Canonical Partition Function for Quantum Ideal Gases: Cycle Decomposition and Cluster Expansion

Overview

This note extends Section 6.2 from Pathria (3rd Edition) and elaborates on the canonical ensemble formulation of quantum ideal gases using cycle decomposition and cluster expansion. We also show the transition to the grand canonical ensemble for easier computation of thermodynamic quantities.

Challenges in Canonical Quantum Partition Function

For a quantum gas of indistinguishable particles, the canonical partition function Z_N cannot be written as $Z_1^N/N!$ due to quantum symmetrization or antisymmetrization. Instead, permutations of particle indices play a central role.

The canonical partition function becomes:

$$Z_N = \frac{1}{N!} \sum_P (\pm 1)^P \mathrm{Tr}(P e^{-\beta H})$$

where P is a permutation, and $(\pm 1)^P$ depends on whether the particles are bosons or fermions.

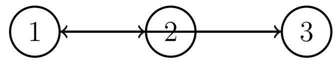
Cycle Decomposition of Permutations

Every permutation can be broken into disjoint cycles. For example:

- $P_1 = (1)(2)(3)$ (identity)
- $P_2 = (1\ 2\ 3)$ (3-cycle)
- $P_3 = (1\ 2)(3)$ (2-cycle + 1-cycle)

Each cycle of length j contributes a factor $Z_1(j\beta)$ to the partition function, interpreted as a single particle evolving for an imaginary time $j\beta$.

Diagrammatic Visualization of Cycle Decomposition



(1 2 3) - A 3-cycle

This cycle corresponds to one term in the permutation sum contributing $Z_1(3\beta)$.

Cycle Expansion of Z_N

Each set of cycle numbers $\{c_j\}$ satisfying $\sum jc_j = N$ contributes:

$$Z_N = \sum_{\{c_j\}} \prod_{j=1}^{N} \frac{1}{c_j! j^{c_j}} [Z_1(j\beta)]^{c_j}$$

This is the exact quantum canonical partition function using permutation cycles. It is valid for both bosons (sign +) and fermions (sign alternates).

Cluster Expansion

Instead of computing Z_N directly, we define the grand partition function:

$$\mathcal{Z}(z, T, V) = \sum_{N=0}^{\infty} z^N Z_N(T, V)$$

Taking the logarithm gives:

$$\ln \mathcal{Z} = \sum_{l=1}^{\infty} b_l z^l$$

where b_l are cluster integrals related to l-particle interactions and statistics.

Grand Canonical Formulation from Canonical Cycles

Substituting the cycle-decomposed Z_N into the grand partition function leads to:

$$\mathcal{Z} = \exp\left[\sum_{j=1}^{\infty} \frac{(\pm 1)^{j+1}}{j} z^j Z_1(j\beta)\right]$$

This is a powerful result: the grand canonical partition function can be computed directly using single-particle quantities and sums over j-cycles.

From this, thermodynamic quantities like N, E, and P follow easily:

$$N = z\frac{\partial \ln \mathcal{Z}}{\partial z}$$
$$E = -\frac{\partial \ln \mathcal{Z}}{\partial \beta}$$

Summary

- Canonical quantum partition functions must account for indistinguishability via permutations.
- Each permutation can be decomposed into cycles, each contributing $Z_1(j\beta)$.
- The cycle expansion of Z_N yields an exact expression, but becomes complex for large N.
- The grand canonical ensemble simplifies analysis via generating functions and leads to cluster expansions.
- The grand partition function naturally encodes quantum statistics using single-particle data.