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Chapter 3

Ergodicity and the Approach to Equilibrium

3.1 References

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  An advanced text with an emphasis on fluids and kinetics.
- R. Balian, *From Macrophysics to Microphysics* (2 vols., Springer-Verlag, 2006)
  A very detailed discussion of the fundamental postulates of statistical mechanics and their implications.

3.2 The Master Equation and the Approach to Equilibrium

3.2.1 Equilibrium

A thermodynamic system typically consists of an enormously large number of constituent particles, a typical 'large number' being Avogadro's number, $N_{\rm A} = 6.02 \times 10^{23}$. Nevertheless, in *equilibrium*, such a system is characterized by a relatively small number of thermodynamic state variables. Thus, while a complete description of a (classical) system would require us to account for $\mathcal{O}(10^{23})$ evolving degrees of freedom, with respect to the physical quantities in which we are interested, the details of the initial conditions are effectively forgotten over some microscopic time scale τ, called the collision time, and over some microscopic distance scale, ℓ, called the mean free path[1]. The equilibrium state is time-independent.

3.2.2 The master equation

Relaxation to equilibrium is often modeled with something called the *master equation*. Let $P_i(t)$ be the probability that the system is in a quantum or classical state i at time t. Then write

$$\frac{dP_i}{dt} = \sum_j \big(W_{ij}\, P_j - W_{ji}\, P_i \big) \quad . \tag{3.1}$$

Here, W_{ij} is the rate at which j makes a transition to i. We assume the state space is finite and of size N, so that $i, j \in \{1, \ldots, N\}$. Note that the diagonal elements W_{ii} (no sum on i) all cancel from the above equation and we may without loss of generality set $W_{ii} = 0 \;\forall\; i$. We may recast the master equation in the form

$$\frac{dP_i}{dt} = -\sum_j \Gamma_{ij}\, P_j \quad , \tag{3.2}$$

where

$$\Gamma_{ij} = \begin{cases} -W_{ij} & \text{if } i \neq j \\ \sum_k{}' W_{kj} & \text{if } i = j \end{cases} \quad , \tag{3.3}$$

where the prime on the sum indicates that $k = j$ is to be excluded. The constraints on the W_{ij} are that $W_{ij} \geq 0$ for all i, j, and we set each $W_{ii} = 0$. Fermi's Golden Rule of quantum mechanics says that

$$W_{ij} = \frac{2\pi}{\hbar} \left| \langle\, i \,|\, \hat{V} \,|\, j \,\rangle \right|^2 \varrho(E_i) \quad , \tag{3.4}$$

with $i \neq j$, where $\hat{H}_0 \,|\, i \,\rangle = E_i \,|\, i \,\rangle$, $\hat{V}$ is an additional potential which leads to transitions, and $\varrho(E_i)$ is the density of final states at energy E_i. The fact that $W_{ij} \geq 0$ means that if each $P_i(t = 0) \geq 0$, then $P_i(t) \geq 0$ for all $t \geq 0$. To see this, suppose that at some time $t > 0$ one of the probabilities P_i is crossing zero and about to become negative. But then eqn. 3.1 says that $\dot{P}_i(t) = \sum_j W_{ij} P_j(t) \geq 0$. So $P_i(t)$ can never become negative.

[1] Exceptions involve quantities which are conserved by collisions, such as overall particle number, momentum, and energy. These quantities relax to equilibrium in a special way called *hydrodynamics*.

3.2.3 Solution to the master equation

If the transition rates W_{ij} are themselves time-independent, then we may formally write

$$P_i(t) = \left(e^{-\Gamma t}\right)_{ij} P_j(0) \quad . \tag{3.5}$$

Here we have used the Einstein 'summation convention' in which repeated indices are summed over (in this case, the j index). Note that $\sum_i \Gamma_{ij} = 0$, which says that the total probability $\sum_i P_i$ is conserved:

$$\frac{d}{dt}\sum_i P_i = -\sum_{i,j} \Gamma_{ij}\, P_j = -\sum_j \left(P_j \sum_i \Gamma_{ij} \right) = 0 \quad . \tag{3.6}$$

We conclude that $\boldsymbol{L}^1 = (1\ ,\ 1\ ,\ \ldots\ ,\ 1)$ is a left eigenvector of Γ with eigenvalue $\lambda = 0$. The corresponding right eigenvector, which we write as $\boldsymbol{R}^1$ with $R^1_i = P^{\rm eq}_i$, satisfies $\sum_j \Gamma_{ij} R^1_j = 0$, and is a stationary (*i.e.* time independent) solution to the master equation. The $N \times N$ matrix Γ_{ij} is real but not necessarily symmetric. For such a matrix, the left eigenvectors L^α_i and the right eigenvectors R^β_j satisfy

$$L^\alpha_i\, \Gamma_{ij} = \lambda_\alpha\, L^\alpha_j \qquad , \qquad \Gamma_{ij}\, R^\beta_j = \lambda_\beta\, R^\beta_i \quad , \tag{3.7}$$

but in general are not related by a simple transpose operation as they are for real symmetric matrices. We denote the right and left eigenvectors by $|\, R^\alpha \,\rangle$ and $\langle\, L^\alpha \,|$, which are column vectors and row vectors, respectively. Thus $\Gamma\,|\, R^\alpha\,\rangle = \lambda_\alpha |\, R^\alpha\,\rangle$ and $\langle\, L^\alpha\,|\,\Gamma = \langle\, L^\alpha\,|\,\lambda_\alpha$, the second of which may be written as $\Gamma^{\mathsf T}\,|\, L^\alpha\,\rangle = \lambda_\alpha\,|\, L^\alpha\,\rangle$, where the column vector $|\, L^\alpha\,\rangle$ is the transpose of the row vector $\langle\, L^\alpha\,|$ and $\Gamma^{\mathsf T}$ is the matrix transpose of Γ. The characteristic polynomial is the same in both cases:

$$F(\lambda) \equiv \det\,(\lambda - \Gamma) = \det\,(\lambda - \Gamma^{\mathsf T}) \quad , \tag{3.8}$$

which means that the left and right eigenvalues are the same. Note also that $\big[F(\lambda)\big]^* = F(\lambda^*)$, hence the eigenvalues are either real or appear in complex conjugate pairs. Multiplying the eigenvector equation for L^α on the right by R^β_j and summing over j, and multiplying the eigenvector equation for R^β on the left by L^α_i and summing over i, and subtracting the two results yields $(\lambda_\alpha - \lambda_\beta)\,\langle\, L^\alpha\,|\,R^\beta\,\rangle = 0$, where the inner product is now $\langle\, L^\alpha\,|\,R^\beta\,\rangle = \sum_i L^\alpha_i\, R^\beta_i$ with no complex conjugation on the bra vector. We may now demand $\langle\, L^\alpha\,|\,R^\beta\,\rangle = \delta^{\alpha\beta}$, which is our eigenvector normalization condition. As discussed above in §3.7, in the event that Γ contains nontrivial Jordan blocks, its eigenvectors do not span. However, this is a nongeneric state of affairs, and here we assume that Γ contains no nontrivial Jordan blocks. In the generic case, there are no Jordan blocks and we have the spectral decomposition

$$\Gamma = \sum_{a=1}^N \lambda_a\, |\, R^a\,\rangle\langle\, L^a\,| \qquad \Rightarrow \qquad \Gamma_{ij} = \sum_{a=1}^N \lambda_a\, R^a_i\, L^a_j \quad . \tag{3.9}$$

We have seen that $\langle\, L\,| = (1\ ,\ 1\ ,\ \ldots\ ,\ 1)$ is a left eigenvector of the matrix Γ with eigenvalue $\lambda = 0$, since $\sum_i \Gamma_{ij} = 0$. We do not know *a priori* the corresponding right eigenvector, which depends on other details of Γ_{ij}. We reiterate that *generically* a matrix which is not normal has spanning eigenvectors, *i.e.*

the existence of nontrivial Jordan blocks is nongeneric. Assuming that the eigenvectors of Γ span, then, let's expand the probability distribution $P_i(t)$ in the right eigenvectors of Γ, writing

$$P_i(t) = \sum_\alpha C_\alpha(t)\, R_i^\alpha \quad , \tag{3.10}$$

where $\alpha \in \{1, \ldots, N\}$. Then

$$\frac{dP_i}{dt} = \sum_\alpha \frac{dC_\alpha}{dt}\, R_i^\alpha = -\Gamma_{ij}\, P_j = -\sum_\alpha C_\alpha\, \Gamma_{ij}\, R_j^\alpha = -\sum_\alpha \lambda_\alpha\, C_\alpha\, R_i^\alpha \quad . \tag{3.11}$$

Contracting on the index i with L_i^β, we have $\dot C_\beta = -\lambda_\beta\, C_\beta$ and thus $C_\beta(t) = C_\beta(0)\, e^{-\lambda_\beta t}$. Hence, we have the formal solution

$$P_i(t) = \sum_\alpha C_\alpha(0)\, e^{-\lambda_\alpha t}\, R_i^\alpha \quad . \tag{3.12}$$

Let $\alpha = 1$ correspond to the left eigenvector $\langle\, L^1 \,| = (1\ ,\ 1\ ,\ \ldots\ ,\ 1)$. The corresponding eigenvalue is $\lambda_1 = 0$. It is now easy to see that $\mathsf{Re}\,(\lambda_\alpha) > 0$ for all $\alpha > 1$, or else the probabilities will become negative[2]. For suppose $\mathsf{Re}\,(\lambda_\alpha) < 0$ for some α. Then as $t \to \infty$, the sum in eqn. 3.12 will be dominated by the term for which λ_α has the largest negative real part; all other contributions will be subleading. But we must have $\sum_i R_i^\alpha = 0$ since $|\!|\, R^\alpha \,\rangle\!\rangle$ must be orthogonal to the left eigenvector $\langle\, L^1 \,|$. Therefore, at least one component of R_i^α (*i.e.* for some value of i) must have a negative real part, which means a negative probability![3] As we have already proven that an initial nonnegative distribution $\{P_i(t=0)\}$ will remain nonnegative under the evolution of the master equation, we conclude that $P_i(t) \to P_i^{\rm eq}$ as $t \to \infty$, relaxing to the $\lambda = 0$ right eigenvector, with $\mathsf{Re}\,(\lambda_\alpha) \geq 0$ for all α.

Detailed balance

In equilibrium, the net *flux* of transitions into a state $|i\rangle$ is equal to the flux of transitions out of $|i\rangle$. The flux of transitions from $|j\rangle$ to $|i\rangle$ is given by the product of the probability π_j for the system to be in the state $|j\rangle$ multiplied by the bare rate W_{ij}. If, for each state $|j\rangle$, the flux from $|i\rangle$ to $|j\rangle$ is equal to the flux from $|j\rangle$ to $|i\rangle$, we say that the rates satisfy the condition of *detailed balance*. In other words,

$$W_{ij}\, \pi_j = W_{ji}\, \pi_i \quad , \tag{3.13}$$

where $\pi_i \equiv P_i^{\rm eq}$ is the equilibrium distribution. Note that this does not say that the bare rates are equal unless $\pi_i = \pi_j$. Assuming $W_{ij} \neq 0$ and $\pi_j \neq 0$, we may divide to obtain

$$\frac{W_{ji}}{W_{ij}} = \frac{\pi_j}{\pi_i} \quad . \tag{3.14}$$

[2]We presume that the eigenvalue $\lambda = 0$ is nondegenerate.

[3]Since the probability $P_i(t)$ is real, if the eigenvalue with the smallest (*i.e.* largest negative) real part is complex, there will be a corresponding complex conjugate eigenvalue, and summing over all eigenvectors will result in a real value for $P_i(t)$.

Note that detailed balance is a stronger condition than that required for a stationary solution to the master equation. Recall that $\Gamma_{ij} = -W_{ij}$ for all $i \neq j$. When detailed balance holds, we then have $\Gamma_{ji}\pi_i = \Gamma_{ij}\pi_j \; \forall \; i, j$. But this entails

$$\widetilde{\Gamma}_{ij} \equiv \pi_i^{-1/2}\Gamma_{ij}\pi_j^{1/2} = \widetilde{\Gamma}_{ji} \quad . \tag{3.15}$$

Note that $\widetilde{\Gamma}_{ii} = \Gamma_{ii}$ for the diagonal elements. The real symmetric matrix $\widetilde{\Gamma}$ has real eigenvalues λ_a and a complete and orthonormal set of left/right eigenvectors ϕ_i^a. For the right and left eigenvectors of Γ, we then have $R_j^a = \pi_j^{1/2}\phi_j^a$ and $L_i^a = \pi_i^{-1/2}\phi_i^a$. Since $\sum_i \pi_i^{1/2}\widetilde{\Gamma}_{ij} = 0$, we have that $\pi_i^{1/2}$ is a left eigenvector of $\widetilde{\Gamma}$ with eigenvalue zero. Therefore $R_j^1 = \pi_j$, which is the equilibrium distribution.

Consider an arbitrary nonnegative real upper triangular matrix T with $T_{ij} \geq 0$ for all $1 \leq i < j \leq N$ and where each nonzero element has dimensions of rate (*i.e.* inverse time). Let π_i be a normalized distribution, *i.e.* $\pi_i \geq 0$ for all $i \in \{1, \ldots, n\}$ with $\sum_i \pi_i = 1$. Now define the nonnegative matrix

$$W_{ij} = \begin{cases} \pi_i \, T_{ij} & \text{if} \quad i < j \\ \pi_i \, T_{ji} & \text{if} \quad i > j \end{cases} \quad . \tag{3.16}$$

and take this to be the matrix of transition rates, so that the master equation is as in Eqn. 3.1, *viz.*

$$\frac{dP_i}{dt} = \sum_j \left(W_{ij} \, P_j - W_{ji} \, P_i \right) \quad . \tag{3.17}$$

Since $W_{ij}/W_{ji} = \pi_i/\pi_j$, the matrix W satisfies detailed balance relative to the distribution π. With $\Gamma_{ij} \equiv -W_{ij}$ for $i \neq j$ and $\Gamma_{ii} \equiv \sum_k{}' W_{ki}$ (with $k = i$ excluded from the sum) as before, we recover the form of the master equation $\dot{P}_i = -\sum_j \Gamma_{ij} \, P_j$.

How many parameters does it take to describe a general $N \times N$ transition matrix W_{ij} satisfying detailed balance? Since there are $\frac{1}{2}N(N-1)$ freedoms in T and $N-1$ freedoms in π, we conclude that there are $\frac{1}{2}(N-1)(N+2)$ parameters required to specify W_{ij} . But if we drop the constraint of detailed balance, then all the off-diagonal elements of W_{ij} are independent, corresponding to $N(N-1)$ parameters. Note that we may set $W_{ii} = 0$ for all i.

For the Boltzmann distribution at temperature T, we have $\pi_i = Z^{-1}\exp(-\beta E_i)$ where $\beta = 1/k_{\rm B}T$ and $Z(\beta) = \sum_i \exp(-\beta E_i)$ is the ordinary canonical partition function. To satisfy detailed balance, we could take $W_{ij} = \gamma \, e^{\beta(E_j - E_i)/2}$, with γ a constant having dimensions of inverse time. Or we could choose

$$W_{ij} = \begin{cases} \gamma & \text{if} \quad E_i < E_j \\ \gamma \, e^{\beta(E_j - E_i)} & \text{if} \quad E_i \geq E_j \end{cases} \quad . \tag{3.18}$$

The latter choice is common in Monte Carlo simulations.

If $\Gamma = \Gamma^{\intercal}$ is symmetric, then, up to normalization, the right eigenvectors and left eigenvectors are transposes of each other, hence $P^{\rm eq} = 1/N$, where N is the matrix dimension of Γ. The system then satisfies the conditions of detailed balance. See §3.8 below for an example of this formalism applied to Poisson processes and to a model of radioactive decay.

3.2.4 Boltzmann's $\mathcal{H}$-theorem

Suppose for the moment that Γ is a symmetric matrix, *i.e.* $\Gamma_{ij} = \Gamma_{ji}$. Then construct the function

$$\mathcal{H}(t) = \sum_i P_i(t)\ \log P_i(t) \quad . \tag{3.19}$$

Then

$$\begin{aligned} \frac{d\mathcal{H}}{dt} &= \sum_i \frac{dP_i}{dt}\left(1 + \log P_i\right) = \sum_i \frac{dP_i}{dt}\ \log P_i \\ &= -\sum_{i,j} \Gamma_{ij}\, P_j \log P_i = \sum_{i,j} \Gamma_{ij}\, P_j \big(\log P_j - \log P_i\big) \quad , \end{aligned} \tag{3.20}$$

where we have used $\sum_i \Gamma_{ij} = 0$. Now switch $i \leftrightarrow j$ in the above sum and add the terms to get

$$\frac{d\mathcal{H}}{dt} = \frac{1}{2}\sum_{i,j} \Gamma_{ij}\big(P_i - P_j\big)\ \big(\log P_i - \log P_j\big) \quad . \tag{3.21}$$

Note that the $i = j$ term does not contribute to the sum. For $i \neq j$ we have $\Gamma_{ij} = -W_{ij} \leq 0$, and using the result

$$(x - y)\,(\log x - \log y) \geq 0 \quad , \tag{3.22}$$

we conclude $d\mathcal{H}/dt \leq 0$. In equilibrium, $P_i^{\rm eq}$ is a constant, independent of i. We write

$$P_i^{\rm eq} = \frac{1}{\Omega} \quad , \quad \Omega = \sum_i 1 \quad \Longrightarrow \quad \mathcal{H} = -\log\Omega \quad , \tag{3.23}$$

with $\Omega = N$, the matrix dimension of Γ.

If $\Gamma_{ij} \neq \Gamma_{ji}$, we can still prove a version of the $\mathcal{H}$-theorem *when there is detailed balance*. Define a new symmetric matrix

$$\overline{W}_{ij} \equiv W_{ij}\, P_j^{\rm eq} = W_{ji}\, P_i^{\rm eq} = \overline{W}_{ji} \quad , \tag{3.24}$$

and the generalized $\mathcal{H}$-function,

$$\mathcal{H}(t) \equiv \sum_i P_i(t)\ \log\!\left(\frac{P_i(t)}{P_i^{\rm eq}}\right) \quad . \tag{3.25}$$

Then

$$\begin{aligned} \frac{d\mathcal{H}}{dt} &= -\frac{1}{2}\sum_{i,j}\left(W_{ji}P_i - W_{ij}P_j\right)\ \log\!\left(\frac{W_{ji}P_i}{W_{ij}P_j}\right) \\ &= -\frac{1}{2}\sum_{i,j}\overline{W}_{ij}\left(\frac{P_i}{P_i^{\rm eq}} - \frac{P_j}{P_j^{\rm eq}}\right)\left[\log\!\left(\frac{P_i}{P_i^{\rm eq}}\right) - \log\!\left(\frac{P_j}{P_j^{\rm eq}}\right)\right] \leq 0 \quad . \end{aligned} \tag{3.26}$$

3.2.5 Markov chains

A *Markov chain* is a process which describes transitions of a stochastic variable in time. There are four types to consider, depending on whether the state space is discrete (*i.e.* countable) or continuous (and measurable), and whether the process occurs in discrete time or continuous time. Here we will consider a discrete time Markov chain of a discrete state space. Let $P_i(t)$ be the probability that the system is in state i at time t. The evolution equation is

$$P_i(t+1) = \sum_j Q_{ij}\, P_j(t) \quad . \tag{3.27}$$

Note the similarity to the (continuous time) master equation in eqn. 3.2. Indeed, the master equation is an example of a *continuous time Markov process*. All the elements of the *transition matrix* Q_{ij} are real and nonnegative, and Q_{ij} satisfies $\sum_i Q_{ij} = 1$ so that the total probability $\sum_i P_i(t)$ is conserved. The element Q_{ij} is the *conditional probability* that for the system to evolve to state i at time $t+1$ given that it is in state j at time t, with Q_{ij} independent of t. Iterating eqn. 3.27, we have

$$P_i(t+n) = \left[Q^n\right]_{ij} P_j(t) \quad . \tag{3.28}$$

The transition matrix Q is in general non-normal, meaning $Q\,Q^{\mathsf{T}} \neq Q^{\mathsf{T}}Q$. In such cases the left eigenvectors are in general not simply related to the right eigenvectors at the corresponding eigenvalues, and the eigenvalues are not necessarily real. Under generic circumstances, we may write

$$Q = \sum_{a=1}^{n} \lambda_a \,|\, R^a \,\rangle\langle\, L^a \,| \quad , \tag{3.29}$$

with $|\lambda_a| \leq 1$ for all a. In nongeneric cases, there may be Jordan blocks in the canonical form of Q, which means the eigenvectors do not span – again see §3.7. From the condition $\sum_i Q_{ij} = 1$, we have that $\boldsymbol{L}^1 = (1, 1, \ldots, 1)$ is a left eigenvector corresponding to eigenvalue $\lambda = 1$, and the corresponding right eigenvector $\boldsymbol{R}^1$ is the asymptotic steady state, with $P_j^{\rm eq} = \langle\, j \,|\, R^1 \,\rangle = R_j^1$., here presumed unique. Since $Q \in M_N(\mathbb{R})$, where N is the matrix dimension (which we take here to be finite), if $\lambda \in \mathbb{C}$ is an eigenvalue, then λ^* is also an eigenvalue.

Example

Consider a group of Physics graduate students consisting of three theorists and four experimentalists. Within each group, the students are to be regarded as indistinguishable. Together, the students rent two apartments, A and B. Initially the three theorists live in A and the four experimentalists live in B. Each month, a random occupant of A and a random occupant of B exchange domiciles. Compute the transition matrix Q_{ij} for this Markov chain, and compute the average fraction of the time that B contains two theorists and two experimentalists, averaged over the effectively infinite time it takes the students to get their degrees. *Hint:* Q is a 4×4 matrix.

There are four states available (see Tab. 3.1). Let's compute the transition probabilities. First, we compute the transition probabilities out of state $|\,1\,\rangle$, *i.e.* the matrix elements Q_{j1}. Clearly $Q_{21} = 1$

$\vert\, j\,\rangle$	room A	room B	$g_j^{\rm A}$	$g_j^{\rm B}$	$g_j^{\rm TOT}$
$\vert\, 1\,\rangle$	TTT	EEEE	1	1	1
$\vert\, 2\,\rangle$	TTE	EEET	3	4	12
$\vert\, 3\,\rangle$	TEE	EETT	3	6	18
$\vert\, 4\,\rangle$	EEE	ETTT	1	4	4

Table 3.1: States and their degeneracies.

since we must exchange a theorist (T) for an experimentalist (E). All the other probabilities are zero: $Q_{11} = Q_{31} = Q_{41} = 0$. For transitions out of state $\vert\, 2\,\rangle$, the nonzero elements are

$$Q_{12} = \tfrac{1}{4} \times \tfrac{1}{3} = \tfrac{1}{12} \quad , \quad Q_{22} = \tfrac{3}{4} \times \tfrac{1}{3} + \tfrac{1}{4} \times \tfrac{2}{3} = \tfrac{5}{12} \quad , \quad Q_{32} = \tfrac{1}{2} \quad . \tag{3.30}$$

To compute Q_{12}, we must choose the experimentalist from room A (probability $\frac{1}{3}$) with the theorist from room B (probability $\frac{1}{4}$). For Q_{22}, we can either choose E from A and one of the E's from B, or one of the T's from A and the T from B. This explains the intermediate steps written above. For transitions out of state $\vert\, 3\,\rangle$, the nonzero elements are then $Q_{23} = \frac{1}{3}$, $Q_{33} = \frac{1}{2}$, and $Q_{43} = \frac{1}{6}$. Finally, for transitions out of state $\vert\, 4\,\rangle$, the nonzero elements are $Q_{34} = \frac{3}{4}$ and $Q_{44} = \frac{1}{4}$. The full transition matrix is then

$$Q = \begin{pmatrix} 0 & \frac{1}{12} & 0 & 0 \\ 1 & \frac{5}{12} & \frac{1}{3} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & \frac{3}{4} \\ 0 & 0 & \frac{1}{6} & \frac{1}{4} \end{pmatrix} \quad . \tag{3.31}$$

Note that $\sum_i Q_{ij} = 1$ for all $j = 1, 2, 3, 4$. This guarantees that $\boldsymbol{L}^1 = (1\ ,\ 1\ ,\ 1\ ,\ 1)$ is a left eigenvector of Q with eigenvalue 1. The corresponding right eigenvector is obtained by setting $Q_{ij}\, R_j^1 = R_i^1$. Simultaneously solving these four equations and normalizing so that $\sum_j R_j^1 = 1$, we easily obtain the (transpose of the) right eigenvector $R^{1,\mathsf{T}} = \frac{1}{35}\begin{pmatrix} 1 & 12 & 18 & 4 \end{pmatrix}$. This is the state we converge to after repeated application of the transition matrix Q. If we decompose $Q = \sum_{\alpha=1}^4 \lambda_\alpha \,\vert\, R^\alpha \,\rangle\langle\, L^\alpha \,\vert$, then in the limit $t \to \infty$ we have $Q^t \approx \vert\, R^1 \,\rangle\langle\, L^1 \,\vert$, where $\lambda_1 = 1$, since the remaining eigenvalues are all less than 1 in magnitude[4]. Thus, $Q^t\big\vert_{t\to\infty}$ acts as a *projector* onto the state $\vert\, R^1 \,\rangle$. Whatever the initial set of probabilities $P_j(t=0)$, we must have $\langle\, L^1 \,\vert\, P(0) \,\rangle = \sum_j P_j(0) = 1$. Therefore, $\lim_{t\to\infty} P_j(t) = R_j^1$, from which we have $P_3(\infty) = \frac{18}{35}$. Note that the equilibrium distribution satisfies detailed balance:

$$R_j^1 = \frac{g_j^{\rm TOT}}{\sum_l g_l^{\rm TOT}} \quad . \tag{3.32}$$

[4]One can check that $\lambda_1 = 1$, $\lambda_2 = \frac{5}{12}$, $\lambda_3 = 0$, and $\lambda_4 = -\frac{1}{4}$.

