Thermal States and Gibbs Distributions

Quantum Foundations · Module 9 — Quantum Thermodynamics

Node 9.1

Position in Knowledge Graph

System: Quantum Foundations **Structural Domain:** Quantum Thermodynamics **Node:** 9.1

This is the foundation node of the quantum thermodynamics module. The Gibbs state is the unique density matrix that maximizes von Neumann entropy subject to a fixed expected energy. It is the equilibrium state in quantum statistical mechanics, and it is the structural object on which all subsequent nodes — work, heat, fluctuation theorems, Landauer's principle — are built.

Formal Definition

For a quantum system with Hamiltonian H at inverse temperature $\beta = 1/(k_B T)$, the **thermal state** (or **Gibbs state**) is

$$\rho_\beta = \frac{e^{-\beta H}}{Z(\beta)}, \qquad Z(\beta) = \mathrm{tr}(e^{-\beta H}).$$

The normalization $Z(\beta)$ is the **partition function**. In the energy eigenbasis $\{|n\rangle\}$ with eigenvalues E_n, the Gibbs state is diagonal with populations

$$p_n = \frac{e^{-\beta E_n}}{Z(\beta)}.$$

The thermodynamic free energy is

$$F(\beta) = -\frac{1}{\beta} \log Z(\beta),$$

and entropy, internal energy, and other thermodynamic quantities follow by standard derivatives.

Variational Characterization

The Gibbs state is the unique density matrix that **maximizes the von Neumann entropy** subject to a constraint on the expected energy:

$$\rho_\beta = \arg \max_{\rho : \mathrm{tr}(\rho H) = U} S(\rho).$$

The Lagrange multiplier of the energy constraint is exactly β.

Equivalently, it minimizes the **free energy functional** $F(\rho) = \mathrm{tr}(\rho H) - T\,S(\rho)$. Both characterizations are quantum analogues of the Boltzmann maximum-entropy and Helmholtz minimum-free-energy principles.

Intuition

The Gibbs state is "what you get when a quantum system equilibrates with a thermal bath at temperature T." It has two structural properties that distinguish it from other density matrices:

1. **Diagonal in the energy eigenbasis.** Energy is conserved, so coherences between eigenstates of H are unstable under thermal fluctuations and decay.
2. **Boltzmann-weighted populations.** Energetically lower states are exponentially more likely. The exponential structure is the structural fingerprint of thermal equilibrium.

The Gibbs state is also the **fixed point of any Lindblad dynamics** that satisfies detailed balance with respect to H at temperature T. This connects quantum thermodynamics to the open-system formalism of Module 8.

Structural Role

The Gibbs state organizes the entire module:

- **Quantum work and heat** (9.2) are defined as energy changes during processes that take a system from one Gibbs state to another (or that drive it out of equilibrium).
- **Fluctuation theorems** (9.3) constrain the statistics of work in non-equilibrium processes.
- **Landauer's principle** (9.4) bounds the thermodynamic cost of erasing information in terms of $k_B T \log 2$.
- **Quantum heat engines** (9.5) are cyclic processes between Gibbs states at different temperatures.
- **Resource theories** (9.6) take Gibbs states as the "free" resource and quantify deviations from equilibrium as the costly resource.

Mathematical Development

High and low temperature limits

- $T \to 0$ ($\beta \to \infty$): the Gibbs state collapses onto the ground state (or ground subspace, if degenerate). Thermal fluctuations are suppressed.
- $T \to \infty$ ($\beta \to 0$): the Gibbs state becomes maximally mixed, $\rho_\beta \to I/d$. All energy levels are equally populated.

In between, the populations interpolate exponentially.

Connection to entropy

Substituting the Gibbs state into the von Neumann entropy formula:

$$S(\rho_\beta) = -\sum_n p_n \log p_n = \beta U + \log Z = \beta(U - F).$$

This is exactly the thermodynamic relation $S = (U - F)/T$, now derived from the underlying quantum-mechanical formalism rather than postulated.

Quantum partition function

For a single qubit with $H = \frac{1}{2}\omega Z$:

$$Z(\beta) = e^{-\beta\omega/2} + e^{\beta\omega/2} = 2\cosh(\beta\omega/2),$$

$$\langle E \rangle = -\frac{\partial \log Z}{\partial \beta} = -\frac{\omega}{2}\tanh(\beta\omega/2).$$

In the high-T limit $\langle E \rangle \to 0$ (qubit unbiased); in the low-T limit $\langle E \rangle \to -\omega/2$ (qubit in ground state).

Worked Example

Two-level atom in a thermal bath

Consider a two-level atom with energies 0 and $\hbar\omega$. At temperature T, the populations are

$$p_0 = \frac{1}{1 + e^{-\beta\hbar\omega}}, \qquad p_1 = \frac{e^{-\beta\hbar\omega}}{1 + e^{-\beta\hbar\omega}}.$$

This is the standard Boltzmann distribution. As T increases, p_1 approaches $1/2$; as $T \to 0$, $p_1 \to 0$.

The von Neumann entropy is the binary entropy $H_2(p_1)$, which is exactly the classical Shannon entropy of the population distribution. This is no coincidence: when a state is diagonal in a fixed basis, von Neumann entropy reduces to Shannon entropy.

Cross-Links

- **Module 5.1:** Density matrices — Gibbs states are a particularly important family.
- **Module 7.4:** Von Neumann entropy is the Lagrange-dual quantity that the Gibbs state maximizes.
- **Module 8:** Open-system dynamics with detailed balance converge to the Gibbs state.
- **Statistics:** Maximum entropy principle in classical statistics; the Gibbs state is the quantum analogue.
- **VQA:** Variational quantum eigensolvers minimize $\langle H \rangle$, which is the $T \to 0$ limit of free-energy minimization.

Structural Compression

Invariant: The Gibbs state is the maximum-entropy state at fixed expected energy.

Mechanism: $\rho_\beta = e^{-\beta H}/Z$ — the unique density matrix with this variational property.

Cross-System Echo: Boltzmann distribution in classical statistical mechanics; maximum-entropy distributions in classical information theory. Same structural identity, non-commutative generalization.

Exercises

1. Derive the Gibbs state by maximizing $S(\rho)$ subject to $\mathrm{tr}(\rho) = 1$ and $\mathrm{tr}(\rho H) = U$, using Lagrange multipliers.
2. Compute the partition function and average energy for a harmonic oscillator with $H = \hbar\omega(a^\dagger a + 1/2)$.

3. Show that the Gibbs state is the unique fixed point of any Lindblad evolution that satisfies detailed balance with respect to H at temperature T.
4. Verify that for a diagonal density matrix, von Neumann entropy reduces to Shannon entropy of the population distribution.
5. Show that the free energy $F = U - TS$ is minimized over all density matrices by the Gibbs state, and that the minimum value equals $-k_B T \log Z$.

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Concepts: density-matrix, von-neumann-entropy, variational-principle, expectation-value
Prerequisites: 5.1, 7.4, 2.6
Enables: 9.2, 9.4

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