3.6: Appendices

Appendix I: Formal Solution of the Master Equation

Recall the master equation $\dot{P}_i = -\Gamma_{ij}\,P_j$. The matrix Γ_{ij} is real but not necessarily symmetric. For such a matrix, the left eigenvectors ϕ_i^α and the right eigenvectors ψ_j^β are not the same: general different:

$$\begin{aligned}\phi_i^\alpha\,\Gamma_{ij} &= \lambda_\alpha\,\phi_j^\alpha \\ \Gamma_{ij}\,\psi_j^\beta &= \lambda_\beta\,\psi_i^\beta\ .\end{aligned}$$

Note that the eigenvalue equation for the right eigenvectors is $\Gamma\psi = \lambda\psi$ while that for the left eigenvectors is $\Gamma^t\phi = \lambda\phi$. The characteristic polynomial is the same in both cases:

$$F(\lambda) \equiv det\,(\lambda - \Gamma) = det\,(\lambda - \Gamma^t)\ , \tag{3.6.1}$$

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 ϕ^α on the right by ψ_j^β and summing over j, and multiplying the eigenvector equation for ψ^β on the left by ϕ_i^α and summing over i, and subtracting the two results yields

$$\big(\lambda_\alpha - \lambda_\beta\big)\,\big\langle\,\phi^\alpha\,\big|\,\psi^\beta\,\big\rangle = 0\ , \tag{3.6.2}$$

where the inner product is

$$\big\langle\,\phi\,\big|\,\psi\,\big\rangle = \sum_i \phi_i\,\psi_i\ . \tag{3.6.3}$$

We can now demand

$$\big\langle\,\phi^\alpha\,\big|\,\psi^\beta\,\big\rangle = \delta_{\alpha\beta}\ , \tag{3.6.4}$$

in which case we can write

$$\Gamma = \sum_\alpha \lambda_\alpha\,\big|\,\psi^\alpha\,\big\rangle\big\langle\,\phi^\alpha\,\big| \qquad\Longleftrightarrow\qquad \Gamma_{ij} = \sum_\alpha \lambda_\alpha\,\psi_i^\alpha\,\phi_j^\alpha\ . \tag{3.6.5}$$

We have seen that $\vec{\phi} = (1, 1, \ldots, 1)$ is a left eigenvector 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}. Now let's expand $P_i(t)$ in the right eigenvectors of Γ, writing

$$P_i(t) = \sum_\alpha C_\alpha(t)\,\psi_i^\alpha\ . \tag{3.6.6}$$

Then

$$\begin{aligned}\frac{dP_i}{dt} &= \sum_\alpha \frac{dC_\alpha}{dt}\,\psi_i^\alpha \\ &= -\Gamma_{ij}\,P_j = -\sum_\alpha C_\alpha\,\Gamma_{ij}\,\psi_j^\alpha \\ &= -\sum_\alpha \lambda_\alpha\,C_\alpha\,\psi_i^\alpha\ .\end{aligned}$$

This allows us to write

$$\frac{dC_\alpha}{dt} = -\lambda_\alpha\,C_\alpha \qquad\Longrightarrow\qquad C_\alpha(t) = C_\alpha(0)\,e^{-\lambda_\alpha t}\ . \tag{3.6.7}$$

Hence, we can write

$$P_i(t) = \sum_\alpha C_\alpha(0)\,e^{-\lambda_\alpha t}\,\psi_i^\alpha\ . \tag{3.6.8}$$

It is now easy to see that $Re\,(\lambda_\alpha) \geq 0$ for all λ, or else the probabilities will become negative. For suppose $Re\,(\lambda_\alpha) < 0$ for some α. Then as $t \to \infty$, the sum in Equation 3.6.8 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 $\sum_i \psi_i^\alpha = 0$ since $\big|\,\psi^\alpha\,\big\rangle$ must be orthogonal to the left eigenvector $\vec{\phi}^{\alpha=0} = (1, 1, \ldots, 1)$. Therefore, at least one component of ψ_i^α (for some value of i) must have a negative real part, which means a negative probability![13] 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 $P_i(t) \to P_i^{eq}$ as $t \to \infty$, relaxing to the $\lambda = 0$ right eigenvector, with $Re\,(\lambda_\alpha) \geq 0$ for all α.

