

9 Gases, Liquids; Magnetism

9.1: Quantum harmonic oscillator

The energy levels of a quantum mechanical harmonic oscillator at frequency ω are

$$\varepsilon_n = \hbar\omega \left(\frac{1}{2} + n \right), \quad n = 0, 1, 2, \dots \quad (1)$$

The canonical partition function $Z(T)$ of this a harmonic oscillator frequency ω is

$$Z(T) = \frac{1}{2 \sinh(\hbar\omega/2kT)}.$$

In this exercise we'll take a different look at this calculation: We view each oscillation quantum as a “particle”. The total energy of the system is given by Equation (1) above, but now “ n ” is interpreted as the number of particles.

- (a) Calculate the “canonical partition function” $Z_n(T)$ for a harmonic oscillator with n oscillation quanta.
- (b) Calculate the “grand canonical partition function” $\Xi(T, \mu)$, where μ is the “chemical potential” for the oscillation quanta. [You'll fix the value of μ in part (d) below.]
- (c) Use your answer to (b) to calculate the average energy $\bar{E}(T, \mu)$ and the entropy $S(T, \mu)$ of the harmonic oscillator.
- (d) Calculate the average energy and the entropy from the canonical partition function $Z(T)$. How do your answers compare to those of part (c)? What chemical potential should one choose for the oscillation quanta?

9.2: Entropy of a nonideal gas

Exercise 10.7 from Reif's book

9.3: Equilibrium fluctuations

The grand canonical ensemble describes a system for which the temperature T , the volume V , and the chemical potential μ are fixed. In the grand canonical ensemble, the number of particles N is allowed to fluctuate.

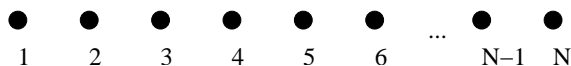
- (a) Express $\text{var } N$ in terms of T , V , μ , and derivatives of the average particle \bar{N} to T , V , and μ .
- (b) Use thermodynamic relations to rewrite your answer in terms of the isothermal compressibility $\kappa = -(1/V)(\partial V/\partial p)_{T,N}$.

9.4: One dimensional paramagnet

In this exercise, you are asked to consider the Ising model in one dimension,

$$H = -\frac{J}{2} \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} - \mu_B B \sum_i \sigma_i,$$

where $\sigma_i = \pm 1$, $i = 1, \dots, N$ (see figure), μ_B is the Bohr magneton, B is the magnetic field, and J is the exchange interaction constant.



For this system, the canonical partition function reads

$$Z = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_N=\pm 1} \exp \left[\frac{J}{2kT} (\sigma_1\sigma_2 + \sigma_2\sigma_3 + \dots + \sigma_{N-1}\sigma_N) \right].$$

Below, you'll show that in one dimension the $J \neq 0$ Ising model at zero magnetic field can be mapped to the $J = 0$ Ising model at nonzero magnetic field. In order to achieve this, instead of using the variables σ_i , $i = 1, 2, \dots, N$ to describe the microscopic state of the magnet, one uses variables τ_i , which are defined as

$$\sigma_1 = \tau_1, \quad \sigma_2 = \tau_1\tau_2, \quad \sigma_3 = \tau_1\tau_2\tau_3, \quad \dots, \quad \sigma_N = \tau_1\tau_2 \dots \tau_N.$$

Each variable τ_i can take values ± 1 , just like the original variables σ_i .

- (a) Express the new variables τ_i in terms of the original variables σ_i .
Hint: Use $\tau_i^2 = \sigma_i^2 = 1$.
- (b) Show that the canonical partition function Z is formally equivalent to that of the $J = 0$ Ising model with a magnetic field once Z is written in terms of the variables τ_i . Use this to calculate Z .

- (c) The same variable change can be used to calculate a “spin-spin correlation function”, which is defined as the average $\overline{\sigma_i \sigma_{i+p}}$. Show that spin-spin correlations decay exponentially with the “distance” p ,

$$\overline{\sigma_i \sigma_{i+p}} = e^{-|p|/\zeta},$$

and find an expression for the “correlation length” ζ .

Hint: Use the fact that $\sigma_i \sigma_{i+p} = \tau_{i+1} \tau_{i+2} \dots \tau_{i+p}$ if $p > 0$. Then argue that the average of a product of τ_i 's factorizes.

Suggested problems for further study:

9.5: Virial expansion

The equation of state of a non-ideal gas can be written in terms of the virial expansion,

$$p = nkT(1 + B_2 n),$$

where $n = N/V$ is the density of gas molecules and B_2 is the second virial coefficient. In lecture we calculated B_2 for a simplified potential between the gas molecules and found a relation of the form

$$B_2 = r_0^3 \left(a - \frac{bu_0}{kT} \right),$$

where r_0 and u_0 are microscopic length and energy scales, respectively, and a and b are positive numerical constants. [FYI: r_0 is the distance between the molecules for which their interaction potential $\mathcal{V}(r)$ is minimal, and $-u_0$ is $\mathcal{V}(r_0) - \mathcal{V}(\infty)$.]

- (a) Find how the mean internal energy \bar{E} of this gas depends on its volume V , i.e., find an expression for $(\partial \bar{E} / \partial V)_T$.
- (b) Explain the sign of your answer to (a).

9.6: Grand canonical ensemble

Consider an ideal gas in a container of volume V and at temperature T .

- (a) Calculate the grand canonical partition function $\Xi(\mu, V, T)$ for this system.

- (b) Make use of the relation $pV = kT \ln \Xi$ to express the chemical potential μ in terms of the pressure p and the temperature T . Compare your answer to that of exercise 8.4c.

9.7: Classical magnet

Exercise 7.14 from Reif's book. Compare your answer to the quantum mechanical result.

9.8: Equilibrium energy fluctuations

Fluctuations of the internal energy in equilibrium are characterized by the mean square fluctuations,

$$\overline{(\Delta E)^2} = \overline{(E - \bar{E})^2}.$$

Calculate the mean square energy fluctuations for the ideal monatomic gas using (a) the canonical ensemble and (b) the grand canonical ensemble. Compare your results.

9.9: Equilibrium magnetization fluctuations

For the Ising model, show that the mean square fluctuations of the magnetization are given by

$$\overline{\Delta M^2} = kT\chi,$$

where χ is the magnetic susceptibility. What can you say about the magnetization fluctuations close to the critical point?

9.10: Heat capacity of an Ising magnet

Consider an Ising model with N lattice spins and no external magnetic field.

- (a) Using the mean-field approximation, find an expression for the internal energy E of the Ising model. Give detailed expressions for $T \gg T_c$, $T \approx T_c$, and $T \ll T_c$.
- (b) What is the behavior of the heat capacity at constant magnetic field C_H in these three temperature limits?
- (c) Make a sketch showing the approximate temperature dependence of C_H .

9.11: One-dimensional Ising model

The one-dimensional Ising model admits an exact solution. We can compare that exact solution to the mean-field solution of the Ising model.

- (a) In one figure, sketch curves of M versus T for different values of the magnetic field H . Do this for the exact solution and for the mean-field solution of the one-dimensional Ising model.
- (b) Calculate the magnetic susceptibility χ for the one-dimensional Ising model. What is its behavior for $T \downarrow 0$?