3.3 Phase Flows in Classical Mechanics

3.3.1 Hamiltonian evolution

The master equation provides us with a semi-phenomenological description of a dynamical system's relaxation to equilibrium. It explicitly breaks time reversal symmetry. Yet the microscopic laws of Nature are (approximately) time-reversal symmetric. How can a system which obeys Hamilton's equations of motion come to equilibrium?

Let's start our investigation by reviewing the basics of Hamiltonian dynamics. Recall the Lagrangian $L = L(q, \dot{q}, t) = T - V$. The Euler-Lagrange equations of motion for the action $S\big[q(t)\big] = \int dt\, L$ are

$$\dot{p}_\sigma = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_\sigma}\right) = \frac{\partial L}{\partial q_\sigma} \quad , \tag{3.33}$$

where p_σ is the canonical momentum conjugate to the generalized coordinate q_σ, *i.e.* $p_\sigma = \partial L/\partial \dot{q}_\sigma$. Here N is the number of degrees of freedom of the system, which is the total number of generalized coordinates.

The Hamiltonian, $H(q, p)$ is obtained by a Legendre transformation,

$$H(q,p) = \sum_{\sigma=1}^{N} p_\sigma\, \dot{q}_\sigma - L \quad . \tag{3.34}$$

Note that the differential of H is given by

$$\begin{aligned} dH &= \sum_{\sigma=1}^{N}\left(p_\sigma\, d\dot{q}_\sigma + \dot{q}_\sigma\, dp_\sigma - \frac{\partial L}{\partial q_\sigma}\, dq_\sigma - \frac{\partial L}{\partial \dot{q}_\sigma}\, d\dot{q}_\sigma\right) - \frac{\partial L}{\partial t}\, dt \\ &= \sum_{\sigma=1}^{N}\left(\dot{q}_\sigma\, dp_\sigma - \frac{\partial L}{\partial q_\sigma}\, dq_\sigma\right) - \frac{\partial L}{\partial t}\, dt \quad . \end{aligned} \tag{3.35}$$

Thus, we obtain Hamilton's equations of motion,

$$\frac{\partial H}{\partial p_\sigma} = \dot{q}_\sigma \quad , \quad \frac{\partial H}{\partial q_\sigma} = -\frac{\partial L}{\partial q_\sigma} = -\dot{p}_\sigma \tag{3.36}$$

and

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t} \quad . \tag{3.37}$$

Define the rank $2N$ vector $\boldsymbol{\varphi}$ by its components,

$$\varphi_i = \begin{cases} q_i & \text{if } 1 \le i \le N \\ p_{i-N} & \text{if } N < i \le 2N \end{cases} \quad . \tag{3.38}$$

Then we may write Hamilton's equations compactly as

$$\dot{\varphi}_i = J_{ij}\, \frac{\partial H}{\partial \varphi_j} \quad , \tag{3.39}$$

where

$$J = \begin{pmatrix} 0_{N\times N} & 1_{N\times N} \\ -1_{N\times N} & 0_{N\times N} \end{pmatrix} \tag{3.40}$$

is a $2N \times 2N$ matrix. Note that $J^{\mathsf{T}} = -J$, *i.e.* J is antisymmetric, and that $J^2 = -1_{2N\times 2N}$.

For any function $F(q, p, t)$, the total time derivative is given by

$$\begin{aligned} \frac{dF}{dt} &= \frac{\partial F}{\partial t} + \sum_{\sigma=1}^{N} \left(\frac{\partial F}{\partial q_\sigma}\frac{dq_\sigma}{dt} + \frac{\partial F}{\partial p_\sigma}\frac{dp_\sigma}{dt} \right) \\ &= \frac{\partial F}{\partial t} + \big\{F, H\big\} \quad , \end{aligned} \tag{3.41}$$

where $\big\{\bullet, \bullet\big\}$ is the *Poisson bracket*,

$$\big\{A, B\big\} = \sum_{\sigma=1}^{N} \left(\frac{\partial A}{\partial q_\sigma}\frac{\partial B}{\partial p_\sigma} - \frac{\partial A}{\partial p_\sigma}\frac{\partial B}{\partial q_\sigma} \right) \quad . \tag{3.42}$$

3.3.2 Dynamical systems and the evolution of phase space volumes

Consider a general dynamical system,

$$\frac{d\boldsymbol{\varphi}}{dt} = \boldsymbol{V}(\boldsymbol{\varphi}) \quad , \tag{3.43}$$

where $\boldsymbol{\varphi}(t)$ is a point in an n-dimensional phase space. Consider now a compact[5] region $\mathcal{R}_0$ in phase space, and consider its evolution under the dynamics. That is, $\mathcal{R}_0$ consists of a set of points $\big\{\boldsymbol{\varphi} \,|\, \boldsymbol{\varphi} \in \mathcal{R}_0\big\}$, and if we regard each $\boldsymbol{\varphi} \in \mathcal{R}_0$ as an initial condition, we can define the time-dependent set $\mathcal{R}(t)$ as the set of points $\boldsymbol{\varphi}(t)$ that *were* in $\mathcal{R}_0$ at time $t = 0$: $\mathcal{R}(t) = \big\{\boldsymbol{\varphi}(t) \,\big|\, \boldsymbol{\varphi}(0) \in \mathcal{R}_0\big\}$.

Now consider the volume $\Omega(t)$ of the set $\mathcal{R}(t)$. We have $\Omega(t) = \int_{\mathcal{R}(t)} d\mu$, where $d\mu = d\varphi_1\, d\varphi_2 \cdots d\varphi_n$ for an n-dimensional phase space. For a Hamiltonian system, $n = 2N$. We then have

$$\Omega(t + dt) = \int\limits_{\mathcal{R}(t+dt)} d\mu' = \int\limits_{\mathcal{R}(t)} d\mu \left| \frac{\partial \varphi_i(t + dt)}{\partial \varphi_j(t)} \right| \quad , \tag{3.44}$$

where

$$\left| \frac{\partial \varphi_i(t + dt)}{\partial \varphi_j(t)} \right| \equiv \frac{\partial(\varphi'_1, \ldots, \varphi'_n)}{\partial(\varphi_1, \ldots, \varphi_n)} \tag{3.45}$$

is a determinant, which is the Jacobian of the transformation from the set of coordinates $\big\{\varphi_i = \varphi_i(t)\big\}$ to the coordinates $\big\{\varphi'_i = \varphi_i(t + dt)\big\}$. But according to the dynamics, we have

$$\varphi_i(t + dt) = \varphi_i(t) + V_i\big(\boldsymbol{\varphi}(t)\big)\, dt + \mathcal{O}(dt^2) \tag{3.46}$$

[5] 'Compact' in the parlance of mathematical analysis means 'closed and bounded'.

and therefore

$$\frac{\partial\varphi_i(t+dt)}{\partial\varphi_j(t)} = \delta_{ij} + \frac{\partial V_i}{\partial\varphi_j}\,dt + \mathcal{O}(dt^2) \quad . \tag{3.47}$$

We now make use of the matrix equality $\log\det M = \mathsf{Tr}\,\log M$, which gives us[6], for small ε,

$$\det\big(1+\varepsilon A\big) = \exp\mathsf{Tr}\,\log\big(1+\varepsilon A\big) = 1 + \varepsilon\;\mathsf{Tr}\,A + \tfrac{1}{2}\,\varepsilon^2\Big(\big(\mathsf{Tr}\,A\big)^2 - \mathsf{Tr}\,(A^2)\Big) + \ldots \tag{3.48}$$

Thus,

$$\Omega(t+dt) = \Omega(t) + \int\limits_{\mathcal{R}(t)} d\mu\;\boldsymbol{\nabla}\cdot\boldsymbol{V}\;dt + \mathcal{O}(dt^2) \quad , \tag{3.49}$$

which says

$$\frac{d\Omega}{dt} = \int\limits_{\mathcal{R}(t)} d\mu\;\boldsymbol{\nabla}\cdot\boldsymbol{V} = \int\limits_{\partial\mathcal{R}(t)} dS\;\hat{\boldsymbol{n}}\cdot\boldsymbol{V} \tag{3.50}$$

Here, the divergence is the *phase space divergence*,

$$\boldsymbol{\nabla}\cdot\boldsymbol{V} = \sum_{i=1}^{n}\frac{\partial V_i}{\partial\varphi_i} \quad , \tag{3.51}$$

and we have used the divergence theorem to convert the volume integral of the divergence to a surface integral of $\hat{\boldsymbol{n}}\cdot\boldsymbol{V}$, where $\hat{\boldsymbol{n}}$ is the surface normal and dS is the differential element of surface area, and $\partial\mathcal{R}$ denotes the boundary of the region $\mathcal{R}$. We see that if $\boldsymbol{\nabla}\cdot\boldsymbol{V} = 0$ everywhere in phase space, then $\Omega(t)$ is a constant, and phase space volumes are *preserved* by the evolution of the system.

For an alternative derivation, consider a function $\varrho(\boldsymbol{\varphi},t)$ which is defined to be the *density* of some collection of points in phase space at phase space position $\boldsymbol{\varphi}$ and time t. This must satisfy the continuity equation,

$$\frac{\partial\varrho}{\partial t} + \boldsymbol{\nabla}\cdot(\varrho\boldsymbol{V}) = 0 \quad . \tag{3.52}$$

This is called the *continuity equation*. It says that 'nobody gets lost'. If we integrate it over a region of phase space $\mathcal{R}$, we have

$$\frac{d}{dt}\int\limits_{\mathcal{R}} d\mu\;\varrho = -\int\limits_{\mathcal{R}} d\mu\;\boldsymbol{\nabla}\cdot(\varrho\boldsymbol{V}) = -\int\limits_{\partial\mathcal{R}} dS\;\hat{\boldsymbol{n}}\cdot(\varrho\boldsymbol{V}) \quad . \tag{3.53}$$

It is perhaps helpful to think of ϱ as a charge density, in which case $\boldsymbol{J} = \varrho\boldsymbol{V}$ is the current density. The above equation then says

$$\frac{dQ_{\mathcal{R}}}{dt} = -\int\limits_{\partial\mathcal{R}} dS\;\hat{\boldsymbol{n}}\cdot\boldsymbol{J} \quad , \tag{3.54}$$

where $Q_{\mathcal{R}}$ is the total charge contained inside the region $\mathcal{R}$. In other words, the rate of increase or decrease of the charge within the region $\mathcal{R}$ is equal to the total integrated current flowing in or out of $\mathcal{R}$ at its boundary.

[6]The equality $\log\det M = \mathsf{Tr}\,\log M$ is most easily proven by bringing the matrix to diagonal form via a similarity transformation, and proving the equality for diagonal matrices.

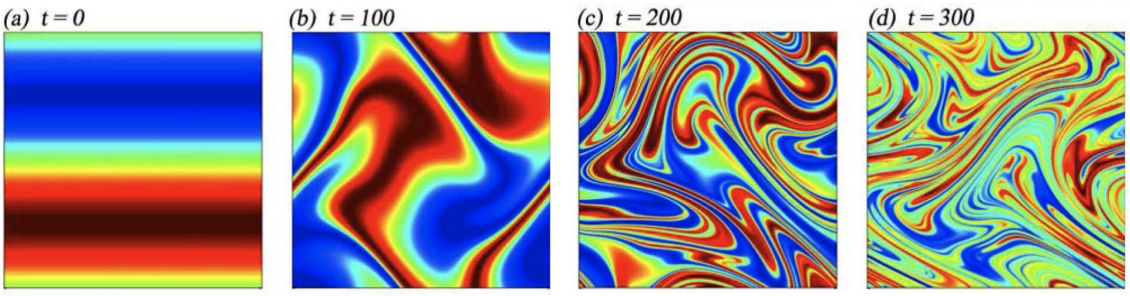


Figure 3.1: Hamiltonian time evolution of a density distribution. Dark red corresponds to $\varrho = 0$ and dark blue to $\varrho = 1$. The local density remains constant in the comoving frame. From D. Saintillan and M. Shelley, *Phys. Fluids* **20**, 123304 (2008).

The Leibniz rule lets us write the continuity equation as

$$\frac{\partial \varrho}{\partial t} + \boldsymbol{V}\cdot\boldsymbol{\nabla}\varrho + \varrho\,\boldsymbol{\nabla}\cdot\boldsymbol{V} = 0 \quad . \tag{3.55}$$

But now suppose that the phase flow is divergenceless, *i.e.* $\boldsymbol{\nabla}\cdot\boldsymbol{V} = 0$. Then we have

$$\frac{D\varrho}{Dt} \equiv \left(\frac{\partial}{\partial t} + \boldsymbol{V}\cdot\boldsymbol{\nabla}\right)\varrho = 0 \quad . \tag{3.56}$$

The combination inside the brackets above is known as the *convective derivative*. It tells us the total rate of change of ϱ for an observer *moving with the phase flow*. That is

$$\begin{aligned}\frac{d}{dt}\,\varrho\big(\boldsymbol{\varphi}(t),t\big) &= \frac{\partial\varrho}{\partial\varphi_i}\,\frac{d\varphi_i}{dt} + \frac{\partial\varrho}{\partial t} \\ &= \sum_{i=1}^{n} V_i\,\frac{\partial\varrho}{\partial\varphi_i} + \frac{\partial\varrho}{\partial t} = \frac{D\varrho}{Dt} \quad .\end{aligned} \tag{3.57}$$

If $D\varrho/Dt = 0$, the local density remains the same during the evolution of the system. If we consider the 'characteristic function'

$$\varrho(\boldsymbol{\varphi}, t=0) = \begin{cases} 1 & \text{if } \boldsymbol{\varphi}\in\mathcal{R}_0 \\ 0 & \text{otherwise}\end{cases} \tag{3.58}$$

then the vanishing of the convective derivative means that the image of the set $\mathcal{R}_0$ under time evolution will always have the same volume.

Hamiltonian evolution in classical mechanics is volume preserving. The equations of motion are

$$\dot q_\sigma = +\frac{\partial H}{\partial p_\sigma} \qquad , \qquad \dot p_\sigma = -\frac{\partial H}{\partial q_\sigma} \tag{3.59}$$

A point in phase space is specified by N positions q_σ and N momenta p_σ, hence the dimension of phase space is $n = 2N$:

$$\boldsymbol{\varphi} = \begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{p}\end{pmatrix} \qquad , \qquad \boldsymbol{V} = \begin{pmatrix}\dot{\boldsymbol{q}}\\ \dot{\boldsymbol{p}}\end{pmatrix} = \begin{pmatrix}+\partial H/\partial\boldsymbol{p}\\ -\partial H/\partial\boldsymbol{q}\end{pmatrix} \quad . \tag{3.60}$$

Hamilton's equations of motion guarantee that the phase space flow is divergenceless:

$$\begin{aligned}\nabla\cdot\boldsymbol{V} &= \sum_{\sigma=1}^{N}\left\{\frac{\partial\dot{q}_\sigma}{\partial q_\sigma}+\frac{\partial\dot{p}\sigma}{\partial p_\sigma}\right\} \\ &= \sum_{\sigma=1}^{N}\left\{\frac{\partial}{\partial q_\sigma}\left(\frac{\partial H}{\partial p_\sigma}\right)+\frac{\partial}{\partial p_\sigma}\left(-\frac{\partial H}{\partial q_\sigma}\right)\right\}=0 \quad .\end{aligned} \tag{3.61}$$

Thus, we have that the convective derivative vanishes, *viz.*

$$\frac{D\varrho}{Dt}\equiv\frac{\partial\varrho}{\partial t}+\boldsymbol{V}\cdot\boldsymbol{\nabla}\varrho=0 \quad , \tag{3.62}$$

for any distribution $\varrho(\boldsymbol{\varphi},t)$ on phase space advected by a Hamiltonian flow. Thus, the value of the density $\varrho(\boldsymbol{\varphi}(t),t)$ is constant, which tells us that the phase flow is *incompressible*. In particular, phase space volumes are preserved.

3.3.3 Liouville's equation and the microcanonical distribution

Let $\varrho(\boldsymbol{\varphi},t)=\varrho(\boldsymbol{q},\boldsymbol{p},t)$ be a distribution on phase space. Assuming the evolution is Hamiltonian, we can write

$$\frac{\partial\varrho}{\partial t}=-\dot{\boldsymbol{\varphi}}\cdot\boldsymbol{\nabla}\varrho=-\big\{\varrho,H\big\} \quad . \tag{3.63}$$

We may also write this as $\partial_t\varrho+i\hat{L}\varrho=0$, where $\hat{L}$ is a differential operator known as the *Liouvillian*:

$$i\hat{L}=\sum_{\sigma=1}^{N}\left\{\frac{\partial H}{\partial p_\sigma}\frac{\partial}{\partial q_\sigma}-\frac{\partial H}{\partial q_\sigma}\frac{\partial}{\partial p_\sigma}\right\} \quad . \tag{3.64}$$

Eqn. 3.63 is known as *Liouville's equation*. Note $i\hat{L}F=\big\{F,H\big\}$ for any function $F(\boldsymbol{\varphi},t)$.

Recall that the evolution of quantum mechanical density matrices satisfies

$$\frac{\partial\hat{\varrho}}{\partial t}=\frac{i}{\hbar}\big[\,\hat{\varrho},\hat{H}\,\big] \quad , \tag{3.65}$$

whence we infer the correspondence

$$\big\{\varrho,H\big\}\to\frac{1}{i\hbar}\big[\,\hat{\varrho},\hat{H}\,\big] \quad . \tag{3.66}$$

Suppose that there is a family of conserved quantities $\Lambda_a(\boldsymbol{\varphi})$, with $a\in\{1,\ldots,k\}$, each of which is conserved by the dynamics of the system. Such conserved quantities might include the components of the total linear momentum (if there is translational invariance), the components of the total angular momentum (if there is rotational invariance), and the Hamiltonian itself (if it is not explicitly time-dependent). Now consider a distribution $\varrho(\boldsymbol{\varphi})=\varrho(\Lambda_1,\Lambda_2,\ldots,\Lambda_k)$ which is a function only of these

various conserved quantities. That Λ_a is conserved entails $\dot{\boldsymbol{\varphi}} \cdot \boldsymbol{\nabla} \Lambda_a = \big\{ \Lambda_a, H \big\} = 0$. Then from the chain rule, we have

$$\dot{\boldsymbol{\varphi}} \cdot \boldsymbol{\nabla} \varrho = \sum_{a=1}^{k} \frac{\partial \varrho}{\partial \Lambda_a} \, \dot{\boldsymbol{\varphi}} \cdot \boldsymbol{\nabla} \Lambda_a = 0 \quad . \tag{3.67}$$

We conclude that any distribution $\varrho(\boldsymbol{\varphi}) = \varrho(\Lambda_1, \Lambda_2, \ldots, \Lambda_k)$ which is a function solely of conserved dynamical quantities is a stationary solution to Liouville's equation.

Clearly the microcanonical distribution,

$$\varrho_E(\boldsymbol{\varphi}) = \frac{\delta\big(E - H(\boldsymbol{\varphi})\big)}{D(E)} = \frac{\delta\big(E - H(\boldsymbol{\varphi})\big)}{\int d\mu \, \delta\big(E - H(\boldsymbol{\varphi})\big)} \quad , \tag{3.68}$$

is a fixed point solution of Liouville's equation. If there were a second conserved quantity, $\Lambda(\boldsymbol{\varphi})$, the generalized microcanonical distribution,

$$\varrho_{E,Q}(\boldsymbol{\varphi}) = \frac{\delta\big(E - H(\boldsymbol{\varphi})\big) \, \delta\big(Q - \Lambda(\boldsymbol{\varphi})\big)}{D(E,Q)} = \frac{\delta\big(E - H(\boldsymbol{\varphi})\big) \, \delta\big(Q - \Lambda(\boldsymbol{\varphi})\big)}{\int d\mu \, \delta\big(E - H(\boldsymbol{\varphi}) \, \delta\big(Q - \Lambda(\boldsymbol{\varphi})\big)} \quad , \tag{3.69}$$

would be a solution to Liouville's equation for arbitrary E and Q.

Similarly, the Gibbs distribution,

$$\varrho_\beta(\boldsymbol{\varphi}) = \frac{1}{Z(\beta)} \, e^{-\beta H(\boldsymbol{\varphi})} \quad , \tag{3.70}$$

where $Z(\beta) = \mathsf{Tr} \, e^{-\beta H(\boldsymbol{\varphi})} = \int d\mu(\boldsymbol{\varphi}) \, e^{-\beta H(\boldsymbol{\varphi})}$ is the partition function, satisfies $\big\{ \varrho_\beta, H \big\} = 0$. In the presence of multiple conserved quantities, one defines the *generalized Gibbs distribution*,

$$\varrho_{\boldsymbol{\beta}}(\boldsymbol{\varphi}) = \frac{1}{Z(\boldsymbol{\beta})} \, \exp\Big(- \sum_{a=1}^{k} \beta_a \, \Lambda_a(\boldsymbol{\varphi}) \Big) \quad , \tag{3.71}$$

where the $\{\Lambda_a(\boldsymbol{\varphi})\}$, with $a \in \{1, \ldots, k\}$, are the conserved quantities, including among them H itself. The coefficients $\{\beta_a\}$ are k Lagrange multipliers enforcing the k conservation constraints $\Lambda_a(\boldsymbol{\varphi}) = Q_a$.

3.4 Irreversibility and Poincaré Recurrence

The dynamics of the master equation describe an approach to equilibrium. These dynamics are irreversible: $dH/dt \leq 0$, where H is Boltzmann's H-function. However, the microscopic laws of physics are (almost) time-reversal invariant[7], so how can we understand the emergence of irreversibility? Furthermore, any dynamics which are deterministic and volume-preserving in a finite phase space exhibit the phenomenon of *Poincaré recurrence*, which guarantees that phase space trajectories are arbitrarily close to periodic if one waits long enough.

[7] Actually, the microscopic laws of physics are *not* time-reversal invariant, but rather are invariant under the product CPT, where C is charge conjugation, P is parity, and T is time reversal.

