

Part I

Quantum System–Bath Interactions and Their Control

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Excerpt

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Equilibration of Large Quantum Systems

The tendency of large systems to evolve to an equilibrium, namely, a stationary state that does not depend on their initial state, is called thermalization. The stationary state of a closed system is described by the *microcanonical ensemble* corresponding to a narrow energy distribution.

Large-system thermalization is commonplace. Yet it appears to contradict the unitarity of quantum mechanics, which requires symmetry with respect to time inversion. This contradiction has not yet been fully reconciled with the fundamental reversibility of quantum mechanics, despite a continuing endeavor that may be traced back to von Neumann's work in 1929. The central paradigm is the eigenstate thermalization hypothesis (ETH) put forward by Srednicki. It relies on the conjecture that a typical (randomly picked) eigenstate of a realistic many-body Hamiltonian yields the same mean value for any reasonable observable as predicted by a microcanonical ensemble with the same total energy. The ETH predicts that almost any superposition of such eigenstates relaxes at long times to a state that is practically indistinguishable from a thermal equilibrium state. Studies of thermalization in closed quantum many-body systems are aimed at bridging unitarity with irreversibility, ergodicity, and the onset of thermodynamic behavior in complex or open systems. Yet the quantum thermalization mechanism and the route to the bridging of quantum and classical descriptions of the world by this mechanism remain enigmatic and are still being debated. However, under generic conditions, one can show that the observables of a large system are governed at long times by a canonical density operator, as detailed in this chapter.

1.1 From Quantum Dynamics to Thermodynamics

In an isolated system with a large but countable number of degrees of freedom (DOF), $1 \ll f < \infty$, governed by an autonomous Hamiltonian H , the spectrum is

discrete (quantized). Its (typically infinitely many) eigenstates $|n\rangle$ ($n = 0, 1, \dots$) possess eigenvalues E_n , ordered as

$$E_0 \leq E_1 \leq E_2 \leq \dots, \quad (1.1)$$

with a bounded ground state energy, $E_0 > -\infty$. The Hamiltonian can then be written as

$$H := \sum_n E_n |n\rangle\langle n|. \quad (1.2)$$

In the presence of energy degeneracy, we may use the projectors onto subspaces of degenerate energies $E_m = E_n$,

$$P_{E_n} := \sum_{E_m=E_n} |m\rangle\langle m|, \quad (1.3)$$

to rewrite the Hamiltonian (1.2) as

$$H = \sum_{E_n} E_n P_{E_n}, \quad (1.4)$$

where \sum_{E_n} is a summation over all *mutually different* E_n values.

1.1.1 Thermodynamic Variables

The number of energy levels below any given E is

$$N(E) := \sum_n \theta(E - E_n), \quad (1.5)$$

the Heaviside (step) function $\theta(x)$ being equal to 1 for $x > 0$ and 0 for $x \leq 0$. The *entropy* associated with this number of levels is defined as

$$S(E) := k_B \ln N(E), \quad (1.6)$$

where k_B is Boltzmann's constant. Commonly, this entropy is an extensive quantity, since it scales for a system with f DOF as

$$S(E)/k_B = O(f). \quad (1.7)$$

Equation (1.5) implies that for macroscopic $f = O(10^{23})$, the level density is staggering even on extremely small energy scales. Hence, the step function $\theta(x)$ in (1.5) may be assumed to be washed out. The level number $N(E)$ then becomes a smooth function of E , whose well-defined derivative represents the density of states

$$\Omega(E) = \sum_n \delta(E - E_n), \quad (1.8)$$

the delta-function $\delta(x) = \theta'(x)$ being also assumed to be washed out over many energy levels.

The *coarse-grained entropy* defined by (1.6) leads to the definition of *temperature*, which applies *whether the system is at equilibrium or not*:

$$T(E) := 1/S'(E). \quad (1.9)$$

In accordance with Nernst's *third law of thermodynamics*, the entropy and temperature converge to zero as the energy approaches the ground-state value, $E \rightarrow E_0$. For macroscopic values of $E - E_0$, the dependence of S on E is logarithmic. It then follows from (1.7) and (1.9) that

$$k_B T(E) = O\left(\frac{E - E_0}{f}\right), \quad (1.10)$$

so that, for any macroscopic energy change ΔE ,

$$T(E + \Delta E) = T(E) \left[1 + O\left(\frac{\Delta E}{E - E_0}\right) \right]. \quad (1.11)$$

All these relations may fail at extremely low temperatures, which are beyond our consideration here (but cf. references in this chapter).

