Appendix

Statistical Ensembles

Equilibrium statistical mechanics forms the foundational basis for thermodynamics, characterizing a system by its Hamiltonian and the nature of its environment (e.g., open or closed) [Grant & Phillips (2013)]. Three primary ensembles are used to describe systems in equilibrium: the microcanonical ensemble, the canonical ensemble, and the grand canonical ensemble [L.Boltzmann (1964); Pathria (1996); Paul M (1995); Zemansky & Dittman (1997)].

Microcanonical Ensemble

The microcanonical ensemble is used for isolated systems with a fixed number of particles N, volume V, and energy E. It represents the most constrained ensemble where the system does not exchange energy or particles with its surroundings. The key thermodynamic potential for this ensemble is the entropy $S(E,V,N)$, which is a function of the energy, volume, and number of particles [K.Huang (2008); Pathria (2016)].

In statistical mechanics, entropy is fundamentally linked to the number of accessible microstates of the system in phase space [Klein (1990); Pathria (1996); Zemansky & Dittman (1997)]. The phase space is a $6N$-dimensional space where each point represents a possible state of the system, defined by the positions $\{q_i\}$ and momenta $\{p_i\}$ of all particles. The entropy S is then defined as:

$$S(E,V,N) = k_B \ln \Omega(E,V,N),$$

where k_B is the Boltzmann constant, and $\Omega(E,V,N)$ is the number of microstates available to the system at a given energy E, volume V, and number of particles N [Bhattacharyajee (2000); Pathria (1996)]. Specifically, $\Omega(E,V,N)$ is the number of states within a narrow energy range E to $E+\delta E$ in phase space, given by:

$$\Omega(E,V,N)=\int \delta(E-H(p,q))\,\mathrm{d}p^N\,\mathrm{d}q^N,$$

where $H(p,q)$ is the Hamiltonian of the system, δ is the Dirac delta function ensuring that the states counted are those with the exact energy E, and $\mathrm{d}p^N\,\mathrm{d}q^N$ represents the differential volume element in phase space [Bhattacharyajee (2000); Zemansky & Dittman (1997)].

Canonical Ensemble

The canonical ensemble is applicable when the system is in thermal contact with a reservoir, allowing for energy exchange at constant volume and particle number [L.Boltzmann (1964)]. It is defined by the temperature $T\equiv\frac{1}{k_B\beta}$, number density $n\equiv\frac{N}{V}$, and volume V. The fundamental thermodynamic potential for this ensemble is the Helmholtz free energy per particle $f_C(\beta,n,V)$ [Sen (2021)].

The partition function $Z(\beta,V,N)$ is the central quantity in the canonical ensemble and is defined as:

$$Z(\beta,V,N)=\frac{1}{h^{3N}N!}\int \mathrm{d}p^N\,\mathrm{d}q^N\,\exp\left(-\beta H(p,q)\right),$$

where $\beta=\frac{1}{k_BT}$ is the inverse temperature, h is the Planck's constant, $H(p,q)$ is the Hamiltonian of the system, and $\mathrm{d}p^N\,\mathrm{d}q^N$ represents the differential volume element in phase space [K.Huang (2008); Pathria (2016)].

The Helmholtz free energy $F(\beta,V,N)$ [Stanley (1971)]is related to the partition function by:

$$F(\beta,V,N)=-k_BT\ln Z(\beta,V,N).$$

The Helmholtz free energy per particle $f_C(\beta,n,V)$ can then be expressed as:

$$f_C(\beta,n,V)=\frac{F(\beta,V,N)}{N}=-\frac{k_BT}{N}\ln Z(\beta,V,N).$$

This relationship shows how the Helmholtz free energy, which determines the equilibrium properties of the system in the canonical ensemble, is derived from the partition function. The Helmholtz free energy is a measure of the work obtainable from a system at constant temperature and volume and is fundamental in predicting how a system responds to changes in its thermodynamic parameters [Klein (1990); Paul M (1995); Stanley (1971)].

Grand Canonical Ensemble

The grand canonical ensemble accommodates not only energy exchange but also particle number exchange with the environment [K.Huang (2008); Pathria (2016); Sen (2021)]. It is parameterized by β, μ (chemical potential), and V. The corresponding thermodynamic potential is the pressure $\mathscr{P}_G(\beta,\mu,V)$. The free energy per particle in the grand canonical ensemble $f_G(\beta,n_G,V)$ can be derived from $\mathscr{P}_G(\beta,\mu,V)$ via a Legendre transformation, where n_G represents the average number density. Similarly, the pressure in the canonical ensemble can be defined by a Legendre transformation as $\mathscr{P}_C = -\partial F_C/\partial V$ [K.Huang (2008); L.Boltzmann (1964)].

Thermodynamic Limit

The thermodynamic limit is defined by $N \to \infty$ at constant n or n_G for the canonical and grand canonical ensembles, respectively [K.Huang (2008)]. Equivalently, this can be expressed as $V \to \infty$ at constant n or n_G [Pathria (1996); Zemansky & Dittman (1997)]. The shape of the system should also be constrained such that all dimensions are of comparable size L, with L/r_0 being large, where r_0 is the average interparticle spacing defined by $4\pi r_0^3/3 = 1$. This limit requires L to be large compared to all other characteristic length scales, such as the interaction range a or the thermal de Broglie wavelength λ [Pathria (1996)]. For Coulomb systems, the screening length replaces a, and at low temperatures, the Fermi length λ_F becomes relevant [Sen (2021)]. In the presence of an external potential, the spatial variations of the potential set another length scale. Near critical points, the correlation length becomes significant, potentially making system-size dependence important even for large systems [Grant & Phillips (2013); Stanley (1971)].