3.4.1 Poincaré recurrence theorem

The proof of the recurrence theorem is simple. Let g_τ be the 'τ-advance mapping' which evolves points in phase space according to Hamilton's equations. Assume that g_τ is invertible and volume-preserving, as is the case for Hamiltonian flow. Further assume that phase space volume is finite. Since energy is preserved in the case of time-independent Hamiltonians, we simply ask that the volume of phase space *at fixed total energy* E be finite, *i.e.*

$$\int d\mu\, \delta\big(E - H(\boldsymbol{q},\boldsymbol{p})\big) < \infty \quad , \tag{3.72}$$

where $d\mu = d\boldsymbol{q}\, d\boldsymbol{p}$ is the phase space uniform integration measure.

Theorem: In any finite neighborhood $\mathcal{R}_0$ of phase space there exists a point $\boldsymbol{\varphi}_0$ which will return to $\mathcal{R}_0$ after m applications of g_τ, where m is finite.

Proof: Assume the theorem fails; we will show this assumption results in a contradiction. Consider the set Υ formed from the union of all sets $g_\tau^k\,\mathcal{R}$ over all k:

$$\Upsilon = \bigcup_{k=0}^{\infty} g_\tau^k\,\mathcal{R}_0 \tag{3.73}$$

We assume that the set $\{g_\tau^k\,\mathcal{R}_0 \,|\, k\in\mathbb{N}_0\}$ is disjoint[8]. The volume of a union of disjoint sets is the sum of the individual volumes. Thus,

$$\mathrm{vol}(\Upsilon) = \sum_{k=0}^{\infty} \mathrm{vol}\big(g_\tau^k\,\mathcal{R}_0\big) = \mathrm{vol}(\mathcal{R}_0)\cdot\sum_{k=0}^{\infty} 1 = \infty \quad , \tag{3.74}$$

since $\mathrm{vol}\big(g_\tau^k\,\mathcal{R}_0\big) = \mathrm{vol}\big(\mathcal{R}_0\big)$ from volume preservation. But clearly Υ is a subset of the entire phase space, hence we have a contradiction, because by assumption phase space is of finite volume.

Thus, the assumption that the set $\{g_\tau^k\,\mathcal{R}_0 \,|\, k\in\mathbb{N}_0\}$ is disjoint fails. This means that there exists some pair of integers k and l, with $k \neq l$, such that $g_\tau^k\,\mathcal{R}_0 \cap g_\tau^l\,\mathcal{R}_0 \neq \emptyset$. Without loss of generality we may assume $k < l$. Apply the inverse g_τ^{-1} to this relation k times to get $g_\tau^{l-k}\,\mathcal{R}_0 \cap \mathcal{R}_0 \neq \emptyset$. Now choose any point $\boldsymbol{\varphi}_1 \in g_\tau^m\,\mathcal{R}_0 \cap \mathcal{R}_0$, where $m = l-k$, and define $\boldsymbol{\varphi}_0 = g_\tau^{-m}\boldsymbol{\varphi}_1$. Then by construction both $\boldsymbol{\varphi}_0$ and $g_\tau^m\,\boldsymbol{\varphi}_0$ lie within $\mathcal{R}_0$ and the theorem is proven.

Poincaré recurrence has remarkable implications. Consider a bottle of perfume which is opened in an otherwise evacuated room, as depicted in fig. 3.3. The perfume molecules evolve according to Hamiltonian evolution. The positions are bounded because physical space is finite. The momenta are bounded because the total energy is conserved, hence no single particle can have a momentum such that $T(\boldsymbol{p}) > E_{\rm TOT}$, where $T(\boldsymbol{p})$ is the single particle kinetic energy function[9]. Thus, phase space, however large, is still bounded. Hamiltonian evolution, as we have seen, is invertible and volume preserving, therefore the system is recurrent. All the molecules must eventually return to the bottle. What's more,

[8] The natural numbers $\mathbb{N}_0$ is the set of non-negative integers $\{0, 1, 2, \ldots\}$.

[9] In the nonrelativistic limit, $T = p^2/2m$. For relativistic particles, we have $T = (p^2c^2 + m^2c^4)^{1/2} - mc^2$.

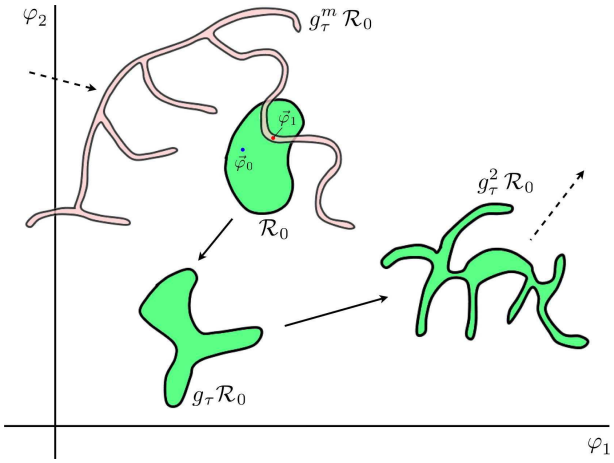


Figure 3.2: Successive images of a set $\mathcal{R}_0$ under the τ-advance mapping g_τ, projected onto a two-dimensional phase plane. The Poincaré recurrence theorem guarantees that if phase space has finite volume, and g_τ is invertible and volume preserving, then for any set $\mathcal{R}_0$ there exists an integer m such that $\mathcal{R}_0 \cap g_\tau^m\,\mathcal{R}_0 \neq \emptyset$.

they all must return with momenta arbitrarily close to their initial momenta![10] In this case, we could define the region $\mathcal{R}_0$ as

$$\mathcal{R}_0 = \big\{(q_1,\ldots,q_r,p_1,\ldots,p_r)\;\big|\;|q_i - q_i^0| \le \Delta q \text{ and } |p_j - p_j^0| \le \Delta p\;\forall\; i,j\big\} \quad , \tag{3.75}$$

which specifies a hypercube in phase space centered about the point $(\boldsymbol{q}^0, \boldsymbol{p}^0)$.

Each of the three central assumptions – finite phase space, invertibility, and volume preservation – is crucial. If any one of these assumptions does not hold, the proof fails. Obviously if phase space is infinite the flow needn't be recurrent since it can keep moving off in a particular direction. Consider next a volume-preserving map which is not invertible. An example might be a mapping $f\colon \mathbb{R} \to \mathbb{R}$ which takes any real number to its fractional part. Thus, $f(\pi) = 0.14159265\ldots$. Let us restrict our attention to intervals of width less than unity. Clearly f is then volume preserving. The action of f on the interval $[2,3)$ is to map it to the interval $[0,1)$. But $[0,1)$ remains fixed under the action of f, so no point within the interval $[2,3)$ will ever return under repeated iterations of f. Thus, f does not exhibit Poincaré recurrence.

Consider next the case of the damped harmonic oscillator. In this case, phase space volumes contract. For a one-dimensional oscillator obeying $\ddot{x} + 2\beta\dot{x} + \Omega_0^2\,x = 0$ one has $\nabla\cdot\boldsymbol{V} = -2\beta < 0$, since $\beta > 0$ for physical damping. Thus the convective derivative is $D_t\varrho = -(\nabla\cdot\boldsymbol{V})\varrho = 2\beta\varrho$ which says that the density increases exponentially in the comoving frame, as $\varrho(t) = e^{2\beta t}\,\varrho(0)$. Thus, phase space volumes collapse: $\Omega(t) = e^{-2\beta t}\,\Omega(0)$, and are not preserved by the dynamics. The proof of recurrence therefore fails. In this case, it is possible for the set Υ to be of finite volume, even if it is the union of an infinite number of sets $g_\tau^k\,\mathcal{R}_0$, because the volumes of these component sets themselves decrease exponentially, as $\mathrm{vol}(g_\tau^n\,\mathcal{R}_0) = e^{-2n\beta\tau}\,\mathrm{vol}(\mathcal{R}_0)$. A damped pendulum, released from rest at some small angle θ_0, will not return arbitrarily close to these initial conditions.

[10] Actually, what the recurrence theorem guarantees is that there is a configuration arbitrarily close to the initial one which recurs, to within the same degree of closeness.

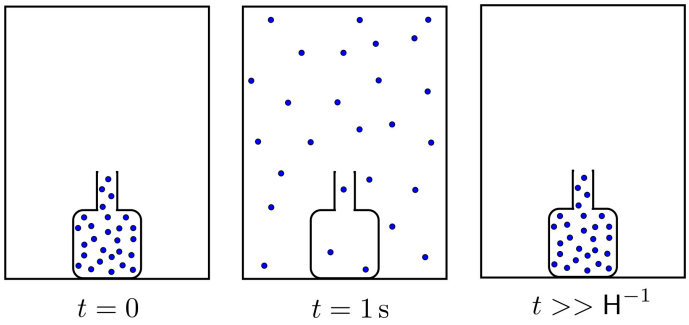


Figure 3.3: Poincaré recurrence guarantees that if we remove the cap from a bottle of perfume in an otherwise evacuated room, all the perfume molecules will eventually return to the bottle! (Here H is the Hubble constant.)

3.4.2 Kac ring model

The implications of the Poincaré recurrence theorem are surprising – even shocking. If one takes a bottle of perfume in a sealed, evacuated room and opens it, the perfume molecules will diffuse throughout the room. The recurrence theorem guarantees that after some finite time T all the molecules will go back inside the bottle (and arbitrarily close to their initial velocities as well). The hitch is that this could take a very long time, *e.g.* much much longer than the age of the Universe.

On less absurd time scales, we know that most systems come to thermodynamic equilibrium. But how can a system both exhibit equilibration *and* Poincaré recurrence? The two concepts seem utterly incompatible!

A beautifully simple model due to Kac shows how a recurrent system can exhibit the phenomenon of equilibration. Consider a ring with N sites. On each site, place a 'spin' which can be in one of two states: up or down. Along the N links of the system, F of them contain 'flippers'. The configuration of the flippers is set at the outset and never changes. The dynamics of the system are as follows: during each time step, every spin moves clockwise a distance of one lattice spacing. Spins which pass through flippers reverse their orientation: up becomes down, and down becomes up.

The 'phase space' for this system consists of 2^N discrete configurations. Since each configuration maps onto a unique image under the evolution of the system, phase space 'volume' is preserved. The evolution is invertible; the inverse is obtained simply by rotating the spins counterclockwise. Figure 3.4 depicts an example configuration for the system, and its first iteration under the dynamics.

Suppose the flippers were not fixed, but moved about randomly. In this case, we could focus on a single spin and determine its configuration probabilistically. Let p_n be the probability that a given spin is in the up configuration at time n. The probability that it is up at time $(n+1)$ is then

$$p_{n+1} = (1-x)\,p_n + x\,(1-p_n) \quad , \tag{3.76}$$

where $x = F/N$ is the fraction of flippers in the system. In words: a spin will be up at time $(n+1)$ if it was up at time n and did not pass through a flipper, or if it was down at time n and did pass through a flipper. If the flipper locations are randomized at each time step, then the probability of flipping is

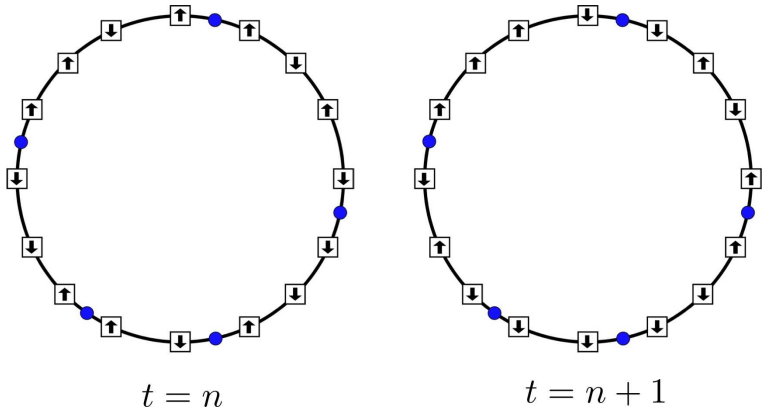


Figure 3.4: Left: A configuration of the Kac ring with $N = 16$ sites and $F = 4$ flippers. The flippers, which live on the links, are represented by blue dots. Right: The ring system after one time step. Evolution proceeds by clockwise rotation. Spins passing through flippers are flipped.

simply $x = F/N$. Equation 3.76 can be solved immediately:

$$p_n = \tfrac{1}{2} + (1-2x)^n \, (p_0 - \tfrac{1}{2}) \quad , \tag{3.77}$$

which decays exponentially to the equilibrium value of $p_{\rm eq} = \frac{1}{2}$ with time scale

$$\tau(x) = -\frac{1}{\log|1-2x|} \quad . \tag{3.78}$$

We identify $\tau(x)$ as the microscopic relaxation time over which local equilibrium is established. If we define the magnetization $m \equiv (N_\uparrow - N_\downarrow)/N$, then $m = 2p - 1$, so $m_n = (1-2x)^n \, m_0$. The equilibrium magnetization is $m_{\rm eq} = 0$. Note that for $\frac{1}{2} < x < 1$ the magnetization reverses sign each time step, as well as decreasing exponentially in magnitude.

The assumption that leads to equation 3.76 is called the *Stosszahlansatz*, a long German word[11] meaning, approximately, 'assumption on the counting of hits'. The resulting dynamics are irreversible: the magnetization inexorably decays to zero. However, the Kac ring model is purely deterministic, and the *Stosszahlansatz* can at best be an approximation to the true dynamics. Clearly the *Stosszahlansatz* fails to account for correlations such as the following: if spin i is flipped at time n, then spin $i+1$ will have been flipped at time $n-1$. Also if spin i is flipped at time n, then it also will be flipped at time $n+N$. Indeed, since the dynamics of the Kac ring model are invertible and volume preserving, it must exhibit Poincaré recurrence. We see this most vividly in figs. 3.5 and 3.6.

The model is trivial to simulate. The results of such a simulation are shown in figure 3.5 for a ring of $N = 2500$ sites, with $F = 500$, 100, and 20 flippers. Note how the magnetization decays and fluctuates about the equilibrium value $m_{\rm eq} = 0$, but that after N iterations m recovers its initial value: $m_N = m_0$. The recurrence time for this system is simply N if F is even, and $2N$ if F is odd, since every spin will then have flipped an even number of times.

[11] Unfortunately, many important physicists were German and we have to put up with a legacy of long German words like *Gedankenexperiment*, *Zitterbewegung*, *Bremsstrahlung*, *Stosszahlansatz*, *Kartoffelsalat*, *etc.*

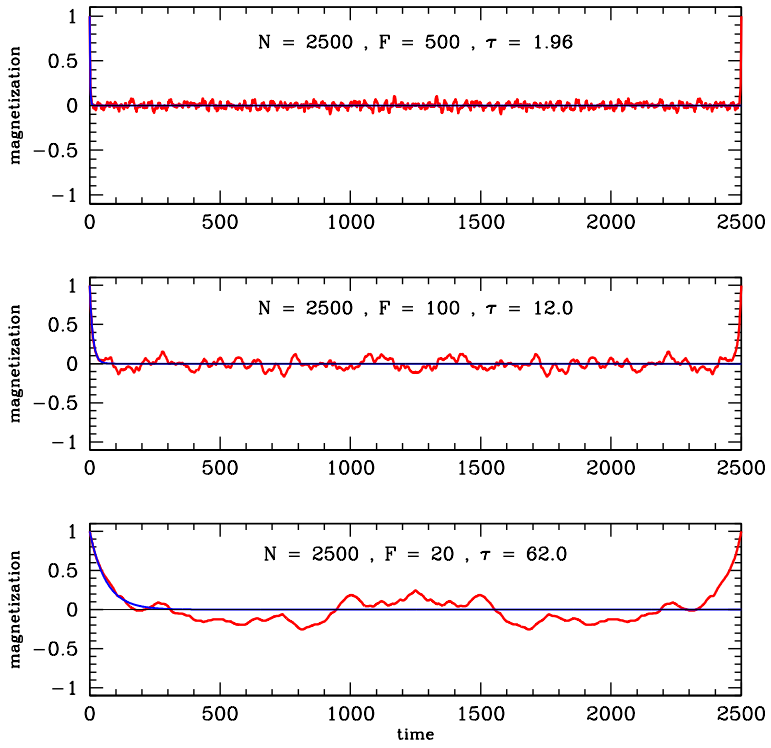


Figure 3.5: Three simulations of the Kac ring model with $N = 2500$ sites and three different concentrations of flippers. The red line shows the magnetization as a function of time, starting from an initial configuration in which 100% of the spins are up. The blue line shows the prediction of the *Stosszahlansatz*, which yields an exponentially decaying magnetization with time constant τ.

In figure 3.6 we plot two other simulations. The middle panel shows what happens when $x > \frac{1}{2}$, so that the magnetization wants to reverse its sign with every iteration. The bottom panel shows a simulation for a larger ring, with $N = 25000$ sites. Note that the fluctuations in m about equilibrium are smaller than in the cases with $N = 1000$ sites. Why? Also, why are the $m(t)$ plots in fig. 3.5 time-reversal symmetric? Is this always a feature of the dynamics?

Finally, for any quenched distribution of flippers, the size of the state space for the ring system is 2^N. The recurrence time is at most $2N$. Thus, in the thermodynamic limit, the dynamics permit only a tiny fraction of the state space to be explored, of order $N \cdot 2^{-N}$.

3.5 Remarks on Ergodic Theory

3.5.1 Definition of ergodicity

A mechanical system evolves according to Hamilton's equations of motion. We have seen how such a system is *recurrent* in the sense of Poincaré. There is a level beyond recurrence called *ergodicity*. In an ergodic system, time averages over intervals $[0, T]$ with $T \to \infty$ may be replaced by phase space

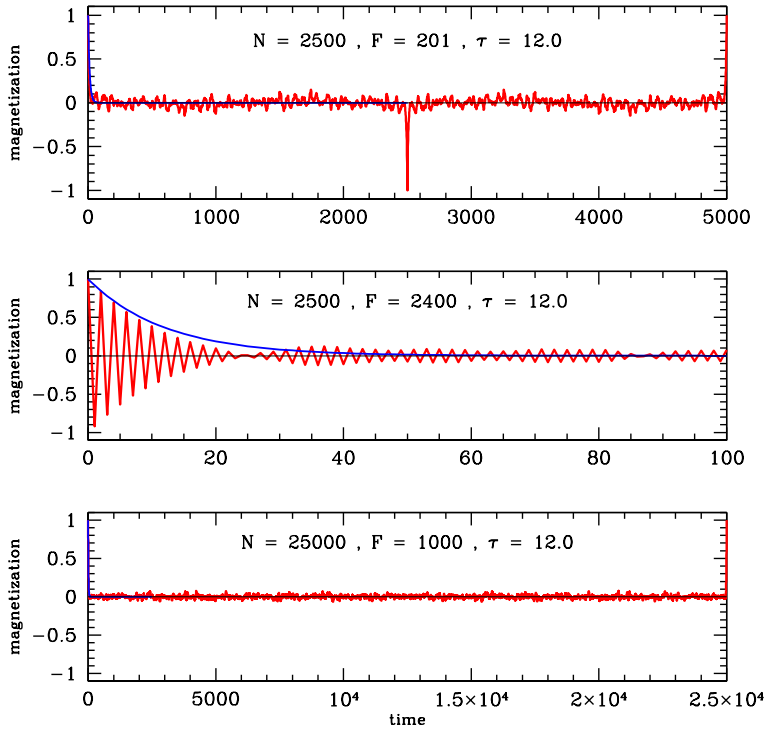


Figure 3.6: Simulations of the Kac ring model. Top: $N = 2500$ sites with $F = 201$ flippers. After 2500 iterations, each spin has flipped an odd number of times, so the recurrence time is $2N$. Middle: $N = 2500$ with $F = 2400$, resulting in a near-complete reversal of the population with every iteration. Bottom: $N = 25000$ with $F = 1000$, showing long time equilibration and dramatic resurgence of the spin population.

averages. The time average of a function $f(\boldsymbol{\varphi})$ is defined as

$$\big\langle f(\boldsymbol{\varphi})\big\rangle_t = \lim_{T\to\infty} \frac{1}{T}\int_0^T dt\, f\big(\boldsymbol{\varphi}(t)\big) \quad . \tag{3.79}$$

For a Hamiltonian system, the *phase space average* of the same function is defined by

$$\big\langle f(\boldsymbol{\varphi})\big\rangle_E = \int d\mu\, f(\boldsymbol{\varphi})\,\delta\big(E - H(\boldsymbol{\varphi})\big) \Big/ \int d\mu\,\delta\big(E - H(\boldsymbol{\varphi})\big) \quad , \tag{3.80}$$

where $H(\boldsymbol{\varphi}) = H(\boldsymbol{q},\boldsymbol{p})$ is the Hamiltonian, and where $\delta(x)$ is the Dirac δ-function. The energy is fixed to be $E = H\big(\boldsymbol{\varphi}(t=0)\big)$. Thus,

$$\text{ergodicity} \quad \Longleftrightarrow \quad \big\langle f(\boldsymbol{\varphi})\big\rangle_t = \big\langle f(\boldsymbol{\varphi})\big\rangle_E \quad , \tag{3.81}$$

for all smooth functions $f(\boldsymbol{\varphi})$ for which $\big\langle f(\boldsymbol{\varphi})\big\rangle_E$ exists and is finite. Note that we do not average over *all* of phase space. Rather, we average only over a hypersurface along which $H(\boldsymbol{\varphi}) = E$ is fixed, *i.e.* over one of the *level sets* of the Hamiltonian function. This is because the dynamics *preserves the energy*.

Ergodicity means that almost all points $\boldsymbol{\varphi}$ will, upon Hamiltonian evolution, move in such a way as to eventually pass through every finite neighborhood on the energy surface, and will spend equal time in equal regions of phase space.

Let Ω denote the entirety of phase space, which is an n-dimensional manifold with $n = 2dN$ for N particles in d space dimensions. Let $\chi_{\mathcal{R}}(\boldsymbol{\varphi})$ be the characteristic function of a region $\mathcal{R} \subset \Omega$:

$$\chi_{\mathcal{R}}(\boldsymbol{\varphi}) = \begin{cases} 1 & \text{if } \boldsymbol{\varphi} \in \mathcal{R} \\ 0 & \text{otherwise} \end{cases} \quad , \tag{3.82}$$

Then

$$\big\langle \chi_{\mathcal{R}}(\boldsymbol{\varphi}) \big\rangle_t = \lim_{T\to\infty} \left(\frac{\text{time spent in } \mathcal{R}}{T} \right) \quad . \tag{3.83}$$

If the system is ergodic, then

$$\big\langle \chi_{\mathcal{R}}(\boldsymbol{\varphi}) \big\rangle_t = P(\mathcal{R}) = \frac{D_{\mathcal{R}}(E)}{D(E)} \quad , \tag{3.84}$$

where $P(\mathcal{R})$ is the *a priori* probability to find $\boldsymbol{\varphi} \in \mathcal{R}$, based solely on the relative volumes of $\mathcal{R}$ and Ω. Here,

$$D(E) = \int\limits_{\Omega} d\mu\, \delta\big(E - H(\boldsymbol{\varphi})\big) \qquad , \qquad D_{\mathcal{R}}(E) = \int\limits_{\mathcal{R}} d\mu\, \delta\big(E - H(\boldsymbol{\varphi})\big). \tag{3.85}$$

$D(E)$ is the *density of states*, and carries the interpretation of the surface area of phase space at energy E Define now the hypersurface $\mathcal{S}_E$ to be the set of points $\boldsymbol{\varphi} \in \Omega$ satisfying $H(\boldsymbol{\varphi}) = E$. We can express $D(E)$ as an integral over $\mathcal{S}_E$ using the *invariant differential surface element* $d\Sigma_E$, defined as follows.. We can write the differential phase space volume $d\mu$ as the product $d\mu = dS_E\, d\zeta_E$, where dS_E is the differential surface element for the level set $\mathcal{S}_E$ and ζ_E is a phase space coordinate locally perpendicular to $\mathcal{S}_E$. We then define[12]

$$d\Sigma_E \equiv \frac{dS_E}{|\boldsymbol{\nabla} H|}\bigg|_{H(\boldsymbol{\varphi})=E} \quad , \tag{3.86}$$

whence we may write $d\mu = dE\, d\Sigma_E$. Note that we may also express $D(E)$ as

$$D(E) = \frac{d}{dE} \int d\mu\, \Theta\big(E - H(\boldsymbol{\varphi})\big) \equiv \frac{d\Omega(E)}{dE} \quad , \tag{3.87}$$

where $\Omega(E) = \int_\Omega d\mu\, \Theta\big(E - H(\boldsymbol{\varphi})\big)$ is the volume of phase space over which $H(\boldsymbol{\varphi}) < E$. If we define $\mathcal{R}_E \equiv \mathcal{R} \cap \mathcal{S}_E$, then we have The density of states for the subset $\mathcal{R}$ is defined as

$$D_{\mathcal{R}}(E) = \int\limits_{\mathcal{R}_E} d\Sigma_E \quad . \tag{3.88}$$

[12]Recall that the phase space coordinates don't all have the same units! N of the coordinates have units of position and N have units of momentum. Furthermore, some may be angles and some angular momenta. However in any case $d\mu$ has units A^N, where A stands for action, *i.e.* $[d\mu] = (\mathrm{ML}^2/\mathrm{T})^N$. Thus while the product $d\mu = dS_E\, d\zeta_E$ has units of A^N, individually the units of dS_E and $d\zeta_E$ vary along the hypersurface $\mathcal{S}_E$! However, the invariant differential surface element $d\Sigma_E$ always has units of A^N/E. To resolve any confusion, one may choose to rescale so that all phase space coordinates are dimensionless.

