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FINAL REPORT ON THE START PROGRAMME

Elements of Statistical Mechanics: A Study of Thermodynamic Ensembles and Particle Distributions

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Abstract

This report delves into the fundamental aspects of statistical ensembles used in thermodynamics to describe macroscopic systems. We examine the microcanonical, canonical, grand canonical, and isobaric ensembles, highlighting their defining parameters and key thermodynamic relations. The study further explores the statistical distributions relevant to these ensembles, including the Fermi-Dirac, Bose-Einstein, and Maxwell-Boltzmann distributions. By understanding these concepts, we gain insights into the behavior of systems at equilibrium and the partition functions that underlie thermodynamic properties. Theoretical derivations are discussed to provide a comprehensive overview of these fundamental principles.

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Chapter 1

Introduction

Statistical mechanics bridges the microscopic and macroscopic worlds, providing a framework to understand thermodynamic properties through statistical methods. In this report, we explore the core statistical ensembles that describe systems in equilibrium. The microcanonical ensemble represents an isolated system with fixed energy, volume, and particle number. The canonical ensemble considers a system in thermal equilibrium with a heat bath, characterized by constant temperature, volume, and particle number. The grand canonical ensemble extends this by allowing particle exchange with a reservoir, leading to constant temperature, volume, and chemical potential. Lastly, the isobaric ensemble describes systems under constant pressure. Each ensemble provides unique insights into system behavior, and understanding their associated distributions, such as the Fermi-Dirac, Bose-Einstein, and Maxwell-Boltzmann distributions, is crucial for analyzing both classical and quantum systems.

Statistical ensembles serve as a cornerstone for predicting and interpreting the properties of complex systems. The microcanonical ensemble is particularly relevant for isolated systems, where its key feature is the conservation of energy. This ensemble is instrumental in deriving the fundamental thermodynamic quantity of entropy and establishing the link between microscopic states and macroscopic observables through the Boltzmann formula. Conversely, the canonical ensemble is indispensable in systems in thermal equilibrium with a reservoir, where it simplifies the treatment of temperature and introduces the concept of free energy as a central thermodynamic potential. The canonical partition function, a pivotal concept in this ensemble, encapsulates all possible microstates and their probabilities, thereby allowing the calculation of thermodynamic quantities like internal energy, entropy, and specific heat.

The grand canonical ensemble extends the flexibility of the canonical ensemble by incorporating the exchange of particles with a reservoir, making it highly applicable to systems where the number of particles is not fixed. This ensemble introduces the chemical potential as a crucial parameter, leading to the derivation of the grand partition function, which facilitates the study of open systems in contact with a particle reservoir. The isobaric ensemble, on the other hand, focuses on systems under constant pressure, often simplifying the analysis of chemical reactions and phase transitions where volume changes are significant. The study of these ensembles is complemented by understanding their associated distributions. The Fermi-Dirac distribution applies to fermions, particles that obey the Pauli exclusion principle, while the Bose-Einstein distribution describes bosons, particles that can occupy the same quantum state. The Maxwell-Boltzmann distribution, applicable in the classical limit, describes the distribution of particle energies in a system at equilibrium. Together, these ensembles and distributions provide a comprehensive framework for analyzing the thermodynamic properties of both classical and quantum systems.

This report aims to provide a detailed exploration of these ensembles and distributions, elucidating their theoretical underpinnings and practical applications. Through a systematic examination of the equations and relations that govern these statistical systems, we endeavor to highlight the relevance and utility of these concepts in modern thermodynamics and statistical mechanics.

Chapter 2

Statistical Ensembles

2.1. Microcanonical Ensemble: (E, N, V)

The statistical entropy is defined as

$$S = -k_B \sum_i P_i \ln P_i, \tag{2.1}$$

where k_B is Boltzmann constant and P_i is the probability of the microstate of the system. The mean value of any quantity is given by the following formula as

$$\langle A \rangle = \sum_i P_i A_i. \tag{2.2}$$

The probabilities of microstates are normalized to unity as

$$\phi = \sum_i P_i - 1 = 0. \tag{2.3}$$

The probabilities P_i of microstates are unknown. They can be found from the principle of maximum entropy:

$$\Phi = S - \lambda\phi, \tag{2.4}$$

$$\frac{\partial \Phi}{\partial P_i} = 0, \tag{2.5}$$

$$\Phi = -k_B \sum_i P_i \ln P_i - \lambda \left(\sum_i P_i - 1 \right), \tag{2.6}$$

where λ is an arbitrary constant.

