

MSc. Non-equilibrium statistical mechanics

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Associate Professor Andy Martin: notes derived from those made by Professor
Andrew Melatos

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Chapter 1

Introduction

1.1 Structure and Origin of Notes

The text is based on an MSc. course originally given by Assoc. Prof. Andrew Melatos. I have added and subtracted from this course where I feel appropriate, but the basic structure remains the same. Ideally students should enter the course having done a third year statistical mechanics course, which focuses on equilibrium statistical mechanics.

In general each week we will have two or three lectures which will be complimented, every other week, by a problem solving class.

1.2 Syllabus

After a revision of equilibrium statistical physics the course is divided into two parts. The first part introduces three practical techniques in nonequilibrium statistical mechanics: Brownian fluctuations, birth-death processes, and kinetic theory. You are likely to encounter these again and again in the course of your research. The second part introduces theory of pattern formation in complex systems. This involves a practical element, namely methods for calculating the stability of nonlinear dynamical systems, as well as a taste of how statistical physics today is being applied to solve biological problems.

- Introduction/Revision
 1. Revision of equilibrium systems: ensembles, phase space density and the Liouville equation.
 2. Probability Distribution Function (PDF).
 3. Central Limit Theorem (CLT)
 4. Entropy in non-equilibrium systems
- Diffusive Processes
 1. Brownian motion, Langevin equation, fluctuation-dissipation theorem.
 2. Markov processes, Chapman-Kolmogorov equation, Fokker-Planck equation, detailed balance and Einstein-Smoluchowski equation.
 3. Boundary problems: Kramers escape problem
- Birth-Death Processes
 1. Master equations.
 2. Applications: predator-prey ecologies, chemical reactions - bistability.
- Kinetic Theory
 1. BBGKY hierarchy, Boltzmann collision integral.
 2. Transport processes, relaxation time - electrical conductivity.
 3. Vlasov equation - Landau damping.
- Stability Far From Equilibrium
 1. Stability of systems of nonlinear ODEs.
 2. Limit cycles, bifurcations, predator-prey ecologies.
- Pattern Formation
 1. Reaction-Diffusion mechanism, 1D and 2D spatial patterns, travelling wave fronts.
 2. Applications: Chemical clock, slime moulds coat patterns.

1.3 Mathematical Preliminaries

You should take the opportunity during the early weeks of the course to look back over your lecture notes from previous mathematics courses and refresh your memory on the following (very useful!) mathematical techniques. Selected references are given for each topic, together with a practice problem or two. The books referred to are J. Mathews and R. L. Walker, 1970, *Mathematical Methods of Physics*, Addison-Wesley (MW70) and D. Zwillinger, 1997, *Handbook of Differential Equations*, Academic (Z97).

- Elementary statistics, including the definitions of moments (mean, standard deviation), autocorrelation functions, probability distributions (e.g. Gaussian), and characteristic functions. (MW70; §14.4 -§14.6; Q14.5-Q14.7.)
- Fourier series and transforms, including the convolution theorem and Parsevals theorem. (MW70; §4.1, §4.2; Q4.3, Q4.4, Q4.8, Q4.9.)
- 1st order partial differential equations, especially the method of characteristics. (Z97; §98, §99.). This is useful when solving master equations.
- 2nd order partial differential equations, especially (i) the diffusion equation and its solution by the spectral method (Fourier transforms), and (ii) the Laplace equation and its solution by orthogonal polynomials. (Z97; §78; MW70; §8.2-§8.4; Q8.1-Q8.4, Q8.6-Q8.10, Q8.18-Q8.20, Q8.22-Q8.24.) This is useful when solving problems in (i) Brownian motion and (ii) pattern formation.
- Solution methods for ordinary differential equations, including by integrating factors, variation of parameters, and eigenfunction expansions. (Z97; §58, §79, §95.)

1.4 Reference Books

There is no single textbook that is suitable for this course. However, below is a set of general references:

- K. Huang, 1987, *Statistical Mechanics*, Wiley. Well written and covers thermodynamics, equilibrium classical and quantum statistical mechanics and phase transitions. Apart from some kinetic theory, it does not discuss non equilibrium systems (however, if you are starting from a base of understanding this text book you are in a good position to start this course).
- N.G. van Kampen, 1992 *Stochastic processes in Physics and Chemistry*, North Holland. Thorough discussion of fluctuations (Brownian motion) and birth and death processes (master equations).
- R. Kubo, N. Today and N. Hashitsume, 1991 *Statistical Physics II: Nonequilibrium Statistical Mechanics*, Springer. Covers similar ground to van Kampen as well as theory of non equilibrium thermodynamics: which are not covered in this course.
- G. Nicolis and I. Prigogine, 1977, *Self-organisation in non equilibrium systems*, Wiley. A classic by the inventors of the theory of pattern formation.
- H.S. Wio, 1994, *An introduction to Stochastic Processes and Nonequilibrium Statistical Physics*, World Scientific. This book is followed closely in parts, especially on stability and pattern formation.

1.5 Assessment

1.5.1 Assignments

You will have four assignments, each worth 10%: giving a total of a 40% contribution to your final mark.

The assignments will be handed out during the course, with \geq two weeks to complete.

1.5.2 Exam

Open Book exam. The exam will be 4 hours and will contribute 60% to the final assessment.

1.6 Contact Details

You can come and see me anytime, but would prefer 2-3 Wednesday (office 613, email: martinam@unimelb.edu.au).

Chapter 2

Equilibrium statistical mechanics

2.1 References

- Most of the material associated with this Chapter can be found on the LMS under *Lecture resources*: Third Year: Equilibrium Lecture Notes.

2.2 Death of the Laplacian dream

The overwhelmingly difficult task of statistical mechanics is to describe the behaviour of N particles economically, when N is large and the particles are mutually interacting. Usually we think in terms of 1 mol of atoms or molecules ($N = 6 \times 10^{23}$). But cooperative behaviour can set in for smallish N too. For example, sand in shallow water develops patterned ripples (stringers) at a threshold surface density as low as $n = 10^5 \text{ cm}^{-2}$. And a capitalist economy like Australia develops highly complex patterns of activity with $N = 10^6$ firms (private and public) and $N = 10^7$ people.

In practice, we can never know the microscopic initial conditions of an N -body system. Furthermore, even if these initial data were known, we could never hope to integrate the N equations of motion. The computational requirements are immense, not just in speed but also in memory, because most systems of this sort are sensitively dependent on initial

conditions and therefore require a computer that represents data internally to enormous precision, lest numerical errors swamp the calculation. For this reason, the mechanistic dream of Laplace is as dead in classical physics as it is (for different reasons) in quantum physics:

Consider an intelligence which, at any instant, could have a knowledge of all forces controlling nature together with the momentary conditions of all the entities of which nature consists. If this intelligence were powerful enough to submit all this data to analysis it would be able to embrace in a single formula the movements of the largest bodies in the universe and those of the lightest atoms; for it nothing would be uncertain; the future and the past would be equally present to its eyes. (Pierre Simon Laplace, 1749-1827)

In response to this dilemma, physicists adopt a statistical description of N -body systems. Macroscopic quantities are calculated from the microscopic dynamics by averaging over huge ensembles consisting of identically prepared systems whose microscopic initial conditions are unknowable yet hugely various. The state of the system is then described probabilistically by a distribution function.

Once a system reaches equilibrium, it has had enough time to fully investigate every nook and cranny in its phase space, with the corollary that every microscopic state of the system of a given energy is equally probable. On the other hand, if a system has not yet reached equilibrium, or indeed cannot ever reach it, this is no longer true; huge chunks of the phase space may have been sampled poorly or not at all. It is the latter kind of system that is the subject of this course.

Before taking our journey into the wonderful world of non equilibrium statistical mechanics we briefly revisit equilibrium systems to place this course into context.

2.3 Equilibrium

2.3.1 Equilibrium and entropy

Thermal equilibrium

Consider two systems (A and B) separated by a wall, which can not exchange energy, volume or particles. For the total ($A + B$) system:

$$E = E_A + E_B, \quad (2.1)$$

$$S = S_A(E_A, V_A, N_A) + S_B(E_B, V_B, N_B). \quad (2.2)$$

Suppose now that the wall is changed to be thermally conducting, so that the systems can exchange energy (but the total system conserves energy). *What will the new E_A and E_B be after the system comes into equilibrium?*. Given that

$$dE = dE_A + dE_B = 0 \rightarrow dE_A = -dE_B \quad (2.3)$$

one finds that

$$dS = \left(\frac{1}{T_A} - \frac{1}{T_B} \right) dE_A. \quad (2.4)$$

Given that at equilibrium entropy is maximised ($dS = 0$) then at equilibrium $T_A = T_B$, i.e. the system is in equilibrium when the two subsystems have the same temperature.

Mechanical equilibrium

Consider two systems (A and B) separated by a wall, which can not exchange energy, volume or particles. For the total ($A + B$) system:

$$E = E_A + E_B, \quad (2.5)$$

$$V = V_A + V_B \quad (2.6)$$

$$S = S_A(E_A, V_A, N_A) + S_B(E_B, V_B, N_B). \quad (2.7)$$

Suppose now that the wall is changed to be thermally conducting and can slide, so that the systems can exchange energy (but the total system conserves energy) and volume (but the

total system conserves volume). Given that

$$dV = dV_A + dV_B = 0 \rightarrow dV_A = -dV_B \quad (2.8)$$

one finds that

$$dS = \left(\frac{1}{T_A} - \frac{1}{T_B} \right) dE_A + \left(\frac{p_A}{T_A} - \frac{p_B}{T_B} \right) dV_A. \quad (2.9)$$

Given that at equilibrium entropy is maximised ($dS = 0$) then at equilibrium $T_A = T_B$ and $p_A = p_B$, i.e. the system is in equilibrium when the two subsystems have the same temperature and pressure.

Chemical equilibrium

Consider two systems (A and B) separated by a wall, which can not exchange energy, volume or particles. For the total ($A + B$) system:

$$E = E_A + E_B, \quad (2.10)$$

$$V = V_A + V_B \quad (2.11)$$

$$N = N_A + N_B \quad (2.12)$$

$$S = S_A(E_A, V_A, N_A) + S_B(E_B, V_B, N_B). \quad (2.13)$$

Suppose now that the wall is changed to be thermally conducting, can slide and is permeable to particles, so that the systems can exchange energy (but the total system conserves energy) and volume (but the total system conserves volume) and particles (but the total system conserves particles). Given that

$$dN = dN_A + dN_B = 0 \rightarrow dN_A = -dN_B \quad (2.14)$$

one finds that

$$dS = \left(\frac{1}{T_A} - \frac{1}{T_B} \right) dE_A + \left(\frac{p_A}{T_A} - \frac{p_B}{T_B} \right) dV_A - \left(\frac{\mu_A}{T_A} - \frac{\mu_B}{T_B} \right) dN_A. \quad (2.15)$$

Given that at equilibrium entropy is maximised ($dS = 0$) then at equilibrium $T_A = T_B$, $p_A = p_B$ and $\mu_A = \mu_B$, i.e. the system is in equilibrium when the two subsystems have the same temperature, pressure and chemical potential.

2.3.2 The ergodic hypothesis

Consider a system of N particles, each with three degrees of freedom, x, y, z . The system is described, in Hamiltonian classical mechanics, by $6N$ degrees of freedom:

$$q_1, q_2, \dots, q_{3N}; p_1, p_2, \dots, p_{3N} \quad (2.16)$$

via

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \text{ and } \dot{q}_i = \frac{\partial H}{\partial p_i} \quad (2.17)$$

which gives the *trajectory* of the system in $\{q_i(t), p_i(t)\}$ in *phase space*.

In general the total energy will be conserved as the system evolves. The condition $H[q_i(t), p_i(t)] = E$ defines a $6N - 1$ dimensional surface in phase space on which the systems trajectory is confined. If one wanted to compute the measured value of some quantity, f , averaged over an interval of time τ , it is:

$$\langle f \rangle = \frac{1}{\tau} \int_{t_0}^{t_0 + \tau} dt f [q_i(t), p_i(t)]. \quad (2.18)$$

In general, for large N , we expect the trajectory to be some horribly complicated curve on the constant energy surface, that we have no way of computing directly. To compute $\langle f \rangle$ we therefore need to make an assumption. The ergodic hypothesis says: *during any time interval τ the location of the system in phase space is equally likely to be anywhere on the surface of constant energy.* Hence

$$\langle f \rangle = \int dq_i dp_i f [q_i, p_i] \rho(q_i, p_i). \quad (2.19)$$

where in the micro canonical ensemble

$$\rho(q_i, p_i) = C \delta(H[q_i, p_i] - E) \quad (2.20)$$

and C is a normalising constant.

By thermodynamics we assume that the macroscopic properties of a system are completely described by a set of a few macroscopic variables, such as E, N and V . If the ergodic hypothesis were not true, there would be parts of phase space with the same E , that never

see each other - i.e. a trajectory in one part would not enter the other and vice versa. One could imagine, therefore, that systems in these two distinct regions of phase space might have different properties and hence they might represent thermodynamically distinguishable states. But this would contradict the assumption that E alone is the important thermodynamic quantity.

Alternatively, if ergodicity fails, there might be some other important macroscopic variable (for example magnetisation) which one overlooked. The disjoint regions of the constant energy surface could correspond to different values of this new macroscopic variable.

In the ensemble theory one abandons any effort to compute thermodynamic properties from the explicitly time dependent trajectory of the system in phase space. Rather one describes the thermodynamic state as represented by a particular ensemble given the density matrix $\rho(q_i, p_i)$.

The ensemble average $\langle f \rangle$ is the value one would find not for a single isolated system moving on its trajectory, but for the average of a collection of systems distributed in phase space according to the density ρ . The ergodic hypothesis asserts that these two types of averages are equal.

$\rho(q_i, p_i)$ can be viewed as the probability density that the system will be found in phase space at $\{q_i(t), p_i(t)\}$.

Equilibrium is described by a density matrix which does not change in time. This leads to Liouville's theorem:

2.3.3 Liouville's theorem

For equilibrium we want to see what general condition ρ must satisfy in order that:

$$\frac{\partial \rho}{\partial t} = 0 \quad (2.21)$$

Consider an initial density ρ of points in phase space. As the system is represented by these initial points evolves in time, their trajectories give the density $\rho(t)$ at later times. Think of the points in ρ like particles in a fluid. The probability density ρ must obey a

local conservation equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{v}) = 0, \quad (2.22)$$

where \underline{v} is the velocity vector of the probability current $\rho \underline{v}$, that tells how the points in ρ flow in phase space. \underline{v} is the $6N$ dimensional vector:

$$(\dot{q}_1, \dot{q}_2, \dots, \dot{q}_{3N}; \dot{p}_1, \dot{p}_2, \dots, \dot{p}_{3N}). \quad (2.23)$$

The second term in the continuity equation can be written as

$$\nabla \cdot (\rho \underline{v}) = \sum_{i=1}^{3N} \left[\frac{\partial \rho}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial q_i} \right] = [\rho, H]. \quad (2.24)$$

Equilibrium requires

$$\frac{\partial \rho}{\partial t} = 0 \quad (2.25)$$

so that the ensemble averages to not change in time. Therefore

$$0 = [\rho, H]. \quad (2.26)$$

This condition is met if ρ depends on q_i and p_i only via the function $H[q_i, p_i]$, i.e. $\rho = \rho(H[q_i, p_i])$. The focus of this course is when this is **not** true, i.e. $0 \neq [\rho, H]$.

2.3.4 Using the ergodic hypothesis: An ideal gas

In the microcanonical ensemble, at energy E , an equal weight is given to all systems on the surface in phase space of constant energy: $H[q_i, p_i] = E$. To count the number of such states on the energy surface we define the density of states:

$$g(E) = \int \frac{dq_i dp_i}{h^{3N}} \delta(H[q_i, p_i] - E), \quad (2.27)$$

where h is a constant with units $q_i p_i$. h^{3N} represents the volume of phase space occupied by one state. Classically, h is totally arbitrary so our thermodynamic results should not depend on it. Quantum mechanically, h turns out to be Planck's constant. At this stage, the factor $1/h^{3N}$ is introduced so that $g(E)$ has the units of $1/J$.

We can now define the number of states in a shell of thickness Δ , about the energy surface E

$$\Omega(E, V, N) = \frac{1}{N!} \int_{E - \frac{\Delta}{2}}^{E + \frac{\Delta}{2}} dE' g(E'). \quad (2.28)$$

Δ is assumed to be $E/N < \Delta \ll E$. It can be thought of as representing the finite accuracy with which one knows E . Our thermodynamic results should not depend on Δ . Both Δ and h are introduced so that Ω is a dimensionless number that we can think of as being the number of microscopic states occupied in the microcanonical ensemble at E .

✓ **Exercise:** Show that for an ideal gas

$$g(E) = \frac{V^N}{h^{3N}} \frac{(2\pi m E)^{3N/2}}{(3N/2 - 1)!} \frac{1}{E} \quad (2.29)$$

and hence

$$\Omega(E) \approx \frac{V^N}{h^{3N} N!} \frac{(2\pi m E)^{3N/2}}{(3N/2 - 1)!} \frac{\Delta}{E}, \quad (2.30)$$

where for large N $\Omega(E)$ is a very rapidly increasing function of E .

Now consider two subsystems (A and B) separated by a wall. Let $g_A(E_A)$ be the density of states of system A , with energy E_A and let $g_B(E_B)$ be the density of states of system B , with energy E_B .

Now suppose the wall is thermally conducting so that energy can be transferred between the two systems. What will be the value of E_A be when the system comes into equilibrium? The total density of system at E_T is

$$g_T(E_T) = \int dE_A g_A(E_A) g_B(E_T - E_A), \quad (2.31)$$

hence the total number of states at E_T is

$$\Omega_T(E_T) = \int \frac{dE_A}{\Delta} \Omega_A(E_A) \Omega_B(E_T - E_A), \quad (2.32)$$

The integrand $\Omega_A(E_A) \Omega_B(E_T - E_A)$:

- $\Omega_A(E_A)$ is a rapidly increasing function of E_A .

- $\Omega_B(E_B)$ is a rapidly increasing function of E_B .
- $\Omega_A(E_T - E_A)$ is a rapidly decreasing function of E_A .
- The product $\Omega_A(E_A)\Omega_B(E_T - E_A)$ has a sharp maximum at some particular value of E_A .

Hence, given that all states with total energy E_T are equally likely. But the value of E_A that one is most likely to find as the energy of system A is the particular value that maximises $\Omega_A(E_A)\Omega_B(E_T - E_A)$. That is, there are more states with this particular value of E_A than with any other value of E_A , and since all microscopic states are equally likely, this value of E_A is most likely.

To determine E_A we use

$$\frac{\partial}{\partial E_A} [\Omega_A(E_A)\Omega_B(E_T - E_A)] = 0, \quad (2.33)$$

resulting in the following condition:

$$\frac{\partial}{\partial E_A} [\ln \Omega_A] = \frac{\partial}{\partial E_B} [\ln \Omega_B]. \quad (2.34)$$

From thermodynamics we know that the equilibrium value of E_A is determined by

$$\frac{1}{T_A} = \frac{\partial S_A}{\partial E_A} = \frac{\partial S_B}{\partial E_B} = \frac{1}{T_B}. \quad (2.35)$$

Therefore following Boltzmann we identify $S(E) = k_B \ln \Omega(E)$.

Given that we now have an expression for the number of states in an ideal gas, Eq. (2.30) it is possible to derive an expression for the entropy:

$$S \approx Nk_B \left\{ \frac{5}{2} + \ln \left[\frac{V}{h^3} \left(\frac{4\pi m E}{3N} \right)^{3/2} \right] \right\}. \quad (2.36)$$

From the entropy one can then derive pertinent thermodynamic quantities such as

$$\frac{1}{T} = \frac{\partial S}{\partial E} = \frac{3}{2} N k_B \frac{1}{E} \rightarrow E = \frac{3}{2} N k_B T \quad (2.37)$$

$$\frac{p}{T} = \frac{\partial S}{\partial V} = N k_B \frac{1}{V} \rightarrow pV = N k_B T. \quad (2.38)$$

In this section on equilibrium we have revisited some of the pillars underpinning the application of statistical mechanics to equilibrium systems and looked at some simple examples. Two pillars in particular have been pertinent: (i) At equilibrium there is a universal function (entropy) which is maximised and (ii) all points in phase space are linked and as such one can map between time averages and ensemble averages.

Unfortunately for non-equilibrium systems there is no single function such as entropy, which exhibits a certain condition (i.e. being maximised) that can be used to characterise the properties of non-equilibrium systems in a universal manner and there is no reason to suppose that in non-equilibrium systems that all points in phase space are linked. As such we need to come up with alternative avenues to investigate non-equilibrium systems. In general these approaches tend to be system specific and rely on considering the fundamental processes governing the properties of the system and casting this in a suitable mathematical framework. The aim of this course is to introduce you to some of the elegant (and sometimes not so elegant) methodologies which can be applied.

Chapter 3

Non-Equilibrium statistical mechanics: Introduction to fundamental ideas

3.1 References

- Most of the material associated with this Chapter can be found on the LMS under *Lecture resources*: Third Year: Equilibrium Lecture Notes.

3.2 Probability distribution function

3.2.1 General definition

The *probability distribution function* (pdf) of a random variable quantifies the relative probabilities attached to different outcomes, when that random variable is sampled. Suppose x is a random variable, with or without any physical significance. Then its pdf, denoted by $p(x)$, is defined such that $p(x)dx$ equals the probability that a sample of x lies in the

range $(x, x + dx)$. Normalisation guarantees

$$\int_{-\infty}^{\infty} dx p(x) = 1. \quad (3.1)$$

In practical problems, it is important to think carefully about what *a sample* means. For example, if a physical quantity $y(t)$ is varying extremely rapidly but continuously with time t , it is not a random variable, but measurements of $y(t)$ at equally spaced time intervals might well be random, with the pdf determined by the details of the experiment (e.g. time between measurements, duration of a single measurement, etc...). If x is a discrete random variable, then its pdf is a sum of delta functions weighted by the probabilities of each discrete outcome. For example, the pdf of a fair die is $p(x) = [\delta(x - 1) + \dots + \delta(x - 6)]/6$.

3.2.2 N-particle distribution function (Gibbs ensemble)

Consider a large number of systems prepared under identical macroscopic (not microscopic, of course) experimental conditions. An example is a huge (say $N!$) ensemble of jars of gas, each containing N molecules, all prepared at the same temperature and pressure. The probability of finding a system in the ensemble in a volume $d^{3N}xd^{3N}p$ around (x, p) at time t is given by

$$f_N(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N; \mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_N; t) d^3\mathbf{x}_1 \dots d^3\mathbf{x}_N d^3\mathbf{p}_1 \dots d^3\mathbf{p}_N \rightarrow f_N(x, p) d^{3N} x d^{3N} p, \quad (3.2)$$

where (x, p) is a particular arrangement of N particles. Equivalently, $f_N(x, p, t) d^{3N} x d^{3N} p$ is the fraction of jars of gas in the ensemble whose internal state at the instant t lies within a volume $d^{3N} x d^{3N} p$ around (x, p) . **The Gibbs ensemble is useful formally but not practically.**

3.2.3 Microscopic phase space density

Consider a single system of N particles, e.g. a single jar of gas then $f(\mathbf{x}, \mathbf{p}, t) d^3\mathbf{x} d^3\mathbf{p}$ is the probability of finding a particle (i.e. fraction of particles) in a volume $d^3\mathbf{x} d^3\mathbf{p}$ around (\mathbf{x}, \mathbf{p}) at time t . If we know the exact positions $\mathbf{x}_i(t)$ and momenta $\mathbf{p}_i(t)$ of the N particles

as functions of time t (impossible in practice, of course), then we can write

$$f(\mathbf{x}, \mathbf{p}, t) = \frac{1}{N} \sum_{i=1}^N \delta[\mathbf{x} - \mathbf{x}_i(t)] \delta[\mathbf{p} - \mathbf{p}_i(t)]. \quad (3.3)$$

In other words, if you *bin* the pdf sufficiently finely, you obtain either zero or one particle per bin. As you coarsen your binning, the bins fill up progressively until there are no holes and the pdf becomes continuous. The microscopic phase space density lives in a six-dimensional phase space instead of a $6N$ dimensional one. More useful! But it contains less information; f_N tells you exactly where all N particles are, and their momenta, up to the uncertainty in microscopic initial conditions, whereas f only gives the distribution of positions and momenta overall, without distinguishing between individual particles.

3.3 Equilibrium systems

- $f_N(t, x, p)$ independent of t (in practice, this also means the system is stable; if the environment nudges it, it quickly relaxes back to a steady state)
- isolated system or system in contact with a heat bath
- *simple*. No long-range, cooperative behaviour (except for phase transitions, which are themselves a non-equilibrium process), no evolution macroscopically (by definition)
- entropy S increases or remains constant with time: $dS/dt \geq 0$.
- pdfs of internal variables are Gaussian or something like Gaussian (except at phase transitions)

3.3.1 An example: a jar of gas

A classic example of an equilibrium system is a sealed jar of gas held at a constant temperature T . A schematic drawing of the system occupies the top left panel in Figure 3.1. The jar has a close-fitting but moveable lid, to which we connect a strain gauge, which measures the net force $F(t)$ on the lid as a function of time t .

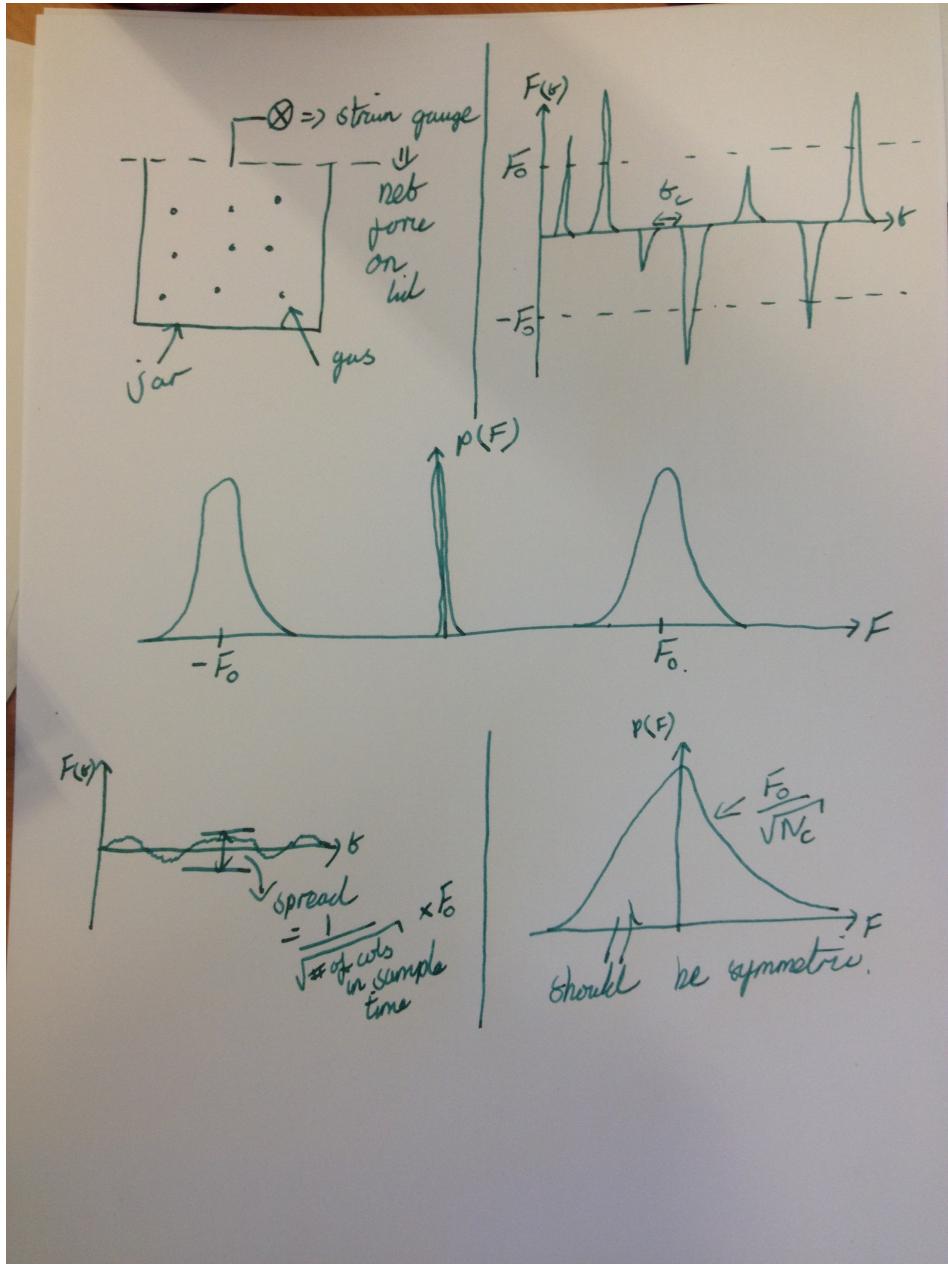


Figure 3.1. Top Left: schematic of jar with strain gauge. Top Right: for ideal (perfect) resolution the net force on the lid as a function of time. Middle: for perfect resolution the pdf of F . Bottom Left: For time broadened measurement the source as a function of time. Bottom Right: the pdf of F for broadened measurements.

