NE334 Assignment 3
Due December 3, 2024

Question 1.

Calculate the equilibrium constant K_p for the gaseous reaction

$$2\mathrm{HI}(g) \quad \rightleftharpoons \quad \mathrm{H_2}(g) + \mathrm{I_2}(g)$$

using the following spectroscopic data (from Herzberg and Huber):

molecule	$\mathrm{H_2}(^1\Sigma_g^+)$	$\mathrm{I_2}(^1\Sigma_g^+)$	$\mathrm{HI}(^1\Sigma^+)$
$B_e\,/\mathrm{cm}^{-1}$	60.853	0.0373	6.4264
$\overline{\nu}_{\mathrm{osc}}\,/\mathrm{cm}^{-1}$	4401.21	214.50	2309.01
$D_0\,/\mathrm{eV}$	4.47813	1.54238	3.0541

Plot $K_p(T)$ as a function of temperature for temperatures varying from 300 K to 3000 K. In particular compare your calculated values with those given by Taylor and Crist [*J. Amer. Chem. Soc.* **63**, 1377 (1941)].

Question 2.

Consider a box into which particles can be placed in a set of 10 single- particle states. For simplicity, assume that each state has energy 0.

(a) What is the value for the molecular partition function if the box contains only a single particle?

(b) What values do you obtain for the partition function if the box contains one of: two distinguishable particles, two identical bosons, two identical fermions?

(c) What value does the canonical partition function $Z_N = \frac{z^N}{N!}$ take?

(d) What are the probabilities for finding both particles in the same single-particle state in each of the three cases (i.e. distinguishable particles, bosons, fermions)?