3.5.2 The microcanonical ensemble

The distribution,

$$\varrho_E(\boldsymbol{\varphi}) = \frac{\delta\big(E - H(\boldsymbol{\varphi})\big)}{D(E)} = \frac{\delta\big(E - H(\boldsymbol{\varphi})\big)}{\int d\mu\, \delta\big(E - H(\boldsymbol{\varphi})\big)} \quad , \tag{3.89}$$

defines the *microcanonical ensemble* (μCE) of Gibbs. We could also write

$$\big\langle f(\boldsymbol{\varphi})\big\rangle_E = \frac{1}{D(E)} \int\limits_{\mathcal{S}_E} d\Sigma_E\, f(\boldsymbol{\varphi}) \quad , \tag{3.90}$$

integrating over the hypersurface $\mathcal{S}_E$ rather than the entire phase space.

3.5.3 Ergodicity and mixing

Just because a system is ergodic, it doesn't necessarily mean that $\varrho(\varphi, t) \to \varrho^{\rm eq}(\boldsymbol{\varphi})$, for consider the following motion on the toroidal space $\big\{\boldsymbol{\varphi} = (q,p)\,\big|\, 0 \le q < 1 \quad , \; 0 \le p < 1\big\}$, where we identify opposite edges, *i.e.* we impose periodic boundary conditions. We also take q and p to be dimensionless, for simplicity of notation. Let the dynamics be given by $\dot q = 1$ and $\dot p = \alpha$. The motion is then $q(t) = q_0 + t$ and $p(t) = p_0 + \alpha t$. Thus the phase curves are given by $p = p_0 + \alpha(q - q_0)$.

Now consider the average of some function $f(q,p)$. We can write $f(q,p)$ in terms of its Fourier transform,

$$f(q,p) = \sum_{m,n} \hat f_{m,n}\, e^{2\pi i(mq+np)} \quad . \tag{3.91}$$

We have, then,

$$f\big(q(t),p(t)\big) = \sum_{m,n} \hat f_{m,n}\, e^{2\pi i(mq_0+np_0)}\, e^{2\pi i(m+\alpha n)t} \quad . \tag{3.92}$$

We can now perform the time average of f:

$$\begin{aligned} \big\langle f(q,p)\big\rangle_t &= \hat f_{0,0} + \lim_{T\to\infty}\, \frac{1}{T} {\sum_{m,n}}' \hat f_{m,n}\, e^{2\pi i(mq_0+np_0)}\, \frac{e^{2\pi i(m+\alpha n)T} - 1}{2\pi i(m+\alpha n)} \\ &= \hat f_{0,0} \quad \text{if } \alpha \notin \mathbb{Q} \quad . \end{aligned} \tag{3.93}$$

Clearly,

$$\big\langle f(q,p)\big\rangle_E = \int\limits_0^1 dq \int\limits_0^1 dp\, f(q,p) = \hat f_{0,0} = \big\langle f(q,p)\big\rangle_t \quad , \tag{3.94}$$

so the system is ergodic. However, if $\alpha = r/s$ with $r, s \in \mathbb{Z}$ and $\gcd(r,s) = 1$ (*i.e.* r and s are relatively prime), then $\exp\big\{2\pi i(m+\alpha n)t\big\} = 1$ whenever $(m,n) = (kr, -ks)$ for any $k \in \mathbb{Z}$. Thus,

$$\big\langle f(q,p)\big\rangle_t = \sum_{k=-\infty}^{\infty} \hat f_{kr,-ks}\, e^{2\pi ik(rq_0 - sp_0)} \quad , \tag{3.95}$$

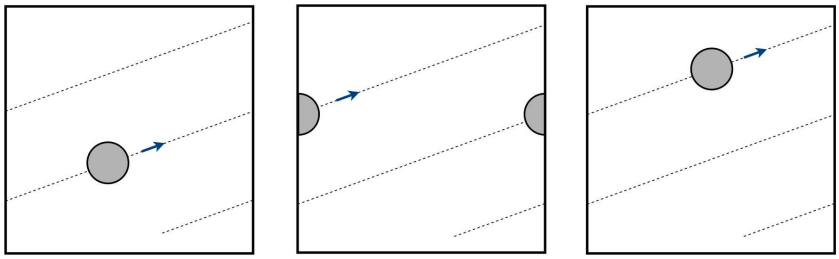


Figure 3.7: Constant phase space velocity at an irrational angle over a toroidal phase space is ergodic, but not mixing. A circle remains a circle, and a blob remains a blob.

which is not the same as $\big\langle f(q,p)\big\rangle_{\mu\rm CE} = \hat{f}_{0,0}$.

The situation is depicted in fig. 3.7. If we start with the characteristic function of a disc,

$$\varrho(q,p,t=0) = \Theta\big(a^2 - (q-q_0)^2 - (p-p_0)^2\big) \quad , \tag{3.96}$$

then it remains the characteristic function of a disc:

$$\varrho(q,p,t) = \Theta\big(a^2 - (q-q_0-t)^2 - (p-p_0-\alpha t)^2\big) \quad , \tag{3.97}$$

For an example of a transition to ergodicity in a simple dynamical Hamiltonian model, see §3.10.

A stronger condition one could impose is the following. Let A and B be subsets of $\mathcal{S}_E$. Define the *measure*

$$\nu(A) = \frac{\int d\Sigma_E\, \chi_A(\boldsymbol{\varphi})}{\int d\Sigma_E} = \frac{D_A(E)}{D(E)} \quad , \tag{3.98}$$

where $\chi_A(\boldsymbol{\varphi})$ is the characteristic function of A. The measure of a set A is the fraction of the energy surface $\mathcal{S}_E$ covered by A. This means $\nu(\mathcal{S}_E) = 1$, since $\mathcal{S}_E$ is the entire phase space at energy E. Now let g be a volume-preserving map on phase space. Given two measurable sets A and B, we say that a system is *mixing* if

$$\text{mixing} \qquad \Longleftrightarrow \qquad \lim_{n\to\infty} \nu\Big(g^n A \cap B\Big) = \nu(A)\,\nu(B) \quad . \tag{3.99}$$

In other words, the fraction of B covered by the $n^{\rm th}$ iterate of A, *i.e.* $g^n A$, is, as $n \to \infty$, simply the fraction of $\mathcal{S}_E$ covered by A. The iterated map g^n distorts the region A so severely that it eventually spreads out 'evenly' over the entire energy hypersurface. Of course by 'evenly' we mean 'with respect to any finite length scale', because at the very smallest scales, the phase space density is still locally constant as one evolves with the dynamics.

Mixing means that

$$\begin{aligned}\big\langle f(\boldsymbol{\varphi})\big\rangle &= \int d\mu\, \varrho(\boldsymbol{\varphi},t)\, f(\boldsymbol{\varphi}) \xrightarrow[t\to\infty]{} \int d\mu\, f(\boldsymbol{\varphi})\, \delta\big(E - H(\boldsymbol{\varphi})\big) \Big/ \int d\mu\, \delta\big(E - H(\boldsymbol{\varphi})\big) \\ &\equiv \mathsf{Tr}\Big[f(\boldsymbol{\varphi})\, \delta\big(E - H(\boldsymbol{\varphi})\big)\Big] \Big/ \mathsf{Tr}\Big[\delta\big(E - H(\boldsymbol{\varphi})\big)\Big] \quad .\end{aligned} \tag{3.100}$$

Physically, we can imagine regions of phase space being successively stretched and folded. During the stretching process, the volume is preserved, so the successive stretch and fold operations map phase space back onto itself.

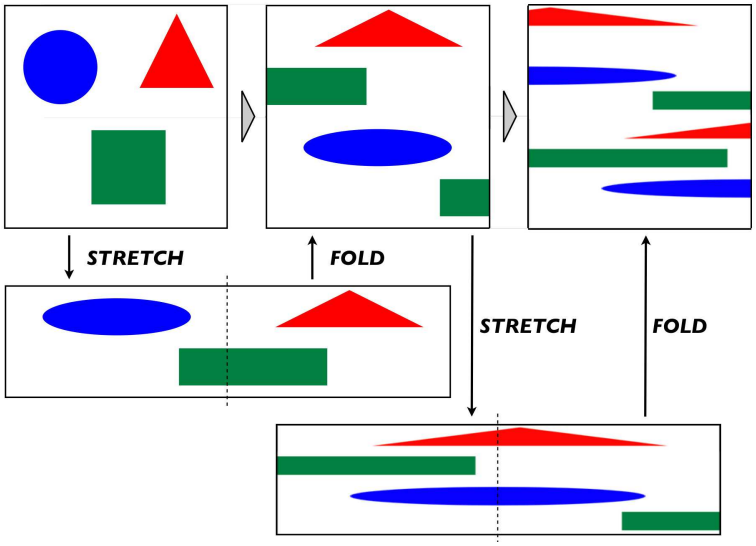


Figure 3.8: The baker's transformation is a successive stretching, cutting, and restacking.

An example of a mixing system is the *baker's transformation*, depicted in fig. 3.8, and defined by

$$g(q,p) = \begin{cases} \left(2q\,,\,\frac{1}{2}p\right) & \text{if} \quad 0 \le q < \frac{1}{2} \\ \left(2q-1\,,\,\frac{1}{2}p+\frac{1}{2}\right) & \text{if} \quad \frac{1}{2} \le q < 1 \end{cases} \quad . \tag{3.101}$$

Note that g is invertible and volume-preserving. The baker's transformation consists of an initial stretch in which q is expanded by a factor of two and p is contracted by a factor of two, which preserves the total volume. The system is then mapped back onto the original area by cutting and restacking, which we can call a 'fold'. The inverse transformation is accomplished by stretching first in the vertical (p) direction and squashing in the horizontal (q) direction, followed by a slicing and restacking. Explicitly,

$$g^{-1}(q,p) = \begin{cases} \left(\frac{1}{2}q\,,\,2p\right) & \text{if} \quad 0 \le p < \frac{1}{2} \\ \left(\frac{1}{2}q+\frac{1}{2}\,,\,2p-1\right) & \text{if} \quad \frac{1}{2} \le p < 1 \end{cases} \quad . \tag{3.102}$$

Another example of a mixing system is Arnold's 'cat map'[13]

$$g(q,p) = \big(\,[q+p]\,,\,[q+2p]\,\big) \quad , \tag{3.103}$$

where $[x]$ denotes the fractional part of x. One can write this in matrix form as

$$\begin{pmatrix} q' \\ p' \end{pmatrix} = \overbrace{\begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}}^{M} \begin{pmatrix} q \\ p \end{pmatrix} \mod \mathbb{Z}^2 \quad . \tag{3.104}$$

The matrix M is very special because it has integer entries and its determinant is $\det M = 1$. This means

[13] The cat map gets its name from its initial application, by Arnold, to the image of a cat's face.

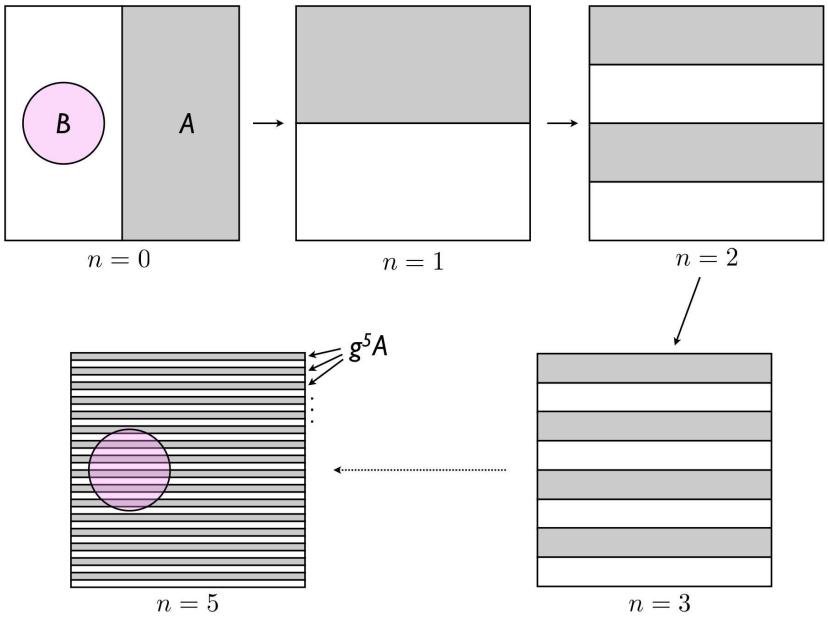


Figure 3.9: The multiply iterated baker's transformation. The set A covers half the phase space and its area is preserved under the map. Initially, the fraction of B covered by A is zero. After many iterations, the fraction of B covered by g^nA approaches $\frac{1}{2}$.

that the inverse also has integer entries. The inverse transformation is then

$$\begin{pmatrix} q \\ p \end{pmatrix} = \overbrace{\begin{pmatrix} 2 & -1 \\ -1 & 1 \end{pmatrix}}^{M^{-1}} \begin{pmatrix} q' \\ p' \end{pmatrix} \mod \mathbb{Z}^2 \quad . \tag{3.105}$$

Now for something cool. Suppose that our image consists of a set of discrete points at $(n_1/k\,,\,n_2/k)$, where the denominator $k \in \mathbb{Z}$ is fixed, and where n_1 and n_2 range over the set $\{1, \ldots, k\}$. Clearly g and its inverse preserve this set, since the entries of M and M^{-1} are integers. If there are two possibilities for each pixel (say off and on, or black and white), then there are $2^{(k^2)}$ possible images, and the cat map will map us invertibly from one image to another. Therefore it must exhibit Poincaré recurrence! This phenomenon is demonstrated vividly in fig. 3.10, which shows a $k = 150$ pixel (square) image of a cat subjected to the iterated cat map. The image is stretched and folded with each successive application of the cat map, but after 300 iterations the image is restored! How can this be if the cat map is mixing? The point is that only the discrete set of points $(n_1/k\,,\,n_2/k)$ is periodic. Points with different denominators will exhibit a different periodicity, and points with irrational coordinates will in general never return to their exact initial conditions, although recurrence says they will come arbitrarily close, given enough iterations. The baker's transformation is also different in this respect, since the denominator of the p coordinate is doubled upon each successive iteration.

The student should now contemplate the hierarchy of dynamical systems depicted in fig. 3.11, understanding the characteristic features of each successive refinement[14].

[14]There is something beyond mixing, called a *K-system*. A K-system has positive Kolmogorov-Sinai entropy.

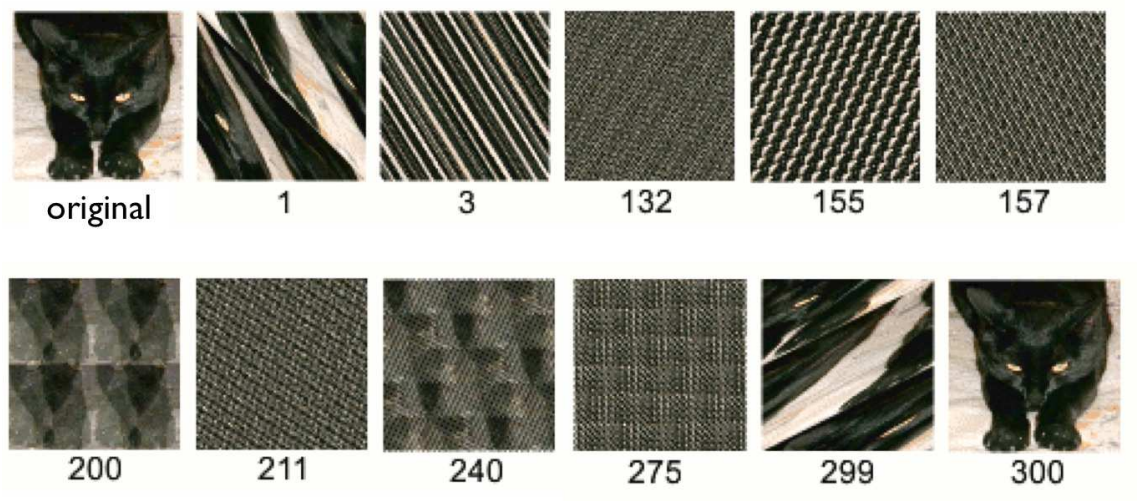


Figure 3.10: The Arnold cat map applied to an image of 150×150 pixels. After 300 iterations, the image repeats itself. (*Source: Wikipedia*)

3.6 Thermalization of Quantum Systems

3.6.1 Quantum dephasing

Thermalization of quantum systems is fundamentally different from that of classical systems. Whereas time evolution in classical mechanics is in general a nonlinear dynamical system, the Schrödinger equation for time evolution in quantum mechanics is linear: $i\hbar\,\partial\Psi/\partial t = \hat{H}\Psi$, where $\hat{H}$ is a many-body Hamiltonian. In classical mechanics, the thermal state is constructed by time evolution – this is the content of the ergodic theorem. In quantum mechanics, as we shall see, the thermal distribution must be encoded in the eigenstates themselves.

Let us assume an initial condition at $t = 0$ with $|\Psi(0)\rangle = \sum_\alpha C_\alpha\,|\Psi_\alpha\rangle$, where $\big\{|\,\Psi_\alpha\,\rangle\big\}$ is an orthonormal eigenbasis for $\hat{H}$ satisfying $\hat{H}\,|\Psi_\alpha\rangle = E_\alpha\,|\Psi_\alpha\rangle$. The expansion coefficients satisfy $C_\alpha = \langle\Psi_\alpha|\Psi(0)\rangle$ and $\sum_\alpha |C_\alpha|^2 = 1$. Normalization requires $\langle\,\Psi(0)\,|\,\Psi(0)\,\rangle = \sum_\alpha |C_\alpha|^2 = 1$.

The time evolution of $|\Psi\rangle$ is then given by

$$|\Psi(t)\rangle = \sum_\alpha C_\alpha\, e^{-iE_\alpha t/\hbar}\,|\Psi_\alpha\rangle \quad . \tag{3.106}$$

The energy is distributed according to the time-independent function

$$P(E) = \langle\,\Psi(t)\,|\,\delta(E-\hat{H})\,|\,\Psi(t)\,\rangle = \sum_\alpha |C_\alpha|^2\,\delta(E-E_\alpha) \quad . \tag{3.107}$$

For such a system, closed orbits separate exponentially in time, and consequently the Liouvillian L has a Lebesgue spectrum with denumerably infinite multiplicity.

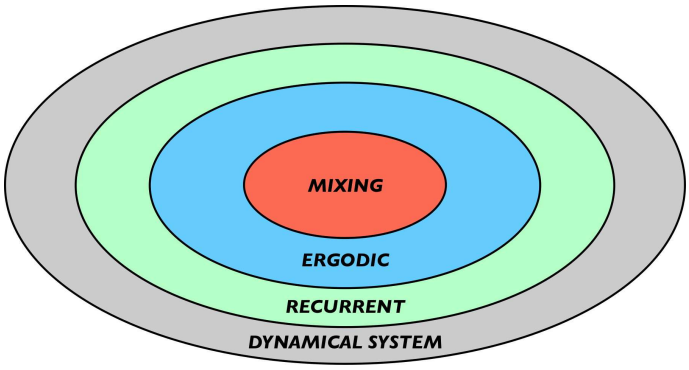


Figure 3.11: The hierarchy of dynamical systems.

Thus, the average energy is time-independent and is given by

$$\langle E \rangle = \langle\, \Psi(t) \,|\, \hat{H} \,|\, \Psi(t) \,\rangle = \int\limits_{-\infty}^{\infty} dE\, P(E)\, E = \sum_\alpha |C_\alpha|^2\, E_\alpha \quad . \tag{3.108}$$

The root mean square fluctuations of the energy are given by

$$(\Delta E)_{\rm rms} = \Big\langle \big(E - \langle E \rangle\big)^2 \Big\rangle^{1/2} = \sqrt{\sum_\alpha |C_\alpha|^2\, E_\alpha^2 - \Big(\sum_\alpha |C_\alpha|^2\, E_\alpha\Big)^2} \quad . \tag{3.109}$$

Typically we assume that the distribution $P(E)$ is narrowly peaked about $\langle E \rangle$, such that $(\Delta E)_{\rm rms} \ll \langle E \rangle - E_0$, where E_0 is the ground state energy. Note that $P(E) = 0$ for $E < E_0$, *i.e.* the eigenspectrum of $\hat{H}$ is bounded from below.

Now consider a general quantum observable described by an operator $\mathcal{A}$. We have

$$\langle \mathcal{A}(t) \rangle = \langle\, \Psi(t) \,|\, \mathcal{A} \,|\, \Psi(t) \,\rangle = \sum_{\alpha,\beta} C_\alpha^*\, C_\beta\, e^{i(E_\alpha - E_\beta)t/\hbar}\, \mathcal{A}_{\alpha\beta} \quad , \tag{3.110}$$

where $\mathcal{A}_{\alpha\beta} = \langle\, \Psi_\alpha \,|\, \mathcal{A} \,|\, \Psi_\beta \,\rangle$. In the limit of large times, we have

$$\langle \mathcal{A} \rangle_t \equiv \lim_{T\to\infty} \frac{1}{T} \int\limits_0^T dt\, \langle \mathcal{A}(t) \rangle = \sum_\alpha |C_\alpha|^2\, \mathcal{A}_{\alpha\alpha} \quad . \tag{3.111}$$

This implies that all coherence between different eigenstates is lost in the long time limit, due to *dephasing*. Note though that there is a subtlety here associated with the order of limits, for if we take the thermodynamic limit first, then for systems with a continuous spectrum the energy gaps $|E_\alpha - E_\beta|$ become arbitrarily small. In many-body systems, the smallest energy gaps typically are exponentially small in the system size, which means that we must average over absurdly long times in order for the coherences between different eigenstates separated by an exponentially small gap to cancel.

3.6.2 Eigenstate thermalization hypothesis

The essential ideas behind the *eigenstate thermalization hypothesis* (ETH) were described independently by J. Deutsch (1991) and by M. Srednicki (1994). The argument goes as follows. If the total energy is the only conserved quantity, and if $\mathcal{A}$ is a local, translationally-invariant, few-body operator, then the time average $\langle \mathcal{A} \rangle$ is given by its microcanonical value,

$$\langle \mathcal{A} \rangle_t = \sum_\alpha |C_\alpha|^2 \, \mathcal{A}_{\alpha\alpha} = \frac{\sum_\alpha \mathcal{A}_{\alpha\alpha} \, \Theta(E_\alpha \in I)}{\sum_\alpha \Theta(E_\alpha \in I)} \equiv \langle \mathcal{A} \rangle_E, \tag{3.112}$$

where $I = \big[E, E + \Delta E\big]$ is an energy interval of width ΔE. So once again, time averages are micro canonical averages[15].