Fundamentally, $F(t)$ is a continuous function of time. It evolves deterministically, not stochastically, in response to the motions of the gas molecules, which satisfy Newtons Laws. The top right panel of Figure 3.1 displays the measured $F(t)$ assuming that the strain gauge is a perfect device, offering infinite time resolution and output precision. In between molecular collisions, the lid feels no net force. During a collision, the net force spikes positively (molecule inside jar strikes lid) or negatively (molecule outside jar strikes lid). The spikes have characteristic height $F_0 = (3mk_B T)^{1/2}/t_c$, where m is the molecular mass, and t_c is the duration of a collision. But there is a fairly wide spread of heights, of order F_0 , because the underlying Maxwell-Boltzmann momentum distribution has width $\sim (3mk_B T)^{1/2}$.

In any realistic experiment, $F(t)$ is measured at discrete times t_1, t_2, \dots . Furthermore, the measurements are not instantaneous in practice; each one takes a time τ , during which the temporal average of $F(t)$ is effectively measured. Measurements F_1, F_2, \dots made in this way constitute samples of a random variable F to a good approximation. It is then reasonable to ask: what is the pdf $p(F)$ of F ?

The answer depends on how fine-grained the measurements are. If the gauge samples $F(t)$ more frequently than the time between collisions, $p(F)$ is the sum of a delta function at $F = 0$ and two broad distributions (width $\sim F_0$) peaked near $\pm F_0$, as drawn in the middle panel of Figure 3.1. The average net force $\langle F \rangle = \int dF F p(F)$ is zero, while the average force exerted by molecules inside the jar (computed from half the null samples in the delta function plus the samples in the right-hand peak) must equal the mean pressure P_0 multiplied by the lids area A_0 . At this level of fine-graining, the lid constantly jumps up and down, like a boiling pot, because the random force varies stochastically over a range whose width is comparable to the central value.

Now suppose that the gauge samples $F(t)$ less frequently than the time between collisions, and also suppose that τ is much greater than t_c . Under these conditions, a random sample of F is the temporal average of the forces from many collisions (and the quiet times between them). The central limit theorem, introduced in Section 3.6, guarantees that $p(F)$ is narrowly peaked about its average value F_0 , if the number of collisions during each sample is large. (Additionally, the delta peak at $F = 0$ goes away.) Quantitatively, if there are N_c

collisions during a time τ , the width of $p(F)$ about F_0 (i.e. the square root of the variance; see Section 3.6) is of order $\sim N^{-1/2}F_0$. This is drawn schematically in the lower right panel of Figure 3.1; the lower left panel shows the corresponding force samples. This conforms with normal experience; the lid on a gas-filled jar does not jump up and down like crazy.

In a similar way, the total internal energy E of the gas at any instant equals $\langle E \rangle = 3/2Nk_B T$ on average, but the variance of the total internal energy equals $\langle E^2 \rangle - \langle E \rangle^2 = \langle E \rangle^2/N$. Note that here N is the total number of particles (you are summing together all of them to get E , not just the ones colliding with the lid of the container).

The central limit theorem does not apply in the same way in non-equilibrium systems. There, large spreads in internal random variables like F are the norm. We discuss this key difference further in Section 3.6.

3.4 Nonequilibrium systems

- $f_N(t, x, p)$ depends on t .
- open system: exchanges mass and energy with environment.
- *complex*. Formation of macroscopic dissipative structures in space and time when huge numbers of particles cooperate over macroscopic distances. Examples include turbulent eddies in high-Reynolds-number flow, biomolecules produced in driven chemical reactions, firms created within economies, and the big one living organisms.
- Nonlinear equations of motion for the macroscopic fields, e.g. $\mathbf{v} \cdot \nabla \mathbf{v}$ in the Navier Stokes equation describing a turbulent fluid.
- Entropy can increase or decrease.

You need to be far from equilibrium to assemble something even moderately complicated. By way of illustration, an embarrassingly simple protein built from 100 amino acids can be assembled in $\sim 20^{100}$ ways, as there are 20 unique amino acids in nature. Even if thermal fluctuations induce structural changes every 10^{-12} s, it would take the protein $\sim 10^{118}$ s

(age of universe $\sim 10^{17}$ s) to explore the phase space fully and settle down to its observed structure. In contrast, far from equilibrium, huge chunks of the phase space are never explored. An essential component of far-from-equilibrium dynamics is the process of natural selection, described beautifully in J. Dawkinss book *The Blind Watchmaker*.

Far-from-equilibrium systems can be classified according to whether or not they are capable of reaching equilibrium once sufficient time has elapsed. For example, a bucket of water eventually settles to equilibrium. If it is refrigerated, it turns to ice: a phase transition which is not an equilibrium process. Once the transition is completed, the bucket of ice settles to a new equilibrium. Likewise, we expect life on earth to eventually reach a state of statistical equilibrium (assuming, unrealistically, that it is exposed to a constant solar energy flux). However, certain systems can never reach equilibrium, no matter how hard they try!

✓ **Exercise:** Show that N self-gravitating point masses can never reach equilibrium for $N > 2$ because the volume of phase space available to the system (at fixed E) is infinite. (T. Padmanabhan, *Astrophysical Journal* **344**, 848 (1989)).

3.4.1 An example: sand piles

Consider a sand pile which is built up by dropping individual grains of sand onto a table. Over time a pile of grains will grow and as additional grains fall onto the pile one of two things can happen: either the number of grains on the table will go from N to $N+1$ or some grains can fall off (through an avalanche process), such that N goes to $N + 1 - S$, where S is the number of grains of sand which fall off. An attempt to schematically elucidate this system is shown in Fig. 3.2 (left). The question we want to consider is what is $N(t)$ (the number of grains for sand in the pile as a function of time) or $S(t)$ (the number of grains of sand which fall of the table as function of time) and what is $p(N)$ (the probability of finding N particles on the table) or $p(S)$ (the probability of S grains falling of the table).

In general what happens is that after a pile has built up the addition of an extra grain can result in avalanches. The outcome of an avalanche (reorganisation of the sand

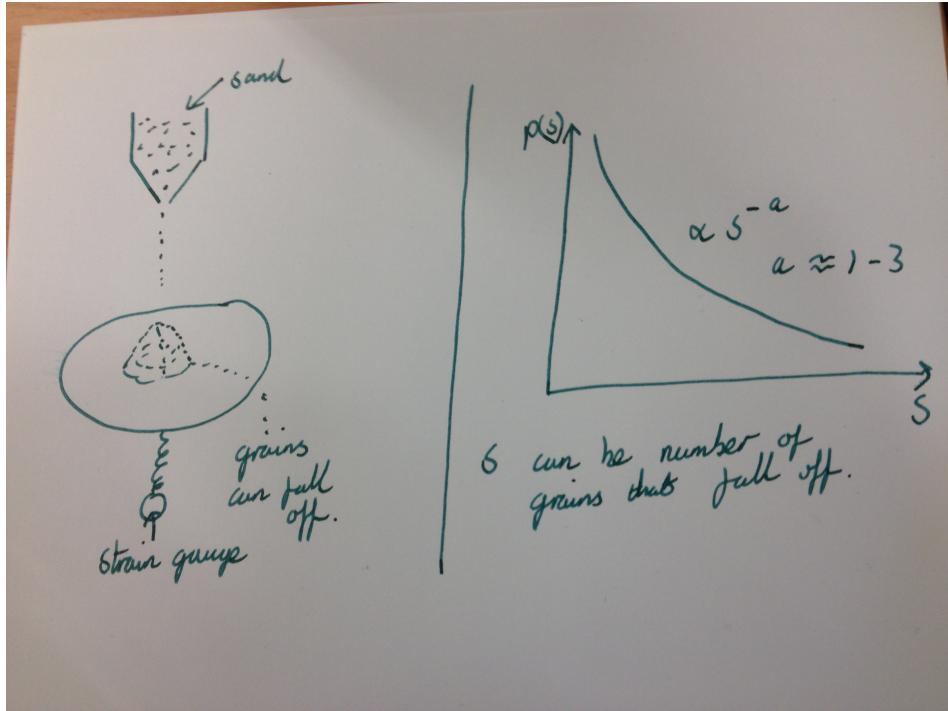


Figure 3.2. Left: Schematic of sandpile *experiment*. Right: Sketch of the pdf $p(S)$, i.e. the pdf for the number of grains falling off the table.

pile) is that 0 or 1 or 2 etc grains will fall off the table. In general bigger avalanches are rarer than small ones. This is a self organising critical system: the pile builds up to a critical slope then fluctuates around that. A sketch of typical results are shown in Fig. 3.2 (right) for the probability of a certain number of grains of sand falling off the pile ($p(S)$). It is a power law, i.e. scale free: stretch S by k and the statistics don't change ($p(kS)/p(S) = (kS)^{-a}/S^{-a} = k^{-a}$).

How this is solved is via an autonoma numerical code (you can find a copy of the code on the LMS), also see Wiesenfeld *et al.*, Journal of Statistical Physics **54**, 1441 (1989). In general the code is constructed in the following manner:

- Define the number of sites on which the sand can fall.
- Define the critical local gradient to trigger local falling.
- Define the total number of grains of sand which will be dropped.
- Choose a random site on which to drop a grain of sand.

- Check that local gradient is below the critical gradient. If so drop another grain of sand.
- If local gradient above critical value then allow grain to fall choose random number of grains to tumble: note that the maximum number that can tumble is between zero and the magnitude of the number of particles on the site you are interested in minus the number of particles on the site they are tumbling to. Then check local gradients of other sites in vicinity and repeat until avalanche has finished. Note should check how many grains have fallen off the table. Then drop another grain of sand.
- From this can build up a pdf for the number of grains which have fallen off the sandpile.

3.5 Global properties of distributions

3.5.1 Moments

There are many ways to represent the information contained in a probability distribution function $p(x)$. Perhaps the most common are the moments of $p(x)$. The n^{th} moment m_n is defined as the average of x^n , i.e.

$$m_n = \langle x^n \rangle = \int_{-\infty}^{\infty} dx x^n p(x). \quad (3.4)$$

The zeroth moment always equals unity for a properly normalised pdf. For a simple, singly peaked pdf, the mean m_1 tells us reliably about the central tendency, and the variance $\sigma^2 = m_2 - m_1^2$ is a measure of the spread around the central tendency. One can generate the moments from the characteristic function, which is simply the Fourier transform of the pdf,

$$\phi(k) = \int_{-\infty}^{\infty} dx \exp(-ikx) p(x). \quad (3.5)$$

The characteristic function can equally be regarded as the average $\langle \exp(-ikx) \rangle$. By differentiating under the integral sign with respect to k , one finds the generating relation

$$m_n = \langle x^n \rangle = i^n \frac{d^n \phi(k)}{dk^n} \Big|_{k=0} \quad (3.6)$$

Likewise, by expanding $\exp(-ikx)$ as a Taylor series about $k = 0$, one can reconstruct the characteristic function as

$$p(k) = \sum_{n=0}^{\infty} \frac{(-ik)^n m_n}{n!}, \quad (3.7)$$

where normalisation always ensures $p(k = 0) = 1$.

The above results suggest that a pdf can always be reconstructed from its moments, simply by computing $p(k)$ and inverting the Fourier transform. Although this procedure does work sometimes in practice, at least to a fair approximation, it should be undertaken with caution for two reasons. First, two different pdfs can have exactly the same moments. (Can you come up with an example?). This is a general problem with Taylor expansions (remember the Taylor series of $\exp(-1/x^2)$). Second, when reconstructing a pdf from empirical data, it is always better to bin the data directly (or make a cumulative distribution if you do not have many data points) rather than compute a string of moments, because high-order moments are notoriously unreliable without a huge time series at ones disposal. This is because of the statistics of rare events in the tails of distributions, which we discuss below.

3.5.2 Cumulants

A variant of the moments are the *cumulants* of a pdf, which are generated by differentiating the logarithm of the characteristic function. The n^{th} cumulant is defined as

$$c_n = i^n \left. \frac{d^n \ln p(k)}{dk^n} \right|_{k=0} \quad (3.8)$$

The characteristic function can then be reconstructed according to

$$\ln p(k) = \sum_{n=0}^{\infty} \frac{(-ik)^n c_n}{n!}. \quad (3.9)$$

✓ **Exercise:** Prove that, if $c_3 = c_4 = \dots = 0$, then $p(x)$ is a gaussian with mean c_1 and variance c_2 , i.e.

$$p(x) = \frac{1}{\sqrt{2\pi c_2}} \exp \left[-(x - c_1)^2 / 2c_2 \right]. \quad (3.10)$$

3.5.3 Rare events

The most interesting outcomes of a stochastic process are often the rarest, yet they are often poorly understood. Rare outcomes can have an outsized impact on the host system; think of the implosion of the credit derivatives bubble in financial markets in 2008 and 2009 as an example. Their statistics are often misjudged because empirical data are skimpy or non-existent, precisely because the events are rare, and because the underlying pdf is usually not a simple extension of the observed pdf of frequent events. In the credit bubble, for example, market participants assumed that extreme losses obey Gaussian statistics, just like moderate losses. Under this assumption, creditors felt confident that events like those that actually transpired would occur once in a million years! This very assumption introduced correlations into the system and fattened the tails of the pdf of loss events into a power law, making a once-in-a-million-year crash a near certainty to occur once every ten years. (This story is told informatively and entertainingly by journalist Gillian Tett in *Fools Gold*.) We look at the all-important difference between Gaussian and power-law statistics in the next section below.

Given a known underlying pdf $p(x)$, which decreases monotonically at large x , so that large- x events are rare, it is reasonable to ask what the distribution of rare events actually is. Suppose we make N draws x_1, \dots, x_N from $p(x)$ and let x_{\max} denote the maximum of these N values. Loosely speaking, as there is only one maximum and N values, we expect the probability of drawing x_{\max} to be of order $1/N$. For large N , this probability is small. Note that the probability that there will be some maximum is obviously unity; but the probability that it has the particular value $(x_{\max}, x_{\max} + dx_{\max})$ is of order $1/N$.

What is the pdf of x_{\max} ? Clearly, it depends on N as well as $p(x)$. Let $P(y)$ be the cumulative probability that x_{\max} is less than y . This equals the probability that all the N draws produce values less than y . By the elementary product rule of probabilities, we have

$$P(y) = \left[\int_{-\infty}^y dx p(x) \right]^N = \exp \left\{ N \ln \left[1 - \int_y^{\infty} dx p(x) \right] \right\}. \quad (3.11)$$

Assuming that large- x events are rare, the integral in square brackets in Eq. (3.11) is small,

and to leading order ($\ln[1 - x] \approx -x - x^2/2\dots$) we can write

$$P(y) \approx \exp \left[-N \int_y^\infty dx p(x) \right]. \quad (3.12)$$

This confirms that the probability of the median rare event is of order $1/N$, as common sense suggests; more precisely, the median rare event $y_{1/2}$ has probability

$$\int_{y_{1/2}}^\infty dx p(x) = \frac{\ln 2}{N}. \quad (3.13)$$

To get the pdf of x_{\max} , one simply differentiates the cumulative probability distribution according to $p(x_{\max}) = dP(y)/dy|_{x_{\max}}$.

- ✓ **Exercise:** Show, numerically, that Figure 3.3 is a representative sketch of the cumulative distribution of rare events drawn from a Gaussian (top curve) and power-law (bottom curve) distributions, generated from the exact result: Eq. (3.11).

How does the size of the median rare event scale with N ? As an example, let us consider the exponential distribution $p(x) = a^{-1} \exp(-x/a)$. Substituting into Eq. (3.13), we obtain $y_{1/2} \approx a \ln N$ for large N .

- ✓ **Exercise:** In a similar way, show that one has $y_{1/2} \propto (\ln N)^{1/2}$ for a Gaussian and $y_{1/2} \propto N^{1/\mu}$ for a power law $p(x) \propto x^{-\mu}$.

The results of the above exercise show that systems with power-law pdfs exhibit huge fluctuations about the central tendency, unlike systems with exponential tails pdfs. For example, the following two random variables have the same mean (zero) and variance (a^2), with pdfs

$$p(x) = \frac{1}{\sqrt{2\pi a^2}} \exp \left[-x^2/2a^2 \right]. \quad (3.14)$$

and

$$p(x) = \begin{cases} \frac{\mu-1}{2a} \left(\frac{\mu-3}{\mu-1} \right)^{(\mu-1)/2} \left(\frac{|x|}{a} \right)^{-\mu} & \text{for } |x| > a\sqrt{\left(\frac{\mu-3}{\mu-1} \right)} \\ 0 & \text{for } |x| \leq a\sqrt{\left(\frac{\mu-3}{\mu-1} \right)} \end{cases} \quad (3.15)$$

respectively (note: need $\mu > 3$ to ensure the variance exists). But their respective median rare events are very different, as shown in Fig. 3.3.

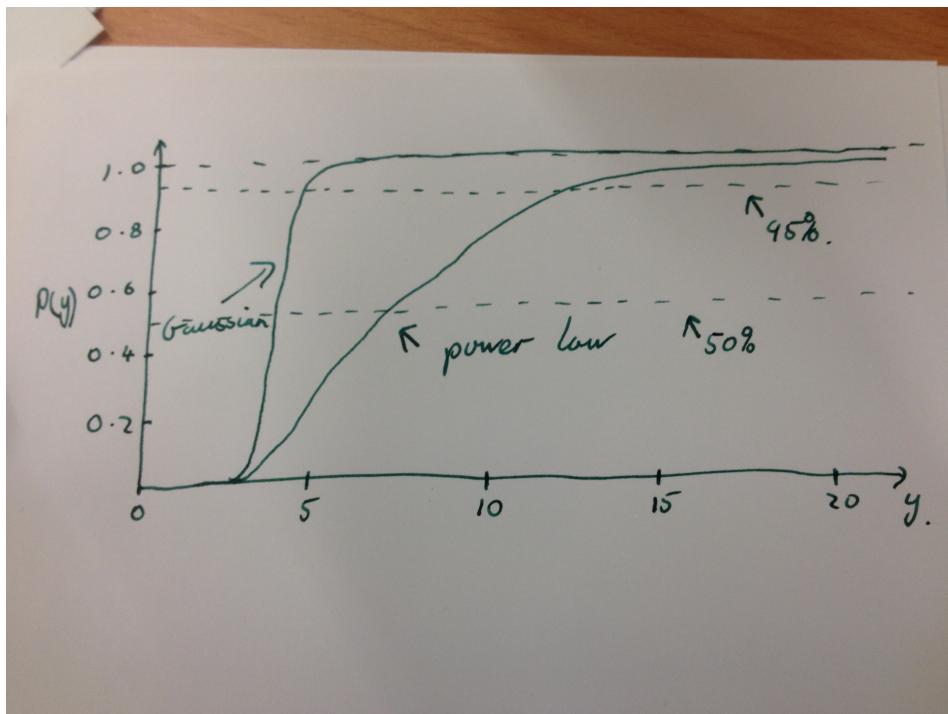


Figure 3.3. Sketch of the cumulative distribution of rare events for a Gaussian and $\mu = 3$ power law with the same variance and $N = 10^4$. The 50% and 95% confidence levels are shown as dashed horizontal lines; we find $y_{95\%} = 3\sigma$ and 12σ for the Gaussian and power law respectively.

3.6 Central limit theorem

3.6.1 Statement of proof

Suppose x_1, \dots, x_N are independent, identically distributed (iid) random variables with mean μ and variance σ^2 . Then the pdf of the normalised sum

$$X = \frac{x_1 + \dots + x_N - N\mu}{\sqrt{N}\sigma} \quad (3.16)$$

approaches a gaussian:

$$p(X) = \frac{1}{\sqrt{2\pi}} \exp[-X^2/2] \quad (3.17)$$

with zero mean and unit variance in the limit $N \rightarrow \infty$.

The central limit theorem formalises the common experience that a large number (say, $N = 10^6$) of rolls of a single die are distributed fairly widely about the mean 3.5, with variance 2.9, but their sum is distributed very narrowly about the mean 3.5×10^6 , with the square root of the variance 2.9×10^3 . Note that the square root of the variance of the sum increases in absolute terms ($\propto N^{1/2}$), but it decreases as a fraction of the mean ($\propto N^{-1/2}$).

- ✓ **Exercise:** Show explicitly that if $p(x)$ is a zero-mean Gaussian with variance σ^2 then the pdf of $y = x_1 + \dots + x_N$ is also a zero-mean Gaussian, with variance $N\sigma^2$.
- ✓ **Exercise:** Let x_1, \dots, x_N be N positive definite, iid random variables.

- Show that the pdf of their product $X = x_1 \dots x_N$ approaches

$$p(X) = \frac{1}{X \sqrt{2\pi\sigma_1^2}} \exp[-(\ln X - \mu_1)^2/(2N\sigma_1^2)], \quad (3.18)$$

with $\mu_1 = \langle \ln x_1 \rangle$ and $\sigma_1^2 = \langle (\ln x_1)^2 \rangle - \langle \ln x_1 \rangle^2$. Equation (3.18) is called a log-normal distribution.

- Explain why it is easy to confuse Eq. (3.18) with a power law.

The central limit theorem can be proved as follows. If $x = x_1 + x_2$ is the sum of two independent (but not necessarily identical) random variables, with pdfs $p_1(x_1)$ and $p_2(x_2)$

respectively, then the pdf $p(x)$ is given by the convolution integral

$$p(x) = \int_{-\infty}^{\infty} dx_1 p_1(x_1) p_2(x - x_1). \quad (3.19)$$

This is proved in two ways in the next subsection and can be extended easily to the sum of N variables by induction. The Fourier transform of Eq. (3.19) is $p(k) = p_1(k)p_2(k)$. Extending this result to N iid variables, each with pdf $p_1(x_i)$, we find that the characteristic function of the pdf $p(y)$ of $y = x_1 + \dots + x_N$ is given by

$$p(k) = [p_1(k)]^N = \exp \left[-ikc_1 N - \frac{k^2 c_2 N}{2} + \frac{ik^3 c_3 N}{6} + \dots \right], \quad (3.20)$$

where we have used the cumulate expansion of $p_1(k)$ (see Eq. (3.9)).

By inspection, the first two terms in the exponential are the characteristic function of a Gaussian with mean $Nc_1 = N\mu$ and variance $Nc_2 = N\sigma^2$. To find the leading order deviation from a Gaussian, we presume (verified a posteriori) that the third and later terms in the exponential are small. Taylor expanding to leading order, and inverting the Fourier transform, we get

$$p(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \exp[ikx] \left(1 + \frac{ik^3 c_3 N}{6} + \dots \right) \exp \left(-ikc_1 N - \frac{k^2 c_2 N}{2} \right) \quad (3.21)$$

$$= \frac{1}{2\pi} \left(1 - \frac{c_3 N}{6} \frac{d^3}{dx^3} + \dots \right) \int_{-\infty}^{\infty} dk \exp[ikx] \exp \left(-ikc_1 N - \frac{k^2 c_2 N}{2} \right) \quad (3.22)$$

$$= \left(1 - \frac{c_3 N}{6} \frac{d^3}{dx^3} + \dots \right) \frac{1}{\sqrt{2\pi N c_2}} \exp \left[\frac{-(x - Nc_1)^2}{2Nc_2} \right]. \quad (3.23)$$

Usually, the approach to a Gaussian is proved by showing that the probability weight in the tail $x \geq z$ over and above a Gaussian decreases with N . Integrating, one obtains

$$\begin{aligned} \int_{-\infty}^z dx p(x) &= \frac{1}{\sqrt{2\pi N c_2}} \int_{-\infty}^z -Nc_1 dx \exp \left[\frac{-x^2}{2Nc_2} \right] \\ &+ \frac{c_3}{6c_2 \sqrt{2\pi N c_2}} \left[1 - \frac{(z - Nc_1)^2}{Nc_2} \right] \exp \left[-\frac{(z - Nc_1)^2}{2Nc_2} \right] + \dots \end{aligned} \quad (3.24)$$

For many power-law distributions, c_3 and higher cumulants are infinite, and the fractional deviation is large over a much wider range that depends logarithmically on N . We examine this further below, in section 3.6.3.

$p_1(x)$	σ^2 exists?	tail	$q(y)$
exponential	yes	$\exp(-x^a)$	good gaussian for $< N^{2/3}\sigma$ or $N^{3/4}\sigma$
steep power law	yes	$ x ^{-a}$ with $a \geq 3$	gaussian with fat tails $> (N \ln N)^{1/2}\sigma$
shallow power law	no	$ x ^{-a}$ with $a < 3$	Levy

Table 3.1. Central limit theorem for different kinds of pdfs.

3.6.2 Convolution theorem for sums of random variables

This theorem, used in the proof of the central limit theorem, can be proved in two ways.

First proof. Let $x = x_1 + x_2$. Then $p(x)dx$ is defined as the probability that x lies in the range $(x, x + dx)$. This in turn equals the sum, over all possible values of x_1 , that x_1 lies in the range $(x_1, x_1 + dx_1)$, multiplied by the probability that x_2 equals $x - x_1$, i.e. $p_1(x_1)dx_1 \times p_2(x - x_1)dx_2$. For any particular fixed value of x_1 in the sum, we have $dx_2 = d(x - x_1) = dx$ and hence

$$p(x) = \int_{-\infty}^{\infty} dx_1 p_1(x_1) p_2(x - x_1). \quad (3.25)$$

Second proof. Take any function $f(x_1, x_2)$; it need not be the sum. Then f is a random variable if x_1 and x_2 are. Let $q(x_1, x_2)$ be the pdf of $f(x_1, x_2)$. Then the characteristic function is

$$q(k) = \sum_{n=0}^{\infty} \frac{(-ik)^n \langle f^n \rangle}{n!} = \int dx_1 \int dx_2 \exp[-ikf(x_1, x_2)] p_1(x_1) p_2(x_2), \quad (3.26)$$

where we have used Eq. (3.7) and the moments ($\langle f^n \rangle$) have been written out explicitly and reassembled the Taylor series into the exponential. As a simple corollary, for $f(x_1, x_2) = x_1 + x_2$, the Fourier integral separates and we have $q(k) = p_1(k)p_2(k)$.

✓ **Exercise:** If x_1 and x_2 are random variables with pdfs $p_1(x_1)$ and $p_2(x_2)$ respectively, prove that the pdf of their product $x = x_1 x_2$ is given by

$$p(x) = \int_{-\infty}^{\infty} dx_1 \frac{p_1(x_1) p_2(x/x_1)}{|x_1|}. \quad (3.27)$$

3.6.3 Wild versus mild pdfs

Benoit Mandelbrot divided probability distribution functions into two classes: mild and wild. Mild distributions include well behaved distributions with exponential tails, like

Poisson or Gaussian distributions, whose moments are all well defined, and where large fluctuations occur extremely (i.e. exponentially) rarely. Wild distributions, on the other hand, usually feature a power-law tail. Some or all of their moments are ill defined, and large fluctuations occur rarely, but not ridiculously so. For example, the Gutenberg-Richter law for the distribution of earthquake energies E , given by $p(E) \propto E^{-1.5}$, is a wild distribution; the mean $\langle E \rangle$ and standard deviation are not defined formally (although of course the size of the Earth places an upper limit on E and hence $\langle E \rangle$), and large events (e.g. San Francisco 1906) recur within a human lifetime.