1.1.2 States and Dynamics

A quantum mechanical state of the system is given by a density operator $\rho(t)$, whose evolution,

$$\rho(t) = U_t \rho(0) U_t^\dagger, \quad (1.12)$$

is governed by the unitary propagator

$$U_t := \exp(-iHt/\hbar) = \sum_n \exp(-iE_n t/\hbar) |n\rangle\langle n|. \quad (1.13)$$

Equations (1.12) and (1.13) yield, for an arbitrary initial state $\rho(0)$,

$$\rho(t) = \sum_{m,n} \rho_{mn}(0) e^{-i(E_m - E_n)t/\hbar} |m\rangle\langle n|, \quad (1.14)$$

where $\sum_{m,n}$ is a summation over all $m, n = 0, 1, 2, \dots$, $\rho_{mn}(t) := \langle m|\rho(t)|n\rangle$ being the matrix elements of $\rho(t)$.

The ensemble-averaged occupation probability p_{E_n} of an eigenvalue E_n is given by the expectation value of the projector (1.3) onto the corresponding eigenspace,

$$p_{E_n} := \text{Tr}[P_{E_n} \rho(t)] = \sum_{E_m=E_n} \rho_{mm}(t) = \sum_{E_m=E_n} p_m, \quad (1.15)$$

where the level population p_n is the time-independent expectation value of the observable $|n\rangle\langle n|$,

$$p_n := \text{Tr} [|n\rangle\langle n| \rho(t)] = \rho_{nn}(t) = \rho_{nn}(0), \quad (1.16)$$

normalized by

$$1 = \text{Tr} \rho(t) = \sum_n \rho_{nn}(t) = \sum_n p_n = \sum_{E_n} p_{E_n}. \quad (1.17)$$

In what follows, we shall employ the energy basis in which all the non-diagonal elements of $P_{E_n} \rho(0) P_{E_n}$ vanish,

$$\rho_{mn}(0) = 0 \quad \text{if} \quad m \neq n \quad \text{and} \quad E_m = E_n. \quad (1.18)$$

1.2 The Problem of Equilibration for Physical Observables

The statistical ensemble $\rho(t)$ is not stationary at short t if $\rho(0)$ is out of equilibrium. Yet, if the right-hand side of (1.14) initially depends on t , it cannot approach at large t any time-independent “equilibrium ensemble.” Furthermore, any mixed state $\rho(t)$ returns arbitrarily “near” its initial state $\rho(0)$ at certain times t (analogously, but not identically, to pure-state Poincaré recurrences). In what follows, we examine the apparent contradiction of such recurrences with equilibration.

According to (1.14), there exists at least one $\rho_{mn}(0) \neq 0$ with

$$\omega := (E_n - E_m)/\hbar \neq 0. \quad (1.19)$$

We consider observables represented by Hermitian operators

$$X = \sum_{m,n} X_{mn} |m\rangle\langle n|, \quad X_{mn} := \langle m|X|n\rangle, \quad (1.20)$$

with expectation values

$$\langle X \rangle(t) := \text{Tr}[\rho(t)X]. \quad (1.21)$$

For the observable that represents an interlevel transition,

$$X = \hat{X} + \hat{X}^\dagger, \quad \hat{X} := |m\rangle\langle n|/\rho_{nn}(0), \quad (1.22)$$

we find from (1.14) that

$$\text{Tr}[\rho(t)X] = 2 \cos(\omega t). \quad (1.23)$$

Thus, the mean value of X in the ensemble $\rho(t)$ exhibits *permanent oscillations*, allowing us to conclude that *quantum mechanics and equilibration are, in general,*

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incompatible. Nevertheless, as shown below, equilibration can approximately hold true for a restricted class of observables X and initial conditions $\rho(0)$.

A measurement of an observable X may be assumed to yield a finite range of possible outcomes,

$$\Delta_X := \max_{\mathcal{H}} \langle \psi | X | \psi \rangle - \min_{\mathcal{H}} \langle \psi | X | \psi \rangle = x_{\max} - x_{\min}, \quad (1.24)$$

where the maximization and minimization are over all normalized vectors in the pertinent Hilbert space \mathcal{H} , $|\psi\rangle \in \mathcal{H}$, so that x_{\max} and x_{\min} are the largest and smallest eigenvalues of X , respectively.