Appendix II: 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

$$W_{mn} = \begin{cases} 0 & if\ m \geq n \\ n\gamma & if\ m = n-1 \\ 0 & if\ m < n-1\ . \end{cases} \tag{3.6.9}$$

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

$$\frac{dP_n}{dt} = (n+1)\,\gamma\,P_{n+1} - n\,\gamma\,P_n\ . \tag{3.6.10}$$

The interpretation here is as follows: let $\big|\,n\,\big\rangle$ denote a state in which n atoms are excited. Then $P_n(t) = \big|\langle\,\psi(t)\,|\,n\,\rangle\big|^2$. 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

$$N(t) = \sum_{n=0}^{\infty} n\,P_n(t)\ . \tag{3.6.11}$$

Note that

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

Thus,

$$N(t) = N(0)\,e^{-\gamma t}\ . \tag{3.6.12}$$

The relaxation time is $\tau = \gamma^{-1}$, and the equilibrium distribution is

$$P_n^{eq} = \delta_{n,0}\ . \tag{3.6.13}$$

Note that this satisfies detailed balance.

We can go a bit farther here. Let us define

$$P(z,t) \equiv \sum_{n=0}^{\infty} z^n\,P_n(t)\ . \tag{3.6.14}$$

This is sometimes called a *generating function*. Then

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

Thus,

$$\frac{1}{\gamma}\frac{\partial P}{\partial t} - (1-z)\frac{\partial P}{\partial z} = 0\ . \tag{3.6.15}$$

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

$$P(z,t) = f\big(\gamma t - \ln(1-z)\big)\ . \tag{3.6.16}$$

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

$$P(z,t) = P\big(1 + (z-1)\, e^{-\gamma t}\ ,\ 0\big)\ . \tag{3.6.17}$$

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

$$N(t) = \sum_{n=0}^{\infty} n\, P_n(t) = \frac{\partial P}{\partial z}\Big|_{z=1} = \ e^{-\gamma t}\, P(1,0) = N(0)\, e^{-\gamma t}\ . \tag{3.6.18}$$

Appendix III: 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

$$H = \frac{P^2}{2M} + \frac{p^2}{2m} + MgX + mgx\ , \tag{3.6.19}$$

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

- 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

  $$\bar{H} = \frac{1}{2}\bar{P}^2 + \bar{X} + \frac{\bar{p}^2}{2r} + r\bar{x}\ , \tag{3.6.20}$$

  with $r = m/M$, and with equations of motion $d\bar{X}/dt = \partial\bar{H}/\partial\bar{P}$, (Here the bar indicates dimensionless variables: $\bar{P} = P/P_0$, $\bar{t}\ = t/\tau_0$,) What special dynamical consequences hold for $r = 1$?
- Compute the microcanonical average piston height $\langle X\rangle$. The analogous dynamical average is

  $$\langle X\rangle_t = \lim_{T\to\infty}\frac{1}{T}\int_0^T\! dt\ X(t)\ . \tag{3.6.21}$$

  When computing microcanonical averages, it is helpful to use the Laplace transform, discussed toward the end of §3.3 of the notes. (It is possible to compute the microcanonical average by more brute force methods as well.)
- Compute the microcanonical average of the rate of collisions between the ball and the floor. Show that this is given by

  $$\Big\langle \sum_i \delta(t-t_i)\Big\rangle = \big\langle \Theta(v)\, v\, \delta(x-0^+)\big\rangle\ . \tag{3.6.22}$$

  The analogous dynamical average is

  $$\langle \gamma\rangle_t = \lim_{T\to\infty}\frac{1}{T}\int_0^T\! dt\ \sum_i \delta(t-t_i)\ , \tag{3.6.23}$$

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

- How do your results change if you do not enforce the dynamical constraint $X \geq x$?
- 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 Figure 3.6.1.