Do all random variables approach a Gaussian equally quickly when summed? No! Table 3.1 summarizes the possible outcomes. If the variance exists and the tail is exponential (a mild pdf), then the central limit theorem gives a Gaussian pdf for y out to a distance $\propto N^{2/3}\sigma$ (if $c_3 \neq 0$) or $\propto N^{3/4}$ (if $c_3 = 0$ and $c_4 \neq 0$). If the variance exists and the tail is a power law, the central limit theorem strictly holds as $N \rightarrow \infty$, but in practice the deviations from a Gaussian occur just a few σ from the core, even for huge values of N . If the variance doesn't exist (a wild pdf), not even the core of $q(y)$ is a Gaussian; instead, the pdf approaches a Levy distribution. These are very important in modern physics (e.g. econophysics) but the mathematical details are outside the scope of this course (see book by Sornette, Chapter 4). (The case $a = 3$ is a transition case; it gives a gaussian, not Levy).

Note that in all cases the characteristic function is the product via the convolution theorem, so you can always compute the pdf of the summed variable exactly by inverting the Fourier transform of $p_1(k)^N$ if you are worried. This will usually be done numerically.

3.6.4 Multivariate gaussian distributions

The concept of a Gaussian distribution can be generalised to several variables. The joint pdf for n Gaussian random variables $\mathbf{x} = (x_1, \dots, x_n)$ is given by

$$p(\mathbf{x}) = \frac{1}{(\sqrt{2\pi})^n |\det(\sigma_{ij})|^{1/2}} \exp[-(x_i - \mu_i)(\sigma^{-1})_{ij}(x_j - \mu_j)/2] \quad (3.28)$$

where $\mu_i = \langle x_i \rangle$ is the mean of the i^{th} variable and $\sigma_{ij} = \langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle$ is the *covariance matrix*.

The characteristic function $p(\mathbf{k}) = p(k_1, \dots, k_n)$ is also a multivariate Gaussian, with prefactor unity as needed for normalisation:

$$p(\mathbf{k}) = \exp(ik_i\mu_i - k_i\sigma_{ij}k_j/2). \quad (3.29)$$

The moments are computed from

$$\langle x_1^{a_1} \dots x_n^{a_n} \rangle = i^{a_1+ \dots + a_n} \left. \frac{\partial^{a_1+ \dots + a_n} p(\mathbf{k})}{\partial k^{a_1} \dots \partial k^{a_n}} \right|_{\mathbf{k}=0} \quad (3.30)$$

✓ **Exercise:** (J. Mathews and R. L. Walker 1970, *Mathematical Methods of Physics*, Section 14.6) Let $n(t)$ be the noise in a gravitational wave detector (say). Assume that the noise is a stationary, Gaussian random process, with zero mean, variance σ^2 , and autocorrelation function $G(t' - t) = \langle n(t)n(t') \rangle$.

- Show that the characteristic function of the joint pdf of the three variables $x_1 = n(t)$, $x_2 = n(t + \tau)$, $x_3 = n(t + \tau')$ is given by

$$p(\mathbf{k}) = \exp[-\sigma^2 k_1^2/2 + G(\tau)k_1k_2 - G(\tau')k_1k_3 - \sigma^2 k_2^2/2 - G(\tau - \tau')k_2k_3 - \sigma^2 k_3^2/2] \quad (3.31)$$

- What is the corresponding pdf $p(\mathbf{x})$?
- Show that the autocorrelation function of the *noise power* is

$$\langle n(t)^2 n(t')^2 \rangle = \sigma^4 + 2G(t' - t)^2. \quad (3.32)$$

Relations like this lie behind the photon counting statistics in interferometers of the Twiss-Hanbury Brown type, e.g. in radio telescopes.

3.7 Transition to equilibrium

As noted above, it is a generally observed fact that systems in equilibrium tend to have mild probability distribution functions, e.g. Maxwell-Boltzmann distribution in a classical gas in contact with a heat bath. In contrast, far-from-equilibrium systems have wild probability distribution functions, e.g. earthquake power laws. It is reasonable to postulate that the probability distribution function of a system transforms from a power law to a Gaussian as it approaches equilibrium. Here we show why.

3.7.1 Equilibrium: gaussian energy fluctuations

Consider, first, a system S , composed of $N \gg 1$ particles, which is in thermal equilibrium with a heat bath at temperature T , i.e. it has been in contact with the heat bath for a very long time. If you measure the total energy E of the system S over and over again, common experience dictates that you will measure an extremely narrow range of values. Indeed, $p(E)$ is a Gaussian, centred at $\langle E \rangle$ and with standard deviation $N^{-1/2}k_B T$. Needless to say, $p(E)$ does not obey the Boltzmann law, $\exp(-E/k_B T)$, unlike the microstates; for if it did, measurements of E would bounce around like crazy, by amounts of order $\sim k_B T$, against common experience.

How do we derive $p(E)$? As usual, we prepare a huge ensemble of $M \gg 1$ copies of the system S , prepared under identical macroscopic conditions. At some time t , we take a snapshot of all the system copies. (If the system is ergodic, this is equivalent to measuring one system over and over again.) This gives us M microstates, each microstate being a snapshot of the N particles in the system, with total energies U_1, U_2, \dots, U_M . Boltzmann then tells us that we have $p(U_i) = \exp(-\beta U_i)/Z$, with $Z = \sum_i \exp(-\beta U_i)$, for all the microstates. But the macroscopic energy is $E = (U_1 + \dots + U_M)/M$, i.e. it is the sum of $M \gg 1$ random variables (due to random initial microscopic conditions for each jar in the ensemble), all independent and identically distributed (according to Boltzmann). So the central limit theorem applies, yielding the Gaussian we expect.

3.7.2 Nonequilibrium: power law energy fluctuations

Now suppose that $x = x_1 + \dots + x_N$ is the sum of N independent, identically distributed random variables whose individual distributions $p_1(x)$ have zero mean (for simplicity) and are power laws at large $|x|$, i.e. $p_1(x) \sim Cx^{-(1+\mu)}$ as $|x| \rightarrow \infty$. Provided that $p_1(x)$ has finite variance σ , which requires $\mu > 2$, the central limit theorem does apply; that is, in the limit $N \rightarrow \infty$, the pdf of x , denoted by $p_N(x)$, approaches a Gaussian with zero mean (in this special case) and variance $N^{1/2}$. However, the gaussianity of $p_N(x)$ breaks down quickly for $x \geq N^{1/2}\sigma$. Formally, the deviation from a Gaussian can be expanded in powers

of $N^{-1/2}$:

$$\frac{1}{\sqrt{2\pi}} \exp[-x^2/2] (N^{-1/2}Q_1(x) + N^{-1}Q_2(x) + \dots), \quad (3.33)$$

where x is suitably normalised, c_3 is the third-order cumulant, and one can work out $Q_1(x) = c_3(1 - x^2)/6$. This expansion does not make sense for the power-law case, because all cumulants with order greater than $1 + \mu$ are infinite.

Let us now see where gaussianity breaks down. Near $x = 0$ we know that the central limit theorem always applies. Therefore we have $p_N(x) = (2\pi N\sigma^2)^{-1/2} \exp[-x^2/(2N\sigma^2)]$ for small x .

On the other hand, at large x , we have $p_N(x) \approx Np_1(x)$. This is because $p_N(x)$ is an N -fold convolution of $p_1(x)$ with itself, leading to a straight multiplication for $x \rightarrow \infty$. The result for $p_N(x)$ follows by induction from the result for $p_2(x)$:

$$p_2(x) = \int_{-\infty}^{\infty} dx' p_1(x') p_1(x - x') \quad (3.34)$$

$$\approx \int_{-m\sigma}^{m\sigma} dx' p_1(x') p_1(x - x') + \int_{x-m\sigma}^{x+m\sigma} dx' p_1(x') p_1(x - x') \quad (3.35)$$

$$\approx p_1(x) + p_1(x), \quad (3.36)$$

where m equals a few, and the second line follows for $x \gg \sigma$ because the integrand is a negligible product of two small numbers except when the argument of one or other of the $p_1(x)$ is small.

For $p_1(x) \sim Cx^{-(1+\mu)}$ as $x \rightarrow \infty$, the transition between the two regimes occurs at $x = x_0$ given by

$$(2\pi N\sigma^2)^{-1/2} \exp[-x_0^2/2N\sigma^2] \approx NCx_0^{-(1+\mu)}. \quad (3.37)$$

Assuming logarithms are roughly constant, we make a first guess $x_0 \approx N^{1/2}\sigma$. Substituting this guess into the RHS and reevaluating, we arrive at the corrected estimate

$$x_0 \approx (N \ln N)^{1/2}\sigma. \quad (3.38)$$

In other words, the power-law tail begins to assert itself only $(\ln N)^{1/2}$ half widths away from the Gaussian core. Even for $N \sim 10^{23}$ this is only a factor of 7.

3.8 Entropy

$$S(t) = -k_B \int d^{3N}x d^{3N}p f_N(x, p, t) \ln f_N(x, p, t) \quad (3.39)$$

In equilibrium (but not away from equilibrium), $S(t)$ is independent of t and can be written in terms of macroscopic variables like N , V (volume), T , U (internal energy), In a closed system, $S(t)$ increases with time as equilibrium is approached, and attains its maximum value at equilibrium. This is not true in open systems.

3.8.1 Phase-space dissipation function

An alternative approach to entropy involves the evolution of phase-space volumes. It has been elaborated by Crookes, Evans, and Searles, among others. For an excellent review of the ideas involved, see E. M. Sevick *et al.*, Ann. Rev. Phys. Chem. **59**, 603 (2008), and references therein. This section draws heavily this paper.

Consider a dynamical system described by the two-dimensional phase space (q, p) , with $\dot{q} = Q(t, q, p)$ and $\dot{p} = P(t, q, p)$. The system is not necessarily Hamiltonian. Consider a bundle of trajectories occupying a phase-space volume $\Delta q_0 \Delta p_0$ around the point (q_0, p_0) at time t_0 . Then it is easy to show that the phase-space volume occupied at $t_0 + \Delta t$ is

$$\Delta q_0 \Delta p_0 \left[1 + \Delta t \left(\frac{\partial Q}{\partial q} + \frac{\partial P}{\partial p} \right)_{(q_0, p_0)} + (\Delta t)^2 \left(\frac{\partial Q}{\partial q} \frac{\partial P}{\partial p} - \frac{\partial P}{\partial q} \frac{\partial Q}{\partial p} \right)_{(q_0, p_0)} \right]. \quad (3.40)$$

Hence the rate of change of the volume is proportional to the volume. Taking $\Delta t \rightarrow 0$, we obtain

$$\frac{d \ln \Delta q \Delta p}{dt} = \frac{\partial Q}{\partial q} + \frac{\partial P}{\partial p}. \quad (3.41)$$

Generalizing to a $2n$ -dimensional phase space $(q_1, \dots, q_n, p_1, \dots, p_n)$, we can relate the initial (at time t_i) and final (at time t_f) volumes along a trajectory by

$$\frac{d\Gamma(t_f)}{d\Gamma(t_i)} = \exp \left\{ \int_{t_i}^{t_f} ds \Lambda[s, q_1(s), \dots, q_n(s), p_1(s), \dots, p_n(s)] \right\} \quad (3.42)$$

with

$$\Lambda(s) = \frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i}, \quad (3.43)$$

where repeated indices imply summation. Note that an initially infinitesimal trajectory bundle remains infinitesimal. In a Hamiltonian system, we have $\Lambda(s) = \partial^2 H / \partial q_i \partial p_i - \partial^2 H / \partial p_i \partial q_i = 0$, and the phase-space volume is strictly conserved (even though it distorts with time). In contrast, most far-from-equilibrium systems are either dissipative (subject to external forces that cannot be expressed as gradients of a potential) or thermostatted (one or more degrees of freedom constrained). Either way, they are not Hamiltonian systems; for example, a system experiencing a dissipative force F satisfies a modified version of Lagrange's equations:

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = \mathbf{F} \cdot \frac{\partial \mathbf{x}}{\partial q_i}, \quad (3.44)$$

and a system in contact with a heat bath at temperature T can be shown to have $\Lambda(s) = \dot{Q}_h(s)/k_B T$, where $\dot{Q}_h(s)$ is the rate at which the system gains heat. Hence the phase-space volume increases or decreases exponentially along trajectories, depending on the sign of $\Lambda(s)$. Needless to say, exponential changes must not be treated lightly!

3.8.2 Macroscopic irreversibility

One of the deeply surprising features of Nature is that macroscopic systems exhibit irreversible dynamics, even when their microscopic equations of motion are fully time-reversible. In the thermodynamic limit (large systems in equilibrium), we explain this tendency in terms of entropy and the Second Law of Thermodynamics. Recently, however, detailed studies of nanoscale systems like protein motors and artificial nano-machines show that the tendency towards macroscopic irreversibility is either partial or completely absent. If the work performed during the duty cycle of a machine is comparable to the thermal energy per degree of freedom, the machine may well run backwards for a while - possibly a long while. There is no equivalent to the Second Law for small, driven systems.

Figure 3.4 depicts a bundle of forward trajectories emanating from the infinitesimal volume $d\Gamma_0$ initially and terminating in the infinitesimal volume $d\Gamma_t$ at time t . Also drawn are

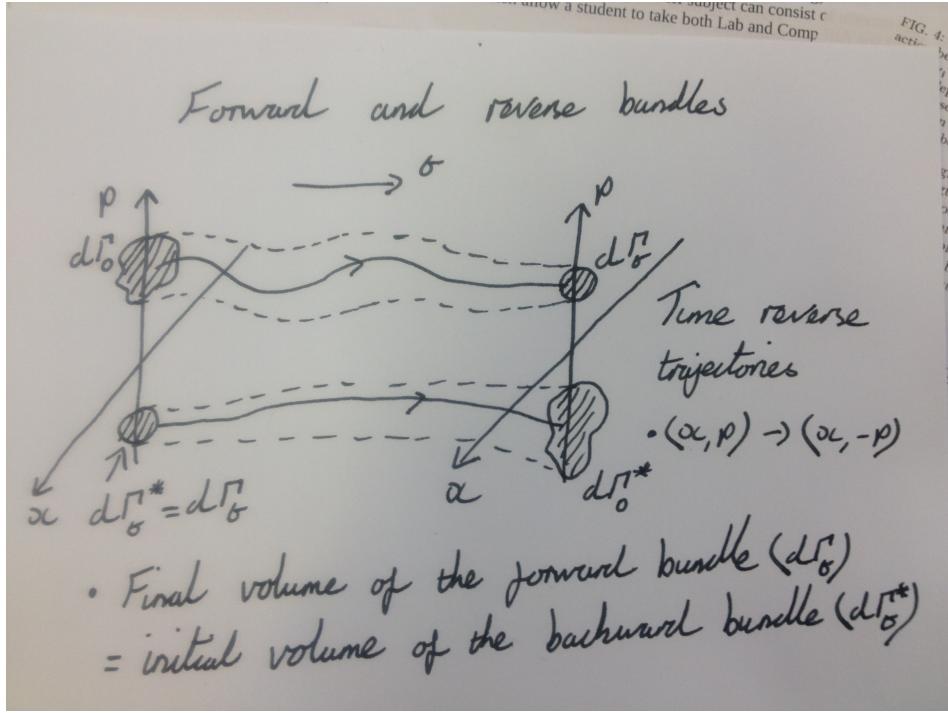


Figure 3.4. Schematic of forward (upper) and time-reverse (lower) bundle trajectories. The forward trajectory starts with volume $d\Gamma_0$ and terminates with volume Γ_t . The time-reversed trajectory starts with volume $d\Gamma_t^*$ and terminates with volume $d\Gamma_0^*$.

the time-reversed trajectories (under the transformation $q \rightarrow q, p \rightarrow -p$), which start from the volume $d\Gamma_t^*$ and end in the volume $d\Gamma_0^*$. Whether or not the process is macroscopically reversible, we always have $d\Gamma_t = d\Gamma_t^*$.

Let us now define the dissipation function $\Omega_t(\Gamma_0)$ such that $\exp[\Omega_t(\Gamma_0)]$ equals the ratio of the probabilities of the forward and reverse trajectory bundles. $\Omega_t(\Gamma_0)$ measures the rate of entropy production and hence provides a quantitative measure of irreversibility. We can then write

$$\Omega_t(\Gamma_0) = \ln \left[\frac{f(\Gamma_0, 0)d\Gamma_0}{f(\Gamma_t^*, 0)d\Gamma_t^*} \right] \quad (3.45)$$

$$= \ln \left[\frac{f(\Gamma_0, 0)}{f(\Gamma_t^*, 0)} \right] - \int_0^t ds \Lambda(s), \quad (3.46)$$

where in the first line, the probability of a trajectory bundle is the microscopic phase-space density at the starting point multiplied by the phase-space volume at the starting point (after that, the dynamics is completely deterministic). The second line follows from $d\Gamma_t = d\Gamma_t^*$ and Eq. (3.42).

A system undergoes a macroscopically reversible process if the probabilities of the forward and reverse bundles are equal, i.e. $\Omega_t(\Gamma_0) = 0$. We also get a nice relation between $f(\Gamma_0, 0)$, $f(\Gamma_t^*, 0)$ and $\Lambda(s)$ in this situation. Strictly speaking, macroscopic reversibility also requires the system to be ergodically consistent, with $f(\Gamma_t^*) \neq 0$ for all Γ_0 , so that the starting point of the reverse trajectory bundle is actually occupied by particles.

If $\Omega_t(\Gamma_0)$ is positive for any given trajectory, then its corresponding reverse trajectory is less likely to be seen (by definition) in any particular measurement of the system; the opposite is true if $\Omega_t(\Gamma_0)$ is negative. If $\langle \Omega_t(\Gamma_0) \rangle$ is positive after ensemble averaging over many measurements, then the macroscopic dynamics moves in the forward direction, otherwise it moves in the reverse direction.

3.8.3 Evans-Searles fluctuation theorem

Consider all trajectories starting in $d\Gamma_0$. The fraction $p[\Omega_t(\Gamma_0) = A]dA$ that end up with $\Omega_t(\Gamma_0)$ in the range $(A, A + dA)$ is given by

$$p(\Omega_t = A) = \int d\Gamma_0 \delta [\Omega_t(\Gamma_0) - A] f(\Gamma_0, 0). \quad (3.47)$$

Likewise, the fraction of trajectories starting in $d\Gamma_0$ that end up with $\Omega_t(\Gamma_0)$ in the range $(-A, -A + dA)$ is given by

$$p(\Omega_t = -A) = \int d\Gamma_0 \delta [\Omega_t(\Gamma_0) + A] f(\Gamma_0, 0) \quad (3.48)$$

$$= \int d\Gamma_t^* \delta [\Omega_t(\Gamma_t^*) + A] f(\Gamma_t^*, 0) \quad (3.49)$$

$$= \int d\Gamma_0 \delta [\Omega_t(\Gamma_t^*) + A] f(\Gamma_0, 0) \exp[-\Omega_t(\Gamma_0)] \quad (3.50)$$

$$= \int d\Gamma_0 \delta [-\Omega_t(\Gamma_0) + A] f(\Gamma_0, 0) \exp[-\Omega_t(\Gamma_0)] \quad (3.51)$$

$$= \exp(-A)p(\Omega_t = A). \quad (3.52)$$

The steps in the above derivation are justified as follows. The second line follows from the first, because Γ_0 and Γ_t^* are dummy variables of integration. The third line follows from the second by applying Eq. (3.45). The fourth line follows from the third, because the definition

of $\Omega_t(\Gamma_t^*)$ implies

$$\Omega_t(\Gamma_t^*) = \ln \left[\frac{f(\Gamma_t^*, 0) d\Gamma_t^*}{f(\Gamma_0, 0) d\Gamma_0} \right] \quad (3.53)$$

$$= -\Omega_t(\Gamma_0). \quad (3.54)$$

Equation (3.52) is called the Evans-Searles fluctuation theorem. It states that, in any given forward-reverse pair of trajectories with $\Omega_t \neq 0$, one trajectory is favoured exponentially over the other. The favouritism becomes ever more overwhelming, as the system grows in size and Ω_t increases. Note that $p(\Omega_t = A)$ and $p(\Omega_t = -A)$ describe two groups of trajectories starting from the same point in phase space but ending up in different places.

We can now calculate the ensemble average of $\Omega_t(\Gamma_0)$ over all its possible values A , weighted by their probabilities:

$$\langle \Omega_t(\Gamma_0) \rangle = \int_{-\infty}^{\infty} dA A p(\Omega_t = A). \quad (3.55)$$

Splitting the domain of integration into positive and negative parts and applying Eq. (3.52) we find

$$\langle \Omega_t(\Gamma_0) \rangle = \int_0^{\infty} dA A (1 - e^{-A}) p(\Omega_t = A). \quad (3.56)$$

As all factors in the integrand are non-negative, so is the integral as a whole. This is a restatement of the Second Law of Thermodynamics. Note that it is only true in equilibrium, when there is enough time to sample all possible trajectories and hence all possible A values. In a far-from-equilibrium situation, only a subset of trajectories is sampled, and the ensemble average can take either sign.

Equation (3.52) has been verified experimentally by observing a single colloidal particle vibrating in an optical trap. A related result is the Crookes fluctuation theorem, which relates the probability of the work done along forward and reverse trajectories joining two states far from equilibrium to the equilibrium change in free energy between the same two states. Crookes's theorem has been verified experimentally by stretching a single RNA molecule and watching it unfold; see Colin *et al.*, Nature **437**, 231 (2005).

3.9 Problems

1. **Two up:** An illegal experiment is performed, whose probability of success is p . If the experiment is repeated N times, the probability of n successes is given by the famous *binomial distribution*,

$$P_N(n) = {}^N C_n p^n (1-p)^{N-n} \quad (3.57)$$

where ${}^N C_n = N!/[n!(N-n)!]$ is the number of unordered ways to select n objects from N .

- (a) Convince yourself by simple counting that Eq. (3.57) is correct.
- (b) Let x be a binary random variable that equals unity when the experiment succeeds and zero when it fails. Write down the pdf $p(x)$ and prove that the characteristic function is

$$p(k) = 1 - p + pe^{-ik}. \quad (3.58)$$

- (c) Let x_1, \dots, x_N be the output from N identical repetitions of the experiment. From Eq. (3.57) and the convolution theorem, prove that the pdf $q(y)$ of the sum $y = x_1 + \dots + x_N$ is

$$q(y) = \sum_{n=0}^N P_N(n) \delta(y - n). \quad (3.59)$$

- (d) The central limit theorem guarantees that $q(y)$ approaches a Gaussian in the limit $N \rightarrow \infty$. Verify this directly by expanding Eq. (3.59) to leading order using Stirlings approximation: $m! \approx m^m e^{-m} (2\pi m)^{1/2}$. You should find

$$P_N(n) \approx \left[\frac{N}{2\pi n(N-n)} \right]^{1/2} \left(\frac{Np}{n} \right)^n \left[\frac{N(1-p)}{N-n} \right]^{N-n} \quad (3.60)$$

Argue that the second factor in Eq. (3.60) is tiny for $n > Np$ in the limit $N \rightarrow \infty$ and that the third factor is tiny for $n < Np$. Near $n = Np$, show that the factors reduce to

$$\left(\frac{Np}{n} \right)^n \approx \exp \left[-(n - Np) - \frac{(n - Np)^2}{2Np} \right] \quad (3.61)$$

$$\left[\frac{N(1-p)}{N-n} \right]^{N-n} \approx \exp \left[n - Np - \frac{(n - Np)^2}{2N(1-p)} \right] \quad (3.62)$$

to order $\mathcal{O}(1/N)$ in the exponentials, leading to the final result

$$P_N(n) \approx \frac{1}{\sqrt{2\pi Np(1-p)}} \exp\left[-\frac{(n-Np)^2}{2Np(1-p)}\right]. \quad (3.63)$$

- (e) Does the variance of y match the prediction of the central limit theorem?
2. **Investment beta:** A tropical island is the home of two businesses: a sun-cream shop, and an umbrella shop. Every day that the sun shines, the sun-cream shop makes a percentage return r_c on capital, while the umbrella shop makes zero return. Every day that it rains, the umbrella shop makes a percentage return r_u on capital, while the sun-cream shop makes zero return. The probability of a sunny (rainy) day is q ($1 - q$) respectively.
- Barnacle Bob invests a fraction λ of his capital in the sun-cream shop and the remainder in the umbrella shop. After n days,
- (a) What is the pdf of his total return?
 - (b) What value of λ minimises the fluctuations in his returns (i.e. minimises his beta in the lingo of investment professionals)?
 - (c) What is his expected return when the fluctuations are minimised?
3. **Sand piles:** (P. Bak, C. Tang and K. Wiesenfeld, Physical Review Letters, **59**, 381 (1987); H. J. Jensen 1998, *Self-Organized Criticality*, Cambridge University Press: Cambridge). Construct a cellular automaton of a two-dimensional sand pile on a square $N \times N$ grid. Initialize the slope z_{ij} at each cell (i, j) with a random value between 0 and 1. At each big time step, add one unit of slope to a random cell (i', j') . If the cell goes supercritical as a result, with $z_{i'j'} > z_c = 1$, reduce $z_{i'j'}$ by one unit and increment the slopes at the four nearest neighbours $(i' \pm 1, j' \pm 1)$ by $1/4$ units each. Keep doing this until all the cells are subcritical again. Count the units of slope that *fall off* the outer boundary of the pile; their total s is the size of the avalanche. Repeat.
- (a) Show that the pdf of the avalanche sizes is a power law $p(s) \propto s^{-a}$ in the domain $1 \leq s \leq N^2 z_c$. What is a ? Quote your answer with an error bar.

- (b) Show that the pdf of the waiting times is an exponential, with $p(\Delta t) = \tau^{-1} \exp(-\Delta t/\tau)$. What is τ , in units of the big time step?
- (c) Verify that, over the long term, the automaton adjusts itself to obey $\langle s \rangle = \dot{s}\langle \Delta t \rangle$, where \dot{s} is the rate at which slope is added to the system from outside.
- (d) Is there a correlation between the size s of an avalanche and the waiting time Δt to the previous or next avalanche?
- (e) How does $p(s)$ compare with the pdf of total size s' (i.e. the total number of toppled grains in an avalanche, whether or not they fall off the edge)? Can you relate your result to the mean residence time of a grain in the pile?

4. Forest fires: The following idealised model (B. Drossel and F. Schwabl, Physical Review Letters **69**, 1629 (1992)) aims to describe the sporadic ignition and sometimes uncontrolled spread of forest fires. It has become an archetype of a particular class of self-organised critical systems. There is an ongoing debate about how faithfully it captures the spread of real forest fires, but its utility as a toy model is undeniable.

Consider a two-dimensional square lattice with periodic boundary conditions. Each site on the lattice occupies one of three states at any instant: black (empty), green (unburnt trees), or red (burning trees). Initially, it contains a random mixture of empty and green sites. At each time step, the lattice is updated according to the following rules:

- a red site becomes black;
- a green site becomes red if one of its neighbours is red, otherwise it becomes red with probability f ;
- a black site becomes green with probability p .

- (a) Justify the above rules on a common-sense basis in the context of forest fires.
- (b) Implement the forest fire model as a cellular automaton. Note that the rules are executed in one shot (synchronously) at each time step.
- (c) What is the probability density function (pdf) of fire sizes, s (s is defined as the total number of red cells after some fixed time). It is a stochastic variable,

because it is different in different realisations of the system (e.g. with different initial conditions)), in the following regimes:

- $f = 0, p = 1/2$.
- $0 < p \ll f \ll 1$.
- $0 < f \ll p \ll 1$.

- (d) How does the system behave qualitatively in each of the above regimes? Account for your results physically.
- (e) What is the distribution of waiting times between fires for an individual cell in the system?
- (f) Denote the fractions of green and red sites by $x_g(t)$, and $x_r(t)$ respectively. Show that we have

$$\frac{dx_g}{dt} = -fx_g - 4x_gx_r + p(1 - x_g - x_r) \quad (3.64)$$

$$\frac{dx_r}{dt} = -x_r + fx_g + 4x_gx_r. \quad (3.65)$$

- (g) Calculate the steady-state fraction of fires. How does it compare with the output of your automaton?