But how is it that this is the case? The hypothesis of Deutsch and of Srednicki is that thermalization in isolated and bounded quantum systems occurs *at the level of individual eigenstates*. That is, for all eigenstates $|\Psi_\alpha\rangle$ with $E_\alpha \in I$, one has $\mathcal{A}_{\alpha\alpha} = \langle \mathcal{A} \rangle_{E_\alpha}$. This means that *thermal information is encoded in each eigenstate*. This is called the *eigenstate thermalization hypothesis* (ETH).

An equivalent version of the ETH is the following scenario. Suppose we have an infinite or extremely large quantum system U (the 'universe') fixed in an eigenstate $|\Psi_\alpha\rangle$. Then form the projection operator $P_\alpha = |\Psi_\alpha\rangle\langle\Psi_\alpha|$. Projection operators satisfy $P^2 = P$ and their eigenspectrum consists of one unit eigenvalue $\lambda = 1$ and the rest of the eigenvalues are zero[16]. Now consider a partition of $U = W \cup S$, where $W \gg S$. We imagine S to be the 'system' and W the 'world'. We can always decompose the state $|\Psi_\alpha\rangle$ in a complete product basis for W and S, *viz.*

$$|\Psi_\alpha\rangle = \sum_{i=1}^{N_W} \sum_{j=1}^{N_S} \Phi_{ij}^\alpha \, |\psi_i^W\rangle \otimes |\psi_j^S\rangle \quad . \tag{3.113}$$

Here $N_{W/S}$ is the size of the basis for W/S. The *reduced density matrix* for S is defined as

$$\varrho_S = \operatorname*{Tr}_W P_\alpha = \sum_{j,j'=1}^{N_S} \left(\sum_{i=1}^{N_W} \Phi_{ij}^\alpha \, \Phi_{ij'}^\alpha \right) |\psi_j^S\rangle\langle\psi_{j'}^S| \quad . \tag{3.114}$$

The claim is that ϱ_S approximates a *thermal density matrix* on S, *i.e.*

$$\varrho_S \approx \frac{1}{Z_S} \, e^{-\beta \hat{H}_S} \quad , \tag{3.115}$$

where $\hat{H}_S$ is some local Hamiltonian on S and $Z_S = \mathrm{Tr} \; e^{-\beta \hat{H}_S}$, so that ϱ_S is normalized with $\mathrm{Tr} \, \varrho_S = 1$. A number of issues remain to be clarified:

[15] This also presumes a sufficiently narrow energy distribution and smooth, approximately constant diagonal matrix elements.

[16] More generally, we could project onto a K-dimensional subspace, in which case there would be K eigenvalues of $+1$ and $N - K$ eigenvalues of 0, where N is the dimension of the entire vector space.

(i) What do we mean by "approximates"?

(ii) What do we mean by $\hat{H}_S$?

(iii) What do we mean by the temperature T?

We address these in reverse order. The temperature T of an eigenstate $|\Psi_\alpha\rangle$ of a Hamiltonian $\hat{H}$ is defined by setting its energy density E_α/V_U to the thermal energy density, *i.e.*

$$\frac{E_\alpha}{V} = \frac{1}{V}\,\frac{\mathsf{Tr}\ \hat{H}\, e^{-\beta\hat{H}}}{\mathsf{Tr}\ e^{-\beta\hat{H}}} \quad . \tag{3.116}$$

Here, $\hat{H} = \hat{H}_U$ is the full Hamiltonian of the universe $U = W \cup S$, and $V = V_U$. Our intuition is that $\hat{H}_S$ should reflect a restriction of the original Hamiltonian $\hat{H}_U$ to the system S. What should be done, though, about the interface parts of $\hat{H}_U$ which link S and W? For lattice Hamiltonians, we can simply but somewhat arbitrarily cut all the bonds coupling S and W. But we could easily imagine some other prescription, such as halving the coupling strength along all such interface bonds. Indeed, the definition of H_S is somewhat arbitrary. However, so long as we use ϱ_S to compute averages of *local operators* which lie sufficiently far from the boundary of S, the precise details of how we truncate $\hat{H}_U$ to $\hat{H}_S$ are unimportant. This brings us to the first issue: the approximation of ϱ_S by its Gibbs form in eqn. 3.115 is only valid when we consider averages of local operators lying within the bulk of S. This means that we must only examine operators whose support is confined to regions greater than some distance ξ_T from ∂S, where ξ_T is a *thermal correlation length*. This, in turn, requires that $L_S \gg \xi_T$, *i.e.* the region S is very large on the scale of ξ_T. How do we define ξ_T? For a model such as the Ising model, it can be taken to be the usual correlation length obtained from the spin-spin correlation function $\langle \sigma_{\boldsymbol{r}}\, \sigma_{\boldsymbol{r}'} \rangle_T$. More generally, we may choose the largest correlation length from among the correlators of all the independent local operators in our system. Again, the requirement is that $\exp(-d_\partial(\boldsymbol{r})/\xi_T) \ll 1$, where $d_\partial(\boldsymbol{r})$ is the shortest distance from the location of our local operator $\mathcal{O}_{\boldsymbol{r}}$ to the boundary of S. At criticality, the exponential is replaced by a power law $(d_\partial(\boldsymbol{r})/a)^{-p}$, where p is a critical exponent and a is a microscopic scale, with $d_\partial(\boldsymbol{r}) \gg a$. Another implicit assumption here is that $V_S \ll V_W$. For a general $|\,\Psi\,\rangle$, the reduced density matrix and entanglement entropy can be expressed using the machinery of the singular value decomposition theorem, and are discussed in the appendix §3.6.4.

3.6.3 Entanglement and entanglement entropy

The *von Neumann entanglement entropy* between S and W is defined to be

$$S_{\rm vN} = -\,\mathsf{Tr}\ \varrho_S \log \varrho_S = -\sum_j \lambda_j \log \lambda_j \quad , \tag{3.117}$$

where $\{\lambda_j\}$ are the eigenvalues of the reduced density matrix ϱ_S. Each eigenvalue λ_j lies on the unit interval $[0,1]$, subject to normalization $\sum_j \lambda_j = 1$. For the special case of a *pure state*, the density matrix is a projection operator, *i.e.* $\varrho = |\Psi\rangle\langle\Psi|$, as we have assumed for the universe $U = W \cup S$. Pure state density matrices have a single nonzero eigenvalue $\lambda_1 = 1$, corresponding to the eigenvector $|\Psi\rangle$, with all other eigenvalues $\lambda_{j>1} = 0$. In general, even when the full density matrix of the system is a projector,

i.e. when $\varrho = |\Psi\rangle\langle\Psi|$ where $|\Psi\rangle$ lies in the Hilbert space for U, the reduced density matrix $\varrho_S = \mathsf{Tr}_W \varrho$ does not correspond to a pure state. *I.e.*, as stated above, ϱ_S has a spectrum of eigenvalues $\{\lambda_j\}$ each of which lies on the interval $[0, 1]$, subject to normalization $\sum_j \lambda_j = 1$. If $|\Psi\rangle = |\phi_W\rangle \otimes |\chi_S\rangle$ factors, then the reduced density matrix $\varrho_S = \mathsf{Tr}_W |\Psi\rangle\langle\Psi| = |\chi_S\rangle\langle\chi_S|$ is pure, and $S_{\rm vN} = 0$. One then has that W and S are *unentangled*.

For a simple example, consider a system consisting of two spin-$\frac{1}{2}$ objects, with wavefunction

$$|\,\Psi\,\rangle = \alpha\,|\uparrow\downarrow\rangle + \beta\,|\downarrow\uparrow\rangle \tag{3.118}$$

and with $|\alpha|^2 + |\beta|^2 = 1$. Then the two spin density matrix is

$$\varrho = |\alpha|^2\,|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\beta|^2\,|\downarrow\uparrow\rangle\langle\downarrow\uparrow| + \alpha\beta^*\,|\uparrow\downarrow\rangle\langle\downarrow\uparrow| + \alpha^*\beta\,|\downarrow\uparrow\rangle\langle\uparrow\downarrow| \quad . \tag{3.119}$$

Taking the trace over the first spin, the reduced density matrix $\tilde{\varrho}$ is given by

$$\tilde{\varrho} = \operatorname*{\mathsf{Tr}}_1 \varrho = |\alpha|^2\,|\downarrow\rangle\langle\downarrow| + |\beta|^2\,|\uparrow\rangle\langle\uparrow| = \begin{pmatrix} |\beta|^2 & 0 \\ 0 & |\alpha|^2 \end{pmatrix} \quad . \tag{3.120}$$

The entanglement entropy is then

$$S_{\rm vN} = -|\alpha|^2 \log|\alpha|^2 - |\beta|^2 \log|\beta|^2 \quad , \tag{3.121}$$

and if our initial state is a singlet with $\alpha = \frac{1}{\sqrt{2}}$ and $\beta = -\frac{1}{\sqrt{2}}$, we obtain $S_{\rm vN} = \log 2$.[17]

3.6.4 Singular value decomposition and entanglement

Consider a quantum system whose wavefunction may be expressed as a vector in a Hilbert space $\mathcal{H}$ where $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ is a direct product of Hilbert subspaces. For example, $\mathcal{H}$ could be the Hilbert space for K spins, and $\mathcal{H}_{A,B}$ disjoint Hilbert spaces for K_A and K_B spins, respectively, with $K = K_A + K_B$. Now consider orthonormal basis states $|\,\psi_a^A\,\rangle$ and $|\,\psi_b^B\,\rangle$ on $\mathcal{H}_{A,B}$, where $a \in \{1, \ldots, N_A\}$ and $b \in \{1, \ldots, N_B\}$, where $N_{A,B}$ are the dimensions of $\mathcal{H}_{A,B}$. Any wavefunction $|\,\Psi\,\rangle \in \mathcal{H}$ can then be expressed as

$$|\,\Psi\,\rangle = \sum_{a=1}^{N_A} \sum_{b=1}^{N_B} \Psi_{ab}\,|\,\psi_a^A\,\rangle \otimes |\,\psi_b^B\,\rangle \quad , \tag{3.122}$$

where Ψ_{ab} is a complex $N_A \times N_B$ matrix. Any such matrix has a *singular value decomposition* [18] given by $\Psi = UDV^{\mathsf{T}}$, where (i) U is a complex rectangular matrix of dimensions $N_A \times N_{\rm s}$ satisfying $U^\dagger U = \mathbb{I}_{N_{\rm s} \times N_{\rm s}}$, (ii) D is a square diagonal matrix of dimensions $N_{\rm s} \times N_{\rm s}$ with positive real entries, (iii) V is a complex rectangular matrix of dimensions $N_B \times N_{\rm s}$ satisfying $V^\dagger V = \mathbb{I}_{N_{\rm s} \times N_{\rm s}}$, and (iv) $N_{\rm s} \le \mathsf{min}(N_A, N_B)$. Writing $D = \mathsf{diag}\{d_1, \ldots, d_{N_{\rm s}}\}$ with $p \in \{1, \ldots, N_{\rm s}\}$ the *singular values*, we obtain

$$|\,\Psi\,\rangle = \sum_{p=1}^{N_{\rm s}} d_p\,|\,\chi_p^A\,\rangle \otimes |\,\chi_p^B\,\rangle \quad , \tag{3.123}$$

[17] In fact, any initial state with $\alpha = \frac{1}{\sqrt{2}}$ and $\beta = \frac{1}{\sqrt{2}}\,e^{i\delta}$ will have entanglement entropy $\log 2$, independent of δ.

[18] See §3.7.2 below as well.

where

$$|\,\chi_p^A\,\rangle = \sum_{a=1}^{N_A} U_{ap}\,|\,\psi_a^A\,\rangle \qquad , \qquad |\,\chi_p^B\,\rangle = \sum_{b=1}^{N_B} V_{bp}\,|\,\psi_b^B\,\rangle \quad . \tag{3.124}$$

Note that $\langle\,\chi_a^A\,|\,\chi_{a'}^A\,\rangle = \delta_{aa'}$ and $\langle\,\chi_b^B\,|\,\chi_{b'}^B\,\rangle = \delta_{bb'}$.

If we trace out over the B degrees of freedom, the reduced density matrices on A and B are

$$\begin{aligned}\varrho_A &= \operatorname*{Tr}_B |\,\Psi\,\rangle\langle\,\Psi\,| = \sum_{p=1}^{N_{\rm s}} d_p^2\,|\,\chi_p^A\,\rangle\langle\,\chi_p^A\,| \\ \varrho_B &= \operatorname*{Tr}_A |\,\Psi\,\rangle\langle\,\Psi\,| = \sum_{p=1}^{N_{\rm s}} d_p^2\,|\,\chi_p^B\,\rangle\langle\,\chi_p^B\,|\end{aligned} \tag{3.125}$$

Since $\mathsf{Tr}\,\varrho_A = \mathsf{Tr}\,\varrho_B = 1$, we must have that the squares of the singular values sum to unity: $\sum_{p=1}^{N_{\rm s}} d_p^2 = 1$. The entanglement entropy is then

$$S_{\rm vN} \equiv S_A = S_B = -\sum_{p=1}^{N_{\rm s}} d_p^2 \log(d_p^2) \quad . \tag{3.126}$$

Writing $d_p \equiv \exp(-\xi_p/2)$, we have

$$\varrho_A = \sum_{p=1}^{N_{\rm s}} e^{-\xi_p}\,|\,\chi_p^A\,\rangle\langle\,\chi_p^A\,| \equiv e^{-\hat{K}} \quad , \tag{3.127}$$

and we identify the *entanglement Hamiltonian* as

$$\hat{K} \equiv \sum_{p=1}^{N_{\rm s}} \xi_p\,|\,\chi_p^A\,\rangle\langle\,\chi_p^A\,| \quad , \tag{3.128}$$

with $\sum_{p=1}^{N_{\rm s}} \exp(-\xi_p) = 1$. Thus, $\mathsf{spec}(\hat{K}) = \{\xi_1, \ldots, \xi_{N_{\rm s}}\}$ is the spectrum of eigenvalues of the entanglement Hamiltonian. In the language of eqn. 3.115, we have $\hat{K} = \beta\hat{H}_S + k_{\rm B}T \log Z_S$, with $A = S$ and $B = W$. In general there is no guarantee that the entanglement Hamiltonian $\hat{K}$ is local. For thermalizing local systems, however, sufficiently small subsystems are expected to have reduced density matrices that approach the corresponding thermal reduced density matrices.

3.6.5 Digression on random matrices

Random matrices are elements of a particular *ensemble* which is specified by a *symmetry class*. The probability distribution for a random matrix H is

$$P_\beta(H) = C_\beta\, e^{-\beta\,\mathsf{Tr}\,(H^2)/2} \quad , \tag{3.129}$$

with C_β a normalization constant, and where $\beta = 1$ for real symmetric, $\beta = 2$ for complex Hermitian, and $\beta = 4$ for quaternion real Hermitian Gaussian ensembles. These are respectively called the Gaussian Orthogonal Ensemble (GOE), Gaussian Unitary Ensemble (GUE), and Gaussian Symplectic Ensemble (GSE), and comprise the 'classical' random matrix ensembles (there are others). They are so named because the ensembles remain invariant under orthogonal $\mathsf{O}(N)$, unitary $\mathsf{U}(N)$, and symplectic $\mathsf{Sp}(2N)$ transformations, respectively, where N is the dimension[19]. The Gaussian probability distributions in eqn. 3.129 possess these invariances, although the invariances themselves do not require a Gaussian distribution[20]. The three ensembles correspond, respectively, to time-reversal invariant systems with integer spin (GOE), systems with no time-reversal invariance (GUE), and time-reversal invariant systems with half-odd-integer spin (GSE). The matrix elements of H in each of these ensembles take the form

$$H_{mn} = \begin{cases} H^{(0)}_{mn} & \text{(GOE)} \\ H^{(0)}_{mn} + iH^{(1)}_{mn} & \text{(GUE)} \\ H^{(0)}_{mn}\,\mathbb{1} + H^{(1)}_{mn}\,\mathbb{i} + H^{(2)}_{mn}\,\mathbb{j} + H^{(3)}_{mn}\,\mathbb{k} & \text{(GSE)} \end{cases} , \tag{3.130}$$

with $m \le n$, where $H^{(\mu)}_{mn} \in \mathbb{R}$ for $\mu \in \{0,1,2,3\}$, $H^{(0)}_{nm} = H^{(0)}_{mn}$, and $H^{(r)}_{nm} = -H^{(r)}_{mn}$ for $r \in \{1,2,3\}$. Here, $\{\mathbb{i},\mathbb{j},\mathbb{k}\}$ are the quaternions (see below). The measure dH in these three ensembles is defined as

$$dH = \begin{cases} \prod_{j\le k} dH^{(0)}_{jk} & \text{(GOE)} \\ \prod_{j\le k} dH^{(0)}_{jk} \prod_{m<n} dH^{(1)}_{mn} & \text{(GUE)} \\ \prod_{j\le k} dH^{(0)}_{jk} \prod_{m<n} \prod_{r=1}^{3} dH^{(r)}_{mn} & \text{(GSE)} \end{cases} . \tag{3.131}$$

The standard reference on the subject is M. L. Mehta, *Random Matrices*, 3rd ed. (Academic Press, 2004)[21]. One can then compute

$$\langle H_{ij} H_{mn} \rangle = \begin{cases} \frac{1}{2}\delta_{in}\delta_{jm} + \frac{1}{2}\delta_{im}\delta_{jn} & \text{(GOE)} \\ \frac{1}{2}\delta_{in}\delta_{jm} & \text{(GUE)} \\ \frac{1}{2}\delta_{in}\delta_{jm} - \frac{1}{4}\delta_{im}\delta_{jn} & \text{(GSE)} \end{cases} . \tag{3.132}$$

For each ensemble, the representative matrices have real eigenvalues λ_j whose joint probability distribution is given by (see Mehta)[22]

$$\mathcal{P}_\beta(\lambda_1, \ldots, \lambda_N) = \mathcal{C}_\beta \prod_{j<k}^{N} |\lambda_j - \lambda_k|^\beta \prod_{l=1}^{N} e^{-\beta\lambda_l^2/2} \quad . \tag{3.133}$$

[19] For quaternionic matrices, expressing each quaternionic number as a 2×2 matrix (see below), the matrix rank becomes $2N$.

[20] More general distributions respecting these invariances are of the form $P(H) \propto e^{\mathsf{Tr}\, V(H)}$ where $V(H) = V(S^{-1}HS)$ and S an element of $\mathsf{O}(N)$ or $\mathsf{U}(N)$ or $\mathsf{Sp}(2N)$ as the case requires.

[21] I once saw a review which said that Mehta's book has gotten worse with each subsequent edition. In my opinion there is some truth to this! The first edition was less detailed than others (259 → 562 → 706 pp.), but what has been gained in completeness seems to have been lost in readability.

[22] For the GSE, each eigenvalue is doubly degenerate due to Kramers' theorem, a consequence of time-reversal invariance and half-odd-integer spin.

Remarkably, the density of states $\sigma(\lambda)$ of the eigenvalues for each ensemble follows the Wigner semicircle law in the large-N limit,

$$\sigma(\lambda) = \frac{1}{\pi}\sqrt{2N-\lambda^2}\,\Theta(2N-\lambda^2) \quad . \tag{3.134}$$

Note that $\int\limits_{-\infty}^{\infty} d\lambda\,\sigma(\lambda) = N$.

A few words about quaternionic numbers

A *complex quaternionic number* q is written as $q = a\,\mathbb{1} + b\,\mathbb{i} + c\,\mathbb{j} + d\,\mathbb{k}$, where $a, b, c, d \in \mathbb{C}$ and $\{\mathbb{i}, \mathbb{j}, \mathbb{k}\}$ are the quaternions: $\mathbb{i}^2 = \mathbb{j}^2 = \mathbb{k}^2 = -\mathbb{1}$ and $\mathbb{ij} = -\mathbb{ji} = \mathbb{k}$, $\mathbb{jk} = -\mathbb{kj} = \mathbb{i}$, and $\mathbb{ki} = -\mathbb{ik} = \mathbb{j}$. In a *real quaternionic number* we have $a, b, c, d \in \mathbb{R}$. The quaternionic algebra is satisfied if we take $\mathbb{1}$ as the 2×2 unit matrix and $(\mathbb{i}, \mathbb{j}, \mathbb{k}) = (iZ, iY, iX)$, where $\{X, Y, Z\}$ are the Pauli matrices. We may then express each quaternionic number q as a 2×2 matrix, *viz.*

$$q = a\mathbb{1} + b\,\mathbb{i} + c\,\mathbb{j} + d\,\mathbb{k} = \begin{pmatrix} a+ib & c+id \\ -c+id & a-ib \end{pmatrix} \quad . \tag{3.135}$$

There are three conjugacy operations defined for quaternions: complex conjugation q^*, quaternion conjugation $\bar{q}$, and Hermitian conjugation $q^\dagger$:

$$\begin{aligned} q^* &= a^*\,\mathbb{1} + b^*\,\mathbb{i} + c^*\,\mathbb{j} + d^*\,\mathbb{k} = \begin{pmatrix} a^*+ib^* & c^*+id^* \\ -c^*+id^* & a^*-ib^* \end{pmatrix} \\ \bar{q} &= a\mathbb{1} - b\,\mathbb{i} - c\,\mathbb{j} - d\,\mathbb{k} = \begin{pmatrix} a-ib & -c-id \\ c-id & a+ib \end{pmatrix} \\ q^\dagger &= a^*\,\mathbb{1} - b^*\,\mathbb{i} - c^*\,\mathbb{j} - d^*\,\mathbb{k} = \begin{pmatrix} a^*-ib^* & -c^*-id^* \\ c^*-id^* & a^*+ib^* \end{pmatrix} \quad ; \end{aligned} \tag{3.136}$$

note that $q^\dagger = \bar{q}^*$. If $q^* = q$ then q is said to be *real*; if $q = \bar{q}$ then q is said to be a *scalar*. Note that if $q = q^\dagger$ then q is an ordinary Hermitian 2×2 matrix. The set of real quaternionic numbers q is denoted by the symbol $\mathbb{H}$. Unlike the reals $\mathbb{R}$ and complex numbers $\mathbb{C}$, $\mathbb{H}$ is not a field because multiplication within $\mathbb{H}$ is not commutative. Rather, we say that $\mathbb{H}$ is *an associative division algebra* over the real numbers. One may now check that for $q \in \mathbb{H}$,

$$|q|^2 \equiv q\bar{q} = \bar{q}q = (a^2+b^2+c^2+d^2)\,\mathbb{1} = \begin{pmatrix} a^2+b^2+c^2+d^2 & 0 \\ 0 & a^2+b^2+c^2+d^2 \end{pmatrix} \quad . \tag{3.137}$$

Let a quaternionic matrix Q have elements $q_{mn} = a_{mn}\,\mathbb{1} + b_{mn}\,\mathbb{i} + c_{mn}\mathbb{j} + d_{mn}\,\mathbb{k}$. If Q is Hermitian and quaternion real, then $q_{nm} = \bar{q}_{mn}$. This entails that the real matrices a, b, c, d satisfy $a = a^{\mathsf{T}}$, $b = -b^{\mathsf{T}}$, $c = -c^{\mathsf{T}}$, and $d = -d^{\mathsf{T}}$. Take care, however, when computing the quaternionic trace, since $\mathsf{Tr}\,\mathbb{1} \equiv 1$ even though the $\mathbb{1}$ on the LHS may be regarded as a 2×2 matrix.

