Ideal Gases Partition Functions Mastery of Fundamentals Questions
CH353 – Prof. Wu

Here are some questions to test your mastery of the fundamentals of ideal gases and partition functions used in statistical mechanics. Once you’ve mastered the material, you should be able to answer these questions without reference to your notes or textbook.

For Ideal Gases and Partition Functions:

1. Write down the equation for the partition function of an ideal gas, Q, in terms of the molecular partition function, q. Explain why this equation has the form it does.
2. Which quantum systems are used to model each degree of freedom in the molecular partition function?
3. Which molecular parameters enter into the translational partition function? Into the rotational partition function? Vibrational? Electronic?
4. Explain why only the translational partition function depends on volume.
5. Explain qualitatively why the sum in q can be approximated by an integral for the translational and rotational partition functions. Under which situations would this approximation fail to be accurate?
6. At room temperature, which degrees of freedom (translational, rotational, vibrational and electronic) in a typical molecule will be found in an excited state?
7. How high does the temperature have to be before the electronic degrees of freedom contribute significantly to the heat capacity? How about for the other degrees of freedom (translation, rotation, vibration)?
8. What is a vibrational temperature? A rotational temperature?
9. Explain why the heat capacity for an ideal gas can be decomposed into a sum of individual contributions from translation, rotation, vibration and electronic.
10. Explain qualitatively why the heat capacity for a monatomic ideal gas is a constant with respect to temperature (neglecting electronic degrees of freedom), but not for a diatomic ideal gas.
11. Why is the vibrational partition function a product of partition functions for each vibrational mode? How many vibrational modes are there for a molecule of N atoms?

In addition, you should feel comfortable doing problems like those that have been assigned in homework. Here are some additional problems you should feel comfortable doing once you’ve mastered the material.

1. For a system with a finite number of states, why does the heat capacity approach zero as the temperature goes to infinity? Why does the heat capacity approach zero as the temperature goes to zero?
2. Given a vibrational temperature or frequency, calculate the population of the different vibrational states.
3. Given a molecule, determine its symmetry number, and identify how it affects the rotational partition function.
4. Given a molecule, write down its partition function in terms of molecular parameters such as mass, moment of inertia, vibrational frequencies, etc.