5. **Ants at war:** (M. W. Moffett, Scientific America **305**, 84 (2011)) Every day, the worlds ants engage in vast, anonymous battles, in which the casualties per month can run into the millions along fronts which stretch over many kilometers. In a fascinating article distilling many years of painstaking (and sometimes painful!) observations, Moffett describes the various tactics and social structures which distinguish different ant species in their approach to war. Examples include roaming in packs (marauder ants) versus defending entrenched nests (weaver ants), entering protracted battles (larger colonies) versus staging preemptive tournaments (smaller colonies), and committing different members of the colony (e.g. large/small, old/young, sterile/fertile) to battle according to subtle cost-benefit considerations which are resolved collectively.

In this question, we model ant warfare as a self-organized critical system. You are asked to build a cellular automaton that captures some of the dynamics described by

Moffett in idealized form, with the aim of quantifying some of his hypotheses about the ants collective behavior. The rules of the automaton should incorporate the following features of a self-organized critical system:

- A spatial grid
- A slow, global driver, i.e. positive natural population growth (births per unit time exceeding natural deaths per unit time);
- Local dissipation, i.e. war-related deaths;
- Self-regulation to a critical state, in which the total number of ants is steady over the long term, although there may be fluctuations (even large ones) about the long-term average.

Moffett observed that marauder ant workers (serving as soldiers) vary in size more than any other species. The minors are relatively feeble but also relatively cheap to maintain, so they are produced in large numbers and sent as cannon fodder to the front line. The majors are more lethal than the minors but more expensive to maintain; they tend to hang back and commit only when the threat is extreme. What overall advantage does this size segregation confer in battle, and what is the optimal ratio of majors to minors?

To answer this question, implement the following cellular automaton in your favourite computer language. Consider a square grid populated by ants from two warring colonies (tribes), red and blue. Each cell contains ants from one tribe only (they kill each other until one prevails). For simplicity, assume that each cell is in one of three states: empty, populated by minors, or populated by majors. At each time step, update every cell simultaneously according to the following algorithm:

- An empty cell becomes populated with probability p , majors are $f < 1$ times as likely to be born as minors, and red and blue births are equally likely;
- A cell of minors becomes empty when surrounded by at least one enemy minor or major;

- A cell of majors becomes empty when surrounded by four minors or at least one major.

Run your automaton starting with all the cells empty.

- Justify the above rules briefly in the context of Moffetts article.
- Plot the probability density functions (pdfs) for the number of deaths per time step of majors, s_+ , and minors, s_- , in the following regimes:

- $f = 1/4, p = 1/2?$
- $0 < p \ll f \ll 1?$
- $0 < f \ll p \ll 1?$

Your answers should be the same (within statistical error) for the red and blue tribes.

- How does the system behave qualitatively in each of the above regimes? Interpret your results physically.
- How do your results change if f is different for the red and blue tribes?
- In ant societies, the workers (soldiers) are sterile. In human societies, soldiers reproduce. According to Moffett, there is some anthropological evidence that successful human warriors tend to have more offspring. By replacing the majors and minors in the automaton with young (strong, fertile) and old (weak, infertile) soldiers (as per Cassills field observations cited by Moffett) and tweaking the rules to incorporate the reproductive advantage and a fight-or-flight option, estimate how large that advantage must be before it makes sense for young soldiers to stand and fight instead of fleeing.

- Cancer growth:** A fascinating branch of research in the life sciences today is systems biology. Its practitioners seek to construct predictive, quantitative models of complex biological systems by modelling how the fundamental elements (e.g. cells) interact and communicate via metabolic and signalling networks. An outstanding question in this area, and a classic example of spatio-temporal pattern formation, is how tumours

emerge naturally from the dynamics of the immune system's surveillance network. Phenomenological models for tumour growth abound. For example, Gompertz showed that the volume V of a tumour evolves with time t exponentially according to the law

$$V = V_0 \exp \left[\frac{A}{B} (1 - e^{-Bt}) \right], \quad (3.66)$$

where V_0 is the initial volume, and A and B are rate constants determined empirically. It is pertinent to ask whether such empirical laws can be derived theoretically from the underlying ordinary or partial differential equations describing the surveillance network dynamics. In this question, we model the growth of tumours with a cellular automaton. We begin by following closely the classic work by Qi, Zheng, Du and An, *Journal of Theoretical Biology* **161**, 1 (1993).

Consider a simple model in which a piece of tissue is divided into a regular, square grid of compartments. At any instant, every compartment contains one of the following: a normal cell N , a cancerous cell C , a cytotoxic complex E , or a dead cancerous cell D . In addition, every compartment contains an effector E_0 which is dormant in the N , C , or D states and active in the E state. Effectors are the sentinels of the immune system's surveillance network. When activated, they bind to a cancerous cell and emit chemical signals that recruit other cytotoxic entities (?assassins?) to the site. Macrophages, for example, are cytotoxic; they kill cells by engulfing and digesting them.

The myriad processes in the immune system can be reduced to the following simplified network.



The first equation, which was not included by Qi et al. (1993), describes random mutations, which convert a normal cell into a cancerous one. The second equation

describes the proliferation of the cancer, i.e. a cancerous cell ?infects? one of its neighbours. The third and fourth equations describe the two-stage assassination of a cancerous cell: the effector binds to the cell and recruits assassins, forming a cytotoxic complex; then, its work done, the complex dissolves to leave behind a dead cancerous cell and dormant effector. The last equation describes dissolution of a dead cell and its replacement by a normal cell.

- (a) What plays the role of an external driver, analogous to the source of grains in a sand pile, in the above equations.
- (b) Write down a set of rules for a cellular automaton which implements the above equations, without mutations. State clearly how a compartment is updated at each time step when it occupies the N , C , E , or D state. The proliferation step is limited by C-cell competition for the finite supply of nutrients in vivo (Qi *et al.* 1993). Include competition by setting the proliferation rate to

$$k'_1 = k_1 \left(1 - \frac{q}{4}\right), \quad (3.72)$$

where $q \leq 4$ is the number of C-cell neighbours. This approach is simpler than that prescribed by Qi *et al.* (1993).

- (c) Implement the automaton in a computer programming language of your choice. Your automaton should be synchronous, meaning that every compartment is updated once per time step.
- (d) Starting with a few randomly situated C cells, run the automaton, until it reaches a statistically stationary state. Choose constant values of k_1 , k_2 , k_3 and k_4 from the ranges suggested in Table 1 of Qi *et al.* (1993), with k_1 , k_3 and k_4 greater than k_2 .
 - i. Does the initial rise in tumour volume reproduce Gompertz's law?
 - ii. Why must we choose k_1 , k_3 and k_4 to be greater than k_2 ?
 - iii. By running many realisations of the automaton, starting with the same number of C cells each time, plot $p(x_c)$, the probability density function

(PDF) of x_c , the total number of C cells in the stationary state. Comment on its shape.

- iv. Compute the variance $\text{var}(x_c)$. Interpret your answer in terms of the central limit theorem.
 - v. Derive analytically the mean number of C , E , and D cells in the stationary state?
- (e) Now switch off competition among proliferating C cells ($k'_1 = k_1$) and take $k_1 = k_2$, so that cytotoxicity balances proliferation. Run many realisations of the automaton, starting with the same number of C cells. Plot the PDF $p(x_c)$ after a fixed, sensibly chosen number of iterations. Comment on its shape.
- (f) Switch on mutations while keeping $k'_1 = k_1 = k_2$ and plot $p(x_c)$.
- i. Show that the system approaches a stationary state, where x_c is independent of k_0 . In this respect, the system resembles a sand pile, whose mean angle of repose does not depend on the rate at which grains are added.
 - ii. Can you derive analytically the mean number of C , E , and D cells in the stationary state?
 - iii. Do you see evidence for avalanches in $p(x_c)$, when the mutations are fast ($k_0 \gg k_1$) or slow ($k_0 \ll k_1$)?
- (g) Switch on competition again. Can you tune k_1 , k_2 , k_3 and k_4 to get avalanches and a power-law PDF?

Chapter 4

Diffusive stochastic processes

4.1 Fluctuations

Given an N -body system, we aim to describe its macroscopic behaviour in terms of just a few variables, such as temperature, pressure, chemical concentration. Consider a Gibbs ensemble of systems prepared under identical macroscopic conditions. When we measure a particular macroscopic variable $A(t)$, we get a slightly different answer for each system in the ensemble, due to the ongoing, rapid, unpredictable transitions between microscopic states in each system.

- Ensemble average: $\langle A(t) \rangle$. The average is over systems in the ensemble, not over t ; in general, for non equilibrium systems, it is a function of t .
- Variance: $\text{var}\{A(t)\} = \langle A(t)^2 \rangle - \langle A(t) \rangle^2$. This measures the fluctuations.

Usually, in equilibrium, the fluctuations are small. For example, suppose we measure the pressure on the lid of a huge number of identically prepared jars of gas (say, using a delicate spring gauge). Our measurements will cluster around a mean pressure P_0 , but there will be some variation about the mean, of order $\delta P \sim N^{-1/2}P_0$, because the number of molecules that strike the lid during the response time of the spring gauge (and their precise momenta) will be slightly different from jar to jar in the ensemble. Generally speaking, if

N particles each have a microscopic property a_i ($1 \leq i \leq N$) whose mean is \bar{a} and variance is σ_a^2 , then a derived macroscopic property $A = \sum_i a_i$ satisfies $\langle A \rangle = N\bar{a}$, $\delta A = N^{1/2}\sigma_a$ by the central limit theorem, and hence $\delta A/\langle A \rangle = N^{-1/2}\sigma_a/\bar{a} \ll 1$.

- ✓ **Exercise:** Estimate δP for a 1 L jar of air at STP if the response time of the strain gauge is 1ms.

In contrast, systems far from equilibrium can have $\delta A \sim \langle A \rangle$ or even $\delta A \gg \langle A \rangle$. Moreover, the fluctuations do not always obey Gaussian statistics, nor does the central limit theorem necessarily hold. Equilibrium systems close to a phase transition can also exhibit large fluctuations (correlated over macroscopic length-scales), e.g. refractive index variations $\delta n \gg 1$ during critical opalescence in a methanol-hexane mixture.

4.1.1 Stationary and ergodic processes

In a *stationary* process, all ensemble averages are independent of time:

$$\langle A(t) \rangle \text{ independent of } t \quad (4.1)$$

$$\langle A(t)A(t') \rangle \text{ depends only on time difference : } t' - t = \tau \quad (4.2)$$

Note that a stationary process is not the same thing as equilibrium. $f_N(t, x, p)$ can still depend on t (i.e. nonequilibrium) even while $\int d^{3N}x d^{3N}p f_N(t, x, p) A(x, p)$ is independent of t for a limited set of macroscopic properties $A(x, p)$ (i.e. stationary).

In an ergodic process, the ensemble average of a quantity equals its average over an infinite time interval:

$$\langle A(t) \rangle_{\text{ensemble}} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_{t-T/2}^{t+T/2} dt' A(t'). \quad (4.3)$$

To illustrate, let us return to our measurement of the pressure on the lid of a jar of gas. Instead of averaging over the whole Gibbs ensemble (many jars) at an instant t , let us pick one jar and plot the pressure registered by our delicate spring gauge as a function of time. Every time a molecule strikes the lid (or a group of molecules if the response time of

the gauge is greater than zero), the gauge will register a blip in pressure. The mean of the pressure-versus-time plot is P_0 , as before, and the variance relative to P_0 (the thickness of the curve) is of order $\delta P \sim N^{-1/2}P_0$.

Ergodicity is often valid in equilibrium and sometimes away from equilibrium. In practice, the ensemble average is nicer to use than the temporal average, because it is easier to work out which operators pass through the angle brackets (almost all do) rather than the $\int dt$ integral.

4.2 One-dimensional random walk

Most features of diffusive stochastic processes are captured in the simple example of a one-dimensional random walk. Imagine a drunk staggering up and down a long street. Suppose the drunk starts his journey at a lamp post (at $x = 0$) at $t = 0$. After contemplating his/her situation for a time Δt , they take a step either north or south along the street. After another time interval Δt , they take another step. And so on and so forth.

Suppose for simplicity, to begin with, that the steps are all of equal length $|\Delta x|$ but are directed north or south with equal probability. Then we know what happens. As time goes by, the drunk tends to move further and further away from the lamp post. In fact, his/her mean unsigned distance from the lamp post grows as $t^{1/2}$ at large t . Another way of saying this is $\langle x(t)^2 \rangle \propto t$. However, at any instant, they are equally likely to be north or south of the lamp post; if a large ensemble of drunks start this journey together, half will be found north of the lamp post at time t , and the other half south. Hence the mean displacement is zero, with $\langle x(t) \rangle = 0$.

What is the probability distribution function $p(x)$ of the positions of the ensemble of drunks? Well, the position of any one drunk at time t is a random variable $x(t) = \Delta x_1 + \dots + \Delta x_N$, where Δx_i is the i^{th} draw of a step from the step-size pdf. Of course the N draws can be thought of as N iid random variables. In the above example, we have a discrete pdf, $p(\Delta x) = [\delta(\Delta x + |\Delta x|) + \delta(\Delta x - |\Delta x|)]/2$, but of course the pdf can be continuous, even north-south biased, in more elaborate examples. By the central limit

theorem, $p(x)$ approaches a Gaussian in the limit $N \rightarrow \infty$, with zero mean and variance $N\Delta|x^2|$ in the above example. Note that the variance can be written as $|\Delta x|^2 t/\Delta t$ using $N = t/\Delta t$. We should be permitted to take time steps as small as possible without breaking the system, so for the variance to remain finite as $\Delta t \rightarrow 0$ we need $|\Delta x| \propto \Delta t^{1/2}$. We come back to this critical point below. Note that because of this scaling, diffusion is faster than the overall drift of the walkers [if $p(\Delta x)$ is skewed] for small t , but at large t the drift (if it is non-zero) takes over.

Now how does the pdf $p(x, t)$ change as a function of time? We know intuitively that as time passes the ensemble of drunks speards out further and further from the lamp post, so this problem does not have an equilibrium solution. But what is the pdf $p(x, t + \Delta t)$ at time step $t + \Delta t$ if we know the pdf $p(x, t)$ at the previous time step?

Well, walkers at position x at time $t + \Delta t$ must have come from positions $x - \Delta x$ at time t , where Δx is the random jump made by each walker in that time step. We now allow for the Δx jumps to have different sizes and a not necessarily symmetric north-south distribution, described by the pdf $p(\Delta x)$. Summing over all the possible Δx values, and using the sum and product rules for probabilities, we get

$$p(x, t + \Delta t) = \int_{-\infty}^{\infty} d(\Delta x) p(x - \Delta x, t) p(\Delta x) \quad (4.4)$$

That is, the probability of ending up at x equals the probability that you were at $x - \Delta x$ previously and made a jump of size Δx , summed over all the possible (mutually exclusive) Δx alternatives. This equation is called a master equation. It is plain common sense (at least, Einstein thought so!).

Now suppose that $\Delta x \propto (\Delta t)^{1/2} \rightarrow 0$ as above. Taylor expanding, we find

$$p(x, t) + \Delta t \frac{\partial p}{\partial t} + \mathcal{O}[(\Delta t)^2] = \int_{-\infty}^{\infty} d(\Delta x) p(\Delta x) \left[p(x, t) - \Delta x \frac{\partial p}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 p}{\partial x^2} \right] + \mathcal{O}[(\Delta x)^3]. \quad (4.5)$$

Now x is fixed in this equation, so it can be taken out of the Δx (jump) integrals, which can then be expressed in terms of the moments of the jumps, i.e.

$$\frac{\partial p}{\partial t} = -\frac{\langle \Delta x \rangle}{\Delta t} \frac{\partial p}{\partial x} + \frac{\langle (\Delta x)^2 \rangle}{2\Delta t} \frac{\partial^2 p}{\partial x^2}. \quad (4.6)$$

The correction terms, of order Δt and $(\Delta x)^3/\Delta t$, both go to zero as $\Delta t \rightarrow 0$, because we have $\langle \Delta x \rangle \propto \Delta t$ and $\langle (\Delta x)^2 \rangle \propto \Delta t$. There is no paradox here; the mean and the variance are independent quantities, just like in the central limit theorem, where both $\langle x \rangle = N\mu$ (drift) and $\langle x^2 \rangle = N\sigma^2$ (dispersion) scale proportional to N (and hence t). Likewise, there is no danger that $\langle \Delta x \rangle / \Delta t$ diverges as $\Delta t \rightarrow 0$, just because we have $\langle (\Delta x)^2 \rangle^{1/2} \propto (\Delta t)^{1/2}$.

✓ **Exercise:** Check all of these properties explicitly for the jump distribution

$$p(\Delta x) = \frac{1}{\sqrt{2\pi}\sigma} \exp[-(\Delta x - \mu)^2/(2\sigma^2)]. \quad (4.7)$$

4.3 Brownian motion

Consider a pollen grain suspended in a liquid. Under a microscope, the pollen grain executes a random walk as it is buffeted by molecules in the liquid. This phenomenon was discovered in 1827 by botanist Robert Brown, who was studying mushroom spores.

✓ **Exercise:** How many molecules strike the grain every second? Take the grain radius to be $a = 1\mu\text{m}$, the number density of H_2O molecules to be $n = 10^{28}\text{m}^{-3}$, and the thermal speed at STP to be $(k_B T/m_{\text{H}_2\text{O}})^{1/2} = 4 \times 10^2\text{m/s}$. (Answer: $3 \times 10^{19}/\text{s}$. The collisions are very frequent and uncorrelated from one instant to the next.)

Standard hydrodynamics states that for a slowly moving pollen grain, of radius a and mass m , moving with velocity \mathbf{v} , the equation of motion is

$$\frac{d\mathbf{v}}{dt} = -\frac{6\pi a\eta}{m}\mathbf{v}, \quad (4.8)$$

i.e. Stokess law for small Reynolds number flow ($\text{Re} = va/\nu$), where η is the dynamic viscosity and ($\nu = \eta/\rho$) is the kinematic viscosity. This equation says that a pollen grain given an initial kick $v(0)$ smoothly (exponentially) decelerates to rest over a time-scale $\gamma^{-1} = m/6\pi a\eta$. Clearly, it does not explain the stochastic jiggling observed under the microscope.

To model Brownian motion, we must acknowledge the existence of fluctuations in the (molecular) liquid. Add a new, stochastic fluctuating force, $\xi(t)$, called the Langevin source or noise term:

$$\frac{d\mathbf{v}(t)}{dt} = -\gamma\mathbf{v}(t) + \xi(t). \quad (4.9)$$

This is the Langevin equation, where the form of the fluctuating force, $\xi(t)$, is system dependent. In fact, we will see later that $\xi(t)$ is not a differentiable function; a special calculus was invented to handle such functions. However, we do know its ensemble-averaged properties:

- if the liquid is in equilibrium, the fluctuating force is stationary and has no preferred direction:

$$\langle \xi_i(t) \rangle = 0 \quad (4.10)$$

- if the correlation time of the fluctuating force τ_i (e.g. duration of a molecular collision or the time between collisions, whichever is greater) is much less than γ^{-1} , as expected for random molecular motion, and if the Cartesian components of the force are uncorrelated, we have

$$\langle \xi_i(t) \xi_j(t') \rangle = 2D\delta_{ij}\delta(t - t') \quad (4.11)$$

This type of fluctuation is called white noise (because its spectrum is flat, as we show below). D will later turn out to be a diffusion coefficient.

- ✓ **Exercise:** If $\xi(t)$ represents a delta-correlated white noise variable, show that the trajectory of that process (e.g. the trajectory of the random walker):

$$W(t) = \int_0^t dt' \xi(t') \quad (4.12)$$

known as a *Wiener process*, has autocorrelation function $\langle W(t)W(t') \rangle = 2D\min(t, t')$.

The Langevin equation, Eq. (4.9) by multiplying by an integrating factor $e^{\gamma t}$ to get:

$$v_i(t) = v_i(0)e^{-\gamma t} + e^{-\gamma t} \int_0^t dt' e^{\gamma t'} \xi_i(t') \quad (4.13)$$

where $v_i(0)$ is the macroscopic initial velocity of the pollen grain. This solution describes one particular realisation in the Gibbs ensemble of identically prepared experiments, i.e. the solution for one particular realisation of the random noise $\xi_i(t)$. To relate it to macroscopic measurements, we take the ensemble average over all these experiments. (Recall that the ensemble average passes through all the integrals.)

$$\langle v_i(t) \rangle = v_i(0)e^{-\gamma t} \quad (4.14)$$

$$\langle v_i(t)v_j(t) \rangle = e^{-2\gamma t} \left[v_i(0)v_j(0) + \int_0^t dt' \int_0^t dt'' e^{\gamma(t'+t'')} \langle \xi_i(t')\xi_j(t'') \rangle \right] \quad (4.15)$$

$$= e^{-2\gamma t} \left[v_i(0)v_j(0) + 2D\delta_{ij} \int_0^t dt' e^{2\gamma t'} \right] \quad (4.16)$$

$$= e^{-2\gamma t} \left[v_i(0)v_j(0) + \frac{2D\delta_{ij}}{\gamma} (e^{2\gamma t} - 1) \right]. \quad (4.17)$$

✓ **Exercise:** The Ornstein-Uhlenbeck process is a stochastic process whose output is coloured noise, i.e. noise that is correlated over a (short) time interval τ_c . If we use the OU process to generate the noise term of our Langevin equation, we get

$$\langle \xi_i(t')\xi_j(t'') \rangle = \frac{2D\delta_{ij}}{\tau_c} e^{-|t'-t''|/\tau_c}. \quad (4.18)$$

Show that this reduces to white noise as $\tau_c \rightarrow 0$. Also show that

$$\langle v_i(t)v_j(t) \rangle = e^{-2\gamma t} \left[v_i(0)v_j(0) + \frac{D\delta_{ij}}{\tau_c(\gamma^2 - \tau_c^{-2})} \left(1 + e^{2\gamma t} - 2e^{(\gamma-\tau_c^{-1})t} + \frac{1-e^{2\gamma t}}{\tau_c\gamma} \right) \right]. \quad (4.19)$$

✓ **Exercise:** Show directly from Eq. (4.13) that the velocity of the pollen grain is correlated with the white-noise Langevin force, and that the correlation time-scale is of order $1/\gamma$.

Answer: $\langle \xi_i(t')v_j(t) \rangle = 2D\delta_{ij}e^{-\gamma(t-t')}$ for $t' < t$; $\langle \xi_i(t')v_j(t) \rangle = 2D\delta_{ij}$ for $t' = t$ (δ -function integrated over half its width); $\langle \xi_i(t')v_j(t) \rangle = 0$ for $t' > t$ (causality).

✓ **Exercise:** Working again directly from Eq. (4.13), compute $\langle \xi_i(t')x_j(t) \rangle$, where we define the displacement $x_j(t) = x_j(0) + \int_0^t dt'' v_j(t'')$.

4.4 Fluctuation-dissipation theorem

Now let us consider a general stationary process, with $G_{ij}(\tau) = \langle \xi_i(t')\xi_j(t'') \rangle$ and $\tau = t'' - t'$. Then

$$\langle v_i(t)v_j(t) \rangle = e^{-2\gamma t} \left[v_i(0)v_j(0) + \int_0^t dt' \int_0^t dt'' e^{\gamma(t'+t'')} G_{ij}(t'' - t') \right] \quad (4.20)$$

$$= e^{-2\gamma t} \left[v_i(0)v_j(0) + \int_0^t dt' \int_{t'}^{t-t'} d\tau e^{\gamma(\tau+2t')} G_{ij}(\tau) \right]. \quad (4.21)$$

Suppose the correlation time of the noise term is very short compared to $1/\gamma$. Then $G_{ij}(\tau)$ is tiny except near $\tau = 0$. We therefore set $e^{\gamma\tau} \approx 1$ and, with minimal error, extend the integration limits to $\int_{-\infty}^{\infty} d\tau$:

$$\langle v_i(t)v_j(t) \rangle \approx e^{-2\gamma t} \left[v_i(0)v_j(0) + \int_0^t dt' e^{2\gamma t'} \int_{-\infty}^{\infty} d\tau G_{ij}(\tau) \right] \quad (4.22)$$

$$= e^{-2\gamma t} \left[v_i(0)v_j(0) + \frac{1}{2\gamma} (e^{2\gamma t} - 1) \int_{-\infty}^{\infty} d\tau G_{ij}(\tau) \right]. \quad (4.23)$$

In statistical equilibrium ($t \rightarrow \infty$),

$$\langle v_i(t)v_j(t) \rangle \rightarrow \frac{1}{2\gamma} \int_{-\infty}^{\infty} d\tau G_{ij}(\tau) \quad (4.24)$$

But we also know that $\langle v_i(t)v_j(t) \rangle = 3k_B T/m$ in thermal equilibrium (each degree of freedom carries mechanical energy $k_B T/2$), implying

$$\gamma = \frac{m}{6k_B T} \int_{-\infty}^{\infty} d\tau G_{ii}(\tau) \quad (4.25)$$

This result, originally due to Einstein, is amazing! It says that the macroscopic viscosity (recall: $\gamma = 6\pi a\eta/m$) is proportional to the correlation function of the microscopic fluctuating force - a seemingly unrelated quantity that doesn't even appear in the hydrodynamic equations. The fluctuation-dissipation theorem is ubiquitous in physics; it operates in any physical system which is lossy yet experiences thermal fluctuations in some microscopic quantity.

✓ **Exercise:** Starting from the equation of motion, show that

$$\frac{d}{dt} \left\langle \frac{1}{2} v_i(t) v_i(t) \right\rangle = -\gamma \langle v_i(t) v_i(t) \rangle + \langle \xi_i(t) v_i(t) \rangle \quad (4.26)$$

and hence argue that, in equilibrium, we have $\langle \xi_i(t) v_i(t) \rangle = 3\gamma k_B T = 3D$. Verify that this agrees with the result calculated directly in a previous exercise in Section 4.3.

4.5 Fluctuation spectra

An equivalent way to express the fluctuation-dissipation theorem is in terms of the spectral breakdown of the fluctuations. To see this, we first need to prove a very useful result called the *Wiener-Khintchine theorem*.

Let $\xi_i(t)$ be a stationary fluctuating force with Fourier transform $\xi(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} \xi_i(t)$. Note it is dangerous to introduce the Fourier transform so casually. A stationary process persists forever into the future and in the past, so it is not square integrable; strictly speaking, its Fourier transform does not exist. We should instead Fourier transform the truncated function $\xi_i^T(t)$, that equals $\xi_i(t)$ for $-T/2 \leq t \leq T/2$ and vanishes elsewhere, and take the limit $T \rightarrow \infty$ (at the end of the calculation). But since we are physicists we shall be sloppy, hence (assuming ξ is real)

$$\langle \xi_i(\omega) \xi_j^*(\omega') \rangle = \int_{-\infty}^{\infty} dt e^{i\omega t} \int_{-\infty}^{\infty} dt' e^{-i\omega' t'} \langle \xi_i(t) \xi_j^*(t') \rangle \quad (4.27)$$

$$= \int_{-\infty}^{\infty} dt e^{i\omega t} \int_{-\infty}^{\infty} d\tau e^{-i\omega'(\tau+t)} G_{ij}(\tau) \quad (4.28)$$

$$= \int_{-\infty}^{\infty} d\tau 2\pi\delta(\omega - \omega') e^{-i\omega'\tau} G_{ij}(\tau) \quad (4.29)$$

$$= 2\pi\delta(\omega - \omega') \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} G_{ij}(\tau) \text{ since } G_{ij}(\tau) = G_{ij}(-\tau) \quad (4.30)$$

$$= 2\pi\delta(\omega - \omega') G_{ij}(\omega). \quad (4.31)$$

Stationarity therefore implies that different frequency components of the fluctuating force are uncorrelated and $\langle \xi_i(\omega) \xi_j^*(\omega') \rangle = 2\pi\delta(\omega - \omega') G_{ij}(\omega)$.