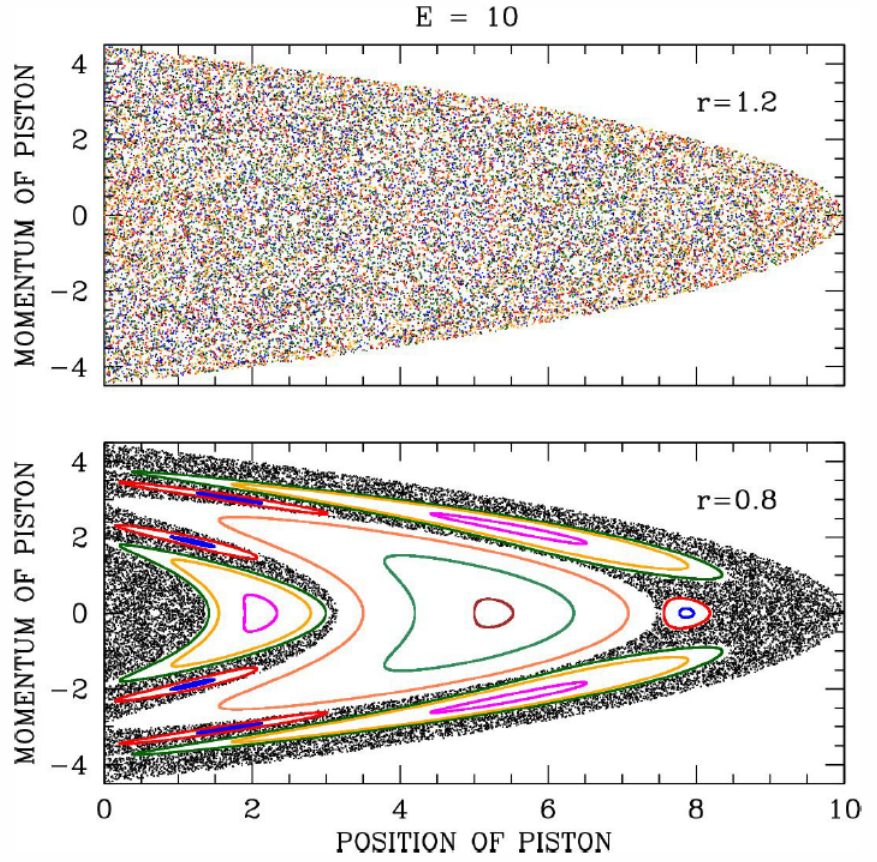

Figure 3.6.1: Poincaré sections for the ball and piston head problem. Each color corresponds to a different initial condition. When the mass ratio $r = m/M$ exceeds unity, the system apparently becomes ergodic.

r	$X(0)$	$\langle X(t)\rangle$	$\langle X\rangle_{\mu ce}$	$\langle \gamma(t)\rangle$	$\langle \gamma\rangle_{\mu ce}$	r	$X(0)$	$\langle X(t)\rangle$	$\langle X\rangle_{\mu ce}$	$\langle \gamma(t)\rangle$	$\langle \gamma\rangle_{\mu ce}$
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

r	$X(0)$	N_b	$\langle X(t)\rangle$	$\langle X\rangle_{\mu ce}$	$\langle \gamma(t)\rangle$	$\langle \gamma\rangle_{\mu ce}$
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

r	$X(0)$	N_b	$\langle X(t)\rangle$	$\langle X\rangle_{\mu ce}$	$\langle \gamma(t)\rangle$	$\langle \gamma\rangle_{\mu ce}$
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

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