When L is not the dominant length scale, the system is considered "small," and the influence of external conditions becomes significant. In such cases, the system's behavior can strongly depend on its environment, such as boundary conditions, external fields, or confinement effects. These factors can lead to deviations from the predictions of thermodynamic formalism, which assumes the thermodynamic limit. While the thermodynamic formalism remains universally applicable, it must be carefully adapted to account for the specific external conditions influencing the system. This discussion primarily focuses on the canonical and grand canonical ensembles, but other ensembles may become relevant depending on the experimental or environmental constraints [Klein (1990); Paul M (1995)].

Example: Ising Model in the Canonical Ensemble

The Ising model is a mathematical model used in statistical mechanics to understand phase transitions, particularly in ferromagnetic systems [Binder et al. (1992); Brush (1967); L.Boltzmann (1964)]. In the canonical ensemble, the system is in thermal equilibrium with a heat bath at a fixed temperature T [K.Huang (2008)]. Here, we explore the properties of the Ising model on a lattice.

Hamiltonian

The Hamiltonian H for the Ising model is given by:

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i, \tag{6.1}$$

where J is the interaction strength between neighboring spins S_i and S_j, h is the external magnetic field, and $\langle i, j \rangle$ denotes summation over nearest-neighbor pairs. Each spin S_i can take values ± 1 [Binder et al. (1992); Brush (1967); Grant & Phillips (2013); Pathria (1996); Stanley (1971)].

Partition Function

The partition function Z for the Ising model in the canonical ensemble is:

$$Z = \sum_{\{S_i\}} e^{-\beta H}, \tag{6.2}$$

where $\beta = \frac{1}{k_B T}$, with k_B being the Boltzmann constant and T the temperature. The sum is over all possible configurations of the spins $\{S_i\}$ [Garg et al. (2013); K.Huang (2008); Pathria (2016)].

Free Energy

The Helmholtz free energy F is related to the partition function by:

$$F = -k_B T \ln Z. \tag{6.3}$$

[Stanley (1971); Zemansky & Dittman (1997)]

Physical Properties

Using the free energy, we can calculate various physical properties.

1. **Average Energy:** The average energy $\langle E \rangle$ is given by:

$$\langle E \rangle = \frac{\partial(\beta F)}{\partial \beta}. \tag{6.4}$$

2. **Magnetization:** The average magnetization $\langle M \rangle$ is:

$$\langle M \rangle = -\frac{\partial F}{\partial h}. \tag{6.5}$$

3. **Susceptibility:** The magnetic susceptibility χ measures the response of the magnetization to the external magnetic field:

$$\chi = -\frac{\partial^2 F}{\partial h^2}. \tag{6.6}$$

4. **Heat Capacity:** The heat capacity C_V at constant volume is:

$$C_V = -\beta^2 \frac{\partial^2 F}{\partial \beta^2}. \tag{6.7}$$

[K.Huang (2008); Paul M (1995); Stanley (1971)]

List of Publications

Published

1. **Pawan Kumar Mishra** and Shradha Mishra, “Active polar flock with birth and death,” *Physics of Fluids*, vol. 34, p. 057110, 2022. DOI: https://doi.org/10.1063/5.0086952.

2. **Pawan Kumar Mishra**, Abhra Puitandy, and Shradha Mishra, "Directional cues affect the collective behaviour of self-propelled particles in one dimension," *Europhysics Letters*, (2024). URL: http://iopscience.iop.org/article/10.1209/0295-5075/ad749c.

3. **Pawan Kumar Mishra**, Ajeya Krishna, and Shradha Mishra, “Active Brownian particles can mimic the pattern of the substrate,” *Soft Materials*, vol. 21, no. 4, pp. 377-387, 2023. DOI: https://doi.org/10.1080/1539445X.2023.2277730.

4*. Partha Sarathi Mondal, **Pawan Kumar Mishra**, and Shradha Mishra, “Ordering kinetics and steady states of XY-model with ferromagnetic and nematic interaction,” *Journal of Physics: Condensed Matter*, vol. 36, p. 285101, 2024. DOI: https://doi.org/10.1088/1361-648X/ad3abe.

5*. **Pawan Kumar Mishra** and Shradha Mishra, “Inhomogeneous active systems,” *PHYSICS NEWS*, vol. 53, pp. 38-41, 2023. URL: https://www.tifr.res.in/~news/V53-12/PN_V53-12. ***(Review article)***

Unpublished

6*. Jayam Joshi, **Pawan Kumar Mishra**, and Shradha Mishra, “Effective Single Particle Theory for Active Systems,” *arXiv preprint*, 2024. URL: https://arxiv.org/abs/2401.02247. ***preprint available*** (2023).

7*. Partha Sarathi Mondal, **Pawan Kumar Mishra**, Tamás Vicsek, and Shradha Mishra, “Dynamical Swirl Structures Powered by Microswimmers in Active Nematics,” *arXiv e-prints*, 2024. URL: https://arxiv.org/abs/2407.XXXX. ***preprint available*** (2024).

8. **Pawan Kumar Mishra**, Partha Sarathi Mondal, and Shradha Mishra, "Polar particles induce strings in liquid crystal," (2024). *Under preparation*.

9*. Partha Sarathi Mondal, **Pawan Kumar Mishra**, Mitali Thorat, Ananya Verma, and Shradha Mishra, "Dynamics of phagocytosis through interplay of forces," URL: http://arxiv.org/abs/2411.12466. ***preprint available*** (2024).. *Submitted*.

10*. Anish Kumar, **Pawan Kumar Mishra**, Riya Singh, Shradha Mishra, and DebaPrasad Giri, "Reinforcement Learning Approach to the One-Dimensional Active Ising Model," (2024). Note: Ready to submit.

Note* 4, 5, 6, 7, 9 and 10 works are not the part of this thesis.

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