We can now re-express the fluctuation-dissipation theorem as follows, in terms of the dc spectral component of the correlation function:

$$\gamma = \frac{m}{6k_B T} \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega\tau} G_{ii}(\omega) \quad (4.32)$$

$$= \frac{m}{6k_B T} \int_{-\infty}^{\infty} d\omega G_{ii}(\omega) \delta(\omega) \quad (4.33)$$

$$= \frac{m}{6k_B T} G_{ii}(\omega = 0). \quad (4.34)$$

The Wiener-Khintchine theorem is also useful when the Langevin equation is difficult to solve directly but easy to solve after Fourier transforming. By way of illustration, let us

examine Brownian motion again. Taking $v_i(0) = 0$ for simplicity, we know from Section 4.3 that the velocity autocorrelation function is given by

$$\langle v_i(t)v_j(t') \rangle = 2D\delta_{ij}e^{-\gamma(t+t')} \int_0^{\min(t,t')} dt'' \int_0^{\min(t,t')} dt''' e^{\gamma(t''+t''')} \delta(t'' - t''') \quad (4.35)$$

$$= \frac{D\delta_{ij}}{\gamma} [e^{-\gamma|t-t'|} - e^{-\gamma(t+t')}], \quad (4.36)$$

where the first line follows from Eq. (4.13) and the fact that $\delta(t'' - t''')$ vanishes for $\min(t, t') \leq t'', t''' \leq \max(t, t')$. The second line follows from the useful formula $\min(a, b) = (a + b - |a| - |b|)$.

If, instead, we proceed by Fourier transforming the Langevin equation of motion first, we obtain

$$v_i(\omega) = \frac{\xi_i(\omega)}{\gamma - i\omega} \quad (4.37)$$

and hence

$$\langle v_i(\omega)v_j^*(\omega') \rangle = \frac{2\pi\delta(\omega - \omega')G_{ij}(\omega)}{(\gamma - i\omega)(\gamma + i\omega')} \quad (4.38)$$

from the Wiener-Khintchine theorem. Writing the velocity autocorrelation function in terms of $v_i(\omega)$, we obtain (remembering that the velocity is real)

$$\langle v_i(t)v_j(t') \rangle = \int \frac{d\omega}{2\pi} \int \frac{d\omega'}{2\pi} e^{i(\omega't' - \omega t)} \langle v_i(\omega)v_j^*(\omega') \rangle \quad (4.39)$$

$$= \int \frac{d\omega}{2\pi} e^{i\omega(t' - t)} \frac{G_{ij}(\omega)}{\gamma^2 + \omega^2}. \quad (4.40)$$

For white noise fluctuations, we have $G_{ij}(\omega) = 2D\delta_{ij}$ and hence

$$\langle v_i(t)v_j(t') \rangle = \frac{D\delta_{ij}}{\gamma} \exp[-\gamma|t - t'|], \quad (4.41)$$

which equals Eq. (4.36) in the limit $t \rightarrow \infty$ and, $t' \rightarrow \infty$, where the initial conditions at $t = 0$ are forgotten; their memory dies away as $e^{-\gamma t}$, as in Eq. (4.13). In order to keep the initial conditions, you should Laplace transform everything instead of Fourier transforming (the Fourier transform assumes an infinite time base without special tricks), and use a Laplace version of the Wiener-Khintchine theorem. Note that diffusive processes cannot be analyzed with initial conditions at $t = -\infty$, an approach which would formally but

incorrectly remove the second term from Eq. (4.36), because their variance can become infinite in many cases when infinite time elapses. Another way of saying this is that the backwards diffusion problem is ill-posed.

✓ **Exercise:** Show that the Langevin equation for a simple harmonic oscillator driven by a white-noise force $\xi_i(t)$,

$$\frac{d^2x_i(t)}{dt^2} + \gamma \frac{dx_i(t)}{dt} + \omega_0^2 x_i(t) = \xi_i(t) \quad (4.42)$$

has an amplitude autocorrelation function in the limit $t \rightarrow \infty$ and $t' \rightarrow \infty$ given by

$$\langle x_i(t)x_j(t') \rangle = \frac{D\delta_{ij}}{\pi} \int d\omega \frac{e^{-i\omega(t-t')}}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2}. \quad (4.43)$$

4.6 Examples

4.6.1 Johnson noise

(Discovered in 1928.) An electric resistor *sitting on a table* spontaneously generates voltage fluctuations across its terminals which can be measured with a sensitive open-circuit voltmeter. The fluctuations occur because electrons jittering thermally inside the resistor are momentarily overrepresented at one end every instant. Naturally, the voltages dissipates heat, which limits their growth.

- Mean square open-circuit noise voltage measured by a noiseless bandpass filter between frequencies f and $f + \Delta f$:

$$\langle V^2 \rangle = 4Rk_B T \Delta f \quad \text{Nyquist theorem} \quad (4.44)$$

- Same power in each Hz of frequency (up to the electron collision frequency 10^{14} Hz). That is, the noise is white; its spectrum is flat, with all colours equally represented. However, no noise can be truly white; the resistor cannot emit infinite power! Non-white noise is called coloured; some frequencies are over-represented.

- Johnson noise is an absolute lower limit on the noise in any circuit.

- Instantaneous voltage $V(t)$ is unpredictable. The probability that it lies in the range $(V, V + dV)$ is $p(V)dV \propto e^{-V^2/(2\langle V^2 \rangle)}dV$.

✓ **Exercise:** How much power does a 1Ω resistor dissipate at room temperature?

4.6.2 Noisy quantum oscillator

(L. Mandel and E. Wolf, *Optical coherence and quantum optics*, §17.4.) Consider a quantum mechanical simple harmonic oscillator, S , with natural frequency ω_0 , that is brought into contact with a thermal reservoir, R , composed of an ensemble of $N \gg 1$ oscillators with natural frequencies ω_n . The Hamiltonian of the coupled system $S + R$ is

$$\hat{H} = \hbar\omega_0 \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) + \sum_n \hbar\omega_n \left[\hat{A}^\dagger(\omega_n) \hat{A}(\omega_n) + \frac{1}{2} \right] + \sum_n \hbar \left[g(\omega_n) \hat{a}^\dagger \hat{A}(\omega_n) + g^*(\omega_n) \hat{A}^\dagger(\omega_n) \hat{a} \right], \quad (4.45)$$

where the three terms give the energies of S , R , and the $S - R$ coupling respectively. Here, $(\hat{a}, \hat{a}^\dagger)$ and $(\hat{A}, \hat{A}^\dagger)$ are the creation and annihilation operators for S and each oscillator in R respectively, and $g(\omega_n)$ measures the coupling between S and the n^{th} oscillator in R .

In the Heisenberg picture, the reservoir oscillators evolve as

$$\frac{d\hat{A}(\omega_n, t)}{dt} = -\frac{i}{\hbar} [\hat{A}(\omega_n, t), \hat{H}] = -i\omega_n \hat{A}(\omega_n, t) - ig^*(\omega_n) \hat{a}(t) \quad (4.46)$$

since the creation and annihilation operators of *different* oscillators commute at any instant t . Similarly, the oscillator S evolves according to

$$\frac{d\hat{a}(t)}{dt} = -\frac{i}{\hbar} [\hat{a}(t), \hat{H}] \quad (4.47)$$

$$= -i\omega_0 \hat{a}(t) - i \sum_n g(\omega_n) \hat{A}(\omega_n, t) \quad (4.48)$$

$$= -i\omega_0 \hat{a}(t) - i \sum_n g(\omega_n) \hat{A}(\omega_n, 0) e^{-i\omega_n t} - \sum_n \int_0^t dt' \hat{a}(t') |g(\omega_n)|^2 e^{-i\omega_n(t-t')}, \quad (4.49)$$

where the last line follows from the middle one by integrating Eq. (4.46) and substituting the result.

As there are a lot of oscillators, all closely spaced in frequency, we can replace the sum by an integral. Defining the density of states $\eta(\omega)d\omega$, to be the number of oscillators with $\omega \leq \omega_n \leq \omega + d\omega$, we obtain

$$\sum_n \int_0^t dt' \hat{a}(t') |g(\omega_n)|^2 e^{-i\omega_n(t-t')} = \int_0^t dt' \hat{a}(t') \int_0^\infty d\omega' \eta(\omega') |g(\omega')|^2 e^{-i\omega'(t-t')}. \quad (4.50)$$

Moreover, as the oscillators in R are spread across a wide range of frequencies (bracketing, ω_0 , in general), the above integral will average internally to zero unless t is very close to t' . In other words, $\eta(\omega')|g(\omega')|^2$ is a slow function of ω' (i.e. it is not strongly peaked at ω_0) compared to $\exp[-i\omega'(t-t')]$, and we can bring it outside the integral. This yields

$$\sum_n \int_0^t dt' \hat{a}(t') |g(\omega_n)|^2 e^{-i\omega_n(t-t')} \approx \pi \eta(\omega_0) |g(\omega_0)|^2 \int_0^t dt' \hat{a}(t') \delta(t' - t) \quad (4.51)$$

$$= \pi \eta(\omega_0) |g(\omega_0)|^2 \hat{a}(t) \quad (4.52)$$

$$= \gamma \hat{a}(t), \quad (4.53)$$

where the first line follows by integrating $\exp[-i\omega'(t-t')]$ over positive frequencies only. The equation of motion for the oscillator S therefore reduces to the Langevin equation

$$\frac{d\hat{a}(t)}{dt} = -i\omega_0 \hat{a}(t) - \gamma \hat{a}(t) - i \sum_n g(\omega_n) \hat{A}(\omega_n, 0) e^{-i\omega_n t}. \quad (4.54)$$

The second term, which physically corresponds to damping, is proportional to $|g(\omega_0)|^2$ and hence the correlation amplitude of the fluctuations in the system, i.e. the stochastic couplings $g(\omega_n)$ of the $N \gg 1$ oscillators in R . It is another example of the *fluctuation-dissipation theorem*; macroscopic damping is generated by microscopic noise. The third term, the Langevin source, fluctuates because $\sum_n \exp(i\omega_n t)$ changes rapidly with t (indeed, it is δ correlated) due to the huge number of frequencies represented.

4.7 Fokker-Planck equation

4.7.1 Markov process

Definition: a stochastic process whose value ξ_{n+1} at the next measuring time t_{n+1} depends only on its value ξ_n at the present measuring time t_n .

Define $p(a|b)da db$ to be the probability density that a is true, in the range $(a, a + da)$, given that b is true, in the range $(b, b + db)$, for a continuous variable. Clearly, for a Markov process, we must have

$$p(\xi_{n+1}|\xi_n \xi_{n-1} \dots \xi_0) = p(\xi_{n+1}|\xi_n). \quad (4.55)$$

✓ **Exercise:** For a Markov process, given that $\xi(t)$ takes on the values $\xi_0, \xi_1 \dots \xi_n$, show that the probability density is given by

$$p(\xi_n|\xi_{n-1})p(\xi_{n-1}|\xi_{n-2})p(\xi_{n-2}|\xi_{n-3}) \dots p(\xi_1|\xi_0) \times p(\xi_0), \quad (4.56)$$

where $p(\xi_0)$ is the probability density of the initial value ξ_0 .

Examples of Markovian and non-Markovian processes

1. A coin toss does not even depend on ξ_{n-1} let alone $\xi_{n-2}, \xi_{n-3}, \dots$, hence even *simpler* than Markovian, actually called a *Bernoulli trial*:

$$p(\xi_n|\xi_{n-1}) = \frac{1}{2}\delta(\xi_n - 1) + \frac{1}{2}\delta(\xi_n + 1). \quad (4.57)$$

2. The sum of coin tosses: $X_n = \sum_{i=1}^n \xi_i$ is Markovian, i.e. it depends on X_{n-1} but no previous value:

$$p(X_n|X_{n-1}) = \frac{1}{2}\delta(X_n - X_{n-1} - 1) + \frac{1}{2}\delta(X_n - X_{n-1} + 1). \quad (4.58)$$

3. A continuous function $\xi(t)$ cannot be a Markov process because ξ_n depends on $\xi'(t_{n-1})$ which in turn depends on ξ_{n-2} :

$$\xi_n \approx \xi_{n-1} + \Delta t \xi'(t_{n-1}) \approx \xi_{n-1} + \Delta t \frac{\xi_{n-1} - \xi_{n-2}}{\Delta t} + \dots \quad (4.59)$$

However, many continuous functions (i.e. physical processes) are approximately Markovian, e.g. Brownian motion.

4.7.2 Chapman-Kolmogorov equation

Before deriving the Fokker-Planck equation we will first derive the Chapman-Kolmogorov equation, which will be used in the subsequent analysis of some of the properties of the Fokker-Planck equation. Consider the probability of the following sequence: ξ_0, ξ_1, ξ_2 at times t_0, t_1, t_2 . The probability of such a sequence occurring can be defined as

$$p(\xi_2\xi_1\xi_0) = p(\xi_2\xi_1|\xi_0)p(\xi_0). \quad (4.60)$$

If the process is Markovian then

$$p(\xi_2\xi_1|\xi_0)p(\xi_0) = p(\xi_2|\xi_1)p(\xi_1|\xi_0)p(\xi_0). \quad (4.61)$$

Hence for Markovian processes $p(\xi_2\xi_1|\xi_0) = p(\xi_2|\xi_1)p(\xi_1|\xi_0)$. Integrating over all possible intermediate outcomes ξ_1 results in the Chapman-Kolmogorov equation:

$$p(\xi_2|\xi_0) = \int d\xi_1 p(\xi_2|\xi_1)p(\xi_1|\xi_0). \quad (4.62)$$

Note that this deceptively simple expression is actually a complicated integral equation that mutually relates $p(a|b)$ for all possible a and b . It is hard to solve.

4.7.3 Fokker-Planck equation: derivation

Now consider a Markov process $x(t)$. Define a (conditional) *jump probability* $W(\mathbf{x}, t + \Delta t | \mathbf{x}', t)$ such that W is the probability that the process jumps from state x' at time t to x at time $t + \Delta t$. Then

$$p(\mathbf{x}, t + \Delta t) = \int d\mathbf{x}' W(\mathbf{x}, t + \Delta t | \mathbf{x}', t) p(\mathbf{x}', t) \quad (4.63)$$

$$= \int d\boldsymbol{\eta} W(\mathbf{x}, t + \Delta t | \mathbf{x} - \boldsymbol{\eta}, t) p(\mathbf{x} - \boldsymbol{\eta}, t) \quad (4.64)$$

$$= \int d\boldsymbol{\eta} W(\mathbf{x} - \boldsymbol{\eta} + \boldsymbol{\eta}, t + \Delta t | \mathbf{x} - \boldsymbol{\eta}, t) p(\mathbf{x} - \boldsymbol{\eta}, t), \quad (4.65)$$

where we have changed variables from \mathbf{x}' to $\boldsymbol{\eta} = \mathbf{x} - \mathbf{x}'$. The integrand is a function of two spatial coordinates: $\mathbf{y} \equiv \mathbf{x} - \boldsymbol{\eta}$ and $\mathbf{z} \equiv \boldsymbol{\eta}$. Suppose we restrict ourselves to small jumps, i.e. small $\boldsymbol{\eta}$. Holding $\mathbf{z} \equiv \boldsymbol{\eta}$ fixed for a moment, we expand the integrand as a Taylor series

about $\mathbf{y} = \mathbf{x}$:

$$\begin{aligned}
W(\mathbf{x} - \boldsymbol{\eta} + \boldsymbol{\eta}, t + \Delta t | \mathbf{x} - \boldsymbol{\eta}, t) p(\mathbf{x} - \boldsymbol{\eta}, t) &\approx W(\mathbf{x} + \boldsymbol{\eta}, t + \Delta t | \mathbf{x}, t) p(\mathbf{x}, t) \\
&+ (-\eta_i) \frac{\partial}{\partial y_i} [W(\mathbf{y} + \boldsymbol{\eta}, t + \Delta t | \mathbf{y}, t) p(\mathbf{y}, t)] \Big|_{\mathbf{y}=\mathbf{x}} \\
&+ \frac{(-\eta_i)(-\eta_j)}{2!} \frac{\partial^2}{\partial y_i \partial y_j} [W(\mathbf{y} + \boldsymbol{\eta}, t + \Delta t | \mathbf{y}, t) p(\mathbf{y}, t)] \Big|_{\mathbf{y}=\mathbf{x}} \\
&+ \dots
\end{aligned} \tag{4.66}$$

Integrate over $\boldsymbol{\eta}$, noting that $\int W(\mathbf{x} + \boldsymbol{\eta}, t + \Delta t | \mathbf{x}, t) = 1$ (the process must jump somewhere) and replacing \mathbf{y} by \mathbf{x} in the derivatives (to clean up the notation):

$$\begin{aligned}
p(\mathbf{x}, t + \Delta t) &= p(\mathbf{x}, t) \\
&- \frac{\partial}{\partial x_i} \int d\boldsymbol{\eta} \eta_i W(\mathbf{x} + \boldsymbol{\eta}, t + \Delta t | \mathbf{x}, t) p(\mathbf{x}, t) \\
&+ \frac{1}{2!} \frac{\partial^2}{\partial x_i \partial x_j} \int d\boldsymbol{\eta} \eta_i \eta_j W(\mathbf{x} + \boldsymbol{\eta}, t + \Delta t | \mathbf{x}, t) p(\mathbf{x}, t) - \dots
\end{aligned} \tag{4.67}$$

This implies

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = \lim_{\Delta t \rightarrow 0} \frac{p(\mathbf{x}, t + \Delta t) - p(\mathbf{x}, t)}{\Delta t} \tag{4.68}$$

$$= -\frac{\partial}{\partial x_i} \left[D_i^{(1)}(\mathbf{x}, t) p(\mathbf{x}, t) \right] + \frac{1}{2!} \frac{\partial^2}{\partial x_i \partial x_j} \left[D_{ij}^{(2)}(\mathbf{x}, t) p(\mathbf{x}, t) \right] - \dots, \tag{4.69}$$

where

$$D_{ijk\dots}^{(n)} \equiv \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int d\boldsymbol{\eta} (\eta_i \eta_j \eta_k \dots) W(\mathbf{x} + \boldsymbol{\eta}, t + \Delta t | \mathbf{x}, t) \tag{4.70}$$

$$= \lim_{\Delta t \rightarrow 0} \left\langle \frac{\Delta x_i \Delta x_j \Delta x_k \dots}{\Delta t} \right\rangle, \tag{4.71}$$

where $\langle \Delta x_i \Delta x_j \Delta x_k \dots \rangle$ is the n^{th} order cumulant. It describes the mean *jump* when the system scatters out of the state \mathbf{x} at time t . The ensemble average is taken over all parameters that govern the scattering process (except the independent variables \mathbf{x} and t , of course). For example, the angular displacement resulting from a two-body Coulomb collision is controlled by the impact parameter, i.e. the distance of closest approach; one must therefore average over the impact parameter in $\langle \dots \rangle$. In the above equations, $\Delta t \rightarrow 0$ means we take Δt to be much smaller than any macroscopic time-scale (e.g. $1/\gamma$ in Brownian motion). But Δt cannot really tend to zero, otherwise the Markovian assumption breaks down. You

can show rigorously that all terms $D_{ijk}^{(3)}$, $D_{ijkl}^{(4)}$ and higher order terms vanish for a Markov process. In this case the Fokker-Planck equation then reads:

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = -\frac{\partial}{\partial x_i} \left[D_i^{(1)}(\mathbf{x}, t) p(\mathbf{x}, t) \right] + \frac{1}{2} \frac{\partial^2}{\partial x_i \partial x_j} \left[D_{ij}^{(2)}(\mathbf{x}, t) p(\mathbf{x}, t) \right]. \quad (4.72)$$

The physical interpretation of the two coefficients $D_i^{(1)}(\mathbf{x}, t)$ and $D_{ij}^{(2)}(\mathbf{x}, t)$ is as follows:

- *Drift coefficient:* $D_i^{(1)}(\mathbf{x}, t) = \langle \Delta x_i / \Delta t \rangle$, often denoted by $A_i(\mathbf{x}, t)$, causes the peak of a unimodal probability distribution to shift to larger x when positive.
- *Diffusion coefficient:* $D_{ij}^{(2)}(\mathbf{x}, t) = \langle \Delta x_i \Delta x_j / \Delta t \rangle$, often denoted by $B_{ij}(\mathbf{x}, t)$, causes the peak of a unimodal probability distribution to broaden (or shrink, under special circumstances).

4.7.4 Linking the Fokker-Planck equation to the Langevin equation

Every Langevin equation has an associated Fokker-Planck equation (but not always vice-versa). Consider the following Langevin equation:

$$\frac{\partial x_i}{\partial t} = A_i(\mathbf{x}, t) + \xi_i(t). \quad (4.73)$$

Over a short time interval, $\Delta t \rightarrow 0$,

$$\Delta x_i = x_i(t + \Delta t) - x_i(t) = A_i(\mathbf{x}, t)\Delta t + \int_t^{t+\Delta t} dt' \xi_i(t'). \quad (4.74)$$

It is vital to note that the integral cannot be approximated by $\xi_i(t)\Delta t$, because the noise is delta correlated and therefore fluctuates wildly even in the tiny interval Δt .

The drift coefficient is defined in the following manner:

$$\langle \Delta x_i \rangle = \langle A_i(\mathbf{x}, t)\Delta t \rangle + \int_t^{t+\Delta t} dt' \langle \xi_i(t') \rangle = A_i(\mathbf{x}, t)\Delta t. \quad (4.75)$$

Hence,

$$D_i^{(1)}(\mathbf{x}, t) = A_i(\mathbf{x}, t). \quad (4.76)$$

The diffusion coefficient is defined in the following manner:

$$\begin{aligned}\langle \Delta x_i \Delta x_j \rangle &= \langle A_i(\mathbf{x}, t) A_j(\mathbf{x}, t) (\Delta t)^2 \rangle \\ &+ A_i(\mathbf{x}, t) \Delta t \int_t^{t+\Delta t} dt' \langle \xi_j(t') \rangle + A_j(\mathbf{x}, t) \Delta t \int_t^{t+\Delta t} dt' \langle \xi_i(t') \rangle \\ &+ \int_t^{t+\Delta t} dt' \int_t^{t+\Delta t} dt'' \langle \xi_i(t') \xi_j(t'') \rangle\end{aligned}\quad (4.77)$$

$$= A_i(\mathbf{x}, t) A_j(\mathbf{x}, t) (\Delta t)^2 + \int_t^{t+\Delta t} dt' \int_t^{t+\Delta t} dt'' G_{ij}(t'' - t'). \quad (4.78)$$

Changing variables from t'' to $\tau = t'' - t'$ gives

$$\langle \Delta x_i \Delta x_j \rangle = A_i(\mathbf{x}, t) A_j(\mathbf{x}, t) (\Delta t)^2 + \int_t^{t+\Delta t} dt' \int_{t-t'}^{t-t'+\Delta t} d\tau G_{ij}(\tau). \quad (4.79)$$

Assuming that the noise is close to δ correlated then

$$\langle \Delta x_i \Delta x_j \rangle \approx A_i(\mathbf{x}, t) A_j(\mathbf{x}, t) (\Delta t)^2 + \int_t^{t+\Delta t} dt' \int_{-\infty}^{\infty} d\tau G_{ij}(\tau) \quad (4.80)$$

$$= A_i(\mathbf{x}, t) A_j(\mathbf{x}, t) (\Delta t)^2 + \Delta t \int_{-\infty}^{\infty} d\tau G_{ij}(\tau) \quad (4.81)$$

Hence,

$$D_{ij}^{(2)}(\mathbf{x}, t) = \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \langle \Delta x_i \Delta x_j \rangle = \int_{-\infty}^{\infty} d\tau G_{ij}(\tau). \quad (4.82)$$

Higher order coefficients $D_{ijk}^{(3)}$ etc. are proportional to Δt , $(\Delta t)^2$, etc. and hence vanish as $\Delta t \rightarrow 0$. For the slightly more general Langevin equation,

$$\frac{\partial x_i}{\partial t} = A_i(\mathbf{x}, t) + B_{ij}(\mathbf{x}, t) \xi_j(t) \quad (4.83)$$

where the noise has unit amplitude, $\langle \xi_i(t) \xi_j(t') \rangle = \delta_{ij} \delta(t - t')$, the corresponding Fokker-Planck equation reads

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = - \frac{\partial}{\partial x_i} [A_i(\mathbf{x}, t)p(\mathbf{x}, t)] + \frac{1}{2} \frac{\partial^2}{\partial x_i \partial x_j} [B_{ik}(\mathbf{x}, t) B_{jk}(\mathbf{x}, t) p(\mathbf{x}, t)]. \quad (4.84)$$

4.7.5 Detailed balance

A Markov process satisfies detailed balance if, in the *steady state* (which may not exist; see section 4.7.7), each possible transition is as likely to occur as its time-reversed version.

For example, in a gas of particles, we have

$$p(\mathbf{x}, \mathbf{v}, t + \Delta t | \mathbf{x}', \mathbf{v}', t) p_s(\mathbf{x}', \mathbf{v}') = p(\mathbf{x}', -\mathbf{v}', t + \Delta t | \mathbf{x}, -\mathbf{v}, t) p_s(\mathbf{x}, \mathbf{v}), \quad (4.85)$$

where p_s is the steady-state probability distribution. For general variables \mathbf{x} (not necessarily spatial coordinates) that transform as $x_i \mapsto \hat{\epsilon}x_i$, $\hat{\epsilon} = \pm 1$, under time reversal, detailed balance is satisfied if and only if the following three conditions are met

1. $W(\mathbf{x}|\mathbf{x}')p_s(\mathbf{x}') = W(\hat{\epsilon}\mathbf{x}'|\hat{\epsilon}\mathbf{x})p_s(\mathbf{x})$;
2. $\hat{\epsilon}A_i(\hat{\epsilon}\mathbf{x})p_s(\mathbf{x}) = -A_i(\mathbf{x})p_s(\mathbf{x}) + \partial[B_{ij}(\mathbf{x})p_s(\mathbf{x})]/\partial x_j$. Note that $\hat{\epsilon}A_i$ is the i^{th} component of \mathbf{A} multiplied by ± 1 depending on how the i^{th} component of \mathbf{x} transforms.
3. $\hat{\epsilon}\hat{\epsilon}B_{ij}(\hat{\epsilon}\mathbf{x}) = B_{ij}(\mathbf{x})$. Note that $\hat{\epsilon}\hat{\epsilon}B_{ij}$ is the $(i,j)^{\text{th}}$ component of the matrix \mathbf{B} multiplied by ± 1 depending on how x_i transforms, then multiplied again by ± 1 depending on how x_j transforms.

✓ **Exercise:** Check that 1-dimensional Brownian motion in a potential (see section 4.7.6) satisfies detailed balance from the three conditions above. The stationary distribution for this problem is

$$p_s(x, v) \propto \exp[-m\Phi(x)/k_B T - mv^2/2k_B T]. \quad (4.86)$$

4.7.6 Einstein-Smoluchowski equation

If the relaxation time of one or more variables in the Fokker-Planck equation is very short, then the equations governing these variables quickly relax to a state with $d/dt = 0$ (for those variables) while the other variables are effectively constant over the relaxation time-scale. This situation is referred to as adiabatic elimination: the fast variables are slaved to the slow ones.

An important example is Brownian motion in a potential $\Phi(\mathbf{x})$. Note that position (of the pollen grain, say) is what one normally measures in such an experiment; it is very hard to measure the rapidly relaxed velocity. Therefore we now attempt to calculate how the pollen grain diffuses spatially:

$$\frac{dx_i}{dt} = v_i \quad (4.87)$$

$$\frac{dv_i}{dt} = -\gamma v_i - \frac{\partial \Phi}{\partial x_i} + \left(\frac{2k_B T \gamma}{m} \right)^{1/2} \xi_i(t), \quad (4.88)$$

with ξ_i being δ -correlated with unit amplitude. If γ is large (compared to the spatial diffusion timescale, to be calculated below) or, equivalently, if m is small, the relaxation of \mathbf{v} occurs very rapidly and we quickly get $d\mathbf{v}/dt \rightarrow 0$ before \mathbf{x} has a chance to change much:

$$\frac{dx_i}{dt} = v_i = \frac{1}{\gamma} \left[-\frac{\partial \Phi}{\partial x_i} + \left(\frac{2k_B T \gamma}{m} \right)^{1/2} \xi_i(t) \right]. \quad (4.89)$$

The corresponding Fokker-Planck equation for the probability distribution $q(\mathbf{x}, t)$, integrated over velocity \mathbf{v} , has $A_i = -\gamma^{-1} \partial \Phi / \partial x_i$ and $B_{ij} = (2k_B T / m \gamma)^{1/2} \delta_{ij}$:

$$\frac{\partial q(\mathbf{x}, t)}{\partial t} = \frac{1}{\gamma} \frac{\partial}{\partial x_i} \left[\frac{\partial \Phi(\mathbf{x})}{\partial x_i} q(\mathbf{x}, t) \right] + \frac{k_B T}{m \gamma} \frac{\partial^2}{\partial x_i \partial x_i} [q(\mathbf{x}, t)]. \quad (4.90)$$

This is the *Einstein-Smoluchowski* equation. It describes spatial diffusion and is valid if the time taken by the Brownian particle to diffuse a characteristic distance l satisfies $m \gamma l^2 / k_B T \gg \gamma^{-1}$.