$$\frac{\partial \Phi}{\partial P_i} = -k_B - k_B \ln P_i - \lambda = 0, \tag{2.7}$$

$$P_i = \exp\left(-\frac{\lambda}{k_B} - 1 \right), \tag{2.8}$$

$$\sum_i \delta(E_i - E)\delta(V_i - V)\delta_{N_i,N} \exp\left(-\frac{\lambda}{k_B} - 1 \right) = 1. \tag{2.9}$$

Define

$$W = \sum_i \delta(E_i - E)\delta(V_i - V)\delta_{N_i,N}, \tag{2.10}$$

we have

$$\exp\left(-\frac{\lambda}{k_B} - 1 \right) = \frac{1}{W}. \tag{2.11}$$

Hence,

$$P_i = \frac{1}{W}. \tag{2.12}$$

$$S = -k_B \sum_i \delta(E_i - E)\delta(V_i - V)\delta_{N_i,N} \frac{1}{W} \ln \frac{1}{W} \tag{2.13}$$

$$S = k_B \ln W \quad \text{(Boltzmann formula)} \tag{2.14}$$

From the first law of thermodynamics:

$$dE = TdS - PdV + \mu dN, \tag{2.15}$$

$$dS = \frac{1}{T}dE + \frac{P}{T}dV - \frac{\mu}{T}dN, \tag{2.16}$$

$$S = S(E, V, N), \tag{2.17}$$

$$dS = \left(\frac{\partial S}{\partial E}\right)_{V,N} dE + \left(\frac{\partial S}{\partial V}\right)_{E,N} dV + \left(\frac{\partial S}{\partial N}\right)_{E,V} dN, \tag{2.18}$$

$$\left(\frac{\partial S}{\partial E}\right)_{V,N} = \frac{\partial S(E, V, N)}{\partial E}, \tag{2.19}$$

$$\left(\frac{\partial S}{\partial E}\right)_{V,N} = \frac{1}{T}, \quad \left(\frac{\partial S}{\partial V}\right)_{E,N} = \frac{P}{T}, \quad \left(\frac{\partial S}{\partial N}\right)_{E,V} = -\frac{\mu}{T}, \tag{2.20}$$

$$\frac{1}{T} = k_B \frac{\partial \ln W}{\partial E}, \tag{2.21}$$

$$\frac{P}{T} = k_B \frac{\partial \ln W}{\partial V}, \tag{2.22}$$

$$\frac{\mu}{T} = -k_B \frac{\partial \ln W}{\partial N}. \tag{2.23}$$

2.2. Canonical Ensemble: (T, V, N)

$$S = -k_B \sum_i P_i \ln P_i, \tag{2.24}$$

where k_B is Boltzmann constant and P_i is the probability. The mean value of any quantity is given by the following formula:

$$\langle A \rangle = \sum_i P_i A_i. \tag{2.25}$$

The normalized condition is given by:

$$\varphi = \sum_i P_i - 1 = 0. \tag{2.26}$$

The Free Energy of the canonical ensemble is given by:

$$F(T, V, N) = E - TS, \tag{2.27}$$

$$\sum_i \cdots = \sum_i \delta_{N_i,N} \delta(V_i - V) \cdots \tag{2.28}$$

Apply equation 2.26 for the energy we get:

$$E = \sum_i P_i E_i, \tag{2.29}$$

Hence,

$$F = \sum_i P_i E_i + k_B T \sum_i P_i \ln P_i = \sum_i P_i \left(E_i + k_B T \ln P_i\right), \tag{2.30}$$

$$\Phi = F - \lambda \varphi, \tag{2.31}$$

$$\frac{\partial \Phi}{\partial P_i} = 0. \tag{2.32}$$

So equation 2.32 can be written as:

$$\Phi = \sum_i P_i(E_i + k_B T ln P_i) - \lambda(\sum_i P_i - 1). \tag{2.33}$$

Substitute equation 2.34 in equation 2.33 we get

$$\frac{\partial \Phi}{\partial P_i} = E_i + k_B T + k_B T \ln P_i - \lambda = 0 \tag{2.34}$$

and

$$P_i = \exp(\frac{\lambda}{k_B T} - 1) \exp(\frac{-E_i}{k_B T}), \tag{2.35}$$

$$P_i = \frac{1}{Z} \exp(\frac{-E_i}{k_B T}), \quad Z^{-1} = \exp[\frac{\lambda}{k_B T} - 1]. \tag{2.36}$$

