Sheet 5,

$$S - S_0 = C_V \ln\frac{T}{T_0} + nR\ln\frac{V}{V_0}, \quad \text{with } C_V = \frac{3}{2}k_BN \text{ and } nR = Nk_B,$$

and discuss their differences. You may need the Stirling approximation $\ln N! \approx N\ln N - N$.
(b) Discuss the problem in the entropy expression you obtained in part (a) in the limit $T \to 0$ and provide possible explanations.