4.7.7 Stationary solutions of the Fokker-Planck equation

Conservation of probability implies

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} + \frac{\partial}{\partial x_i} \left\{ A_i(\mathbf{x}, t)p(\mathbf{x}, t) - \frac{1}{2} \frac{\partial}{\partial x_j} [B_{ik}(\mathbf{x}, t)B_{jk}(\mathbf{x}, t)p(\mathbf{x}, t)] \right\} = 0. \quad (4.91)$$

The quantity in braces ($\{\dots\}$) is a probability current, denoted by $J_i(\mathbf{x}, t) = \{\dots\}$. If a stationary solution exists (which is not always the case), then the total flow of probability across any closed surface S (unit normal \mathbf{n}) is zero:

$$\int dS n_i J_i(\mathbf{x}) = 0. \quad (4.92)$$

An example where no nontrivial stationary solution exists is when perfume is released at a point in an infinite volume; it diffuses until $p = 0$ everywhere. However, if the perfume is released in a box with reflecting walls, a nontrivial stationary solution does exist, with $p = (\text{no. of molecules}) / (\text{volume of box})$ everywhere. In other words, the existence of a stationary solution depends not just on the system but also on the boundary conditions. Several kinds of boundary conditions are possible, the most common of which are described below.

4.7.8 Boundary conditions

1. *Reflecting barrier:* Particle can not leave an enclosed region:

$$\mathbf{n} \cdot \mathbf{J}(\mathbf{x}, t) = 0 \text{ zero current through wall} \quad (4.93)$$

2. *Absorbing barrier:* Particle removed from system when it touches the boundary. So the probability of being at the boundary vanishes:

$$p(\mathbf{x}, t) = 0 \text{ for } \mathbf{x} \in S. \quad (4.94)$$

3. *Discontinuity:* Both A_i and B_{ij} can be discontinuous at some surface while still permitting drift and diffusion to occur freely across the surface. Then $J_i(\mathbf{x}, t)$ and $p(\mathbf{x}, t)$ must be continuous across S (i.e. the solutions on both sides must match at S), although $\partial p / \partial x_i$ is not necessarily continuous.
4. *Periodic:* Interval $[a, b]$ whose endpoints are identified with each other; usually A_i and B_{ij} are periodic in this situation as well. Then $J_i(\mathbf{x}, t)$ and $p(\mathbf{x}, t)$ must be periodic.
5. *Infinity:* Normalisation of p usually requires $p \rightarrow 0$ and $\partial p / \partial x_i \rightarrow 0$ as $\mathbf{x} \rightarrow \infty$, as long as there is no inflow or outflow of probability current (e.g. an incoming beam of particles) at infinity.

4.7.9 Backward Fokker-Planck equation

In the previous sections, we interpret the Fokker-Planck equation as an evolution equation for the pdf $p(\mathbf{x}, t)$ subject to the initial condition $p(\mathbf{x}, t)|_{t=t_0}$, as befits a parabolic partial differential equation. Equivalently, we can interpret the Fokker-Planck equation as an evolutionary equation for the conditional probability $p(\mathbf{x}, t|\mathbf{x}_0, t_0)$ for any initial x_0 and t_0 , subject to the initial condition $p(\mathbf{x}, t_0|\mathbf{x}_0, t_0) = \delta(\mathbf{x} - \mathbf{x}_0)$. The initial conditions are manifestly identical via the relation (true for all t by common sense)

$$p(\mathbf{x}, t) = \int d\mathbf{x}_0 p(\mathbf{x}, t|\mathbf{x}_0, t_0) p(\mathbf{x}_0, t_0). \quad (4.95)$$

Under either interpretation, the distribution of initial states at time t_0 [either $p(\mathbf{x}, t_0)$ or $\delta(\mathbf{x} - \mathbf{x}_0)$] is assumed known, and the Fokker-Planck equation predicts the distribution of final states at a later time $t \geq t_0$.

One can also ask: given a known distribution of final states $p(\mathbf{x}, t)$ at time t , what distribution of initial states at a range of earlier times $t_0 \leq t$, could possibly lead to $p(\mathbf{x}, t)$? This question crops up when we wish to calculate the probability that a particle exits a region of state space in a given time (first passage or exit time problems). It reduces to finding an evolution equation for $p(\mathbf{x}, t|\mathbf{x}_0, t_0)$ for $t_0 \leq t$ subject to the initial (actually, final) condition $p(\mathbf{x}, t_0|\mathbf{x}_0, t_0) = \delta(\mathbf{x} - \mathbf{x}_0)$ as above [or equivalent, $p(\mathbf{x}, t_0)$]. This equation, derived below, is called the backwards Fokker-Planck equation to distinguish it from the forward Fokker-Planck equation discussed in previous sections. The two types of Fokker-Planck equation are mathematically equivalent.

To derive the backward Fokker-Planck equation, we apply the Chapman-Kolmogorov equation (section 4.7.2) to all the intermediate states \mathbf{x}' (with $\mathbf{x}' \in V$) at an arbitrary intermediate instant s , with $t_0 \leq s \leq t$:

$$p(\mathbf{x}, t|\mathbf{x}_0, t_0) = \int d\mathbf{x}' p(\mathbf{x}, t|\mathbf{x}', s)p(\mathbf{x}', s|\mathbf{x}_0, t_0). \quad (4.96)$$

The left-hand side is independent of s , implying

$$0 = \frac{\partial p(\mathbf{x}, t|\mathbf{x}_0, t_0)}{\partial s} \quad (4.97)$$

$$= \int_V d\mathbf{x}' \left[\frac{\partial p(\mathbf{x}, t|\mathbf{x}', s)}{\partial s} p(\mathbf{x}', s|\mathbf{x}_0, t_0) + p(\mathbf{x}, t|\mathbf{x}', s) \frac{\partial p(\mathbf{x}', s|\mathbf{x}_0, t_0)}{\partial s} \right] \quad (4.98)$$

$$\begin{aligned} &= \int_V d\mathbf{x}' \left\{ \frac{\partial p(\mathbf{x}, t|\mathbf{x}', s)}{\partial s} p(\mathbf{x}', s|\mathbf{x}_0, t_0) \right. \\ &\quad - p(\mathbf{x}, t|\mathbf{x}', s) \frac{\partial}{\partial x'_i} [A_i(\mathbf{x}', s)p(\mathbf{x}', s|\mathbf{x}_0, t_0)] \\ &\quad \left. + p(\mathbf{x}, t|\mathbf{x}', s) \frac{1}{2} \frac{\partial^2}{\partial x'_i \partial x'_j} [B_{ij}(\mathbf{x}', s)p(\mathbf{x}', s|\mathbf{x}_0, t_0)] \right\} \end{aligned} \quad (4.99)$$

The last line follows from the forward Fokker-Planck equation and $B_{ij}(\mathbf{x}', s) = \sum_k B_{ik}(\mathbf{x}', s)B_{jk}(\mathbf{x}', s)$. We now integrate the second and third terms in Eq. (4.99)

once and twice by parts respectively to obtain

$$\begin{aligned}
0 &= \int_V d\mathbf{x}' \left[\frac{\partial p(\mathbf{x}, t|\mathbf{x}', s)}{\partial s} p(\mathbf{x}', s|\mathbf{x}_0, t_0) \right. \\
&+ \frac{\partial p(\mathbf{x}, t|\mathbf{x}', s)}{\partial x'_i} A_i(\mathbf{x}', s) p(\mathbf{x}', s|\mathbf{x}_0, t_0) \\
&+ \frac{1}{2} \frac{\partial^2 p(\mathbf{x}, t|\mathbf{x}', s)}{\partial x'_i \partial x'_j} [B_{ij}(\mathbf{x}', s) p(\mathbf{x}', s|\mathbf{x}_0, t_0)] \Big] \\
&+ \int_{\partial V} dS'_i p(\mathbf{x}, t|\mathbf{x}', s) \left\{ -A_i(\mathbf{x}', s) p(\mathbf{x}', s|\mathbf{x}_0, t_0) + \frac{1}{2} \frac{\partial}{\partial x'_j} [B_{ij}(\mathbf{x}', s) p(\mathbf{x}', s|\mathbf{x}_0, t_0)] \right\} \\
&- \int_{\partial V} dS'_j \frac{\partial p(\mathbf{x}, t|\mathbf{x}', s)}{\partial x'_i} \frac{1}{2} B_{ij}(\mathbf{x}', s) p(\mathbf{x}', s|\mathbf{x}_0, t_0). \tag{4.100}
\end{aligned}$$

When formulating the backward Fokker-Planck equation, we are free to choose the boundary conditions on $p(\mathbf{x}, t|\mathbf{x}', s)$, so that the surface integrals $\int_{\partial V}$ vanish. A general treatment is given by W. Feller, Ann. Math. **55**, 227 (1952); see also Gardiner, Section 5.2.4. We treat two important special cases below.

1. *Absorbing barrier*: One has $p(\mathbf{x}', s|\mathbf{x}_0, t_0) = 0$ for $\mathbf{x}' \in \partial V$ in the forward Fokker-Planck equation. One also has $p(\mathbf{x}, t|\mathbf{x}', s) = 0$ for $\mathbf{x}' \in \partial V$ by common sense, because if a test particle touches ∂V at time s , it is absorbed; there is zero probability of finding it at $\mathbf{x} \in V$ at some later time $t \geq s$.
2. *Reflecting barrier*: The probability current [fourth and fifth terms in curly braces in Eq. (4.100)] vanishes for $\mathbf{x}' \in V$ in the forward Fokker-Planck equation. In order for the sixth term to also vanish for arbitrary s and hence arbitrary $p(\mathbf{x}', s|\mathbf{x}_0, t_0) \neq 0$, we must have in addition

$$0 = dS'_j \frac{\partial p(\mathbf{x}, t|\mathbf{x}', s)}{\partial x'_i} B_{ij}(\mathbf{x}', s), \tag{4.101}$$

for $\mathbf{x}' \in \partial V$.

With the surface integrals vanishing by construction, Eq. (4.99) tells us that the volume integral \int_V also vanishes. And it does so for arbitrary s and hence arbitrary $p(\mathbf{x}', s|\mathbf{x}_0, t_0)$. This is only possible if one has

$$-\frac{\partial p(\mathbf{x}, t|\mathbf{x}', s)}{\partial s} = A_i(\mathbf{x}', s) \frac{\partial p(\mathbf{x}, t|\mathbf{x}', s)}{\partial x'_i} + \frac{1}{2} B_{ij}(\mathbf{x}', s) \frac{\partial^2 p(\mathbf{x}, t|\mathbf{x}', s)}{\partial x'_i \partial x'_j}. \tag{4.102}$$

Equation (4.102) is the backward Fokker-Planck equation.

First exit time

The probability that a particle initially at $\mathbf{x}_0 \in V$ (at time t_0) is somewhere in V at time t is given by

$$G(t, \mathbf{x}_0, t_0) = \int_V d\mathbf{x} p(\mathbf{x}, t | \mathbf{x}_0, t_0). \quad (4.103)$$

Self-evidently, if all the boundaries are reflecting, $G(t, \mathbf{x}_0, t_0)$ equals unity for all $t \geq t_0$. However, if at least some of the boundaries are absorbing, $G(t, \mathbf{x}_0, t_0)$ decreases monotonically with time, i.e., $\partial G(t, \mathbf{x}_0, t_0) / \partial t \leq 0$ for all t ; once the test particle is absorbed, it leaves the system for good. Hence the cumulative probability (as a function of t) that the test particle is nowhere in V is $1 - G(t, \mathbf{x}_0, t_0)$.

The mean exit time $T(\mathbf{x}_0, t_0)$ is the average of t weighted by the pdf of t :

$$T(\mathbf{x}_0, t_0) = \int_0^\infty dt t \frac{\partial}{\partial t} [1 - G(t, \mathbf{x}_0, t_0)] \quad (4.104)$$

$$= \int_0^\infty dt G(t, \mathbf{x}_0, t_0), \quad (4.105)$$

where the second line follows from the first by integrating by parts, with $G(0, \mathbf{x}_0, t_0) = 1$ and $G(\infty, \mathbf{x}_0, t_0) = 0$.

What equation does $T(\mathbf{x}_0, t_0)$ satisfy? It is built from $p(\mathbf{x}, t | \mathbf{x}_0, t_0)$, with \mathbf{x} and t integrated out, so it is reasonable to guess that it satisfies a backward Fokker-Planck equation (or a close cousin). Indeed, we find

$$-\frac{\partial T(\mathbf{x}_0, t_0)}{\partial t_0} = A_i(\mathbf{x}_0, t_0) \frac{\partial T(\mathbf{x}_0, t_0)}{\partial x_{0i}} + \frac{1}{2} B_{ij}(\mathbf{x}_0, t_0) \frac{\partial^2 T(\mathbf{x}_0, t_0)}{\partial x_{0i} \partial x_{0j}}. \quad (4.106)$$

$T(\mathbf{x}_0, t_0)$ obeys the same boundary condition on ∂V as $p(\mathbf{x}, t | \mathbf{x}_0, t_0)$ does; see above. It is okay if some parts of the boundary are absorbing, while others are reflecting; no extra complications arise.

For the special case of a stationary process, which is invariant under time translation by definition [with $A_i(\mathbf{x}_0, t_0) = A_i(\mathbf{x}_0)$ and $B_{ij}(\mathbf{x}_0, t_0) = B_{ij}(\mathbf{x}_0)$], we have

$$p(\mathbf{x}, t | \mathbf{x}_0, t_0) = p(\mathbf{x}, 0 | \mathbf{x}_0, t_0 - t) \quad (4.107)$$

$$\frac{\partial p(\mathbf{x}, t | \mathbf{x}_0, t_0)}{\partial t} = -\frac{\partial p(\mathbf{x}, 0 | \mathbf{x}_0, t_0 - t)}{\partial t_0} = -\frac{\partial p(\mathbf{x}, t | \mathbf{x}_0, t_0)}{\partial t_0} \quad (4.108)$$

and hence

$$-\frac{\partial T(\mathbf{x}_0, t_0)}{\partial t_0} = -\int_0^\infty dt \frac{\partial G(t, \mathbf{x}_0, t_0)}{\partial t_0} = \int_0^\infty dt \frac{\partial G(t, \mathbf{x}_0, t_0)}{\partial t} \quad (4.109)$$

$$= G(\infty, \mathbf{x}_0, t_0) - G(0, \mathbf{x}_0, t_0) = -1. \quad (4.110)$$

✓ **Exercise:** Show that the n^{th} moment of the exit time, $T_n(\mathbf{x}_0, t_0)$, obeys the recursive backward Fokker-Planck equation:

$$A_i(\mathbf{x}_0) \frac{\partial T_n(\mathbf{x}_0)}{\partial x_{0i}} + \frac{1}{2} B_{ij}(\mathbf{x}_0) \frac{\partial^2 T_n(\mathbf{x}_0)}{\partial x_{0i} \partial x_{0j}} = -n T_{n-1}(\mathbf{x}_0) \quad (4.111)$$

for a stationary process.

4.7.10 Examples

Wiener process on an unbound interval

$$\text{Stochastic differential equation : } \frac{dx}{dt} = \xi(t) \quad (4.112)$$

$$\text{Fokker - Planck equation : } \frac{dp}{dt} = \frac{1}{2} \frac{\partial^2 p}{\partial x^2} \quad (4.113)$$

Solve in an infinite volume, with $p(x, 0) = \delta(x)$, i.e. all particles at the origin initially:

$$p(x, t) = \frac{1}{\sqrt{2\pi t}} e^{-x^2/2t}. \quad (4.114)$$

No stationary solution as $p(x, t) \rightarrow 0$ as $t \rightarrow 0$.

$$\text{Moments : } \langle x \rangle = 0, \quad \langle x^2 \rangle = t. \quad (4.115)$$

Ornstein-Uhlenbeck process with zero probability current

$$\text{Stochastic differential equation : } \frac{dx}{dt} = -\gamma x + D^{1/2} \xi(t) \quad (4.116)$$

$$\text{Fokker - Planck equation : } \frac{dp}{dt} = \frac{\partial \gamma x p}{\partial x} + \frac{D}{2} \frac{\partial^2 p}{\partial x^2} \quad (4.117)$$

Solve in an infinite volume, with $p(x, 0) = \delta(x - x_0)$. Many solution methods are possible; use whatever you please. One method (which does not always work!) is to reduce the Fokker-Planck equation to a first order PDE for the characteristic function

$$\tilde{p}(k, t) = \int_{-\infty}^{\infty} dx e^{-ikx} p(x, t)$$

$$\frac{\partial \tilde{p}}{\partial t} + \gamma k \frac{\partial \tilde{p}}{\partial k} = -\frac{Dk^2 \tilde{p}}{2}, \quad (4.118)$$

which has the following solution:

$$\tilde{p}(k, t) = \exp \left[-\frac{Dk^2}{4\gamma} (1 - e^{-2\gamma t}) - ikx_0 e^{-\gamma t} \right]. \quad (4.119)$$

Taking the inverse fourier transform:

$$p(x, t) = \left[\frac{\pi D}{\gamma} (1 - e^{-2\gamma t}) \right]^{-1/2} \exp \left[\frac{\gamma (x - x_0 e^{-\gamma t})^2}{D(1 - e^{-2\gamma t})} \right]. \quad (4.120)$$

Stationary solution as $t \rightarrow \infty$:

$$p_s(x) = \left[\frac{\pi D}{\gamma} \right]^{-1/2} \exp \left[\frac{\gamma x^2}{D} \right], \quad (4.121)$$

i.e. there is a balance between drag and diffusion in the steady state.

$$\text{Moments : } \langle x \rangle = x_0 e^{-\gamma t}, \quad \langle x^2 \rangle - \langle x \rangle^2 = \frac{D}{2\gamma} (1 - e^{-2\gamma t}). \quad (4.122)$$

✓ **Exercise:** Calculate the temporal correlation function directly from

$$\langle x(t)x(t') \rangle = \int dx_1 dx_2 x_1 x_2 p(x_1, t|x_2, t_2) p(x_2, t_2|x_0, t') = \frac{D}{2\gamma} e^{-\gamma|t-t'|}. \quad (4.123)$$

Hence the steady-state Ornstein-Uhlenbeck process is a physical model of a coloured noise source.

Ornstein-Uhlenbeck process with nonzero probability current

The first integral of the steady-state Fokker-Planck equation is

$$J = \gamma x p_s + \frac{D}{2} \frac{\partial p_s}{\partial x} \quad (4.124)$$

In a one-dimensional geometry, this means that a flux of particles is entering from the left of the system and exiting from the right. [In two or more dimensions, the latter statement

is not necessarily true; you can have an influx through $x = -a$ and an efflux through $y = b$ (say), with zero flux through $x = a$ and $y = -b$.] Integrating over the domain $-a \leq x \leq a$, we obtain

$$p_s(x) = C_2 \exp(-\gamma x^2/D) + \frac{2J}{D} \int_{-a}^x dx' \exp[-\gamma(x^2 - x'^2)/D]. \quad (4.125)$$

The undetermined constant C_2 is fixed by normalization:

$$1 = C_2 \int_{-a}^a dx \exp[-\gamma x^2/D] + \frac{2J}{D} \int_{-a}^a dx \int_{-a}^x dx' \exp[-\gamma(x^2 - x'^2)/D]. \quad (4.126)$$

Interestingly, though, the above equation shows that the process is not normalizable on the interval $(-\infty, \infty)$; the second integral on the right-hand side is logarithmically divergent.

✓ **Exercise:** Prove this, e.g. by changing variable to $(y, y') = (x' + x, x' - x)$.

Physically, the divergence arises because the process wants to produce a Gaussian pdf centred on $x = 0$, whose tails at $x = \pm\infty$ are vanishingly small - too small to support a nonzero flux. Lifting up the pdf by the required amount at the tails also lifts it everywhere else, leading to infinite area under the curve. There are two main sets of boundary conditions which circumvent this problem: (1) inject at $x = 0$ and let the particles escape at $x = \pm\infty$ (check this!), and (2) solve on a finite domain with absorbing boundaries at $x = \pm a$. In the latter case, setting $u = \gamma/D$ for convenience, we obtain

$$p_s(x) = u^{-1/2} \left[e^{u(a^2-x^2)} F(\sqrt{ua}) + F(\sqrt{ua}) \right], \quad (4.127)$$

where $F(x) = e^{-x^2} \int_0^x dy e^{y^2}$ is the Dawson function.

One-dimensional Wiener process with absorbing boundaries

$$\frac{\partial p}{\partial t} = \frac{1}{2} \frac{\partial^2 p}{\partial x^2}, \quad (4.128)$$

with $p(0, t) = p(1, t) = 0$. The eigenfunctions appropriate for absorbing boundaries are $\propto \sin(n\pi x)$, yielding

$$p(x, t) = \sum_{n=1}^{\infty} b_n(t) \sin(n\pi x), \quad (4.129)$$

with

$$\frac{db_n}{dt} = -\lambda_n b_n, \quad (4.130)$$

where $\lambda_n = n^2\pi^2/2$ and hence $b_n(t) = b_n(0)e^{-\lambda_n t}$. The initial condition $p(x, 0) = \delta(x - x_0)$ implies $b_n(0) = 2\sin(n\pi x_0)$. We therefore arrive at the probability distribution

$$p(x, t) = 2 \sum_{n=1}^{\infty} e^{-\lambda_n t} \sin(n\pi x_0) \sin(n\pi x). \quad (4.131)$$

Kramers escape problem

We wish to calculate the average time required for a Brownian particle to escape a potential barrier, e.g. to surmount the activation energy for a chemical reaction. In one dimension, the Fokker-Planck equation for such a system is given by

$$\frac{\partial p(t, x, v)}{\partial t} = -v \frac{\partial p}{\partial x} + U'(x) \frac{\partial p}{\partial v} + \gamma \left[\frac{\partial vp}{\partial v} + \frac{k_B T}{m} \frac{\partial^2 p}{\partial v^2} \right], \quad (4.132)$$

where the potential $U(x)$ has a minimum at $x = a$, a maximum at $x = b > a$, and tends to zero for $x \rightarrow 0$ and $x \rightarrow \infty$.

The Fokker-Planck equation has no analytic solution for general $U(x)$. However, we can get a rough idea of the answer by noting that we usually have $k_B T \ll W = U(b) - U(a)$. (In the opposite limit, the particle escapes immediately). Under these conditions, the escape rate is slow, i.e. $\partial p / \partial t \approx 0$ and the solution is roughly stationary:

$$p_s(x, v) = C \exp \left[-\frac{U(x) + mv^2/2}{k_B T} \right]. \quad (4.133)$$

As the escape rate is slow, the point $x = b$ is an absorbing barrier, with $p_s(x \geq b, v) = 0$; once particles breach the hump of the potential, they slide away to larger x and never return. This fixes the normalisation constant:

$$1 = \int_{-\infty}^{\infty} dv \int_{-\infty}^b dx p_s(x, v) \quad (4.134)$$

and hence

$$C^{-1} = 2\pi k_B T [mU''(a)]^{-1/2} \exp [-U(a)/k_B T]. \quad (4.135)$$

where we have used the fact that $U(x)$ is peaked near $x = a$, such that $U(x) \approx U(a) + U''(a)(x - a)^2/2$.

The *escape time* t_{esc} is inversely proportional to the particle flux through $x = b$:

$$t_{\text{esc}}^{-1} = \int_0^\infty dv v p_s(b, v) \quad (4.136)$$

$$= C e^{U(b)/k_B T} \int_0^\infty dv v e^{-mv^2/2k_B T} \quad (4.137)$$

$$= \frac{1}{2\pi} [U''(a)]^{1/2} \exp[-W/k_B T]. \quad (4.138)$$

The particle oscillates in the potential $U''(a)(x - a)^2/2$, hits the $x = b$ barrier $[U''(a)]^{1/2}/2\pi$ times per second, and has a probability $e^{-W/k_B T}$ each time of breaching the barrier. Note that the rate is exponentially slow since $W \gg k_B T$. This explains why, for instance, cracks and dislocations in a crystal propagate at a speed $\mu\text{m}/\text{yr}$ even though the local sound speed is $\approx \text{km}/\text{s}$.

4.8 Problems

- 1. Circular plantations:** A forest is planted on an infinite plain (*don't you just love theorists*). It starts from a single point and spreads radially in the absence of wind. When the experiment is repeated many times, it is found that, on average, the forest covers an area of 100ha after two years. The position of each tree satisfies a Langevin equation:

$$\frac{dx}{dt} = D^{1/2} \xi_x(t), \quad \frac{dy}{dt} = D^{1/2} \xi_y(t). \quad (4.139)$$

- (a) Evaluate D [Answer 7.96 ha/yr]
- (b) Now suppose the wind blows steadily from the south, i.e. in the positive y direction, causing the trees to move northward at 0.1km/yr. Rewrite the Langevin equation.
- (c) How rapidly does the area increase now?

- 2. Pendulum in air:** A damped pendulum suspended in air has a nonzero rms amplitude of oscillation in equilibrium, due to the impact of air molecules on its bob. Its

motion in one dimension can be described by the Langevin equations:

$$\frac{dx}{dt} = v \quad (4.140)$$

$$\frac{dv}{dt} = -\frac{k}{m}x - \gamma v + D^{1/2}\xi(t), \quad (4.141)$$

where x is the replacement and v is the velocity.

- (a) Write down the Fokker-Planck equation obeyed by the probability distribution function $f(t, x, v)$.

- (b) Derive the evolution equations for the first-order moments $d\langle x' \rangle/dt$ and $d\langle v \rangle/dt$.

The system is closed. What does it describe physically?

- (c) Derive the evolution equations for the second-order moments $\langle x^2 \rangle$, $\langle xv \rangle$, and $\langle v^2 \rangle$.

- (d) Show that we have:

$$\langle x^2 \rangle = D/2\gamma k, \quad \langle v^2 \rangle = D/2\gamma. \quad (4.142)$$

in equilibrium. What is the form of the fluctuation-dissipation theorem in this system?

- (e) Check your answer to the above by solving the steady-state Fokker-Planck equation explicitly.

3. **Bacterial chemotactic motion:** Escherichia coli is an intestinal bacterium with a cylindrical body $1\mu\text{m}$ in diameter and $2\mu\text{m}$ in length. It propels itself via six helical flagella. When the flagella spin counterclockwise, they form a synchronous bundle and the bacterium moves in a straight line (run) with a drift speed of $20\mu\text{m}/\text{s}$. During this run, the bacterium also tumbles due to rotational Brownian motion. When the flagella spin clockwise, the bundle comes apart and the cell moves along an erratic path (tumble) which reorients it randomly. The tumbles exhibit memory or persistence: the mean angle between the new and previous swimming direction is $\approx 62^\circ$.

In this question, we consider the simple situation of the rotational Brownian motion during a run. Let $p(\theta, \phi) \sin \theta d\theta d\phi$ be the probability that the swimming direction

lies in an infinitesimal solid angle about (θ, ϕ) , with $\theta = 0$ along the z axis. Then p satisfies the Foker-Planck equation:

$$\frac{\partial p}{\partial t} = D \left(\frac{\partial^2 p}{\partial \theta^2} + \cot \theta \frac{\partial p}{\partial \theta} \right), \quad (4.143)$$

with $D \approx 0.062/\text{s}$ determined experimentally. For an ensemble of bacteria, all with initial direction $\theta = 0$, show that we have

$$\langle \cos \theta \rangle = \exp(-2Dt). \quad (4.144)$$

4. Compulsive Gambler: Every evening, Andrew visits Reverend Bob's 24-Hour Chapel and Casino in Nevada, bearing $x_0 = \$1000$ in his wallet, the daily takings from his hydroponic tomato farm. He bets compulsively on every turn of the roulette wheel, once per minute, staking $f = 5\%$ of his outstanding capital at every turn and always playing red. He quits when he reaches $x_w = \$2000$ or sinks below the table minimum, $x_m = \$10$.