Now, substituting the last equation in equation 2.26, $\sum_i P_i = 1$, we get

$$Z = \sum_i \delta_{N_i, N} \delta(V_i - V) \exp(\frac{-E_i}{k_B T}), \tag{2.37}$$

Where Z is the partition function for the canonical ensemble. Equation 2.30 can be written as

$$E = \frac{1}{Z} \sum_i \delta_{N_i, N} \delta(V_i - V) \exp(\frac{-E_i}{k_B T}) E_i. \tag{2.38}$$

Hence, eq. 2.28 is calculated as

$$F = \frac{1}{Z} \sum_i \delta_{N_i, N} \delta(V_i - V) \exp(\frac{-E_i}{k_B T})(E_i + k_B T ln(\frac{1}{Z} \exp(\frac{-E_i}{k_B T}))). \tag{2.39}$$

Then,

$$F = -k_B T ln Z. \tag{2.40}$$

From the first law of thermodynamics:

$$dE = TdS - PdV + \mu dN \tag{2.41}$$

and

$$F(T, V, N) = E - TS, \tag{2.42}$$

$$d = \frac{\partial}{\partial T} dT + \frac{\partial}{\partial V} dV + \frac{\partial}{\partial N} dN, \tag{2.43}$$

we have

$$dF = TdS - PdV + \mu dN - TdS - SdT, \tag{2.44}$$

$$dF = -PdV + \mu dN - SdT, \tag{2.45}$$

$$dF = (\frac{\partial F}{\partial T})_{VN} dT + (\frac{\partial F}{\partial V})_{TN} dV + (\frac{\partial F}{\partial N})_{TV} dN. \tag{2.46}$$

By comparing the last two equations we get,

$$S = -\left(\frac{\partial F}{\partial T}\right)_{VN}, \tag{2.47}$$

$$\mu = -\left(\frac{\partial F}{\partial V}\right)_{TN}, \tag{2.48}$$

$$P = -\left(\frac{\partial F}{\partial N}\right)_{TV}, \tag{2.49}$$

$$E = F + TS = F - T(\frac{\partial F}{\partial T})_{VN}. \tag{2.50}$$

Then

$$E = -T^2 \frac{\partial}{\partial T}(\frac{F}{T}). \tag{2.51}$$

So, these quantities entropy S, chemical potential μ, pressure P, and energy E are the thermodynamic relations of the canonical ensemble.

2.3. Grand Canonical Ensemble (T, V, μ)

$$S = -k_B \sum_i P_i \ln P_i, \tag{1}$$

$$\langle A \rangle = \sum_i P_i A_i, \tag{2}$$

$$\Phi = \sum_i P_i - 1 = 0 \quad , \quad \sum_i P_i = 1, \tag{3}$$

$$\Omega = E - TS - \mu N, \tag{4}$$

$$\Phi = \Omega - \lambda \Phi, \tag{5}$$

$$\frac{\partial \Phi}{\partial P_i} = 0, \tag{6}$$

$$E = \sum_i P_i E_i \quad , \quad N = \sum_i P_i N_i,$$

$$\sum ... = \sum \delta(V_i - V) \quad ...$$

Substituting equations (3) and (4) into (5), we obtain

$$\Phi = E - TS - \mu N - \lambda \left(\sum_i P_i - 1 \right)$$

$$= \left[\sum_i P_i E_i - T \left(-k_B \sum_i P_i \ln P_i \right) - \mu \left(\sum_i P_i N_i \right) \right] - \lambda \left(\sum_i P_i - 1 \right),$$

$$\frac{\partial \Phi}{\partial P_i} = E_i + T k_B \ln P_i + k_B T - \mu N_i - \lambda = 0. \tag{7}$$