1.2.1 Equilibration Conditions

The key requirement on the initial condition $\rho(0)$ is that the ensemble-averaged level populations p_n can be split into a locally averaged level *population density* $h(E)$ and “unbiased fluctuations” δp_n , whose average within the interval around E is vanishingly small compared to $h(E)$,

$$p_n = h(E_n) + \delta p_n. \quad (1.25)$$

This requirement should hold within any energy interval, which contains many levels E_n , but is still exceedingly small on any experimentally resolvable scale.

This initial condition is the result of a preparation process, during which the system was still entangled with the outside world. The reduced initial state (at $t = 0$) of the system (obtained by tracing out the outside world) must therefore be a mixed state. Any time-dependent system Hamiltonian will cause the spreading of occupation probabilities over neighboring energy levels. Since the levels are so dense, the spreading *randomizes the* p_n 's in accordance with (1.25). This preparation process stands in contrast to a “sudden” (discontinuous) parametric change of the Hamiltonian, dubbed *quantum quench*.

1.2.2 Energy Density

Let us define the ensemble-averaged energy density

$$\rho(E) := \langle \delta(E - H) \rangle, \quad (1.26)$$

$\rho(E)dE$ being the probability to find an energy value between E and $E + dE$. From (1.16) it follows that

$$\rho(E) = \sum_n p_n \delta(E - E_n). \quad (1.27)$$

The delta-functions in (1.27) are assumed to be “washed out” over many energy levels so that they give rise to a well-defined, smooth energy density. Consistently with (1.25) one then finds that

$$\rho(E) = h(E)\Omega(E). \quad (1.28)$$

Namely, the probability $\rho(E)dE$ of finding an energy between E and $E + dE$ is given by the locally averaged energy-level population $h(E)$ multiplied by the local level density $\Omega(E)$ times the interval dE . It is important that the locally averaged population-density $h(E)$ be independent of the specific choice of the energy interval around E .

1.2.3 Maximal Level Population

Even if the energy levels are populated nonuniformly, we expect from (1.25)–(1.28) that

$$\max_n p_n \simeq 10^{-O(f)}, \quad (1.29)$$

so that $\max_n p_n$ is extremely small.

According to (1.22), the spectrum of X consists of the eigenvalues $x_{\pm} = \pm|\rho_{nm}(0)|^{-1}$ and, for $\dim \mathcal{H} > 2$, of the eigenvalue $x_0 = 0$. From (1.24) we then have

$$\Delta_X = 2|x_{\pm}| > \frac{2}{\max_n p_n}. \quad (1.30)$$

We can deduce from (1.29) that $\Delta_X \geq O(10^f)$. Although the observable (1.22) exhibits persistent oscillations (1.23), such oscillations are beyond the conceivable resolution limit for macroscopic systems ($f \gg 1$). Hence, any realistic measurement will yield one of the three outcomes, x_{\pm} or x_0 .

1.2.4 Equilibrium Ensemble

For an arbitrary $\rho(0)$ evolving according to (1.14), we can show that the corresponding equilibrium ensemble is described by the density operator of the time-averaged ensemble $\rho(t)$,

$$\rho_{\text{eq}} := \overline{\rho(t)}, \quad (1.31)$$

where ρ_{eq} is a nonnegative, Hermitian operator of unit trace.

In the energy basis employed in (1.18), one finds from (1.16) and (1.31) that

$$\rho_{\text{eq}} = \sum_n \rho_{nn}(0)|n\rangle\langle n| = \sum_n p_n |n\rangle\langle n|, \quad (1.32)$$

so that ρ_{eq} is the (time-independent) diagonal part of $\rho(t)$ from (1.14).

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From (1.21) and (1.31) we obtain that the average of $X(t)$ over all times $t > 0$ equals

$$\overline{\langle X \rangle(t)} = \text{Tr}(\rho_{\text{eq}} X). \quad (1.33)$$

Since this equality holds for $X = I$, the unity operator, it follows that the average of $\rho(t)$ over all times $t > 0$ is indistinguishable from ρ_{eq} .