- (a) Research (theoretically) the odds for colour bets in American roulette.
- (b) If Andrew tracks his fortune over the course of each evening and constructs a pdf $p(x, t)$ of his capital x at time t (where $t = 0$ corresponds to when he walks in the door), argue that the pdf obeys the Fokker-Planck equation:

$$\frac{\partial p(x, t)}{\partial t} = \frac{f(1 - 2q)}{\tau} \frac{\partial}{\partial x} [xp(x, t)] + \frac{f^2}{2\tau} \frac{\partial^2}{\partial x^2} [x^2 p(x, t)], \quad (4.145)$$

where $q = 9/19$ and $\tau = 60\text{s}$.

- (c) Argue that the probability that Andrew is still sitting at the table after a time t is given by

$$G(x_0, t) = \int_{x_m}^{x_w} dx' p(x', t | x_0, 0). \quad (4.146)$$

- (d) Show that, if $p(x, t)$ satisfies a homogeneous Fokker-Planck equation of the form

$$\frac{\partial p(x, t)}{\partial t} = -\frac{\partial}{\partial x} [A(x)p(x, t)] + \frac{1}{2} \frac{\partial^2}{\partial x^2} [B(x)^2 p(x, t)], \quad (4.147)$$

the $G(x_0, t)$ satisfies the relation

$$\frac{\partial G(x_0, t)}{\partial t} = A(x_0) \frac{\partial}{\partial x_0} [G(x_0, t)] + \frac{B(x_0)^2}{2} \frac{\partial^2}{\partial x_0^2} [G(x_0, t)], \quad (4.148)$$

- (e) Show on average, Andrew sits at the table every evening for a time

$$T(x_0) = \int_0^\infty dt G(x_0, t) \quad (4.149)$$

and that $T(x_0)$ satisfies

$$-1 = A(x_0) \frac{dT(x_0)}{dx_0} + \frac{B(x_0)^2}{2} \frac{d^2 T(x_0)}{dx_0^2}. \quad (4.150)$$

with the boundary condition $T(x_m) = T(x_w) = 0$.

- (f) Evaluate $T(x_0)$, the average time Andrew spends in the Casino.

Chapter 5

Birth and death processes

5.1 Birth and death

Birth-death processes involve populations of (animate or inanimate!) individuals who make transitions between states. As a result, the occupation numbers of the states change in discrete jumps; individuals in particular states are created or destroyed. Examples include the creation and destruction of quantum mechanical particles (\hat{a} , \hat{a}^\dagger), the production and consumption of molecules in chemical reaction networks, and the birth and death of living organisms.

5.1.1 Predator prey (Lotka-Volterra) ecology

Let X be the prey, A be the preys food, and Y be the predator. (An example would be rabbits, carrots, and foxes respectively.) Simple ecology:



If the populations are large ($N \gg 1$), we can approximate the population densities by continuous variables, e.g. x is the number of prey per unit area of land. The populations

then evolve according to a deterministic system of ODEs known as the Lotka-Volterra equations:

$$\begin{aligned}\frac{dx}{dt} &= k_1ax - k_2xy \\ \frac{dy}{dt} &= k_2xy - k_3y\end{aligned}\tag{5.4}$$

Here, a is the population density of the preys food; it is held constant. In our example, this is equivalent to assuming that the supply of carrots is unaffected by the rabbits eating habits. The term k_1ax is the rate at which the prey feeds and reproduces; it is proportional to the likelihood ax that the prey finds food. The term k_2xy is the rate at which the prey is eaten (and the predator reproduces); it is proportional to the likelihood xy that the prey and predator encounter each other. The term k_3y is the rate at which the predator dies a natural death; plainly, it is proportional to the number of predators.

- ✓ **Exercise:** Common sense suggests that without the process $Y \rightarrow 0$ the total population reaches a constant value; there is no mechanism for removing foxes, but no more foxes can be born after a while, because all the rabbits are being eaten as quickly as they are born. Prove this from Eq. (5.4).
- ✓ **Exercise:** One would expect to find a fourth process in the above ecology, namely $X \xrightarrow{k_4} 0$ (prey dies naturally). Show that this process can be absorbed into the rate k_1 .

Later in the course, we will show that the solutions of Eq. (5.4) are limit cycles that persist indefinitely provided one has $ak_1/k_3 > 0$. This would normally hold true except in a famine, where X 's death rate can be large enough to render k_1 negative; see above exercise. The prey flourish initially; their numbers stimulate multiplication of predators, who subsequently decimate the prey and therefore (ironically) their own food supply; the predators dwindle due to famine, allowing the prey to regenerate in peace and quiet; and the cycle starts anew.

5.1.2 An idealised model

The Lotka-Volterra model makes several unrealistic assumptions:

1. Individuals within the populations are identical.
2. The environment has an infinite carrying capacity.
3. Births and deaths occur instantaneously; consequently, their rates at any instant are functions of the population densities at any instant.

The model can be generalised easily to accommodate diversity within the populations by replacing x, y, \dots by probability distributions $f_X(q), f_Y(q), \dots$, where the populations are subdivided according to some measurable characteristic q .

5.1.3 Environmental carrying capacity

The issue of carrying capacity leads to some interesting mathematics. One simple way to incorporate it is by adding a (negative) nonlinear term to the population evolution equation, causing growth to saturate once the population reaches a certain size. Consider a single species (e.g. humans) for simplicity, with natural birth rate k_1 , i.e. $dx/dt = k_1x$, where x is the population density. In an infinite environment, x grows exponentially, leading to the famous Malthusian (1798) catastrophe, where we are all standing on each others toes! However, as x increases, there is heightened competition for limited resources in a unit area of land, and the death rate (due to disease, famine, and the like) rises in proportion to the probability that individuals encounter each other:

$$\frac{dx}{dt} = k_1x - k_2x^2. \quad (5.5)$$

The solution of this equation, called the logistic equation, is given by

$$x(t) = \frac{x(0) \exp[k_1 t]}{1 + k_2 k_1^{-1} x(0) (\exp[k_1 t] - 1)}. \quad (5.6)$$

It shows explicitly that the population tends to a finite value k_1/k_2 (the carrying capacity). For $x(0) < k_1/2k_2$, the curve has a distinctive *S* shape, known as a sigmoid.

Now consider the situation where the population evolves over discrete time steps (e.g. generations). We replace the logistic equation by its discrete analogue, the logistic map:

$$x_{n+1} = k_1 x_n - k_2 x_n^2. \quad (5.7)$$

This map was first studied in depth by the Australian-born physicist and mathematical biologist Robert May in the 1960s. It is special because it has chaotic solutions. For $3 < k_1 < k'$, the map has a stable solution of period 2; i.e. $x_{n+2} = x_n$ for $n > n_{\min}$. For $k' < k_1 < k''$, the map has a stable solution of period 2^2 . For $k'' < k_1 < k'''$, the stable solution is of period 2^3 , and so on. Finally, for $k_1 > 3.828$, the map generates chaotic sequences of iterates with stable periods of all orders, even and odd! This is the classic period-doubling route to chaos. If you would like to learn more about the intricate mathematical structure of the logistic map, e.g. the fact that its trajectories, taken together, constitute a Cantor set (which is self-similar, or fractal), you should consult any book on chaos, such as Chapter 1 of R. L. Devaney, *An Introduction to Chaotic Dynamical Systems* (1989).

5.1.4 Delays

In physical and chemical systems, transition rates between discrete states commonly depend on the state occupation numbers at the instant of the transition. By contrast, time delays are often built into biological systems, to account for factors like the time to reach sexual maturity, the gestation period, the latent consequences of environmental degradation, the incubation period of diseases, and so on. One interesting consequence of delays is that, when they are not too short or too long (in a sense that can be made precise), they lead naturally to cycles in a population whose evolution would otherwise be monotonic. In his classic book, May applied this idea to explain quantitatively the 35 – 40 day cycles observed painstakingly by Nicholson in local populations of the Australian sheep-blowfly (*Lucilia cuprina*), which takes 11 days to mature from a larva into an adult (R. M. May, *Stability and complexity in model ecosystems*, 1975).

To illustrate the emergence of cycles, consider the simple case of a population in famine,

with $dx(t)/dt = -\pi x(t)/2T$ and hence $x(t) = x(0) \exp(-\pi t/2T)$. If the death rate at time t is instead taken to depend on the population at time $t-T$, to account for the latent effect of environmental degradation (i.e. the death rate today is determined by the toxins released by our ancestors), then we find $dx(t)/dt = -\pi x(t-T)/2T$ and hence $x(t) = x(0) \cos(\pi t/2T)$. A monotonic decline in population is therefore converted into a persistent cycle! Note that cyclic behaviour cannot arise unless the ratio of the e-folding time to the delay (here $2/\pi$) lies in a certain range, as discussed above.

✓ **Exercise:** Verify the cyclic solution by substitution and justify it using common sense.

✓ **Exercise:** For what range of λT does $dx(t)/dt = -\lambda x(t-T)$ admit a cyclic solution?

5.2 Master equations

5.2.1 An example: predator prey ecology

In real N-body systems, the populations fluctuate about deterministic trends. One way to model this is by replacing the continuous ODEs with a master equation describing discrete jumps between states. For the Lotka-Volterra ecology in Sec. 5.1.1, we have

$$p(x \rightarrow x + 1, y \rightarrow y) = k_1 ax \Delta t \quad (5.8)$$

$$p(x \rightarrow x - 1, y \rightarrow y + 1) = k_2 xy \Delta t \quad (5.9)$$

$$p(x \rightarrow x, y \rightarrow y - 1) = k_3 y \Delta t \quad (5.10)$$

$$p(x \rightarrow x, y \rightarrow y) = 1 - (k_1 ax + k_2 xy + k_3 y) \Delta t \quad (5.11)$$

and hence

$$\begin{aligned} p(x, y, t + \Delta t) &= k_1 a(x - 1)p(x - 1, y, t)\Delta t \\ &\quad + k_2(x + 1)(y - 1)p(x + 1, y - 1, t)\Delta t \\ &\quad + k_3(y + 1)p(x, y + 1, t)\Delta t \\ &\quad + [1 - (k_1 ax + k_2 xy + k_3 y) \Delta t] p(x, y, t). \end{aligned} \quad (5.12)$$

Note that the LHS is the probability of being in the state (x, y) at time $t + \Delta t$. So the first term on the RHS describes the transition $(x - 1, y) \rightarrow (x, y)$, via the process $X + A \rightarrow 2X$, and hence is proportional to $a(x - 1)$ rather than ax , as one might naively suppose. Moreover, the fourth term on the RHS describes the status quo $(x, y) \rightarrow (x, y)$ and is therefore the probability that none of the three possible transitions out of the state (x, y) occurs. The probability distribution then evolves according to the master equation

$$\frac{\partial p(x, y, t)}{\partial t} = \frac{p(x, y, t + \Delta t) - p(x, y, t)}{\Delta t}. \quad (5.13)$$

Note that the transitions are Markovian; the current state fully determines the next state in a statistical sense. This may be appropriate in chemical reactions, say, but is less common in ecologies, where history matters.

The master equation does not have a simple solution. This is because, interestingly, it contains the fluctuations within its own solution, unlike the Langevin equation, where the fluctuations are inserted manually via the noise term. In other words, the master equation generates fluctuations as well as secular trends. The (fractional) fluctuations are typically of order $\sim N^{-1/2}$, for a system of N individuals.

- ✓ **Exercise:** Simulate the predator-prey ecology using a Monte Carlo approach. Plot your results on top of the solution of Eq. (5.4) in the $x - y$ plane. Do you see fluctuations around the deterministic solution?

5.2.2 General theory

A master equation is a Chapman-Kolmogorov equation for Markov processes. It governs the evolution of state occupation numbers by summing up the gain and loss probabilities into and out of each state. Chapman-Kolmogorov (see Secs. 4.7.2 and 4.7.3):

$$p(\mathbf{x}, t + \Delta t) = \int d\mathbf{x}' W(\mathbf{x}, t + \Delta t | \mathbf{x}', t) p(\mathbf{x}', t). \quad (5.14)$$

Separately, the integral of jump probabilities over the possible final states is unity. Considering for a moment the reverse (but not time-reversed) jumps $\mathbf{x} \rightarrow \mathbf{x}'$, we have

$$1 = \int d\mathbf{x}' W(\mathbf{x}', t + \Delta t | \mathbf{x}, t) \quad (5.15)$$

and hence

$$p(\mathbf{x}, t) = \int d\mathbf{x}' W(\mathbf{x}', t + \Delta t | \mathbf{x}, t) p(\mathbf{x}, t). \quad (5.16)$$

Combining Eqs. (5.14) and (5.16):

$$\begin{aligned} \frac{\partial p(\mathbf{x}, t)}{\partial t} &= \lim_{\Delta t \rightarrow 0} \frac{p(\mathbf{x}, t + \Delta t) - p(\mathbf{x}, t)}{\Delta t} \\ &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int d\mathbf{x}' [W(\mathbf{x}, t + \Delta t | \mathbf{x}', t) p(\mathbf{x}', t) - W(\mathbf{x}', t + \Delta t | \mathbf{x}, t) p(\mathbf{x}, t)] \end{aligned} \quad (5.17)$$

$$\begin{aligned} &= \lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \int d\mathbf{x}' \{ [W(\mathbf{x}, t + \Delta t | \mathbf{x}', t) - W(\mathbf{x}, t | \mathbf{x}', t)] p(\mathbf{x}', t) \\ &\quad - [W(\mathbf{x}', t + \Delta t | \mathbf{x}, t) - W(\mathbf{x}', t | \mathbf{x}, t)] p(\mathbf{x}, t) \}, \end{aligned} \quad (5.18)$$

where we use $W(\mathbf{x}, t | \mathbf{x}', t) = \delta(\mathbf{x} - \mathbf{x}') = W(\mathbf{x}', t | \mathbf{x}, t)$ since a jump from \mathbf{x} to \mathbf{x}' instantly (i.e. at same t) is impossible unless $\mathbf{x} = \mathbf{x}'$, when it is certain.

Now define the *transition rate* to be the rate of change of the transition probability density:

$$T(\mathbf{x}, \mathbf{x}', t) = \lim_{\Delta t \rightarrow 0} \frac{W(\mathbf{x}, t + \Delta t | \mathbf{x}', t) - W(\mathbf{x}, t | \mathbf{x}', t)}{\Delta t} \quad (5.20)$$

then the Master equation becomes:

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = \int d\mathbf{x}' [T(\mathbf{x}, \mathbf{x}', t) p(\mathbf{x}', t) - T(\mathbf{x}', \mathbf{x}, t) p(\mathbf{x}, t)], \quad (5.21)$$

where the first term describes scattering out of all intermediate states \mathbf{x}' into \mathbf{x} , and the second term describes scattering out of \mathbf{x} into all states \mathbf{x}' . Note that $\int d\mathbf{x} T(\mathbf{x}, \mathbf{x}', t) = 0$ since both W s in the definition integrate to unity (i.e. for each W , there must be a jump to some final state, and there is no loss of probability from the system). Hence the second term in the master equation is zero by construction:

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = \int d\mathbf{x}' T(\mathbf{x}, \mathbf{x}', t) p(\mathbf{x}', t). \quad (5.22)$$

Often, however, the symmetric form, Eq. (5.21), is preferable.

5.3 Examples

5.3.1 Birth and death in a single species

Let X be a species and x be the number of individuals in that species. Suppose individuals are born or die one at a time.

$$x \rightarrow x + 1 \quad T^+(x) = \text{transition rate for birth} \quad (5.23)$$

$$x \rightarrow x - 1 \quad T^-(x) = \text{transition rate for death} \quad (5.24)$$

then

$$\frac{\partial p(x, t)}{\partial t} = T^+(x-1)p(x-1, t) + T^-(x+1)p(x+1, t) - [T^+(x) + T^-(x)]p(x, t), \quad (5.25)$$

where the term in [...] describes removal (by birth or death) out of state x .

There is no general method to solve this master equation for $p(x, t)$ given arbitrary rates $T^\pm(x)$. However, it is possible to obtain the stationary distribution $p_s(x)$ as follows:

$$0 = -T^+(x')p_s(x') + T^-(x'+1)p_s(x'+1) - [-T^+(x'-1)p_s(x'-1) + T^-(x')p_s(x')]. \quad (5.26)$$

Add up from $x' = 0$ to $x' = x-1$, noting that the first two terms at one x' value cancel the last two terms at the next:

$$0 = -T^+(x-1)p_s(x-1) + T^-(x)p_s(x) - [-T^+(-1)p_s(-1) + T^-(0)p_s(0)]. \quad (5.27)$$

Here, $T^-(0)$ vanishes, because individuals cannot die when there are none present, and $p_s(-1)$ vanishes, because one cannot have negative populations. This gives

$$\frac{p_s(x)}{p_s(x-1)} = \frac{T^+(x-1)}{T^-(x)} \quad (5.28)$$

and hence

$$p_s(x) = p_s(0) \prod_{x'=1}^x \frac{T^+(x'-1)}{T^-(x')}. \quad (5.29)$$

We can also calculate how the mean population evolves without solving explicitly for $p(x, t)$:

$$\frac{d}{dt} \langle x(t) \rangle = \sum_{x=0}^{\infty} x \frac{\partial p(x, t)}{\partial t} \quad (5.30)$$

$$\begin{aligned} &= \sum_{x=0}^{\infty} x T^+(x-1)p(x-1, t) + \sum_{x=0}^{\infty} x T^-(x+1)p(x+1, t) \\ &- \sum_{x=0}^{\infty} x [T^+(x) + xT^-(x)] p(x, t) \end{aligned} \quad (5.31)$$

$$\begin{aligned} &= \sum_{x'=-1}^{\infty} (x'+1) T^+(x') p(x', t) + \sum_{x'=1}^{\infty} (x'-1) T^-(x') p(x', t) \\ &- \sum_{x=0}^{\infty} x [T^+(x) + T^-(x)] p(x, t) \end{aligned} \quad (5.32)$$

$$\begin{aligned} &= \sum_{x=0}^{\infty} [(x+1)T^+(x) + (x-1)T^-(x) - xT^+(x) - xT^-(x)] p(x, t) \\ &\quad (5.33) \end{aligned}$$

$$= \langle T^+[x(t)] \rangle - \langle T^-[x(t)] \rangle, \quad (5.34)$$

where we use $p(-1, t) = 0$ and $T^-(0) = 0$ to extend the first two sums in the second-last line. Thus, the continuous variable $x(t)$ achieves a steady state when $\langle T^+(x) \rangle = \langle T^-(x) \rangle$. Compare the discrete situation, where the most likely state (modal value of x) is the one with maximum $p_s(x)$, i.e. the one for which $p_s(x)$ and $p_s(x-1)$ differ as little as possible. This happens when

$$T^+(x-1) = T^-(x), \quad (5.35)$$

i.e. detailed balance: the birth rate into x equals the death rate out of x .

5.3.2 Biomolecular chemical reaction

Consider the following reaction:



with A at a fixed concentration a . The resulting master equation is

$$\frac{\partial p(x, t)}{\partial t} = k_2 a p(x-1, t) + k_1 (x+1) p(x+1, t) - (k_1 x + k_2 a) p(x, t), \quad (5.37)$$

where the first term *consumes* A to produce X : $x - 1 \rightarrow x$, the second term *consumes* X to produce A : $x + 1 \rightarrow x$.

To solve this, we introduce the *generating function*:

$$G(s, t) = \sum_{x=0}^{\infty} s^x p(x, t). \quad (5.38)$$

This is a common technique. It is analogous to a Fourier series but for discrete differential equations.

Now substitute the generating function into the master equation:

$$\frac{\partial G(s, t)}{\partial t} = \sum_{x=0}^{\infty} s^x \frac{\partial p(x, t)}{\partial t} \quad (5.39)$$

$$\begin{aligned} &= k_2 a \sum_{x=0}^{\infty} s^x p(x-1, t) + k_1 \sum_{x=0}^{\infty} s^x (x+1) p(x+1, t) \\ &\quad - k_1 \sum_{x=0}^{\infty} s^x x p(x, t) - k_2 a \sum_{x=0}^{\infty} s^x p(x, t) \end{aligned} \quad (5.40)$$

$$\begin{aligned} &= k_2 a \sum_{x'=-1}^{\infty} s^{x'+1} p(x', t) + k_1 \sum_{x'=1}^{\infty} s^{x'-1} x' p(x', t) \\ &\quad - k_1 \sum_{x=0}^{\infty} s^x x p(x, t) - k_2 a \sum_{x=0}^{\infty} s^x p(x, t) \end{aligned} \quad (5.41)$$

$$= k_2 a (s-1) \sum_{x=0}^{\infty} s^x p(x, t) + k_1 (1-s) \sum_{x=0}^{\infty} s^{x-1} x p(x, t) \quad (5.42)$$

$$= k_2 a (s-1) G(s, t) + k_1 (1-s) \frac{\partial G(s, t)}{\partial s}, \quad (5.43)$$

where we use $p(-1, t) = 0$ in the first term and $x' = 0$ in the second term to extend or cut the sums in the third line.

✓ **Exercise:** Solve Eq. (5.43) by the method of characteristics (or indeed any other method).

Answer:

$$G(s, t) = F[(s-1)e^{-k_1 t}] \exp[(s-1)k_2 a/k_1] \quad (5.44)$$

where F is an arbitrary function determined by the initial conditions

Suppose there are N molecules of species X initially, i.e. $p(x, 0) = \delta_{x,N}$. Then

$$G(s, 0) = \sum_{x=0}^{\infty} s^x p(x, 0) = s^N = F[s - 1] \exp[(s - 1)k_2 a / k_1]. \quad (5.45)$$

Replacing $(s - 1)$ by u , to see what F looks like (univariate function), one finds $F(u) = (u + 1)^N \exp(-uak_2/k_1)$ and hence

$$G(s, t) = [1 + (s - 1)e^{-k_1 t}]^N \exp\left[-\frac{ak_2(s - 1)e^{-k_1 t}}{k_1}\right] \exp\left[\frac{ak_2(s - 1)}{k_1}\right] \quad (5.46)$$

$$= [1 + (s - 1)e^{-k_1 t}]^N \exp\left[\frac{ak_2(s - 1)(1 - e^{-k_1 t})}{k_1}\right]. \quad (5.47)$$

We can expand this expression in powers s^x and infer $p(x, t)$ by equating coefficients:

$$\begin{aligned} p(x, t) &= \exp\left[-\frac{ak_2(1 - e^{-k_1 t})}{k_1}\right] \sum_{r=0}^x \frac{N!}{(N-r)!r!(x-r)!} \left(\frac{k_2 a}{k_1}\right)^{x-r} \\ &\times (1 - e^{-k_1 t})^{N+x-2r} e^{-k_1 t r}. \end{aligned} \quad (5.48)$$

However, the generating function itself is often more useful, as it can be used to compute the moments of x as functions of time directly (see Eq. (5.38)):

$$\langle x(t) \rangle = \left. \frac{\partial G(s, t)}{\partial s} \right|_{s=1} \quad (5.49)$$

$$= \frac{k_2 a}{k_1} (1 - e^{-k_1 t}) + N e^{-k_1 t} \quad (5.50)$$

$$\text{var}[x(t)] = \langle x(t)[x(t) - 1] \rangle + \langle x(t) \rangle - \langle x(t) \rangle^2 \quad (5.51)$$

$$= \left. \frac{\partial^2 G(s, t)}{\partial s^2} \right|_{s=1} + \langle x(t) \rangle - \langle x(t) \rangle^2 \quad (5.52)$$

$$= (N e^{-k_1 t} + k_2 a / k_1) (1 - e^{-k_1 t}) \quad (5.53)$$

✓ **Exercise:** Show that the n^{th} moment obeys

$$\frac{d}{dt} \langle x(t)^n \rangle = n [k_2 a \langle x(t)^{n-1} \rangle - k_1 \langle x(t)^n \rangle]. \quad (5.54)$$

✓ **Exercise:** that the stationary distribution ($t \rightarrow \infty$) is Poissonian (see Sec. 5.5), with

$$G_s(s) = e^{(s-1)k_2 a / k_1} \quad (5.55)$$

$$p_s(x) = e^{-k_2 a / k_1} \frac{1}{x!} \left(\frac{k_2 a}{k_1}\right)^x. \quad (5.56)$$

5.3.3 Autocatalytic chemical reaction: bistability

Now consider the following reaction:



with A at a fixed concentration a . The transition rates are

$$T^+(x) = k_1ax(x-1) + k_3a \quad (5.59)$$

$$T^-(x) = k_2x(x-1)(x-2) + k_4x. \quad (5.60)$$

The most likely stationary state (modal value of x) is given by $T^+(x-1) = T^-(x)$:

$$\frac{k_1a}{k_2} = \frac{x[(x-1)(x-2) + k_4/k_2]}{(x-1)(x-2) + k_3/k_1}. \quad (5.61)$$

Now plot the model concentration x_m as a function of k_1a/k_2 . Clearly, if $k_4/k_2 = k_3/k_1$, the result is a straight line; for every value of k_1a/k_2 , there exists a unique modal concentration $x_m = k_1a/k_2$. However, for $k_4/k_2 > 9k_3/k_1$, the result is a cubic (*S*-shaped) curve; there exists an intermediate range of k_1a/k_2 in which there are three modal concentrations $x'_m < x''_m < x'''_m$ for every value of k_1a/k_2 . As a increases from zero, the system occupies the state x'_m until the lower branch of the *S* curve turns back on itself, at some value a_+ , at which point the system jumps to the upper branch and the state x'''_m (because x''_m is unstable). On the other hand, as a decreases from very large values, the system jumps from the upper branch to the lower branch (again skipping x''_m) at a different concentration $a_- < a_+$. This phenomenon is termed *bistability* and is ubiquitous in far-from-equilibrium systems.

If the rates are in the same ratio ($k_4/k_2 = k_3/k_1$), the stationary distribution (chemical equilibrium) is Poissonian (see Sec. 5.5):

$$p_s(x) = p_s(0) \prod_{x'=1}^x \frac{T^+(x-1)}{T^-(x)} \quad (5.62)$$

$$= p_s(0) \prod_{x'=1}^x \frac{k_1a}{k_2x'} = \frac{p_s(0)}{x!} \left(\frac{k_1a}{k_2}\right)^x. \quad (5.63)$$

5.4 Econophysics

Econophysics is a branch of interdisciplinary science which seeks to apply ideas from statistical physics to predict quantitatively the behaviour of economic systems.

Traditional economics is built on two fundamental principles:

- Systems rapidly come to equilibrium. The law of supply and demand is a classic example of this thesis. As soon as there is a shortfall of supply for a given level of demand, for example, prices rise; this suppresses demand and encourages investment in additional productive capacity to boost supply, until supply and demand are brought back into line. The perfect markets principle (*If you see a ten dollar note on the ground, it cannot exist, because someone has already picked it up*) is another example.
- The equilibrium discovered by a system is the steady state that maximises the systems utility (or, in more sophisticated treatments, the utility of some subset of the system). For example, one might seek to maximise a convex welfare function like the total wealth in the system (e.g. the sum of the squares of the wealths of all its subsystems).

The above principles were noted by Adam Smith in the 1800s, when he studied the operation of commodity markets and described the results in his classic text *The Wealth of Nations*. They were put on a firm mathematical basis as a theory of general equilibrium by John Maynard Keynes in the 1930s. They lead to powerful general theorems, e.g. that free trade (shorn of trade barriers or tariffs) maximises the utility of nations by allowing each nation to exploit its comparative advantages (e.g. in natural endowments) to the fullest.

- ✓ **Exercise:** A consumer, Mr Micawber, is endowed with total income I (his budget constraint). Note income is a misnomer here, because there is no temporal element in the problem, but we stick to the language of traditional economics. Mr Micawber can buy two goods, A and B , selling at prices p_A and p_B respectively (He is a price taker in this problem; no matter how hard he bargains, the price is the price). Let $U(q_A, q_B)$ be the utility function that describes Mr Micawbers relative preference for

the two goods as a function of the amounts q_A and q_B that he buys; as U increases, Mr Micawber feels happier.

