

# ROTATION OF DIATOMIC MOLECULES

FYS2160

SEBASTIAN G. WINTHER-LARSEN  
GITHUB.COM/GREGWINTHER

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## 1. INTRODUCTION

This study shows how to connect a microscopic and macroscopic representation of a canonical system, as system with given  $N$ ,  $V$  and  $T$  (number of particles/-molecules, volume of the system and temperature respectively). A general method can be applied to all canonical systems. First, finding the partition function. Second, one derives a function for Helmholtz free energy. Lastly, the remaining interesting aspects of the system can be found, like the entropy and heat capacity.

## 2. A SIMPLIFIED MODEL SYSTEM

In this simple system we look at a diatomic molecule, which at low temperatures can be in four different states,  $i = 1, 2, 3, 4$ , with energies  $\varepsilon_i = \varepsilon$ ,  $\varepsilon_2 = \varepsilon_3 = \varepsilon_4 = 2\varepsilon$ . In other words, this system has two possible energies,  $\varepsilon$  and  $2\varepsilon$ . The highest energy has a degeneracy of 3.

The partition function is found by the following formula

$$(1) \quad Z = \sum_i e^{-\beta E_i}, \quad \beta = \frac{1}{kT},$$

colloquially, the sum of a special transform of every state. For this system the partition function is

$$(2) \quad Z = e^{-\beta\varepsilon} + 3e^{-2\beta\varepsilon}$$

Now to employ Helmholtz' free energy

$$(3) \quad F = -kT \ln Z.$$

First, computing

$$\begin{aligned} \ln Z &= \ln(e^{-\beta\varepsilon} + 3e^{-2\beta\varepsilon}) = \ln(e^{-\beta\varepsilon}) + \ln(1 + 3e^{-\beta\varepsilon}) \\ &\approx \ln(e^{-\beta\varepsilon}) + \ln(3e^{-\beta\varepsilon}) = -\beta\varepsilon + \ln(3) - \beta\varepsilon = -2\beta\varepsilon + \ln(3) \end{aligned}$$

This is all probably wrong....