Problem Set 2

Advanced Statistical Mechanics

Deadline: Saturday, 30 Esfand, 23:59

1 Density Operator

1.1 Introduction

a) Write a one-page assay about the density operator and make a connection with statistical mechanics.
b) Let ρ be a density operator. Show that $\mathrm{tr}\left(\rho^2\right) \leq 1$, with equality if and only if ρ is a pure state.
c) Suppose a composite of systems A and B is in the state $|a\rangle\,|b\rangle$, where $|a\rangle$ is a pure state of system A, and $|b\rangle$ is a pure state of system B. Show that the reduced density operator of system A alone is a pure state.

1.2 The Schmidt Decomposition

Density operators and the partial trace are just the beginning of a wide array of tools useful for the study of composite quantum systems, which are the heart of quantum information and its applications. One of the additional tools is Schmidt decomposition. Prove the following theorem for the case where A and B have state spaces of the same dimension.

(You can prove it for the general case as a bonus question)

Theorem: Suppose $|\psi\rangle$ is a pure state of a composite system, AB. Then there exist orthonormal states $|i_A\rangle$ for system A, and orthonormal states $|i_B\rangle$ of system B such that

$$|\psi\rangle = \sum_i \lambda_i\,|i_A\rangle\,|i_B\rangle \tag{1}$$

where λ_i are non-negative real numbers satisfying $\sum_i \lambda_i^2 = 1$ known as Schmidt coefficient.

1.3 Thermal Radiation

Assume that the density operator for the radiation mode can be written as

$$\rho = \sum_{n=0}^{\infty} P(n)\,|n\rangle\,\langle n| \tag{2}$$

In the photon number state basis, the density operator has no off-diagonal elements but only diagonal elements, $P(n)$, that give the probability of there being n photons in the radiation mode. From statistical physics we know that for a canonical ensemble the probability for a system at temperature T to have energy E is proportional to $e^{\frac{E}{k_B T}}$. Therefore,

$$P(n) \propto e^{-\frac{\hbar\omega(n+1/2)}{k_B T}} \tag{3}$$

a) Calculate the normalized constant.
b) Show that the average number of photons in the mode equals,

$$\langle n \rangle = \frac{1}{e^{\hbar\omega/k_B T} - 1} \tag{4}$$

The expression for the average photon number is called the Bose-Einstein factor.

1.4 Equivalence of Entropies

Suppose that thermodynamic system S is contacted with a huge bath with temperature T. In terms of statistical mechanics, thermodynamics quantities in thermal equilibrium can be calculated by using probability models. One of the most probability models is the canonical distribution:

$$\rho_{can} = \frac{e^{-\beta\mathcal{H}}}{Z} \tag{5}$$

where $\mathcal{H}$ is the Hamiltonian of the system and Z is the partition function.

Show that the thermodynamic entropy S and the von Neumann entropy H are equivalent in the canonical distribution.

Hint: the von Neumann entropy is defined by:

$$H(\rho_{can}) = -\operatorname{tr}(\rho_{can} \ln \rho_{can}) \tag{6}$$

1.5 Spin 1/2 Particle

Suppose a particle with spin $\frac{1}{2}$ which interacts with a magnetic field $\mathbf{B} = B\hat{n}$. The Hamiltonian of the system is

$$\mathcal{H} = -g\boldsymbol{\sigma} \cdot \boldsymbol{B} \tag{7}$$

and the particle is in equilibrium at temperature T.
a) Calculate the density operator of the particle.
b) Calculate the partition function of the particle.
c) Calculate the expected energy and entropy of the particle.

1.6 Spin 1/2 Particles

Again, suppose two particles with spin $\frac{1}{2}$ which interact with a magnetic field $\mathbf{B} = B\hat{n}$. The Hamiltonian of the system is

$$\mathcal{H} = -g(\boldsymbol{\sigma}_1 \cdot \mathbf{B} + \boldsymbol{\sigma}_2 \cdot \mathbf{B}) - J\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \tag{8}$$

and the particles are in equilibrium at temperature T.
a) Calculate the density operator of the system.
b) Calculate the partition function of the system.
c) Calculate the expected energy and entropy of the system.