Eigenvector statistics

In the limit $N \to \infty$, the eigenvectors of random matrices are independent random vectors in any basis. Let ψ_j^α be the α component of the $j^{\rm th}$ eigenvector of a given random matrix. The probability distribution

for a given eigenvector is given by

$$P\big(\{\psi_j^\alpha, \bar\psi_j^\alpha\}\big) \propto \delta\left(\sum_{\alpha=1}^N |\psi_j^\alpha|^2 - 1\right) \quad , \tag{3.138}$$

where $\bar\psi_j^\alpha = \psi_j^\alpha$ for GOE, $\bar\psi_j^\alpha = \psi_j^{\alpha *}$ for GUE, and $\bar\psi_j^\alpha$ is the quaternion conjugate of ψ_j^α for GSE. For the full joint distribution, mutual orthogonality must also be respected:

$$P\big(\{\psi_j^\alpha, \bar\psi_j^\alpha\}\big) \propto \prod_{j=1}^N \delta\left(\sum_{\alpha=1}^N |\psi_j^\alpha|^2 - 1\right) \prod_{k<l}^N \delta\left(\sum_{\alpha=1}^N \bar\psi_k^\beta \psi_l^\beta\right) \quad . \tag{3.139}$$

It then follows that

$$\begin{aligned}
&\text{GOE}: \quad \langle \psi_i^\alpha \psi_j^\beta \rangle = \frac{1}{N}\,\delta_{ij}\,\delta^{\alpha\beta} \\
&\text{GUE}: \quad \langle \psi_i^\alpha \bar\psi_j^\beta \rangle = \frac{1}{N}\,\delta_{ij}\,\delta^{\alpha\beta} \quad , \quad \langle \psi_i^\alpha \psi_j^\beta \rangle = \langle \bar\psi_i^\alpha \bar\psi_j^\beta \rangle = 0 \\
&\text{GSE}: \quad \langle \psi_i^\alpha \bar\psi_j^\beta \rangle = \frac{1}{N}\,\delta_{ij}\,\delta^{\alpha\beta} \quad , \quad \langle \psi_i^\alpha \psi_j^\beta \rangle = \langle \bar\psi_i^\alpha \bar\psi_j^\beta \rangle = -\frac{1}{2N}\,\delta_{ij}\,\delta^{\alpha\beta} \quad .
\end{aligned} \tag{3.140}$$

Now consider an operator $\hat A = \sum_\alpha A_\alpha \,|\,\alpha\,\rangle\langle\,\alpha\,|$. Let us compute the matrix element of $\hat A$ in the random matrix eigenstates $|\,j\,\rangle$ and $|\,k\,\rangle$:

$$A_{jk} = \langle\, j \,|\, \hat A \,|\, k\,\rangle = \sum_\alpha A_\alpha \,\langle\, j \,|\, \alpha\,\rangle\langle\,\alpha \,|\, k\,\rangle = \sum_\alpha A_\alpha\, \bar\psi_j^\alpha\, \psi_k^\alpha \quad . \tag{3.141}$$

Then

$$\langle A_{jk}\rangle = \sum_\alpha A_\alpha\, \langle \bar\psi_j^\alpha\, \psi_k^\alpha\rangle = \frac{1}{N}\sum_\alpha A_\alpha\,\delta_{jk} = \frac{\mathsf{Tr}\,(\hat A)}{N}\,\delta_{jk} \quad . \tag{3.142}$$

We may also compute

$$\langle A_{jk}\,\bar A_{mn}\rangle = \sum_{\alpha,\beta} A_\alpha\, A_\beta\, \langle \bar\psi_j^\alpha\, \psi_k^\alpha\, \psi_m^\beta\, \bar\psi_n^\beta\rangle \tag{3.143}$$

using Wick's theorem, *viz.*

$$\langle \bar\psi_j^\alpha\, \psi_k^\alpha\, \psi_m^\beta\, \bar\psi_n^\beta\rangle = \langle \bar\psi_j^\alpha\, \psi_k^\alpha\rangle\langle \psi_m^\beta\, \bar\psi_n^\beta\rangle + \langle \bar\psi_j^\alpha\, \psi_m^\beta\rangle\langle \psi_k^\alpha\, \bar\psi_n^\beta\rangle + \langle \bar\psi_j^\alpha\, \bar\psi_n^\beta\rangle\langle \psi_m^\beta\, \psi_k^\alpha\rangle \quad . \tag{3.144}$$

Thus we obtain

$$\begin{aligned}
&\text{GOE}: \quad \langle \bar\psi_j^\alpha\, \psi_k^\alpha\, \psi_m^\beta\, \bar\psi_n^\beta\rangle = \frac{1}{N^2}\left(\delta_{jk}\,\delta_{mn} + \delta_{jm}\,\delta_{kn}\,\delta^{\alpha\beta} + \delta_{jn}\,\delta_{km}\,\delta^{\alpha\beta}\right) \\
&\text{GUE}: \quad \langle \bar\psi_j^\alpha\, \psi_k^\alpha\, \psi_m^\beta\, \bar\psi_n^\beta\rangle = \frac{1}{N^2}\left(\delta_{jk}\,\delta_{mn} + \delta_{jm}\,\delta_{kn}\,\delta^{\alpha\beta}\right) \\
&\text{GSE}: \quad \langle \bar\psi_j^\alpha\, \psi_k^\alpha\, \psi_m^\beta\, \bar\psi_n^\beta\rangle = \frac{1}{N^2}\left(\delta_{jk}\,\delta_{mn} + \delta_{jm}\,\delta_{kn}\,\delta^{\alpha\beta} + \tfrac{1}{4}\,\delta_{jn}\,\delta_{km}\,\delta^{\alpha\beta}\right)
\end{aligned} \tag{3.145}$$

We use these results to obtain the following:

$$\langle |A_{mn}|^2 \rangle - |\langle A_{mn} \rangle|^2 = \frac{\mathsf{Tr}\,(\hat{A}^2)}{N^2} \cdot \begin{cases} 1 + \delta_{mn} & \text{(GOE)} \\ 1 & \text{(GUE)} \\ 1 + \frac{1}{4}\,\delta_{mn} & \text{(GSE)} \end{cases} . \tag{3.146}$$

Thus for off diagonal elements of A the relative ratios GOE : GUE : GSE are $1:1:1$, while for diagonal elements the relative ratios are $2:1:\frac{5}{4}$.

3.6.6 More precise formulation of ETH

More precisely (Srednicki, 1999), ETH is formulated in terms of general matrix elements of local observables in the energy eigenbasis, *viz.*[23]

$$A_{mn} = \langle\, m \,|\, \hat{A} \,|\, n \,\rangle = A(E)\,\delta_{mn} + e^{-S(E)/2}\, f_A(E,\omega)\, R_{mn} \tag{3.147}$$

where $E = \frac{1}{2}(E_m + E_n)$ is an average of the energy eigenvalues, $\omega = E_m - E_n$ is their difference, R_{mn} is a *random matrix* with $\langle R_{mn} \rangle = 0$ and $\mathsf{var}(R_{mn}) \equiv \langle |R_{mn}|^2 \rangle = 1$ (no sum), $S(E)$ is the thermodynamic entropy. Toward the middle of the spectrum, $S(E) \sim \log \mathcal{D}$, where $\mathcal{D}$ is the Hilbert space dimension, *i.e.* the dimension of A. We further assume that $A(E)$ and $f(E,\omega)$ are smooth functions of their arguments. Additionally, one has

$$\begin{aligned} A_{mn} \in \mathbb{R} \quad &: \quad R_{nm} = R_{mn} \quad , \quad f_A(E,-\omega) = f_A(E,\omega) \\ A_{mn} \in \mathbb{C} \quad &: \quad R_{nm} = \bar{R}_{mn} \quad , \quad f_A(E,-\omega) = f_A^*(E,\omega) \quad , \end{aligned} \tag{3.148}$$

for systems with and without time-reversal symmetry, respectively[24].

ETH *versus* random matrix theory

ETH reduces to random matrix theory within a given small energy window. Eqn. 3.147 is to be contrasted with the corresponding result for random matrix theory,

$$A_{mn} = \langle A \rangle\, \delta_{mn} + \sqrt{\frac{\langle A^2 \rangle - \langle A \rangle^2}{\mathcal{D}}}\, R_{mn} \quad , \tag{3.149}$$

where $\langle A \rangle \equiv \mathcal{D}^{-1}\,\mathsf{Tr}\,\hat{A}$ and $\langle A^2 \rangle \equiv \mathcal{D}^{-1}\,\mathsf{Tr}\,(\hat{A}^2)$ so that the averages are over the entire spectrum. Again, $\langle |R_{mn}|^2 \rangle = 1$, with the necessary ensemble-specific adjustments for the diagonal elements as indicated in eqn. 3.146. ETH thus reduces to RMT within any small window which contains $\mathcal{O}(\mathcal{D})$ states.

[23] See the review article by L. D'Alessio, Y. Kafri, A. Polkovnikov, and M. Rigol, *Adv. Phys.*, **65**, 239 (2016) and references therein.

[24] For systems with time reversal symmetry, a real basis is possible for the $T^2 = +1$ class, where T is the eigenvalue of the time reversal operator. The symplectic/Kramers class with $T^2 = -1$ requires a separate treatment.

A consequence of ETH

From ETH it follows that the expectation value of an operator in a Gibbs state $\varrho = Z^{-1}\exp(-\beta H)$ can be replaced by its expectation value in any eigenstate whose energy eigenvalue corresponds to the peak in $D(E)\exp(-\beta E)$, where $D(E)$ is the (many-body) density of states. Such an eigenstate is then called a *representative pure state*[25]. To see this, note

$$\mathsf{Tr}\,(\varrho\hat{A}) \approx \frac{1}{Z}\int dE\; D(E)\, e^{-\beta E} A(E) \approx A(E^*) \quad . \tag{3.150}$$

Here it is assumed that the function $A(E)$ in Eqn. 3.147 is a smooth function of E, and that the distribution $D(E)\exp(-\beta E)$ has a narrow peak centered at $E = E^*$. For example, if

$$D(E) \sim \exp\left(-\frac{(E-E_{\rm c})^2}{2\sigma^2}\right) \quad , \tag{3.151}$$

where the energy variance is extensive, *i.e.* $\sigma^2 \approx wN$ with w a constant and N the total number of particles or the system volume in microscopic units, then $E^*(\beta) \approx E_{\rm c} - \beta\sigma^2$ and the energy density is

$$\varepsilon^*(\beta) \equiv \frac{E^*}{N} \approx \varepsilon_{\rm c} - \beta w \quad , \tag{3.152}$$

where $\varepsilon_{\rm c}$ is the energy density at the center of the spectrum. Eigenstates of H in the vicinity of energy density $\varepsilon^*(\beta)$ are thus representative pure states of the Gibbs density matrix which reproduce expectation values of few body operators. Note that we may obtain $\varepsilon^*(\beta)$ from the expression

$$\varepsilon^*(\beta) = \frac{1}{NZ}\,\mathsf{Tr}\,(\hat{H}e^{-\beta\hat{H}}) \quad . \tag{3.153}$$

3.6.7 When is the ETH true?

There is no rigorous general proof of the ETH. Deutsch showed that the ETH holds for the case of an integrable Hamiltonian weakly perturbed by a single Gaussian random matrix. Horoi *et al.* (1995) showed that nuclear shell model wavefunctions reproduce thermodynamic predictions. Recent numerical work by M. Rigol and collaborators has verified the applicability of the ETH in small interacting boson systems. ETH fails for so-called integrable models, where there are a large number of conserved quantities, which commute with the Hamiltonian. Integrable models are, however, quite special, and as Deutsch showed, integrability is spoiled by weak perturbations, in which case ETH then applies.

ETH also fails in the case of noninteracting disordered systems which exhibit *Anderson localization*. Single particle energy eigenstates ψ_j whose energies ε_j lie within the localized portion of the eigenspectrum decay exponentially, as $|\psi_j(\boldsymbol{r})|^2 \sim \exp\big(-|\boldsymbol{r}-\boldsymbol{r}_j|/\xi(\varepsilon_j)\big)$, where $\boldsymbol{r}_j$ is some position in space associated with ψ_j and $\xi(\varepsilon_j)$ is the *localization length*. Within the localized portion of the spectrum, $\xi(\varepsilon)$ is finite. As ε approaches a *mobility edge*, $\xi(\varepsilon)$ diverges as a power law. In the *delocalized regime*, eigenstates are spatially *extended* and typically decay at worst as a power law[26]. Exponentially localized states are

[25] See V. Khemani, A. Chandran, H. Kim, and S. L. Sondhi, *Phys. Rev. E* **90**, 052133 (2014).

[26] Recall that in systems with no disorder, eigenstates exhibit Bloch periodicity in space.

unable to thermalize with other distantly removed localized states. Of course, all noninteracting systems will violate ETH, because they are integrable. The interacting version of this phenomenon, *many-body localization* (MBL), is a topic of current interest and some controversy in condensed matter and statistical physics. MBL systems also exhibit a large number of conserved quantities, but in contrast to the case of integrable systems, where each conserved quantity is in general expressed in terms of an integral of a local density, in MBL systems the conserved quantities are themselves local, although *emergent*. The emergent nature of locally conserved quantities in MBL systems means that they are not simply expressed in terms of the original local operators of the system, but rather are arrived at via a sequence of local unitary transformations.

Note again that in contrast to the classical case, time evolution of a quantum state does not create the thermal state. Rather, it *reveals* the thermal distribution which is encoded in all eigenstates after sufficient time for dephasing to occur, so that correlations between all the wavefunction expansion coefficients $\{C_\alpha\}$ in $|\Psi(t)\rangle = \sum_\alpha C_\alpha\, e^{-iE_\alpha t/\hbar}\,|\Psi_\alpha\rangle$ for $\alpha \neq \alpha'$ are all lost[27].

3.7 Appendix I: Matrices and Jordan Canonical Form

3.7.1 Normal and non-normal matrices

If a matrix A is normal, meaning $\left[A, A^\dagger\right] = 0$, then it may be diagonalized by a unitary transformation. Indeed, any $n \times n$ matrix A is diagonalizable by a unitary transformation if and only if A is normal. When A is normal, the eigenspaces span, and we may choose $\langle\, L^\alpha \,|\, R^\beta \,\rangle = \delta^{\alpha\beta}$, using Gram-Schmidt in the case of degeneracies.

When A is not normal, while the sum of the dimensions of its eigenspaces generically is equal to its dimension $\dim(A) = n$, this is not guaranteed, and it may be less than n. What is true is that any non-normal complex matrix A can be brought to Jordan canonical form by a similarity transformation $\tilde{A} = Q^{-1} A\, Q$, where Q is invertible and

$$\tilde{A} = \begin{pmatrix} J_1 & 0 & \\ 0 & \ddots & 0 \\ & 0 & J_b \end{pmatrix} \tag{3.154}$$

is block diagonal with b Jordan blocks. Each Jordan block J_α with $\alpha \in \{1, \ldots, b\}$ is of the form

$$J_\alpha = \begin{pmatrix} \lambda_\alpha & 1 & 0 & \\ 0 & \lambda_\alpha & \ddots & 0 \\ & & \ddots & 1 \\ & & 0 & \lambda_\alpha \end{pmatrix} \quad . \tag{3.155}$$

Thus each J_α is tridiagonal, with diagonal elements all given by λ_α and each element directly above the diagonal equal to one. We denote the right and left eigenvectors of $\tilde{A}$ as $|\,\widetilde{R}^\alpha\,\rangle = Q^{-1}\,|\,R^\alpha\,\rangle$ and

[27] To be more precise, "strong ETH" proposes that each bulk eigenstate encodes thermal information, but "weak ETH" allows for exceptional states, such as quantum scars.

$\langle\, \widetilde{L}^\alpha \,| = \langle\, L^\alpha \,| \, Q$, respectively. Each J_α has only one right eigenvector, $\psi^\alpha_j = \delta_{j,1}$, whose corresponding left eigenvector is $\chi^\alpha_j = \delta_{j,n_\alpha}$, where $n_\alpha = \mathsf{dim}(J_\alpha)$. Note $n = \mathsf{dim}(A)$ is the sum of the dimensions of the Jordan blocks, *i.e.* $n = \sum_{\alpha=1}^b n_\alpha$. When $n_\alpha = 1$, the Jordan block is the 1×1 matrix λ_α. For a non-normal matrix A, its eigenvalues λ_α may be complex. However, if all the elements of A are real, then any complex eigenvalues must occur in complex conjugate pairs, because the characteristic polynomial $P(\lambda) = \mathsf{det}(\lambda - A)$ satisfies $\big[P(\lambda)\big]^* = P(\lambda^*)$.

When $\lambda_\alpha \neq \lambda_\beta$, we have $\langle\, L^\alpha \,|\, R^\beta \,\rangle = \langle\, \widetilde{L}^\alpha \,|\, \widetilde{R}^\beta \,\rangle = 0$. For eigenspaces with $n_\alpha = 1$, we may choose $\langle\, L^\alpha \,|\, R^\beta \,\rangle = \langle\, \widetilde{L}^\alpha \,|\, \widetilde{R}^\beta \,\rangle = \delta^{\alpha\beta}$, but for the nontrivial Jordan blocks with $n_\alpha > 1$ we have $\langle\, \widetilde{L}^\alpha \,|\, \widetilde{R}^\alpha \,\rangle = 0$, as we have seen in the previous paragraph, and therefore $\langle\, L^\alpha \,|\, R^\alpha \,\rangle = 0$. Real symmetric matrices are all normal, with no Jordan blocks. For complex symmetric matrices, we may have nontrivial Jordan blocks.

Since $\langle\, L \,|\, R \,\rangle = \langle\, \widetilde{L} \,|\, \widetilde{R} \,\rangle = 0$, we may write

$$A = \bigoplus_{n_\alpha=1} \lambda_\alpha \,|\, R^\alpha \,\rangle\langle\, L^\alpha \,| \bigoplus_{n_\beta>1} Q J_\beta \, Q^{-1} \tag{3.156}$$

and raising A to the k power yields

$$A^k = \bigoplus_{n_\alpha=1} \lambda^k_\alpha \,|\, R^\alpha \,\rangle\langle\, L^\alpha \,| \bigoplus_{n_\beta>1} Q J^k_\beta \, Q^{-1} \quad . \tag{3.157}$$

Note that J^k_β is upper triangular with all diagonal elements given by λ^k_β. Note that for complex symmetric matrices, the left and right eigenvectors are identical and we may write

$$L^\alpha_j = R^\alpha_j \equiv \Psi^\alpha_j \qquad \Rightarrow \qquad \langle\, L^\alpha \,| = \langle\, \Psi^\alpha \,| \quad , \quad |\, R^\alpha \,\rangle = |\, \Psi^\alpha \,\rangle \quad , \tag{3.158}$$

with no complex conjugation, *i.e.* $\langle\, L^\alpha \,|\, j \,\rangle = \langle\, j \,|\, R^\alpha \,\rangle \equiv \Psi^\alpha_j$.

3.7.2 Contrast with singular value decomposition

We now remark upon the difference between the decomposition into Jordan canonical form and the singular value decomposition (SVD), in which we write an $m \times n$ matrix A as $A = U D V^\dagger$, where U is $m \times k$, V is $n \times k$ (hence $V^\dagger$ is $k \times n$), $U^\dagger U = V^\dagger V = \mathbb{I}_{k\times k}$, and $D = \mathsf{diag}(d_1, \ldots, d_k)$ is $k \times k$ with $k \leq \mathsf{min}(m, n)$ and each $d_j > 0$. The elements d_j are the singular values and the columns of U and V are the singular vectors. Note that $A^\dagger A = V D^2 \, V^\dagger$ is $n \times n$ and $A A^\dagger = U D^2 \, U^\dagger$ is $m \times m$. If we define

$$\widetilde{P}(\lambda) = \prod_{j=1}^k \big(\lambda - d_j^2\big) \quad , \tag{3.159}$$

Then

$$P(\lambda) \equiv \mathsf{det}(\lambda - A^\dagger A) = \lambda^{n-k} \widetilde{P}(\lambda) \qquad , \qquad Q(\lambda) \equiv \mathsf{det}(\lambda - A A^\dagger) = \lambda^{m-k} \widetilde{P}(\lambda) \quad . \tag{3.160}$$

For any square $n \times n$ complex matrix A we therefore have two decompositions, via JCF and SVD, *viz.*

$$A = Q J \, Q^{-1} = U D \, V^\dagger \quad , \tag{3.161}$$

where J is the Jordan canonical form of A. When A is normal, its Jordan canonical form is diagonal. Its singular values are $d_j = |\lambda_j|$, and its left and right singular vectors can be chosen to differ only by the phases of the corresponding eigenvalues. In a reduced SVD, $k = \mathsf{rank}(A)$, which need not equal n. Only when A is positive semidefinite Hermitian may one generally take $U = V = Q$.

3.7.3 Examples

Consider the real asymmetric matrix

$$A = \begin{pmatrix} 2a & -4a^2 \\ \frac{1}{4} & 0 \end{pmatrix} \quad , \tag{3.162}$$

where $a \in \mathbb{R}$ is any real number. The characteristic polynomial is $P(\lambda) = \det(\lambda - A) = (\lambda - a)^2$ and there is a single eigenvalue, $\lambda = a$. The right and left eigenvectors are found to be

$$|\, R \,\rangle = \begin{pmatrix} 4a \\ 1 \end{pmatrix} \qquad , \qquad \langle\, L \,| = \begin{pmatrix} \frac{1}{4} & -a \end{pmatrix} \quad , \tag{3.163}$$

where the normalization is arbitrary. Note $\langle\, L \,|\, R \,\rangle = 0$. The matrix A is brought to JCF by the similarity transformation $\tilde{A} = Q^{-1} A\, Q$ with

$$Q = \begin{pmatrix} 4a & 4 \\ 1 & 0 \end{pmatrix} \qquad , \qquad Q^{-1} = \begin{pmatrix} 0 & 1 \\ \frac{1}{4} & -a \end{pmatrix} \qquad , \qquad \tilde{A} = Q^{-1} A\, Q = \begin{pmatrix} a & 1 \\ 0 & a \end{pmatrix} \quad . \tag{3.164}$$

Note that

$$|\, \widetilde{R} \,\rangle = Q^{-1} \,|\, R \,\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad , \qquad \langle\, \widetilde{L} \,| = \langle\, L \,|\, Q = \begin{pmatrix} 0 & 1 \end{pmatrix} \quad , \tag{3.165}$$

and that $\langle\, \widetilde{L} \,|\, \widetilde{R} \,\rangle = 0$.

Adding another row and column to our matrix A, consider the matrix

$$B = \begin{pmatrix} 2a & -4a^2 & 0 \\ \frac{1}{4} & 0 & 0 \\ 0 & 0 & b \end{pmatrix} \quad , \tag{3.166}$$

where both a and b are arbitrary real numbers. Since $\det(\lambda - B) = (\lambda - a)^2\,(\lambda - b)$, B thus has two eigenvalues: $\lambda_1 = a$ and $\lambda_2 = b$. The decomposition of B is then

$$B = Q J_1 Q^{-1} \bigoplus \lambda_2 \,|\, R^2 \,\rangle\langle\, L^2 \,| \quad , \tag{3.167}$$

where $\langle\, L^2 \,| = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix}$ and $|\, R^2 \,\rangle = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix}^{\mathsf{T}}$. Of course, we could mix up the various elements of B by applying a general similarity transformation $B \to B' \equiv SBS^{-1}$, but the JCF of B' would be the same.

3.7.4 Exponentiating Jordan blocks

For a diagonal matrix $M = \mathsf{diag}\{\lambda_1, \ldots, \lambda_n\}$, its exponential is $\exp(Mt) = \mathsf{diag}\{e^{\lambda_1 t}, \ldots, e^{\lambda_n t}\}$. Consider instead the $n \times n$ Jordan block

$$J = \begin{pmatrix} \lambda & 1 & 0 & \\ 0 & \lambda & \ddots & 0 \\ & & \ddots & 1 \\ & & 0 & \lambda \end{pmatrix} \quad . \tag{3.168}$$

We can write

$$J = \lambda I + N \tag{3.169}$$

where $I_{jk} = \delta_{jk}$ is the $n \times n$ identity matrix and $N_{jk} = \delta_{k,j+1}$ has ones along its first superdiagonal (*i.e.* just above its main diagonal) and zeros elsewhere. The matrix N is *nilpotent*, with $N^n = 0$, and thus the exponential series for $\exp(Nt)$ terminates after n terms, *viz.*

$$\exp(Nt) = I + tN + \frac{t^2}{2!} N^2 + \ldots + \frac{t^{n-1}}{(n-1)!} N^{n-1} \quad . \tag{3.170}$$

Since λI commutes with N, we have

$$\exp(Jt) = e^{\lambda t} K \tag{3.171}$$

where

$$K = \exp(Nt) = \begin{pmatrix} 1 & t & t^2/2! & t^3/3! & \cdots & t^{n-1}/(n-1)! \\ 0 & 1 & t & t^2/2! & \cdots & t^{n-2}/(n-2)! \\ 0 & 0 & 1 & t & \cdots & t^{n-3}/(n-3)! \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & t \\ 0 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix} \quad . \tag{3.172}$$

In component notation,

$$K_{jk} = \begin{cases} t^{k-j}/(k-j)! & \text{if } k \geq j \\ 0 & \text{if } k < j \end{cases} \quad . \tag{3.173}$$

3.8 Appendix II: Poisson Processes and Radioactive Decay

Here we consider two examples where the state labels of the master equation denote a number, corresponding to the discrete population of some group. The master equation is

$$\frac{dP_n}{dt} = \sum_m \left(W_{nm} P_m - W_{mn} P_n \right) \quad . \tag{3.174}$$

Thus W_{nm} is the transition rate for the process $|\, m \,\rangle \to |\, n \,\rangle$.