We now estimate the derivation of $\langle X \rangle(t)$ from its time average (1.33). To this end, we define $\tilde{\Delta}_X$, the minimal range of the eigenvalues of the difference between X and *any energy-diagonal operator* $Y := \sum_n y_n |n\rangle\langle n|$ with arbitrary real coefficients y_0, y_1, \dots . Explicitly,

$$\tilde{\Delta}_X := \min_Y [\max_{\mathcal{H}} \langle \psi | X - Y | \psi \rangle - \min_{\mathcal{H}} \langle \psi | X - Y | \psi \rangle]. \quad (1.34)$$

By definition,

$$\tilde{\Delta}_X = 0 \quad \text{if } X = Y. \quad (1.35)$$

From (1.24) and (1.34) we then find that

$$\tilde{\Delta}_X \leq \Delta_X. \quad (1.36)$$

The mean-square deviation of $\langle X \rangle(t)$,

$$\sigma_X^2 := \overline{[\langle X \rangle(t) - \overline{\langle X \rangle(t)}]^2}, \quad (1.37a)$$

can then be shown to be bounded by

$$\sigma_X^2 \leq \tilde{\Delta}_X^2 \text{Tr} \rho_{\text{eq}}^2. \quad (1.37b)$$

The factor $\text{Tr} \rho_{\text{eq}}^2$ in (1.37b) is the purity of the *time-independent* part of $\rho(t)$: $\text{Tr} \rho_{\text{eq}}^2 = \sum_n \rho_{nn}^2(0)$ according to (1.32). While $\rho(t)$ may be a pure state, the purity of ρ_{eq} may be as small as $10^{-O(f)}$ according to (1.29). We then finally obtain

$$\sigma_X^2 \leq \tilde{\Delta}_X^2 \max_n p_{E_n}, \quad (1.38)$$

where p_{E_n} [see (1.15)] is the occupation probability of E_n .

Let us consider $\text{Tr}[\rho(t)X]$ as a *random variable*, generated by sampling the observable at random times t . The probability for $\langle X \rangle(t)$ to deviate from its time average $\overline{\langle X \rangle(t)}$ by more than an infinitesimal quantity δX can then be proven to be bounded by

$$\text{Prob}\{|\text{Tr}[\rho(t)X] - \text{Tr}(\rho_{\text{eq}}X)| \geq \delta X\} \leq \left(\frac{\sigma_X}{\delta X}\right)^2. \quad (1.39)$$

Upon replacing (1.38) by its estimate according to (1.29) and considering (1.39), one arrives at the main result of the present chapter:

$$\text{Prob}\{|\text{Tr}[\rho(t)X] - \text{Tr}(\rho_{\text{eq}}X)| \geq \delta X\} \leq \left(\frac{\tilde{\Delta}_X}{\delta X}\right)^2 10^{-O(f)}. \quad (1.40)$$

This general expression defines the resolution limit δX of $\langle X \rangle(t)$ deviations from equilibrium.

1.3 From Equilibration to Thermalization

According to the present discussion, all observable expectation values (1.21) become practically indistinguishable from

$$\text{Tr}(\rho_{\text{eq}}X) = \sum p_n X_{nn} \quad (1.41)$$

after initial transients have died out. Hence, the arguments raised above imply that for realistic typical observables of macrosystems the problem of equilibration can be considered as settled.

Upon adopting the arguments that support equilibration of experimentally realistic (typical) observables, as per (1.41), we next turn to the key question: To what extent is the equilibrium expectation value of X from (1.41) in agreement with that predicted by the microcanonical ensemble, namely

$$\text{Tr}(\rho^{\text{mic}}X) = \sum p_n^{\text{mic}} X_{nn}? \quad (1.42)$$

Accordingly, are the level populations p_n^{mic} simply equal to a normalization constant if E_n is contained within a small energy interval $[E - \Delta E, E]$? Alternatively, we may ask: Under what conditions does the microcanonical formalism of equilibrium statistical mechanics break down?

The main condition for the microcanonical formalism to be valid is that only E_n within a small energy interval have a nonvanishing occupation probability, namely, the system energy is known to a high precision. We specifically assume that the system energy is known within an uncertainty ΔE that is small, but experimentally realistic.

Another validity condition of the microcanonical formalism is that the expectation values (1.42) must be (practically) independent of the exact choice of the energy interval (i.e., of its upper limit E and its width ΔE). The same conclusion follows from the equivalence of the microcanonical and canonical ensembles (for all energies E), considered as a self-consistency condition for equilibrium