Using eq.(6) and eq.(7), we have

$$P_i = \exp[\frac{\lambda}{k_B T} + \frac{\mu N_i}{k_B T} - \frac{E_i}{k_B T} - 1]. \tag{8}$$

substituting (8) in (3) we get

$$Z = \sum_i \delta(V_i - V) \exp[\frac{\mu N_i}{k_B T} - \frac{E_i}{k_B T}], \quad Z^{-1} = \exp[\frac{\lambda}{k_B T} - 1], \tag{9}$$

where Z is the grand partition function. So, P_i can be written as,

$$P_i = \frac{1}{Z} \exp[\frac{\mu N_i}{k_B T} - \frac{E_i}{k_B T}]. \tag{10}$$

Then, applying Eq.(10) to Eq.(1) and after simplifying the result, we get

$$S = \frac{E}{T} - \frac{\mu N}{T} - k_B \ln \frac{1}{Z}, \tag{11}$$

Substituting into Eq.(4) so, we obtain the grand thermodynamic potential as

$$\Omega = -k_B T \ln Z, \tag{12}$$

2.3.1. Thermodynamic Relations of Grand Canonical Ensemble

From the first law of thermodynamics:

$$dE = TdS - PdV + \mu dN,$$

$$\Omega = E - TS - \mu N,$$

$$d = \frac{\partial}{\partial T} dT + \frac{\partial}{\partial V} dV + \frac{\partial}{\partial N} dN,$$

$$d\Omega = dE - TdS - SdT,$$

$$d\Omega = TdS - PdV + \mu dN - TdS - SdT,$$

$$d\Omega = -PdV + \mu dN - SdT,$$

$$d\Omega = (\frac{\partial \Omega}{\partial T})_{V\mu} dT + (\frac{\partial \Omega}{\partial V})_{T\mu} dV + (\frac{\partial \Omega}{\partial N})_{TV} dN.$$

By comparing the last two equations we get,

- Entropy S

$$S = -(\frac{\partial \Omega}{\partial T})_{V,\mu}. \tag{13}$$

- Pressure P

$$P = -(\frac{\partial \Omega}{\partial V})_{T,\mu}. \tag{14}$$

- Number of Particles N

$$N = -(\frac{\partial \Omega}{\partial \mu})_{T,V}. \tag{15}$$

- Energy of the system E

$$E = \Omega - T(\frac{\partial \Omega}{\partial T})_{V,\mu} - \mu(\frac{\partial \Omega}{\partial \mu})_{T,V}. \tag{16}$$

2.4. Isobaric Ensemble (T, P, N)

$$S = -k_B \sum_i P_i \ln P_i, \tag{1}$$

$$\langle A \rangle = \sum_i P_i A_i, \tag{2}$$

$$\phi = \sum_i P_i - 1 = 0 \quad , \quad \sum_i P_i = 1, \tag{3}$$

$$G = E - TS + PV, \tag{4}$$

$$\Phi = G - \lambda \phi, \tag{5}$$

$$\frac{\partial \Phi}{\partial P_i} = 0, \tag{6}$$

$$V = \sum_i P_i V_i, \quad \sum_i ... = \sum_i \delta_{N_i,N},$$

$$\frac{\partial \Phi}{\partial P_i} = E_i + k_B T + k_B T \ln P_i + PV_i - \lambda = 0.$$

After substitution and simplifying calculations the probability P_i is given by:

$$P_i = \frac{1}{Z}. \exp[-\frac{E_i}{k_B T} - \frac{PV_i}{k_B T}], \tag{7}$$

where Z is the Isobaric Partition Function and is given by

$$Z = \sum_i \delta_{N_i,N} \exp[-\frac{E_i}{k_B T} - \frac{PV_i}{k_B T}]. \tag{8}$$

Hence,

$$S = k_B \ln Z + \frac{E}{T} + \frac{PV}{T}, \tag{9}$$

and

$$G = -k_B T \ln Z. \tag{10}$$

2.4.1. Thermal Relations

From the first law of thermodynamics:

$$dE = TdS - PdV + \mu dN,$$

$$G = E - TS + PV,$$

$$d = \frac{\partial}{\partial T} dT + \frac{\partial}{\partial P} dP + \frac{\partial}{\partial N} dN,$$

$$dG = dE - TdS - SdT + PdV + VdP,$$

$$dG = VdP + \mu dN - SdT,$$

$$dG = (\frac{\partial G}{\partial T})_{NP} dT + (\frac{\partial G}{\partial N})_{TP} dN + (\frac{\partial G}{\partial P})_{TN} dP.$$

