

Symmetric Hamiltonians, Energy Distribution, and Information Efficiency

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Abstract

This document explores the properties of symmetric Hamiltonians with zero-centered average energy, comparing their behavior in the canonical and microcanonical ensembles. We discuss how these systems maximize entropy and minimize free energy, leading to efficient energy and information distributions. Additionally, we analyze the distribution of spin values and the Gini coefficient, providing insights into the uniformity of spin distributions as the system approaches thermal equilibrium. Connections to ecological systems and species richness are also discussed, highlighting the broader applicability of these concepts.

1 Introduction

In statistical mechanics and thermodynamics, the behavior of systems can often be understood by examining their Hamiltonians and the symmetries they exhibit. A particular class of Hamiltonians, characterized by their zero-centered average energy, offers interesting insights into the distribution of energy, the efficiency of information encoding, and the system's stability. This document aims to provide a detailed analysis of these Hamiltonians, comparing their behavior in different thermodynamic ensembles and exploring their implications for energy and information efficiency. Additionally, we draw connections to ecological systems and species richness, demonstrating the broader applicability of these concepts.

2 Symmetric Hamiltonians and Zero-Centered Energy

Consider a Hamiltonian of the form:

$$H = -J \sum_i (s_i - \bar{s}), \quad (1)$$

where $\bar{s} = \frac{1}{N} \sum_i s_i$ is the average spin, and s_i are the individual spin values. This Hamiltonian is symmetric and ensures that the sum of deviations from the average spin is zero:

$$\sum_i (s_i - \bar{s}) = 0. \quad (2)$$

This symmetry implies that the energy distribution is centered around zero.

2.1 Symmetry Properties

The Hamiltonian exhibits several key symmetries,

- **Translation Symmetry in Spin Space:** The Hamiltonian is invariant under a global shift of all spin values by a constant. Mathematically, if $s_i \rightarrow s_i + c$ for all i , then $\bar{s} \rightarrow \bar{s} + c$, and $s_i - \bar{s}$ remains unchanged.
- **Reflection Symmetry:** The Hamiltonian is symmetric under the reflection of spins around the mean value. If $s_i - \bar{s} \rightarrow -(s_i - \bar{s})$, the Hamiltonian remains the same.
- **Global Spin Flip Symmetry (Z2 Symmetry):** For systems where spins can take values ± 1 , the Hamiltonian is invariant under a global flip of all spins. If $s_i \rightarrow -s_i$ for all i , then $\bar{s} \rightarrow -\bar{s}$, and $s_i - \bar{s} \rightarrow -(s_i - \bar{s})$.

3 The Canonical Ensemble

In the canonical ensemble, the system is in thermal equilibrium with a heat bath at temperature T . The probability of the system being in a particular microstate with energy E_i is given by the Boltzmann distribution:

$$P_i = \frac{e^{-\beta E_i}}{Z}, \quad (3)$$

where $\beta = \frac{1}{k_B T}$ and Z is the partition function. The distribution of energies in the canonical ensemble allows for fluctuations around an average energy, influenced by temperature and the coupling constant J .

3.1 Internal Energy U

The internal energy U is the expectation value of the energy, which by symmetry of the Hamiltonian is 0,

$$U = \langle E \rangle = \frac{1}{Z} \sum_i E_i e^{-\beta E_i} \quad (4)$$

$$= 0 \quad (5)$$

3.2 Helmholtz Free Energy F

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

$$F = U - k_B T \ln Z \quad (6)$$

$$= -k_B T \ln Z \quad (7)$$

3.3 Entropy in the Canonical Ensemble

The entropy S quantifies the number of possible microstates Ω consistent with the macroscopic properties of the system, and can be derived from the Helmholtz free energy using the relation,

$$S = - \left(\frac{\partial F}{\partial T} \right)_V \quad (8)$$

We differentiate F with respect to T ,

$$\frac{\partial F}{\partial T} = -k_B \left(\ln Z + T \frac{\partial \ln Z}{\partial T} \right) \quad (9)$$

Next, we differentiate $\ln Z$ with respect to T ,

$$\frac{\partial \ln Z}{\partial T} = \frac{1}{Z} \frac{\partial Z}{\partial T} \quad (10)$$

Now, we differentiate Z with respect to T ,

$$Z = \sum_i e^{-\beta E_i} \quad (11)$$

$$\frac{\partial Z}{\partial T} = \sum_i \frac{\partial}{\partial T} e^{-\beta E_i} \quad (12)$$

$$= \sum_i e^{-\beta E_i} \left(-E_i \frac{\partial \beta}{\partial T} \right) \quad (13)$$

Since $\beta = \frac{1}{k_B T}$,

$$\frac{\partial \beta}{\partial T} = -\frac{1}{k_B T^2} \quad (14)$$

51 Substituting $\frac{\partial \beta}{\partial T}$ into $\frac{\partial Z}{\partial T}$,

$$\frac{\partial Z}{\partial T} = \sum_i e^{-\beta E_i} \left(-E_i \left(-\frac{1}{k_B T^2} \right) \right) \quad (15)$$

$$= \frac{1}{k_B T^2} \sum_i E_i e^{-\beta E_i} \quad (16)$$

52 Substituting $\frac{\partial Z}{\partial T}$ back into $\frac{\partial \ln Z}{\partial T}$,

$$\frac{\partial \ln Z}{\partial T} = \frac{1}{Z} \cdot \frac{1}{k_B T^2} \sum_i E_i e^{-\beta E_i} \quad (17)$$