3.8.1 Poisson process

Consider the *Poisson process*, for which

$$W_{nm} = \begin{cases} \lambda & \text{if } n = m+1 \\ 0 & \text{if } n \neq m+1 \ . \end{cases} \tag{3.175}$$

We then have

$$\frac{dP_n}{dt} = \lambda\big(P_{n-1} - P_n\big) \ . \tag{3.176}$$

The *generating function* $P(z,t) = \sum_{n=0}^{\infty} z^n P_n(t)$ then satisfies

$$\frac{\partial P}{\partial t} = \lambda(z-1)\,P \quad \Rightarrow \quad P(z,t) = e^{(z-1)\lambda t}\,P(z,0) \ . \tag{3.177}$$

If the initial distribution is $P_n(0) = \delta_{n,0}$, then

$$P_n(t) = \frac{(\lambda t)^n}{n!}\,e^{-\lambda t} \ , \tag{3.178}$$

which is known as the *Poisson distribution*. If we define $\alpha \equiv \lambda t$, then from $P_n = \alpha^n\,e^{-\alpha}/n!$ we have

$$\langle n^k \rangle = e^{-\alpha}\left(\alpha\frac{\partial}{\partial\alpha}\right)^k e^{\alpha} \ . \tag{3.179}$$

Thus, $\langle n \rangle = \alpha$, $\langle n^2 \rangle = \alpha^2 + \alpha$, *etc.*

3.8.2 Radioactive decay

Consider a group of atoms, some of which are in an excited state which can undergo nuclear decay. Let $P_n(t)$ be the probability that n atoms are excited at some time t. We then model the decay dynamics by

$$W_{nm} = \begin{cases} 0 & \text{if } n \geq m \\ m\gamma & \text{if } n = m-1 \\ 0 & \text{if } n < m-1 \quad . \end{cases} \tag{3.180}$$

Here, γ is the decay rate of an individual atom, which can be determined from quantum mechanics. The master equation then tells us

$$\frac{dP_n}{dt} = (n+1)\,\gamma\,P_{n+1} - n\,\gamma\,P_n \quad . \tag{3.181}$$

The interpretation here is as follows: let $|\,n\,\rangle$ denote a state in which n atoms are excited. We then have $P_n(t) = \langle\, n\,|\,P(t)\,\rangle$. Then $P_n(t)$ will increase due to spontaneous transitions from $|\,n+1\,\rangle$ to $|\,n\,\rangle$, and will decrease due to spontaneous transitions from $|\,n\,\rangle$ to $|\,n-1\,\rangle$.

The average number of particles in the system is $N(t) = \sum_{n=0}^{\infty} n\, P_n(t)$. Note that

$$\begin{aligned}\frac{dN}{dt} &= \sum_{n=0}^{\infty} n\Big[(n+1)\,\gamma\, P_{n+1} - n\,\gamma\, P_n\Big] \\ &= \gamma\sum_{n=0}^{\infty}\Big[n(n-1)\,P_n - n^2 P_n\Big] = -\gamma\sum_{n=0}^{\infty} n\,P_n = -\gamma\,N \quad .\end{aligned} \tag{3.182}$$

Thus, $N(t) = N(0)\,e^{-\gamma t}$. The relaxation time is $\tau = \gamma^{-1}$, and the equilibrium distribution is $P_n^{\rm eq} = \delta_{n,0}$. Note that this satisfies detailed balance.

We can go a bit farther here. Let us define

$$P(z,t) \equiv \sum_{n=0}^{\infty} z^n\, P_n(t) \quad . \tag{3.183}$$

This is sometimes called a *generating function*. Then

$$\begin{aligned}\frac{\partial P}{\partial t} &= \gamma\sum_{n=0}^{\infty} z^n\Big[(n+1)\,P_{n+1} - n\,P_n\Big] \\ &= \gamma\,\frac{\partial P}{\partial z} - \gamma z\,\frac{\partial P}{\partial z} \quad .\end{aligned} \tag{3.184}$$

Thus,

$$\frac{1}{\gamma}\,\frac{\partial P}{\partial t} - (1-z)\,\frac{\partial P}{\partial z} = 0 \quad . \tag{3.185}$$

We now see that any function $f(\xi)$ satisfies the above equation, where $\xi = \gamma t - \log(1-z)$. Thus, we can write

$$P(z,t) = f\big(\gamma t - \log(1-z)\big) \quad . \tag{3.186}$$

Setting $t = 0$ we have $P(z,0) = f\big(-\log(1-z)\big)$, and inverting this result we obtain $f(u) = P(1-e^{-u}, 0)$, which entails

$$P(z,t) = P\big(1 + (z-1)\,e^{-\gamma t}\,,\,0\big) \quad . \tag{3.187}$$

The total probability is $P(z{=}1,t) = \sum_{n=0}^{\infty} P_n$, which clearly is conserved: $P(1,t) = P(1,0)$. The average particle number is

$$N(t) = \sum_{n=0}^{\infty} n\,P_n(t) = \left.\frac{\partial P}{\partial z}\right|_{z=1} = \left.e^{-\gamma t}\,\frac{\partial P(z,0)}{\partial z}\right|_{z=1} = N(0)\,e^{-\gamma t} \quad . \tag{3.188}$$

3.9 Appendix III: The Markovian Mpemba Effect

3.9.1 Introduction

Intuition and common experience tell us that if we place two objects of identical composition at temperatures $T_{\rm h}$ and $T_{\rm c}$ into the same bath at temperature $T_{\rm b}$, with $T_{\rm h} > T_{\rm c} > T_{\rm b} > 0$, it will take longer for the

hotter object to thermalize to the bath temperature than for the cold object. If you want to make ice, you fill your ice tray with cold water before placing it in the freezer and not with hot water. Yet ca. 350-340 BCE, Aristotle wrote,[28]

"Hail occurs less often in the summer than in spring and autumn, though more often than in winter, because the air is drier in summer; in spring it is still moist, while in autumn it is already becoming moist. Sometimes, as has been said, hail also occurs in late summer, for the same reason. The fact that the water has previously been heated also contributes to the rapidity of its freezing, for it cools more quickly. Hence many people, when they wish to cool water quickly, first place it in the sun. And the people around the Pontus, when they make camp upon the ice for catching fish – for they fish by breaking through the ice – pour hot water around their reeds so that it will freeze more quickly. "

This may be the first mention of what is known today as the *Mpemba effect*, where a given system takes a shorter time to cool down from a hotter initial temperature than from a colder one. Newton's phenomenological law of cooling says

$$\frac{dT}{dt} = -k(T - T_{\rm env}) \quad , \tag{3.189}$$

where $T(t)$ is the temperature of an object in contact with a heat bath at temperature $T_{\rm env}$. The constant $k > 0$ thus determines the cooling rate. We then have

$$T(t) = T_{\rm env} + \big[T(0) - T_{\rm env}\big] e^{-kt} \quad , \tag{3.190}$$

which entails that the Mpemba effect is impossible. The existence of such a phenomenon remains controversial[29].

Here we discuss a demonstrable mathematical phenomenon known as the *Markovian Mpemba effect*[30] (MME) in which an initial thermal probability distribution $p_j(t=0) = \pi_j(T)$ at temperature T is evolved according to the master equation. The equilibrium distribution eventually reached is also thermal, corresponding to a bath temperature $T_{\rm b} < T$. Given an appropriate definition of distance between two distributions, $D[\boldsymbol{p}, \boldsymbol{p}']$, the distance between two thermal distributions $T_{1,2}$ is an increasing function of their temperature difference $|T_1 - T_2|$. Now let $\boldsymbol{p}(t;T)$ be the solution of the master equation subject to the initial conditions $\boldsymbol{p}(t=0,T) = \boldsymbol{\pi}(T)$, the Boltzmann distribution at temperature T. Then for some choices of the rates W_{ij}, it may be that the plots of $D[\boldsymbol{p}(t,T), \boldsymbol{\pi}(T_{\rm b})]$ *versus* t for $T = T_{\rm h}$ and $T = T_{\rm c}$ cross at some time t, and that for asymptotically late times the distribution evolving from the hotter initial state is closer to $\boldsymbol{\pi}(T_{\rm b})$.

The Master equation was introduced in §3.2:

$$\frac{dP_i}{dt} = \sum_j \big(W_{ij}\, P_j - W_{ji}\, P_i\big) = -\Gamma_{ij} P_j \quad , \tag{3.191}$$

with

$$W_{ij} = \gamma \exp\left(\frac{E_j - B_{ij}}{k_{\rm B} T_{\rm b}}\right) \quad , \tag{3.192}$$

[28] Aristotle, *Meteorologica* 1.12, 348b26-349a1.

[29] On the yes side, see, *e.g.*, M. Jeng, *Am. J. Phys.* **74**, 514 (2006). On the no side, H. C. Burridge and P. F. Linden. *Sci Rep.* **6**, 37665 (2016).

[30] Z. Lu and O. Raz, *Proc. Natl. Acad. Sci.* **114**, 5083 (2017).

where $T_{\rm b}$ is the bath temperature and $B_{ij} = B_{ji}$ is the energy barrier that must be overcome in transitioning from $|j\rangle$ to $|i\rangle$. If we take

$$B_{ij} = \begin{cases} E_j & \text{if } i < j \\ E_i & \text{if } i \geq j \end{cases} \quad , \tag{3.193}$$

then W_{ij} is given in eqn. 3.2.3. Recall $\sum_i W_{ij} = 0$ and thus $\langle\, L^1 \,| = (1\ ,\ 1\ ,\ \ldots\ ,\ 1)$ is a left eigenvector of Γ with eigenvalue $\lambda_1 = 0$. The equilibrium distribution at temperature T is given by

$$\pi_i(T) = \frac{1}{Z(T)}\, e^{-E_i/k_{\rm B}T} \quad , \tag{3.194}$$

where $Z(T)$ is the canonical partition function, which guarantees $\sum_i \pi_i = 1$. We assume detailed balance, which entails $W_{ij}\,\pi_j(T_{\rm b}) = W_{ji}\,\pi_i(T_{\rm b})$ and is satisfied by eqns. 3.192 and 3.194 for arbitrary symmetric B_{ij}.

3.9.2 Distance between distributions

Lu and Raz list three desiderata which any distance function $D[\boldsymbol{p}(t), \boldsymbol{\pi}(T_{\rm b})]$ should satisfy:

(i) Under the Master equation dynamics, $D[\boldsymbol{p}(t), \boldsymbol{\pi}(T_{\rm b})]$ should be monotonically decreasing in t.

(ii) For all $T_{\rm h} > R_{\rm c} > R_{\rm b}$, we should have $D[\boldsymbol{\pi}(T_{\rm h}), \boldsymbol{\pi}(T_{\rm b})] > D[\boldsymbol{\pi}(T_{\rm c}), \boldsymbol{\pi}(T_{\rm b})] > 0$.

(iii) $D[\boldsymbol{p}, \boldsymbol{\pi}(T_{\rm b})]$ should be a continuous convex function of the components $\{\pi_i(T_{\rm b})\}$.

One possibility is the Kullback-Leibler divergence,

$$D_{\rm KL}[\boldsymbol{p}, \boldsymbol{\pi}^{\rm b}] = \sum_i p_i \log\Big(\frac{p_i}{\pi_i^{\rm b}}\Big) \quad , \tag{3.195}$$

where $\pi_i^{\rm b} = \pi_i(T_{\rm b})$ is the equilibrium distribution. This is also known as the "relative entropy" of the distributions. Extremizing with respect to $\boldsymbol{p}$ at fixed and normalized $\boldsymbol{\pi}^{\rm b}$ yields $p_i = \pi_i^{\rm b}$. Another possibility is the L^1 distance,

$$D_{L^1}[\boldsymbol{p}, \boldsymbol{\pi}^{\rm b}] = \sum_i |p_i - \pi_i^{\rm b}| \quad , \tag{3.196}$$

where in this case we assume $\boldsymbol{p}'$ is normalized. Again the minimum occurs for $\boldsymbol{p} = \boldsymbol{p}'$, where $D = 0$.

3.9.3 Conditions for the Markovian Mpemba effect

The general solution to the Master equation may be written

$$p_i(t) = \pi_i^{\rm b} + \sum_{a=2}^{N} C_a\, R_i^a\, e^{-\lambda_a t} \quad , \tag{3.197}$$

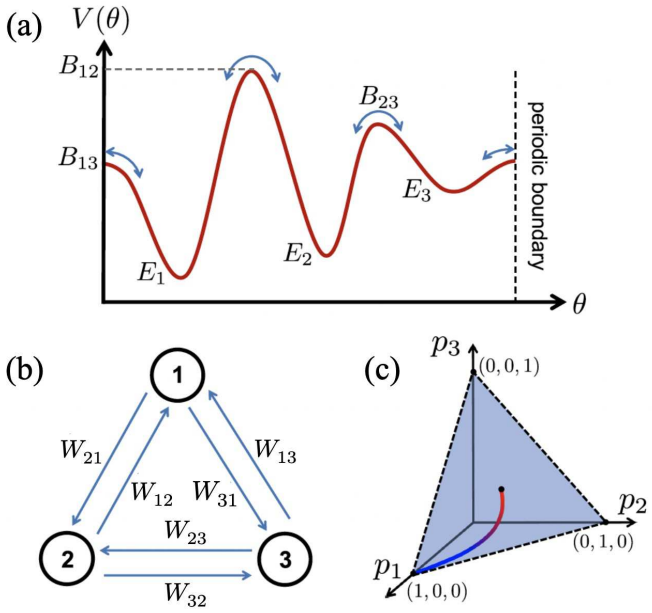


Figure 3.12: Three-state MME from fig. 1 of Lu and Raz (2017). (a) Sketch of potential $V(\theta)$ *versus* coordinate θ in a periodic geometry. (b) Master equation rates. (c) The probability distribution is specified by (p_1, p_2, p_3) where $p_1 + p_2 + p_3 = 1$. The curved line is the set of Boltzmann distributions $\boldsymbol{\pi}(T)$, with $\boldsymbol{\pi}(T = 0) = (1, 0, 0)$ and $\boldsymbol{\pi}(T = \infty) = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$.

where N is the dimension of the state space and $C_a \equiv \langle\, L^a \,|\, p(0) \,\rangle = \sum_j L^a_j p_j(0)$. Again we assume there are no Jordan blocks in the spectral decomposition of Γ. If we order the eigenmodes such that

$$0 = \lambda_1 < \mathsf{Re}\,\lambda_2 < \mathsf{Re}\,\lambda_3 < \cdots < \mathsf{Re}\,\lambda_N \quad , \tag{3.198}$$

then, with $\boldsymbol{p}(0) = \boldsymbol{\pi}(T)$ a Boltzmann distribution at a temperature $T > T_{\rm b}$, we find that at long times the solution is

$$|\, p(t) \,\rangle = |\, \pi^{\rm b} \,\rangle + C_2(T)\, e^{-\lambda_2 t}\, |\, R^2 \,\rangle \quad . \tag{3.199}$$

The MME holds in whenever $|C_2(T)|$ is a decreasing function of T. If $T < T_{\rm b}$, then there is an *inverse Markovian Mpemba effect* whenever $|C_2(T)|$ is an increasing function of T.

3.9.4 Numerical simulation

Lu and Raz (2017) investigated numerically a three-state model with energies $E_1 = 0$, $E_2 = 0.1$, and $E_3 = 0.7$ and barriers $B_{12} = 1.5$, $B_{13} = 0.8$, and $B_{23} = 1.2$. A sketch is shown in fig. 3.12. Evolution of the distribution $\boldsymbol{p}(t)$ starting from hot and cold initial thermal distributions $\boldsymbol{p}(0) = \boldsymbol{\pi}(T^{\rm h,c})$ and their relaxation to the bath temperature $T^{\rm b}$ is shown in fig. 3.13.

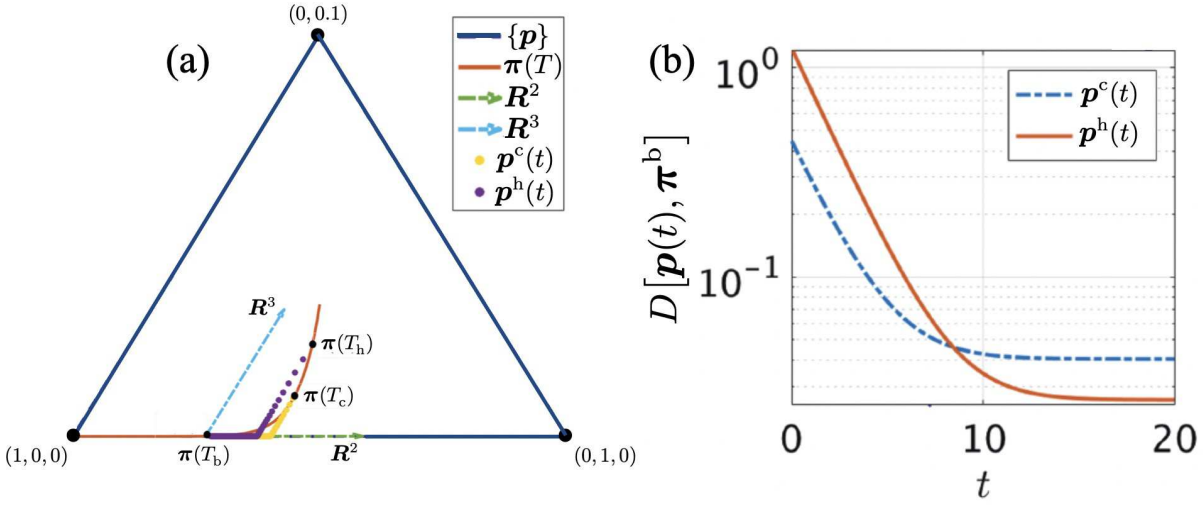


Figure 3.13: Fig. 2 from Lu and Raz (2017). (a) The triangular simplex corresponds to the set of all normalized three-state probability distributions $\boldsymbol{p} = (p_1, p_2, p_3)$. The green and blue dashed lines show the right eigenvectors $\boldsymbol{R}^{2,3}$ of Γ. The dotted lines show the relaxations starting from thermal distributions at $T_{\rm h} = 1.3$ (purple) and $T_{\rm c} = 0.42$ to the bath at $T_{\rm b} = 0.1$. (b) The distances $D_{\rm KL}[\boldsymbol{p}^{\rm h,c}(t), \boldsymbol{\pi}^{\rm b}]$ *versus time*, showing a MME. At late times, the distribution $\boldsymbol{p}^{\rm h}(t)$ is closer to the bath distribution $\boldsymbol{\pi}^{\rm b}$ than $\boldsymbol{p}^{\rm c}(t)$.

3.10 Appendix IV: Transition to Ergodicity in a Simple Model

A ball of mass m executes perfect one-dimensional motion along the symmetry axis of a piston. Above the ball lies a mobile piston head of mass M which slides frictionlessly inside the piston. Both the ball and piston head execute ballistic motion, with two types of collision possible: (i) the ball may bounce off the floor, which is assumed to be infinitely massive and fixed in space, and (ii) the ball and piston head may engage in a one-dimensional elastic collision. The Hamiltonian is

$$H = \frac{P^2}{2M} + \frac{p^2}{2m} + MgX + mgx \quad ,$$

where X is the height of the piston head and x the height of the ball. Another quantity is conserved by the dynamics: $\Theta(X - x)$. *I.e.*, the ball always is below the piston head.

(a) Choose an arbitrary length scale L, and then energy scale $E_0 = MgL$, momentum scale $P_0 = M\sqrt{gL}$, and time scale $\tau_0 = \sqrt{L/g}$. Show that the dimensionless Hamiltonian becomes

$$\bar{H} = \tfrac{1}{2}\bar{P}^2 + \bar{X} + \frac{\bar{p}^2}{2r} + r\bar{x} \quad ,$$

with $r = m/M$, and with equations of motion $d\bar{X}/dt = \partial\bar{H}/\partial\bar{P}$, *etc.* (Here the bar indicates dimensionless variables: $\bar{P} = P/P_0$, $\bar{t} = t/\tau_0$, *etc.*) What special dynamical consequences hold for $r = 1$?

(b) Compute the microcanonical average piston height $\langle X \rangle$. The analogous dynamical average is

$$\langle X \rangle_t = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, X(t) \quad .$$

When computing microcanonical averages, it is helpful to use the Laplace transform, discussed in §4.2.2 of the notes. (It is possible to compute the microcanonical average by more brute force methods as well.)

(c) Compute the microcanonical average of the rate of collisions between the ball and the floor. Show that this is given by

$$\Big\langle \sum_i \delta(t - t_i) \Big\rangle = \big\langle \Theta(v)\, v\, \delta(x - 0^+) \big\rangle \quad .$$

The analogous dynamical average is

$$\langle \gamma \rangle_t = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt \sum_i \delta(t - t_i) \quad ,$$

where $\{t_i\}$ is the set of times at which the ball hits the floor.

(d) How do your results change if you do not enforce the dynamical constraint $X \geq x$?

(e) Write a computer program to simulate this system. The only input should be the mass ratio r (set $\bar{E} = 10$ to fix the energy). You also may wish to input the initial conditions, or perhaps to choose the initial conditions randomly (all satisfying energy conservation, of course!). Have your program compute the microcanonical as well as dynamical averages in parts (b) and (c). Plot out the Poincaré section of P *vs.* X for those times when the ball hits the floor. Investigate this for several values of r. Just to show you that this is interesting, I've plotted some of my own numerical results in fig. 3.14.

Solution:

(a) Once we choose a length scale L (arbitrary), we may define $E_0 = M\,gL$, $P_0 = M\sqrt{gL}$, $V_0 = \sqrt{gL}$, and $\tau_0 = \sqrt{L/g}$ as energy, momentum, velocity, and time scales, respectively, the result follows directly. Rather than write $\bar{P} = P/P_0$ *etc.*, we will drop the bar notation and write

$$H = \tfrac{1}{2}P^2 + X + \frac{p^2}{2r} + rx \quad .$$

(b) What is missing from the Hamiltonian of course is the interaction potential between the ball and the piston head. We assume that both objects are impenetrable, so the potential energy is infinite when the two overlap. We further assume that the ball is a point particle (otherwise reset ground level to minus the diameter of the ball). We can eliminate the interaction potential from H if we enforce that each time $X = x$ the ball and the piston head undergo an elastic collision. From energy and momentum

conservation, it is easy to derive the elastic collision formulae

$$P' = \frac{1-r}{1+r}\,P + \frac{2}{1+r}\,p$$

$$p' = \frac{2r}{1+r}\,P - \frac{1-r}{1+r}\,p \quad .$$

We can now answer the last question from part (a). When $r = 1$, we have that $P' = p$ and $p' = P$, *i.e.* the ball and piston simply exchange momenta. The problem is then equivalent to two identical particles elastically bouncing off the bottom of the piston, and moving through each other as if they were completely transparent. When the trajectories cross, however, the particles exchange identities.