By comparing the last two equations we get,

- Chemical Potential μ

$$\mu = -(\frac{\partial G}{\partial N})_{T,P}. \tag{11}$$

- Entropy S

$$S = -(\frac{\partial G}{\partial T})_{N,P}. \tag{12}$$

- Volume V

$$V = -(\frac{\partial G}{\partial P})_{T,N}. \tag{13}$$

- Energy of the system E

$$E = G - T(\frac{\partial G}{\partial T})_{N,P} - P(\frac{\partial G}{\partial P})_{T,N}. \tag{14}$$

Chapter 3

Statistical Distributions for Grand Canonical Ensemble

3.1. Fermi-Dirac Distribution (Fermions)

3.1.1. Grand Partition Function for Fermions

The grand partition function is given by:

$$Z(T,V,\mu)=\sum_i \delta(V_i-V)\exp[\beta(\mu N_i-E_i)] \tag{3.1}$$

and

$$E_i \Longrightarrow \sum_p n_p\epsilon_p,$$

$$N_i \Longrightarrow \sum_p n_p,$$

$$\epsilon_p=\sqrt{\vec{p}^2+m^2},$$

$$p_j=\frac{2\pi\hbar}{L}n_j, \quad n_j=0,\pm1,\pm2,\ldots, \quad j=1,2,3, \quad L=V^{\frac{1}{3}}.$$

Hence, after substitution and simplification the grand partition function can be written as

$$Z=\sum_{\{n_p\}}\exp[\beta\sum_p n_p(\mu-\epsilon_p)], \quad n_p=0,1. \tag{3.2}$$

Simplifying, we get

$$Z=\prod_p\sum_{n_p=0}^{1}\exp(\beta(\mu-\epsilon_p)n_p). \tag{3.3}$$

Then,

$$Z=\prod_p[1+\exp(\beta(\mu-\epsilon_p))] \tag{3.4}$$

And the grand potential is

$$\Omega=-\frac{1}{\beta}\ln Z \tag{3.5}$$

Substitute Z in Ω we get:

$$\Omega=-\frac{1}{\beta}\ln\left[\prod_p[1+\exp(\beta(\mu-\epsilon_p))]\right]. \tag{3.6}$$

After simplifying we get,

$$\Omega=-\frac{1}{\beta}\sum_p\ln[1+\exp(\beta(\mu-\epsilon_p))] \tag{3.7}$$

Where Ω is the thermodynamic potential for ideal gas for Fermions.

3.1.2. Mean Occupation Numbers

From the grand partition function eq.(3.4) and the mean value equation, the mean occupation numbers for Fermions can be calcultes as

$$<n_{p'}>=\frac{1}{Z}\sum_{\{n_p\}}\exp[\beta\sum_p n_p(\mu-\epsilon_p)]n_{p'} \tag{3.8}$$

Then,

$$<n_p>=\frac{\sum\limits_{n_p=0}^{1}\exp[\beta\sum\limits_p n_p(\mu-\epsilon_p)]n_p}{\sum\limits_{n_p=0}^{1}\exp[\beta\sum\limits_p n_p(\mu-\epsilon_p)]}, \tag{3.9}$$

by simplifying the equation, we have

$$< n_p >= \frac{1}{\exp[\beta(\epsilon_p - \mu)] + 1}. \tag{3.10}$$

3.1.3. Thermodynamic Quantities for Grand Canonical Ensemble for Fermions

Entropy can be drived from the following equation:

$$S = -(\frac{\partial \Omega}{\partial T})_{V,\mu}. \tag{3.11}$$

So, substitute and simplify we get,

$$S = k_B \sum_p \ln[1 + \exp(\beta(\mu - \epsilon_p))] - \frac{1}{T} \sum_p \frac{(\mu - \epsilon_p)}{\exp(\beta(\epsilon_p - \mu)) + 1}. \tag{3.12}$$

Then,

$$\Omega = E - TS - \mu N. \tag{3.13}$$

The pressure can be derived from the following equation:

$$P = -(\frac{\partial \Omega}{\partial V})_{T,\mu}. \tag{14}$$

So, substitute Ω and simplify the equation, we get

$$P = \frac{1}{3V} \sum_p \frac{p^2 c^2}{\epsilon_p} < n_p >, \tag{3.14}$$

where p is the momentum.
The number of particles for Fermions can be calculated from the following equation:

$$N = -(\frac{\partial \Omega}{\partial \mu})_{T,V}. \tag{3.15}$$

So,

$$N = \sum_p \frac{1}{\exp(\beta(\epsilon_p - \mu)) + 1} = \sum_p < n_p > . \tag{3.16}$$