$$= \frac{1}{k_B T^2} \langle E \rangle \quad (18)$$

53 where $\langle E \rangle = \frac{1}{Z} \sum_i E_i e^{-\beta E_i}$. Finally, substituting $\frac{\partial \ln Z}{\partial T}$ back into $\frac{\partial F}{\partial T}$,

$$\frac{\partial F}{\partial T} = -k_B \left(\ln Z + T \cdot \frac{1}{k_B T^2} \langle E \rangle \right) \quad (19)$$

$$= -k_B \ln Z - \frac{\langle E \rangle}{T} \quad (20)$$

54 Giving the expression for entropy,

$$S = - \left(\frac{\partial F}{\partial T} \right)_V \quad (21)$$

$$= k_B \ln Z + \frac{\langle E \rangle}{T} \quad (22)$$

$$= k_B \ln Z \quad (23)$$

55 3.4 Relation to Gibbs Entropy Formula

56 From the canonical ensemble the probability of a configuration at a given energy is,

$$P_i = \frac{e^{-\beta E_i}}{Z} \quad (24)$$

57 Substituting P_i into the Gibbs entropy formula,

$$(25)$$

$$S = -k_B \sum_i P_i \ln P_i \quad (26)$$

58 Simplify the expression,

$$(27)$$

$$S = -k_B \sum_i \left(\frac{e^{-\beta E_i}}{Z} \right) \ln \left(\frac{e^{-\beta E_i}}{Z} \right) \quad (28)$$

$$= -k_B \sum_i \left(\frac{e^{-\beta E_i}}{Z} \right) (-\beta E_i - \ln Z) \quad (29)$$

$$= k_B \sum_i \left(\frac{e^{-\beta E_i}}{Z} \right) (\beta E_i + \ln Z) \quad (30)$$

59 Separate the terms,

$$S = k_B \beta \sum_i \left(\frac{E_i e^{-\beta E_i}}{Z} \right) + k_B \ln Z \sum_i \left(\frac{e^{-\beta E_i}}{Z} \right) \quad (31)$$

$$= k_B \beta \langle E \rangle + k_B \ln Z \quad (32)$$

60 Given that $\beta = \frac{1}{k_B T}$,

(33)

$$S = \frac{\langle E \rangle}{T} + k_B \ln Z \quad (34)$$

61 and for $\langle E \rangle = 0$,

$$S = k_B \ln Z \quad (35)$$

62 This derivation shows the relation to the Gibbs entropy formula for the canonical ensemble, and for a
63 symmetric Hamiltonian with zero-centered average energy the entropy depends solely on the partition
64 function Z .

65 Only in the infinite limit of the number of lattice sites, N , does $\langle E \rangle = 0$. For a finite lattice the
66 average energy is fluctuates about 0.

67 3.5 Entropy for Finite Lattice Size with $\langle E \rangle = 0$

68 For a finite lattice size, the average energy $\langle E \rangle$ is not exactly zero, and there are energy fluctuations.
69 We define δE as the standard deviation of the energy,

$$\sigma_E^2 = \delta E = \sqrt{\langle E^2 \rangle - \langle E \rangle^2}. \quad (36)$$

70 Substituting δE into the entropy expression, we have,

$$S = k_B \ln Z + \frac{\delta E}{T} \quad (37)$$

71 Therefore, the entropy for a finite lattice size, including energy fluctuations, is,

$$S = k_B \ln Z + \frac{1}{T} \sqrt{\langle E^2 \rangle - \langle E \rangle^2} \quad (38)$$

$$S = k_B \ln Z + \frac{\sigma_E^2}{T} \quad (39)$$

72 3.6 Distribution of Spin Values and the Gini Coefficient

73 As the system reaches equilibrium, the distribution of spin values becomes more uniform, reflecting the
74 maximization of entropy and minimization of free energy. The Gini coefficient is a measure of inequality
75 in the distribution of spin values:

$$G = \frac{\sum_{i=1}^n \sum_{j=1}^n |s_i - s_j|}{2n \sum_{i=1}^n s_i}. \quad (40)$$

76 At thermal equilibrium, the Gini coefficient approaches zero, indicating a uniform distribution of spin
77 values.

78 4 Connections to Ecology and Species Richness

79 The principles of energy distribution, stability, and information efficiency have direct analogies in ecology,
80 particularly in the context of species richness and biodiversity.

81 4.1 Energy Flow in Ecosystems

82 Energy flows through ecosystems via trophic levels, from primary producers to herbivores, carnivores,
83 and decomposers. The efficiency of energy transfer between trophic levels impacts the distribution of
84 energy within the ecosystem.

4.2 Productivity and Biodiversity

Areas with higher primary productivity often support greater species richness due to the availability of more energy and resources. This is analogous to systems with higher energy levels supporting a broader range of states.

4.3 Metabolic Theory of Ecology

The metabolic theory of ecology links energy metabolism to biodiversity patterns, explaining how energy availability and metabolic constraints influence species richness.

4.4 Ecosystem Stability

Biodiversity contributes to ecosystem stability, similar to how entropy maximization leads to stable energy distributions. Diverse ecosystems can better absorb disturbances and maintain function, reflecting the stability observed in thermodynamic systems at equilibrium.

5 Conclusion

The analysis of symmetric Hamiltonians with zero-centered average energy reveals important insights into the behavior of physical systems. By comparing their behavior in the canonical and microcanonical ensembles, we understand how these systems maximize entropy and minimize free energy, leading to efficient energy and information distributions. The approach to thermal equilibrium results in a uniform distribution of spin values, minimizing the Gini coefficient and demonstrating the balance and efficiency inherent in these systems. The connections to ecological systems further highlight the broader applicability of these concepts, offering a unified framework for understanding stability, energy distribution, and information efficiency in both physical and ecological contexts.

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