Averages within the microcanonical ensemble are normally performed with respect to the phase space distribution

$$\varrho(\boldsymbol{\varphi}) = \frac{\delta\big(E - H(\boldsymbol{\varphi})\big)}{\mathsf{Tr}\;\delta\big(E - H(\boldsymbol{\varphi})\big)} \quad ,$$

where $\boldsymbol{\varphi} = (P, X, p, x)$, and

$$\mathsf{Tr}\;F(\boldsymbol{\varphi}) = \int\limits_{-\infty}^{\infty} dP \int\limits_{0}^{\infty} dX \int\limits_{-\infty}^{\infty} dp \int\limits_{0}^{\infty} dx\; F(P, X, p, x) \quad .$$

Since $X \geq x$ is a dynamical constraint, we should define an appropriately restricted microcanonical average:

$$\big\langle F(\boldsymbol{\varphi})\big\rangle_{\mu\text{ce}} \equiv \widetilde{\mathsf{Tr}}\,\Big[F(\boldsymbol{\varphi})\,\delta\big(E - H(\boldsymbol{\varphi})\big)\Big] \Big/ \widetilde{\mathsf{Tr}}\,\delta\big(E - H(\boldsymbol{\varphi})\big)$$

where

$$\widetilde{\mathsf{Tr}}\,F(\boldsymbol{\varphi}) \equiv \int\limits_{-\infty}^{\infty} dP \int\limits_{0}^{\infty} dX \int\limits_{-\infty}^{\infty} dp \int\limits_{0}^{X} dx\; F(P, X, p, x)$$

is the modified trace. Note that the integral over x has an upper limit of X rather than ∞, since the region of phase space with $x > X$ is *dynamically inaccessible*.

When computing the traces, we shall make use of the following result from the theory of Laplace transforms. The Laplace transform of a function $K(E)$ is

$$\widehat{K}(\beta) = \int\limits_{0}^{\infty} dE\; K(E)\, e^{-\beta E} \quad .$$

The inverse Laplace transform is given by

$$K(E) = \int\limits_{c-i\infty}^{c+i\infty} \frac{d\beta}{2\pi i}\;\widehat{K}(\beta)\, e^{\beta E} \quad ,$$

where the integration contour, which is a line extending from $\beta = c - i\infty$ to $\beta = c + i\infty$, lies to the right of any singularities of $\widehat{K}(\beta)$ in the complex β-plane. For this problem, all we shall need is the following:

$$K(E) = \frac{E^{t-1}}{\Gamma(t)} \quad \Longleftrightarrow \quad \widehat{K}(\beta) = \beta^{-t} \quad .$$

For a proof, see §4.2.2 of the lecture notes.

We're now ready to compute the microcanonical average of X. We have

$$\langle X \rangle = \frac{N(E)}{D(E)} \quad ,$$

where $N(E) = \widetilde{\mathsf{Tr}}\left[X\,\delta(E-H)\right]$ and $D(E) = \widetilde{\mathsf{Tr}}\,\delta(E-H)$. Let's first compute $D(E)$. To do this, we compute the Laplace transform $\widehat{D}(\beta)$:

$$\begin{aligned}
\widehat{D}(\beta) &= \widetilde{\mathsf{Tr}}\, e^{-\beta H} \\
&= \int\limits_{-\infty}^{\infty} dP\, e^{-\beta P^2/2} \int\limits_{-\infty}^{\infty} dp\, e^{-\beta p^2/2r} \int\limits_{0}^{\infty} dX\, e^{-\beta X} \int\limits_{0}^{X} dx\, e^{-\beta r x} \\
&= \frac{2\pi\sqrt{r}}{\beta} \int\limits_{0}^{\infty} dX\, e^{-\beta X} \left(\frac{1 - e^{-\beta r X}}{\beta r} \right) = \frac{\sqrt{r}}{1+r} \cdot \frac{2\pi}{\beta^3} \quad .
\end{aligned}$$

Similarly for $\widehat{N}(\beta)$ we have

$$\begin{aligned}
\widehat{N}(\beta) &= \widetilde{\mathsf{Tr}}\, X\, e^{-\beta H} \\
&= \int\limits_{-\infty}^{\infty} dP\, e^{-\beta P^2/2} \int\limits_{-\infty}^{\infty} dp\, e^{-\beta p^2/2r} \int\limits_{0}^{\infty} dX\, X\, e^{-\beta X} \int\limits_{0}^{X} dx\, e^{-\beta r x} \\
&= \frac{2\pi\sqrt{r}}{\beta} \int\limits_{0}^{\infty} dX\, X\, e^{-\beta X} \left(\frac{1 - e^{-\beta r X}}{\beta r} \right) = \frac{(2+r)\, r^{3/2}}{(1+r)^2} \cdot \frac{2\pi}{\beta^4} \quad .
\end{aligned}$$

Taking the inverse Laplace transform, we then have

$$D(E) = \frac{\sqrt{r}}{1+r} \cdot \pi E^2 \qquad , \qquad N(E) = \frac{(2+r)\,\sqrt{r}}{(1+r)^2} \cdot \tfrac{1}{3}\pi E^3 \quad .$$

We then have

$$\langle X \rangle = \frac{N(E)}{D(E)} = \left(\frac{2+r}{1+r} \right) \cdot \tfrac{1}{3} E \quad .$$

The 'brute force' evaluation of the integrals isn't so bad either. We have

$$D(E) = \int\limits_{-\infty}^{\infty} dP \int\limits_{0}^{\infty} dX \int\limits_{-\infty}^{\infty} dp \int\limits_{0}^{X} dx\, \delta\big(\tfrac{1}{2}P^2 + \tfrac{1}{2r}p^2 + X + rx - E\big) \quad .$$

To evaluate, define $P = \sqrt{2}\,u_x$ and $p = \sqrt{2r}\,u_y$. Then we have $dP\,dp = 2\sqrt{r}\,du_x\,du_y$ and $\frac{1}{2}P^2 + \frac{1}{2r}\,p^2 = u_x^2 + u_y^2$. Now convert to 2D polar coordinates with $w \equiv u_x^2 + u_y^2$. Thus,

$$\begin{aligned} D(E) &= 2\pi\sqrt{r}\int_0^\infty dw \int_0^\infty dX \int_0^X dx\;\delta\big(w + X + rx - E\big) \\ &= \frac{2\pi}{\sqrt{r}}\int_0^\infty dw \int_0^\infty dX \int_0^X dx\;\;\Theta(E - w - X)\,\Theta(X + rX - E + w) \\ &= \frac{2\pi}{\sqrt{r}}\int_0^E dw \int_{\frac{E-w}{1+r}}^{E-w} dX = \frac{2\pi\sqrt{r}}{1+r}\int_0^E dq\;q = \frac{\sqrt{r}}{1+r}\cdot\pi E^2 \quad , \end{aligned}$$

with $q = E - w$. Similarly,

$$\begin{aligned} N(E) &= 2\pi\sqrt{r}\int_0^\infty dw \int_0^\infty dX\;X \int_0^X dx\;\delta\big(w + X + rx - E\big) \\ &= \frac{2\pi}{\sqrt{r}}\int_0^\infty dw \int_0^\infty dX\;X \int_0^X dx\;\;\Theta(E - w - X)\,\Theta(X + rX - E + w) \\ &= \frac{2\pi}{\sqrt{r}}\int_0^E dw \int_{\frac{E-w}{1+r}}^{E-w} dX\;X = \frac{2\pi}{\sqrt{r}}\int_0^E dq\left(1 - \frac{1}{(1+r)^2}\right)\cdot\tfrac{1}{2}q^2 = \left(\frac{2+r}{1+r}\right)\cdot\frac{\sqrt{r}}{1+r}\cdot\tfrac{1}{3}\pi E^3 \quad . \end{aligned}$$

(c) Using the general result

$$\delta\big(F(x) - A\big) = \sum_i \frac{\delta(x - x_i)}{\big|F'(x_i)\big|} \quad ,$$

where $F(x_i) = A$, we recover the desired expression. We should be careful not to double count, so to avoid this difficulty we can evaluate $\delta(t - t_i^+)$, where $t_i^+ = t_i + 0^+$ is infinitesimally later than t_i. The point here is that when $t = t_i^+$ we have $p = r\,v > 0$ (*i.e.* just after hitting the bottom). Similarly, at times $t = t_i^-$ we have $p < 0$ (*i.e.* just prior to hitting the bottom). Note $v = p/r$. Again we write $\gamma(E) = N(E)/D(E)$, this time with

$$N(E) = \widetilde{\mathsf{Tr}}\left[\Theta(p)\,r^{-1}p\,\delta(x - 0^+)\,\delta(E - H)\right] \quad .$$

The Laplace transform is

$$\begin{aligned} \widehat{N}(\beta) &= \int_{-\infty}^\infty dP\,e^{-\beta P^2/2}\int_0^\infty dp\;r^{-1}\,p\,e^{-\beta p^2/2r}\int_0^\infty dX\,e^{-\beta X} \\ &= \sqrt{\frac{2\pi}{\beta}}\cdot\frac{1}{\beta}\cdot\frac{1}{\beta} = \sqrt{2\pi}\,\beta^{-5/2} \quad . \end{aligned}$$

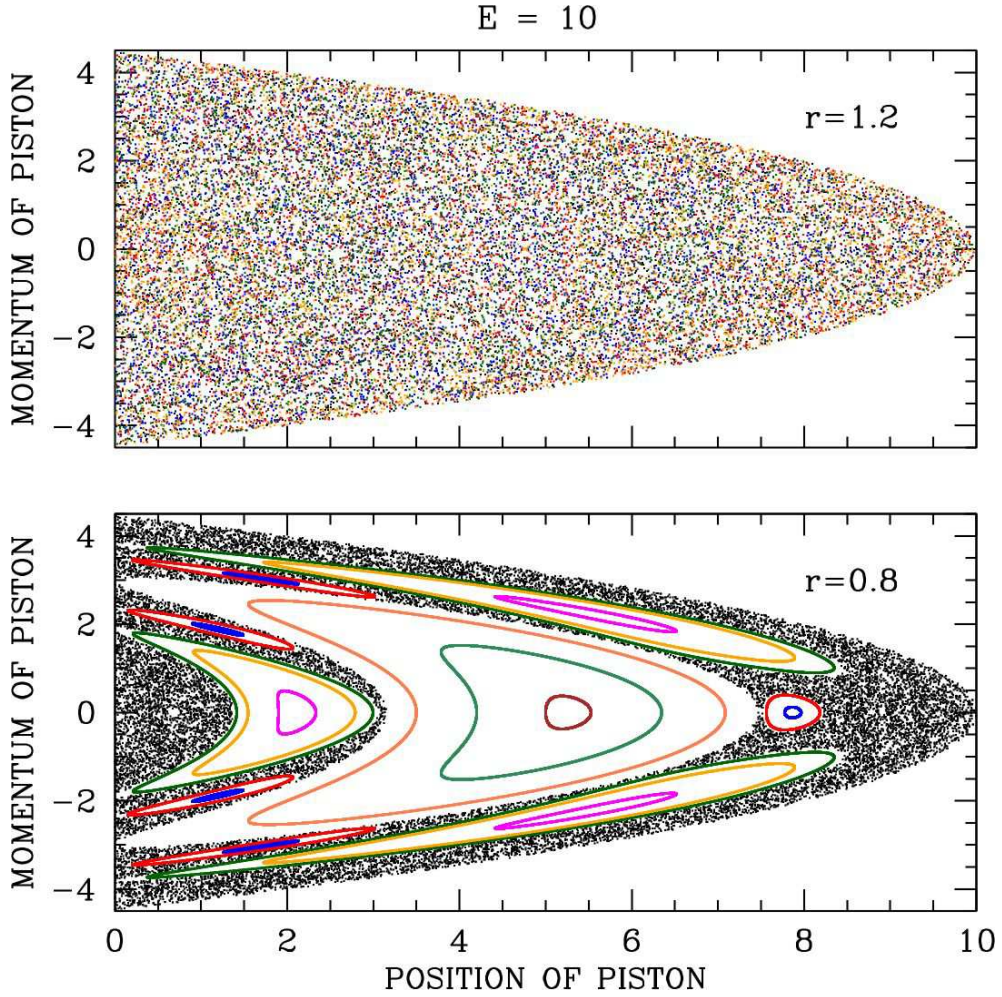


Figure 3.14: Poincaré sections for the ball and piston head problem. Each color corresponds to a different initial condition. When the mass ratio $r = m/M$ exceeds unity, the system apparently becomes ergodic.

Thus, $N(E) = \frac{4\sqrt{2}}{3}\,E^{3/2}$ and

$$\langle\gamma\rangle = \frac{N(E)}{D(E)} = \frac{4\sqrt{2}}{3\pi}\left(\frac{1+r}{\sqrt{r}}\right)E^{-1/2} \quad .$$

(d) When the constraint $X \geq x$ is removed, we integrate over all phase space. We then have

$$\begin{aligned}\widehat{D}(\beta) &= \mathsf{Tr}\; e^{-\beta H} \\ &= \int\limits_{-\infty}^{\infty} dP\, e^{-\beta P^2/2} \int\limits_{-\infty}^{\infty} dp\, e^{-\beta p^2/2r} \int\limits_{0}^{\infty} dX\, e^{-\beta X} \int\limits_{0}^{\infty} dx\, e^{-\beta r x} = \frac{2\pi\sqrt{r}}{\beta^3} \quad .\end{aligned}$$

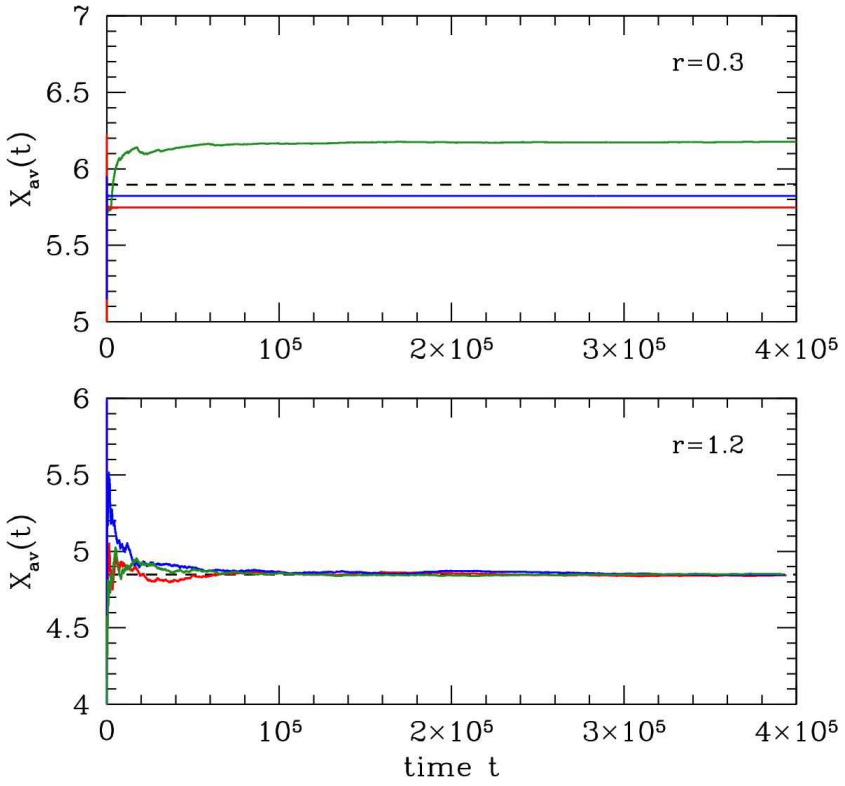


Figure 3.15: Long time running numerical averages $X_{\rm av}(t) \equiv t^{-1}\int_0^t dt' X(t')$ for $r = 0.3$ (top) and $r = 1.2$ (bottom), each for three different initial conditions, with $E = 10$ in all cases. Note how in the $r = 0.3$ case the long time average is dependent on the initial condition, while the $r = 1.2$ case is ergodic and hence independent of initial conditions. The dashed black line shows the restricted microcanonical average, $\langle X\rangle_{\mu\rm ce} = \frac{(2+r)}{(1+r)}\cdot\frac{1}{3}E$.

r	$X(0)$	$\langle X(t)\rangle$	$\langle X\rangle_{\mu\rm ce}$	$\langle\gamma(t)\rangle$	$\langle\gamma\rangle_{\mu\rm ce}$	r	$X(0)$	$\langle X(t)\rangle$	$\langle X\rangle_{\mu\rm ce}$	$\langle\gamma(t)\rangle$	$\langle\gamma\rangle_{\mu\rm ce}$
0.3	0.1	6.1743	5.8974	0.5283	0.4505	1.2	0.1	4.8509	4.8545	0.3816	0.3812
0.3	1.0	5.7303	5.8974	0.4170	0.4505	1.2	1.0	4.8479	4.8545	0.3811	0.3812
0.3	3.0	5.7876	5.8974	0.4217	0.4505	1.2	3.0	4.8493	4.8545	0.3813	0.3812
0.3	5.0	5.8231	5.8974	0.4228	0.4505	1.2	5.0	4.8482	4.8545	0.3813	0.3812
0.3	7.0	5.8227	5.8974	0.4228	0.4505	1.2	7.0	4.8472	4.8545	0.3808	0.3812
0.3	9.0	5.8016	5.8974	0.4234	0.4505	1.2	9.0	4.8466	4.8545	0.3808	0.3812
0.3	9.9	6.1539	5.8974	0.5249	0.4505	1.2	9.9	4.8444	4.8545	0.3807	0.3812

Table 3.2: Comparison of time averages and microcanonical ensemble averages for $r = 0.3$ and $r = 1.2$. Initial conditions are $P(0) = x(0) = 0$, with $X(0)$ given in the table and $E = 10$. Averages were performed over a period extending for $N_{\rm b} = 10^7$ bounces.

For part (b) we would then have

$$\widehat{N}(\beta) = \mathrm{Tr}\ X\, e^{-\beta H} = \int_{-\infty}^{\infty} dP\, e^{-\beta P^2/2} \int_{-\infty}^{\infty} dp\, e^{-\beta p^2/2r} \int_0^{\infty} dX\, X\, e^{-\beta X} \int_0^{\infty} dx\, e^{-\beta r x} = \frac{2\pi\sqrt{r}}{\beta^4} \quad .$$

The respective inverse Laplace transforms are $D(E) = \pi\sqrt{r}\,E^2$ and $N(E) = \frac{1}{3}\pi\sqrt{r}\,E^3$. The microcanonical average of X would then be $\langle X\rangle = \frac{1}{3}E$. Using the restricted phase space, we obtained a value which is greater than this by a factor of $(2+r)/(1+r)$. That the restricted average gives a larger value makes good sense, since X is not allowed to descend below x in that case. For part (c), we would obtain the same result for $N(E)$ since $x = 0$ in the average. We would then obtain

$$\langle\gamma\rangle = \tfrac{4\sqrt{2}}{3\pi}\, r^{-1/2}\, E^{-1/2} \quad .$$

The restricted microcanonical average yields a rate which is larger by a factor $1 + r$. Again, it makes good sense that the restricted average should yield a higher rate, since the ball is not allowed to attain a height greater than the instantaneous value of X.

(e) It is straightforward to simulate the dynamics. So long as $0 < x(t) < X(t)$, we have

$$\dot{X} = P \quad , \quad \dot{P} = -1 \quad , \quad \dot{x} = \frac{p}{r} \quad , \quad \dot{p} = -r \quad .$$

Starting at an arbitrary time t_0, these equations are integrated to yield

$$\begin{aligned} X(t) &= X(t_0) + P(t_0)\,(t-t_0) - \tfrac{1}{2}(t-t_0)^2 \\ P(t) &= P(t_0) - (t-t_0) \\ x(t) &= x(t_0) + \frac{p(t_0)}{r}\,(t-t_0) - \tfrac{1}{2}(t-t_0)^2 \\ p(t) &= p(t_0) - r(t-t_0) \quad . \end{aligned}$$

We must stop the evolution when one of two things happens. The first possibility is a bounce at $t = t_{\rm b}$, meaning $x(t_{\rm b}) = 0$. The momentum $p(t)$ changes discontinuously at the bounce, with $p(t_{\rm b}^+) = -p(t_{\rm b}^-)$, and where $p(t_{\rm b}^-) < 0$ necessarily. The second possibility is a collision at $t = t_{\rm c}$, meaning $X(t_{\rm c}) = x(t_{\rm c})$. Integrating across the collision, we must conserve both energy and momentum. This means

$$P(t_{\rm c}^+) = \frac{1-r}{1+r}\,P(t_{\rm c}^-) + \frac{2}{1+r}\,p(t_{\rm c}^-)$$

$$p(t_{\rm c}^+) = \frac{2r}{1+r}\,P(t_{\rm c}^-) - \frac{1-r}{1+r}\,p(t_{\rm c}^-) \quad .$$

In the following tables I report on the results of numerical simulations, comparing dynamical averages with (restricted) phase space averages within the microcanonical ensemble. For $r = 0.3$ the microcanonical averages poorly approximate the dynamical averages, and the dynamical averages are dependent on the initial conditions, indicating that the system is not ergodic. For $r = 1.2$, the agreement between

r	$X(0)$	$N_{\rm b}$	$\langle X(t)\rangle$	$\langle X\rangle_{\mu{\rm ce}}$	$\langle\gamma(t)\rangle$	$\langle\gamma\rangle_{\mu{\rm ce}}$
1.2	7.0	10^4	4.8054892	4.8484848	0.37560388	0.38118510
1.2	7.0	10^5	4.8436969	4.8484848	0.38120356	0.38118510
1.2	7.0	10^6	4.8479414	4.8484848	0.38122778	0.38118510
1.2	7.0	10^7	4.8471686	4.8484848	0.38083749	0.38118510
1.2	7.0	10^8	4.8485825	4.8484848	0.38116282	0.38118510
1.2	7.0	10^9	4.8486682	4.8484848	0.38120259	0.38118510
1.2	1.0	10^9	4.8485381	4.8484848	0.38118069	0.38118510
1.2	9.9	10^9	4.8484886	4.8484848	0.38116295	0.38118510

Table 3.3: Comparison of time averages and microcanonical ensemble averages for $r = 1.2$, with $N_{\rm b}$ ranging from 10^4 to 10^9.

dynamical and microcanonical averages generally improves with averaging time. Indeed, it has been shown by N. I. Chernov, *Physica D* **53**, 233 (1991), building on the work of M. P. Wojtkowski, *Comm. Math. Phys.* **126**, 507 (1990) that this system is ergodic for $r > 1$. Wojtkowski also showed that this system is equivalent to the *wedge billiard*, in which a single point particle of mass m bounces inside a two-dimensional wedge-shaped region $\big\{(\mathsf{x},\mathsf{y})\,\big|\,\mathsf{x}\ge 0\,,\ \mathsf{y}\ge \mathsf{x}\,\mathrm{ctn}\,\phi\big\}$ for some fixed angle $\phi = \tan^{-1}\sqrt{\frac{m}{M}}$. To see this, pass to relative ($\mathcal{X}$) and center-of-mass ($\mathcal{Y}$) coordinates,

$$\mathcal{X} = X - x \qquad\qquad \mathcal{P}_x = \frac{mP - Mp}{M+m}$$
$$\mathcal{Y} = \frac{MX + mx}{M+m} \qquad\qquad \mathcal{P}_y = P + p \quad .$$

Then

$$H = \frac{(M+m)\,\mathcal{P}_x^2}{2Mm} + \frac{\mathcal{P}_y^2}{2(M+m)} + (M+m)\,g\mathcal{Y} \quad .$$

There are two constraints. One requires $X \ge x$, *i.e.* $\mathcal{X} \ge 0$. The second requires $x > 0$, *i.e.*

$$x = \mathcal{Y} - \frac{M}{M+m}\,\mathcal{X} \ge 0 \quad .$$

Now define $\mathsf{x} \equiv \mathcal{X}$, $\mathsf{p}_x \equiv \mathcal{P}_x$, and rescale $\mathsf{y} \equiv \frac{M+m}{\sqrt{Mm}}\,\mathcal{Y}$ and $\mathsf{p}_y \equiv \frac{\sqrt{Mm}}{M+m}\,\mathcal{P}_y$ to obtain

$$H = \frac{1}{2\mu}\big(\mathsf{p}_x^2 + \mathsf{p}_y^2\big) + \mathsf{M}g\mathsf{y}$$

with $\mu = \frac{Mm}{M+m}$ the familiar reduced mass and $\mathsf{M} = \sqrt{Mm}$. The constraints are then $\mathsf{x} \ge 0$ and $\mathsf{y} \ge \sqrt{\frac{M}{m}}\,\mathsf{x}$.