The energy of the system for Fermions is given by

$$E = \Omega - T(\frac{\partial \Omega}{\partial T})_{V,\mu} - \mu(\frac{\partial \Omega}{\partial \mu})_{T,V}. \tag{16}$$

By substitution and simplification, the final form of the energy is given by

$$E = \sum_p \epsilon_p n_p. \tag{3.17}$$

3.2. Bose-Einstein Distribution (Bosons)

3.2.1. Grand Partition Function for Bosons

$$Z = \sum_{\{n_p\}} \exp[\beta \sum_p^{\infty} n_p(\mu - \epsilon_p)], \quad n_p = 0, 1, 2, ..., \infty, \tag{3.18}$$

$$Z = \prod_p \sum_{n_p=0}^{\infty} \exp[\beta n_p(\mu - \epsilon_p)]. \tag{3.19}$$

This sum is in the form of geometric series.

$$\sum_{k=0}^{\infty} r^k = \frac{1}{1 - r}. \tag{3.20}$$

Thus,

$$\sum_{n_p=0}^{\infty} \exp[\beta n_p(\mu - \epsilon_p)] = [1 - \exp[\beta(\mu - \epsilon_p)]^{-1}. \tag{3.21}$$

So, the partition function can be calculated as:

$$Z = \prod_p [1 - \exp(\beta(\mu - \epsilon_p))]^{-1}. \tag{3.22}$$

So, the thermodynamic potential for an ideal gas for Bosons is given by

$$\Omega = \frac{1}{\beta} \sum_p \ln[1 - \exp(\beta(\mu - \epsilon_p))]. \tag{3.23}$$

3.2.2. Mean Occupation Numbers

$$< n_{p'} >= \frac{1}{Z} \sum_{\{n_p\}} \exp[\beta \sum_p n_p(\mu - \epsilon_p)] n_{p'}, \tag{3.24}$$

$$< n_p >= \frac{\sum\limits_{n_p=0}^{\infty} n_p \exp[\beta n_p(\mu - \epsilon_p)]}{\sum\limits_{n_p=0}^{\infty} \exp[\beta n_p(\mu - \epsilon_p)]}, \tag{3.25}$$

$$< n_p >= \frac{1}{\exp[\beta(\epsilon_p - \mu)] - 1} \tag{3.26}$$

and

$$N = \sum_p < n_p >= \sum_p \frac{1}{\exp[\beta(\epsilon_p - \mu)] - 1} \tag{3.27}$$

where N is the main occupation number for Bosons.

3.2.3. Thermodynamic Quantities for Grand Canonical Ensemble for Bosons

Entropy can be derived from the following equation:

$$S = -(\frac{\partial \Omega}{\partial T})_{V,\mu}. \tag{3.28}$$

So, substitute Ω and simplify we get,

$$S = -k_B \sum_p \ln[1 - \exp(\beta(\mu - \epsilon_p))] - \frac{E}{.} T + \frac{\mu N}{T} \tag{3.29}$$

Then,

$$\Omega = E - TS - \mu N. \tag{3.30}$$

The pressure can be derived from the following equation:

$$P = -(\frac{\partial \Omega}{\partial V})_{T,\mu}. \tag{3.31}$$

So, substitute Ω and simplify the equation, we get

$$P = \frac{1}{3V} \sum_p < n_p > \frac{p^2 c^2}{\epsilon_{n_p}}. \tag{3.32}$$

Where c is the speed of light and p is the momentum. The number of particles for Bosons can be calculated from the following equation:

$$N = -(\frac{\partial \Omega}{\partial \mu})_{T,V}. \tag{3.33}$$

Then,

$$N = \sum_p < n_p >= \sum_p \frac{1}{\exp[\beta(\epsilon_p - \mu)] - 1}. \tag{3.34}$$

The energy of the system for Bosons is given by

$$E = \Omega - T(\frac{\partial \Omega}{\partial T})_{V,\mu} - \mu(\frac{\partial \Omega}{\partial \mu})_{T,V}. \tag{3.35}$$

By substitution and simplification, the final form of the energy is given by

$$E = \sum_p \epsilon_p n_p. \tag{3.36}$$

3.3. Maxwell-Boltzmann Distribution

3.3.1. Grand Partition Function for Maxwell-Boltzmann Statistics

$$Z = \sum_{\{n_p\}} \frac{1}{\prod_p n_p!} \exp[\beta \sum_p^{\infty} n_p(\mu - \epsilon_p], \quad n_p = 0, 1, 2, \ldots, \infty, \tag{3.37}$$

$$Z = \prod_p \sum_{n_p=0}^{\infty} \frac{1}{n_p!} \exp[\beta n_p(\mu - \epsilon_p)] \tag{3.38}$$

and

$$\exp(x) = \sum_{k=0}^{\infty} \frac{x^k}{k!}. \tag{3.39}$$

After simplification, the grand partition function for Maxwell-Boltzmann is given by:

$$Z = \prod_p [\exp(\exp(\beta(\mu - \epsilon_p)))]. \tag{3.40}$$

So, the thermodynamic potential for an ideal gas for Maxwell-Boltzmann is given by

$$\Omega = -\frac{1}{\beta} \sum_p \exp(\beta(\mu - \epsilon_p)). \tag{3.41}$$

3.3.2. Mean Occupation Numbers

$$< n_{p'} >= \frac{1}{Z} \sum_{\{n_p\}} \frac{1}{\prod_p n_p!} \exp[\beta(\mu - \epsilon_p)] n_{p'}, \tag{3.42}$$

$$< n_p >= \frac{\sum\limits_{n_p=0}^{\infty} \frac{1}{n_p!} \exp[\beta n_p(\mu - \epsilon_p)] n_p}{\sum\limits_{n_p=0}^{\infty} \frac{1}{n_p!} \exp[\beta n_p(\mu - \epsilon_p)]}, \tag{3.43}$$

$$\sum_{n_p=0}^{\infty} \frac{1}{n_p!} \exp[\beta n_p(\mu - \epsilon_p)] n_p = \exp[\beta(\mu - \epsilon_p)] \sum_{m=0}^{\infty} \frac{\exp[\beta m(\mu - \epsilon_p)]}{m!}, \tag{3.44}$$

$$< n_p >= \exp(\beta(\mu - \epsilon_p)) \tag{3.45}$$

and

$$N = \sum_p < n_p >= \sum_p \exp(\beta(\mu - \epsilon_p)) \tag{3.46}$$

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3.3.3. Thermodynamic Quantities for Grand Canonical Ensemble for Maxwell-Boltzmann

Entropy can be derived from the following equation:

$$S = -(\frac{\partial \Omega}{\partial T})_{V,\mu}. \tag{3.47}$$

So, substitute Ω and simplify we get,

$$S = k_B \sum_p \exp(\beta(\mu - \epsilon_p)) - \frac{1}{T}[-E + \mu N]. \tag{3.48}$$

Thus,

$$\Omega = E - TS - \mu N. \tag{3.49}$$

The pressure can be derived from the following equation:

$$P = -(\frac{\partial \Omega}{\partial V})_{T,\mu}. \tag{3.50}$$

So, substitute Ω and simplify the equation we get,

$$P = \frac{1}{3V} \sum_p < n_p > \frac{p^2 c^2}{\epsilon_p}. \tag{3.51}$$

The number of particles for Bosons can be calculated from the following equation:

$$N = -(\frac{\partial \Omega}{\partial \mu})_{T,V}. \tag{3.52}$$

Then,

$$N = \sum_p \exp(\beta(\mu - \epsilon_p)) = \sum_p < n_p > . \tag{3.53}$$

The energy of the system for Maxwell-Boltzmann is given by

$$E = \Omega - T(\frac{\partial \Omega}{\partial T})_{V,\mu} - \mu(\frac{\partial \Omega}{\partial \mu})_{T,V}. \tag{3.54}$$

By substitution and simplification, the final form of the energy is given by

$$E = \sum_p \epsilon_p n_p. \tag{3.55}$$

3.4. Conclusion

This report has outlined the fundamental statistical ensembles that are pivotal in the field of thermodynamics and statistical mechanics. By analyzing the microcanonical, canonical, grand canonical, and isobaric ensembles, we have provided a detailed understanding of their thermodynamic relations and the partition functions essential for describing system properties. The study of Fermi-Dirac, Bose-Einstein, and Maxwell-Boltzmann distributions has revealed how different particles obey different statistical laws, influencing their thermodynamic behavior. The theoretical formulations and derived equations underscore the significance of these ensembles and distributions in predicting and interpreting the physical properties of various systems. As we continue to explore complex systems, the principles discussed here remain foundational to advancements in statistical mechanics.

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