- Show that Mr Micawber maximizes his utility subject to his budget constraint at the point (q_A^*, q_B^*) where

$$\frac{p_A}{p_B} = \frac{(\partial U / \partial q_A)_{q_A^*, q_B^*}}{(\partial U / \partial q_B)_{q_A^*, q_B^*}}. \quad (5.64)$$

- Show that, in most situations, (q_A^*, q_B^*) lies at the point on the $q_A - q_B$ plane where the budget constraint is tangent to the contours of the utility function (known as indifference curves in traditional economics). What are the exceptions?
- Show that, at (q_A^*, q_B^*) , the next incremental dollar spent on each good yields the same increment in utility. (This increment is called marginal utility by economists.)
- Evaluate all the above results explicitly for a Cobb-Douglas utility function of the form $U(q_A, q_B) = q_A^a q_B^b$.

✓ **Exercise:** Look up the statements and proofs of the First and Second Fundamental Theorems of Welfare Economics. Comment on the assumptions they make.

Of course, the fundamental principles above are not always satisfied, or at least not on time-scales of interest. A cursory look at the economy around you will reveal many examples of systems that are far from equilibrium, e.g. housing and stock market bubbles, secular changes in the wealth held by the top/bottom deciles of our society, transformative technological breakthroughs which disrupt established commercial networks, and so on. Some of these non-equilibrium behaviours are exogenous, i.e. triggered by external shocks. Some are endogenous, e.g. caused by delays in the transmission of information or resources through the system. Sec. 5.1.4 contains an example of how a simple delay in a linear population model can turn exponential decay into a limit cycle.

More subtly, it is assumed that the rational actions of individual agents inevitably lead to utility maximisation for the system as a whole. While this may be true in certain situations, it is certainly not true in general. A classic example from behavioural economics is the

Prisoners Dilemma. Two spies, Shaken and Stirred, are secluded in separate cells. Their captors do not have sufficient proof of their guilt. If both stay loyal, they are imprisoned for one year on some minor pretext. If Shaken betrays Stirred while Stirred stays loyal, Shaken is set free and Stirred is imprisoned for ten years (or vice versa). If both betray each other, they are imprisoned for five years. From the perspective of both individuals, rational self-interest impels them to betray each other, leaving them worse off than if they had taken a broader view and cooperated. (You may wish to ponder how this resembles a game of chicken.) A fascinating account of how these games are rife in the animal kingdom as well as social settings, and how the best strategies depend on whether you are playing the game once or many times (building trust and learning cooperation through tit-for-tat punishment), can be found in the classic book Evolution and the *Theory of Games*, by John Maynard-Smith (1982).

5.4.1 Asset exchange models

In econophysics, a favourite tool for studying these issues is the agent-based simulation, wherein many agents behave according to simple (indeed, simplistic) microscopic rules, whose iterated execution leads to a macroscopic behaviour of the system. The rules may simply be postulated, or they may distil the results of controlled social experiments carried out by behavioural scientists. Under this approach, global properties like equilibrium and utility maximization are emergent phenomena, which arise naturally in a statistical sense (if they exist at all) without being put in by hand.

For more details, see S. Ispolatov, P. L. Krapivsky and S. Redner 1998, European Physics Journal B **2**, 267276.

Additive exchange

Consider a system of many agents who pair up at random at each time step Δt and exchange a fixed parcel of wealth Δw . We work in units where $\Delta t = \Delta w = 1$, and assume

that initially every agent has one unit of wealth. Therefore subsequently the wealth w of each agent is quantized in non-negative integer units.

Let $p(w, t)$ be the number of agents with wealth w . There are two ways to add to the number of agents with wealth w : (i) an agent with wealth $w + 1$ gives one unit of wealth to his counterparty; or (ii) an agent with wealth $w - 1$ receives one unit of wealth from his counterparty. As outcomes (i) and (ii) are equally probable, the transition rate is given by

$$T(w, w', t) = (\delta_{w,w'-1} + \delta_{w,w'+1})N(t)/2, \quad (5.65)$$

where

$$N(t) = \sum_{w=1}^{\infty} p(w, t) \quad (5.66)$$

is the total number of agents. From the discrete form of the master equation Eq. (5.22), we obtain

$$\frac{\partial p(w, t)}{\partial t} = -N(t)p(w, t) + [p(w+1, t) + p(w-1, t)]N(t)/2, \quad (5.67)$$

where the first term is the rate of loss from the state w (which occurs with unit probability over the time step $\Delta t = 1$; agents with wealth w will always move away from w after one time step, whether they are givers or receivers) and the second term is the rate of gain into the state w from all other intermediate states w' via processes (i) or (ii). This equation is written down in the mean-field approximation, where the probability of a transaction occurring (say involving a giver with wealth w) is proportional to $N(t)$ because they are sure to find a counterparty from the rest of the population and do not care whom [we assume $N(t)$ is large so $N(t) - 1 \approx N(t)$]. It is vital to realise that $N(t)$ is a function of time, i.e. it is not conserved; when agents get down to just one unit of wealth and are forced to give it away in an exchange, they have zero wealth and drop out of the system (in the language of Fokker-Planck equations, there is an absorbing boundary at $w = 0$).

Make the change of variables from t to T via

$$T = \int_0^t dt' N(t'). \quad (5.68)$$

This leads to

$$\frac{\partial p(w, T)}{\partial T} = p(w + 1, T) + p(w - 1, T) - 2p(w, T), \quad (5.69)$$

with boundary condition $p(0, T) = 0$ for all T (bankrupts leave the system). If in addition we impose initial conditions $p(w, 0) = \delta_{w,1}$, i.e. every agent starts with one unit of wealth, then we can show from recursion relations for Bessel functions that

$$p(w, T) = e^{-2T} [I_{w-1}(2T) - I_{w+1}(2T)], \quad (5.70)$$

where I_n is the modified Bessel function of order n . Summing over all w , we get

$$N(T) = e^{-2T} [I_0(2T) - I_2(2T) + I_1(2T) - I_3(2T) + I_2(2T) - I_4(2T) + \dots] \quad (5.71)$$

$$= e^{-2T} [I_0(2T) + I_1(2T)]. \quad (5.72)$$

We now substitute into the change-of-variable definition to get $T(t)$ and hence $p(w, t)$. For large T and t , we have

$$p(w, t) \approx (4\pi T^3)^{-1/2} w \exp[-w^2/(4T)], \quad (5.73)$$

$$N(T) \approx (\pi T)^{-1/2}, \quad (5.74)$$

$$t \approx (4\pi T^3/9)^{1/2}, \quad (5.75)$$

and hence

$$p(w, t) \approx \frac{w}{3t} \exp \left[- \left(\frac{\pi}{144} \right)^{1/3} \frac{w^2}{t^{2/3}} \right]. \quad (5.76)$$

This can be written in the self-similar scaling form $\propto N(t)^2 f[awN(t)]$, with $f(x) = xe^{-x^2}$. It describes a diffusive process with $\langle w^2 \rangle \propto t^{2/3}$, much like a standard Wiener process except that the diffusion proceeds slower at large t .

Multiplicative exchange

Now consider a more realistic asset exchange process, in which the transfer amount is a fixed fraction of the wealths of the participating agents. Think about investing in the stockmarket; you are constrained to buy/sell at most your total wealth (neglecting

borrowings), no more; and, for most people, each buy/sell transaction comprises a small fraction of their total wealth. Likewise, transactions involving the earning of some kind of interest (bank interest, stock dividend, rent) are usually levied as a proportion of the value of the underlying asset (explicitly so for bank interest, effectively so for stock dividends and rent, whose rates of return are typically 2% to 5% per annum). In this section, we consider a special type of multiplicative asset transfer: the giver scheme, where a fraction f of the givers wealth is exchanged at each transaction.

In this system, the total wealth is conserved; no agent ever ends up with so little wealth that they cannot participate in a transaction, unlike in additive schemes. Hence the wealth pdf $p(w, t)$ has constant unit normalisation.

There are two ways to increase the number of agents in the state w . (i) A giver with wealth $w/(1 - f)$ surrenders a fraction f of his/her wealth and ends up with wealth w . In this case, the wealth of the counterparty is irrelevant to the probability of occurrence, which is proportional to the number of givers with wealth $w(1 - f)$; a suitable counterparty always exists. The factor $[2(1 - f)]^{-1}$ is needed to normalise everything properly; if we integrate this process in isolation over all w , we must get 1/2, since half the agents are givers at each time step. (ii) A receiver with wealth $w - fw'$ encounters a giver with wealth w' . In this case, the probability of occurrence is proportional to the product of the number of givers with wealth $w - fw'$ and the number of receivers with wealth w' ; given w and f , only a subset of agents are suitable counterparties. Mathematically, we write

$$\frac{\partial p(w, t)}{\partial t} = -p(w, t) + \frac{1}{2(1 - f)} p\left(\frac{w}{1 - f}, t\right) + \frac{1}{2} \int_0^{w/f} dw' p(w - fw', t) p(w', t) \quad (5.77)$$

$$= -p(w, t) + \frac{1}{2(1 - f)} p\left(\frac{w}{1 - f}, t\right) + \frac{1}{2f} \int_0^w du p\left(\frac{w - u}{f}, t\right) p(u, t), \quad (5.78)$$

where the last line follows from the second last line by changing variables to $u = w - fw'$ in the integral and noting that $p(u, t) = 0$ for $u < 0$.

It is not easy to solve Eq. (5.78) analytically. Numerical solutions show that for values of $0 < f \leq 0.5$ and $0.5 < f \leq 1$; the solutions agree with the results from agent-based

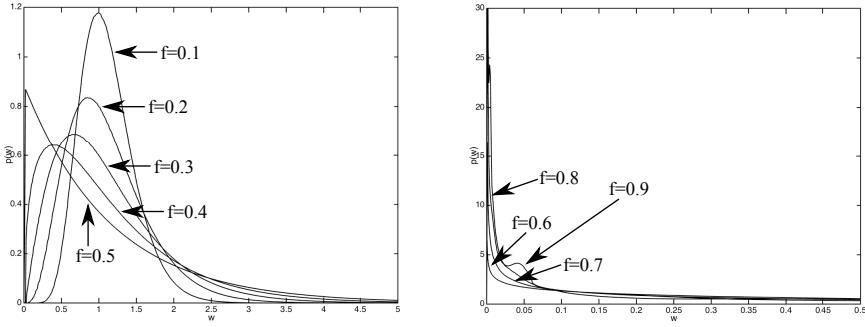


Figure 5.1. Wealth pdf, as determined from Eq. (5.78). Left: $f = 0.1, 0.2, 0.3, 0.4, 0.5$. Right: $f = 0.6, 0.7, 0.8, 0.9$ (note the scale of the x-axis in the two plots differs by an order of magnitude)

simulations. In all cases, a stationary distribution $p_s(w)$ is reached after a few tens of time steps, because the typical gain from an interaction is much smaller than the typical loss for a rich agent, while the opposite holds true for a poor agent. The stationary distribution can be solved for by Laplace transforming (in w) the master equation (5.78) to give

$$0 = -2g_s(z) + g_s(z - fz) + g_s(z)g_s(fz) \quad (5.79)$$

for $g_s(z) = \int_0^\infty dw e^{-zw} p_s(w)$.

✓ **Exercise:** Confirm that for $f = 1/2$ we have $g_s(z) = (1 + \mu z)^{-1}$ and hence $p_s(z) = \mu^{-1} \exp(-w/\mu)$, where μ is the mean wealth.

The solutions in Figure 5.1 are qualitatively different for $f < 1/2$ and $f > 1/2$. In the former regime, they are mild (egalitarian): strongly peaked, with an exponential tail at large w and a power-law rise with positive exponent at small w . In the latter regime, they are wild, diverging as a power law with a negative exponent at small w (and an exponential tail still at large w). Curiously, oscillations (this may well be a numerical artifact) are overlaid on the power law for $f > 1/2$, which are most visible as f approaches unity.

The moments of $p(w, t)$ confirm the approach to a steady state. By multiplying both sides of Eq. (5.78) by w and w^2 and integrating over all w , we find $d\mu/dt = 0$, as expected for a conservative system. The variance obeys

$$\sigma^2(t) = \left[\sigma^2(0) - \frac{f\mu^2}{1-f} \right] \exp[-f(1-f)t] + \frac{f\mu^2}{1-f}. \quad (5.80)$$

✓ **Exercise:** Prove Eq. (5.80).

A fascinating characteristic of the giver scheme is that the Boltzmann entropy, Eq. (3.39) does not increase monotonically with time, even though the system appears to have all the properties of a system to which the Boltzmann H theorem applies: it is closed and conservative (wealth is neither created nor destroyed), just like momentum redistribution in an ideal gas. However, the asymmetry built into the giver scheme, namely that the transfer amount is proportional to the givers wealth, means that the microscopic dynamics are not symmetric under time reversal; the rules of the system, applied repeatedly, suck up entropy. For more details and some numerical examples, please consult A. Sokolov, A. Melatos, and T. Kieu, European Physics Journal B **76**, 637 (2010).

5.5 A note on the Poisson distribution

In Secs. 5.3.2, the time-dependent probability distribution $p(x, t)$ is Poissonian as well as the stationary distribution. This provides the rationale behind a useful technique for generating Fokker-Planck equations from master equations.

Let us consider the example in Sec. 5.3.2, but starting with a Poisson ($\neq \delta_{x,N}$) distribution:

$$p(x, 0) = e^{-\alpha_0} c_0^x / x! \quad (5.81)$$

$$G(s, 0) = e^{-\alpha_0} \sum_{x=0}^{\infty} [s\alpha_0]^x / x! = \exp[(s - 1)\alpha_0]. \quad (5.82)$$

Then $F(u)$ changes to $F(u) = e^{\alpha_0 u} e^{-uk_2 a/k_1}$ and hence

$$G(s, t) = \exp \left[(s - 1)e^{-k_1 t} \left(\alpha_0 - \frac{ak_2}{k_1} \right) \right] \exp \left[(s - 1) \frac{ak_2}{k_1} t \right] \quad (5.83)$$

$$= \exp \left[(s - 1) \left(\alpha_0 e^{-k_1 t} + \frac{ak_2}{k_1} (1 - e^{-k_1 t}) \right) \right] \quad (5.84)$$

which also corresponds to a Poisson distribution

$$p(x, 0) = e^{-\alpha(t)} \alpha(t)^x / x!, \quad (5.85)$$

with

$$\alpha(t) = \frac{ak_2}{k_1} + \left(\alpha_0 - \frac{ak_2}{k_1} \right) e^{-k_1 t}, \quad (5.86)$$

where $\alpha(t)$ is the solution of the deterministic equation for the first moment, $dx/dt = k_2 a - k_1 x$, given $x(0) = \alpha_0$.

For a general master equation of the sort that arises in chemical reactions, we follow a similar approach. Assume that the probability distribution can be expanded as a product of Poissons, one for each species:

$$p(x_1, \dots, x_n, t) = \int d\alpha_1 \dots d\alpha_n \prod_j \frac{1}{x_j!} e^{-\alpha_j} \alpha_j^{x_j} f(\alpha_1, \dots, \alpha_n, t) \quad (5.87)$$

$$G(s_1, \dots, s_n, t) = \int d\alpha_1 \dots d\alpha_n \left[\sum_j (s_j - 1) \alpha_j \right] f(\alpha_1, \dots, \alpha_n, t). \quad (5.88)$$

Then substitute the above generating function into your master equation, do the α_j integrals (by parts, discarding surface terms), and equate coefficients of the exponential to get a PDE for $f(\alpha_1, \dots, \alpha_n, t)$.

5.6 Problems

1. **Continuous random walk:** A drunken sailor is confined to move along a line. At any instant, there is a probability α per unit time that he steps to the left, and an equal probability that he steps to the right. We do not necessarily have $\alpha dt = 1/2$; the sailor may not take a step during the time interval dt . The steps are all of equal length h . Let x denote the position of the sailor from the origin, measured as an integer number of steps.

- (a) Explain why the probability distribution $p(x, t)$ satisfies a master equation of the form

$$\frac{\partial p(x, t)}{\partial t} = \alpha [p(x+1, t) + p(x-1, t) - 2p(x, t)]. \quad (5.89)$$

- (b) Show that the generating function is given by

$$G(s, t) = \sum_{x=-\infty}^{\infty} s^x p(x, t) = \exp[\alpha t(s - 2 + s^{-1})]. \quad (5.90)$$

Note: the negative values of x are perfectly acceptable here, unlike in birth-death problems where population numbers cannot be negative.

Hint: the constant of integration is fixed by normalisation of the probability.

- (c) Verify that $\langle x \rangle = 0$ and $\langle x^2 \rangle = 2\alpha t$, as expected for an unbiased random walk.
- (d) By expanding the right-hand side in a Taylor series about $s = 0$, and treating the negative x values by symmetry, show that the probability distribution is

$$p(x, t) = \exp[-2\alpha t] I_x(4\alpha t), \quad (5.91)$$

where I_x is the modified Bessel function of order x .

2. **Predator-prey ecologies far from extinction:** Consider the Lotka-Volterra ecology described in Sec. 5.1.1 in the regime where the prey and predator populations are large, i.e. $x \gg 1$ and $y \gg 1$.

Argue that the probability distribution, $p(x, y, t)$, satisfies the following master equation:

$$\begin{aligned} \frac{\partial p(x, y, t)}{\partial t} &= k_1 a(x-1)p(x-1, y, t) + k_2(x+1)(y-1)p(x+1, y-1, t) \\ &\quad + k_3(y+1)p(x, y+1, t) - (k_1 a x + k_2 x y + k_3 y)p(x, y, t) \end{aligned} \quad (5.92)$$

3. **Dissociation of Oxygen molecules:** In the stratosphere and mesosphere of the Earth, between altitudes of 30 km and 90 km, solar ultraviolet radiation dissociates oxygen molecules (O_2) to form oxygen atoms (O). An oxygen atom and molecule can then combine to form an ozone molecule in an excited state (O_3^*). In turn, the excited ozone molecule decomposes into its original constituents, unless it collides promptly with some other atmospheric molecule, which carries away the excess energy. The forward and reverse reactions



proceed with rate coefficients k_1 and k_2 respectively.

- (a) Show that the master equation obeyed by the joint probability distribution function $p(x_0, x_3, t)$ of the atomic oxygen (x_0) and ozone (x_3) populations, assuming that the O_2 population is fixed at x_2 , is given by

$$\begin{aligned}\frac{\partial p(x_0, x_3, t)}{\partial t} &= k_1 x_2 (x_0 + 1) p(x_0 + 1, x_3 - 1, t) + k_2 (x_3 + 1) p(x_0 - 1, x_3 + 1, t) \\ &\quad - (k_1 x_2 x_0 + k_2 x_3) p(x_0, x_3, t).\end{aligned}\quad (5.95)$$

- (b) Derive the first-order partial differential equation satisfied by the generating function

$$G(t, s_0, s_3) = \sum_{x_0=0}^{\infty} \sum_{x_3=0}^{\infty} s_0^{x_0} s_3^{x_3} p(x_0, x_3, t). \quad (5.96)$$

You should find

$$\frac{\partial G}{\partial t} = k_1 x_2 (s_3 - s_0) \frac{\partial G}{\partial s_0} + k_2 (s_0 - s_3) \frac{\partial G}{\partial s_3}. \quad (5.97)$$

- (c) Assuming that there are exactly p oxygen atoms and zero ozone molecules initially, the solution for the above equation is

$$G(t, s_0, s_3) = \left[\frac{(k_2 s_0 + k_1 x_2 s_3) (1 - e^{-\beta t})}{\beta} + s_0 e^{-\beta t} \right]^p, \quad (5.98)$$

with $\beta = k_2 + k_1 x_1$. What is the mean number of ozone molecules in equilibrium ($t \rightarrow \infty$)?

- (d) Calculate the covariance $\langle x_0 x_3 \rangle$ at equilibrium?

- (e) Are the numbers of oxygen atoms and ozone molecules correlated, anti-correlated, or uncorrelated at equilibrium? Explain the result physically.

- 4. Superannuation:** It is never too soon to plan your superannuation strategy! Some respected economists predict that asset prices will decline steadily in real terms (i.e. after inflation) over the next few decades, as the world's population hits environmental capacity constraints and stabilises for the first time since the Industrial Revolution. At the same time, higher volatility is expected to become the norm in investment markets, as the financial industry grows its share of the economy. In this environment, what should you do to ensure that you maintain access to the essentials ? fine wine, say,

and adventure holidays ? as you live to a ripe old age? Below we show that the answer to this question is *be lucky*.

Let $x(t)$ be a random variable denoting the dollar balance of your retirement fund as a function of time, t , measured in years. Every year, you deposit a fixed sum $\lambda > 0$ into the fund. The fund is invested in a mix of stocks and bonds. It earns interest at a fluctuating rate $\alpha + \eta(t)$ per annum, where α is the steady, underlying rate of return (which can be positive or negative), and $\eta(t)$ is a stochastic variable of Langevin type which obeys stationary Gaussian statistics with $\langle \eta(t) \rangle = 0$, $\langle \eta(t)\eta(t') \rangle = 2D\delta(t-t')$, with $D > 0$.

- (a) Justify the following Langevin equation describing the evolution of $x(t)$:

$$\frac{\partial x(t)}{\partial t} = x(t) [\alpha + \eta(t)] + \lambda. \quad (5.99)$$

- (b) By introducing an integrating factor, or otherwise, explicitly solve Langevin equation (for a fund starting with zero balance)

$$x(t) = \lambda \exp \left[\int_0^t dt' (\alpha + \eta(t')) \right] \int_0^t dt'' \exp \left[- \int_0^{t''} dt' (\alpha + \eta(t')) \right]. \quad (5.100)$$

- (c) Show that the mean balance is given by

$$\langle x(t) \rangle = \frac{\lambda}{\alpha + D} [\exp[(\alpha + D)t] - 1]. \quad (5.101)$$

Note that the system must self-regulate, such that $\langle x(t) \rangle$ (and hence the total money in the system after inflation) does not diverge in the long term ($t \rightarrow \infty$). This requires $\alpha + D < 0$.

- (d) Let $q(u, t)$ be the probability distribution function of the logarithmic balances $u = \ln(x)$ of an ensemble of retirement funds. Write down the Langevin equation for u and thereby show that the associated Fokker-Planck equation takes the form

$$\frac{\partial q(u, t)}{\partial t} = -\frac{\partial}{\partial u} [(\lambda \exp(-u) + \alpha) q(u, t)] + D \frac{\partial^2 q(u, t)}{\partial u^2}. \quad (5.102)$$

- (e) Explain why the system self-imposes a reflecting boundary at $x = 0$.
(f) Use the boundary condition from part (e) to solve for the steady-state distribution.

- (g) Relate $p_s(x)$, the steady-state probability distribution function of x , to $q_s(u)$.
- (h) Sketch $p_s(x)$ and comment on its properties.
- (i) If the system self-regulates to be marginally stable, i.e. $\alpha + D$ adjusts to be slightly negative, what happens to the dispersion, $\text{var}(x)$, as $t \rightarrow \infty$?
- (j) Comment briefly on what all this means in practice for policy makers seeking to design a viable superannuation system.

Chapter 6

Kinetic theory

6.1 Bogoliubov, Born, Green, Kirkwood and Yvon (BBGKY) hierarchy

Given a large number of systems prepared under identical macroscopic (but not microscopic) conditions, we define $f_N(t, x, p)d^{3N}xd^{3N}p$ to be the probability of finding a system in the ensemble in a volume $d^{3N}xd^{3N}p$ around (x, p) at time t . This N -particle distribution function obeys Liouville's equation:

$$\frac{\partial f_N}{\partial t} + \frac{\partial H}{\partial p_i} \frac{\partial f_N}{\partial x_i} - \frac{\partial H}{\partial x_i} \frac{\partial f_N}{\partial p_i} = 0. \quad (6.1)$$

Liouville's equation is complicated and unwieldy; it contains all the statistical information in the system apart from the (unknowable) microscopic initial conditions.

Bogoliubov, Born, Green, Kirkwood, and Yvon (BBGKY) simplified Liouville's equation by expressing f_1 in terms of f_2 , f_2 in terms of f_3 , and so on, up to f_{N-1} in terms of f_N . This procedure entails an expansion in the multiplicity of interparticle interactions:

$$\begin{aligned} f_1 &\text{ is determined by 2 - body interactions only} \\ f_2 &\text{ is determined by 3 - body interactions only} \\ &\quad \text{etc} \end{aligned} \quad (6.2)$$

Above some multiplicity, the likelihood of multiple-body interactions (collisions) becomes

very small, because it is rare to find the requisite particles in the same place at the same time. Hence we can truncate the hierarchy. The multiplicity where this becomes possible depends on the density of the system. For example, only 2-body collisions are important in a dilute gas, whereas higher-order correlations are crucial in, say, water. (The statistical mechanics of H₂O remains unsolved.)

A nice derivation of the BBGKY hierarchy can be found in K. Huang, 1987, *Statistical Mechanics*, Sec. 3.5. Please refer to it. The main steps are outlined below.

Assume the Hamiltonian takes the form:

$$H = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{i=1}^N U(\mathbf{x}_i) + \sum_{i=1}^N \sum_{j>i} V(|\mathbf{x}_i - \mathbf{x}_j|), \quad (6.3)$$

where $U(\mathbf{x}_i)$ is the mean potential at the position of the i^{th} body and $V(|\mathbf{x}_i - \mathbf{x}_j|)$ is the inter-body potential. Note that H does not involve $U(\mathbf{x}_i)$ away from the N bodies, i.e. there is no self-interaction of the mean field with itself. Then we get

$$\frac{\partial H}{\partial \mathbf{p}_i} = \frac{\mathbf{p}_i}{m} \quad (6.4)$$

$$\frac{\partial H}{\partial \mathbf{x}_i} = \frac{\partial U(\mathbf{x}_i)}{\partial \mathbf{x}_i} + \sum_{j=1, j \neq i}^N \frac{\partial V(|\mathbf{x}_i - \mathbf{x}_j|)}{\partial \mathbf{x}_i}. \quad (6.5)$$

Denote the first and second terms on the RHS of Eq. (6.5) by $-\mathbf{F}_i$ and $-\sum \mathbf{K}_{ij}$ respectively.

The second term is derived from H as follows:

$$\frac{\partial}{\partial \mathbf{x}_i} \left[\frac{1}{2} \sum_{j \neq k} V(|\mathbf{x}_j - \mathbf{x}_k|) \right] = \frac{1}{2} \sum_{j \neq k} \frac{\partial V(|\mathbf{x}_j - \mathbf{x}_k|)}{\partial \mathbf{x}_i} (\delta_{ij} + \delta_{ik}) \quad (6.6)$$

$$= \frac{1}{2} \sum_{k=1, k \neq i}^N \frac{\partial V(|\mathbf{x}_i - \mathbf{x}_k|)}{\partial \mathbf{x}_i} + \frac{1}{2} \sum_{j=1, j \neq i}^N \frac{\partial V(|\mathbf{x}_j - \mathbf{x}_i|)}{\partial \mathbf{x}_i}. \quad (6.7)$$

Can now rewrite Liouville's theorem as

$$\left[\frac{\partial}{\partial t} + \hat{h}_N(x, p) \right] f_N(t, x, p) = 0, \quad (6.8)$$

with

$$\hat{h}_N(x, p) = \sum_{i=1}^N S_i + \sum_{i,j=1, j \neq i}^N P_{ij} \quad (6.9)$$

and

$$S_i = \frac{\mathbf{p}_i}{m} \cdot \frac{\partial}{\partial \mathbf{x}_i} + \mathbf{F}_i \cdot \frac{\partial}{\partial \mathbf{p}_i}, \quad (6.10)$$

$$P_{ij} = \mathbf{K}_{ij} \cdot \frac{\partial}{\partial \mathbf{p}_i} + \mathbf{K}_{ji} \cdot \frac{\partial}{\partial \mathbf{p}_j}. \quad (6.11)$$

The single-particle distribution function (also known as the microscopic phase space density) of N indistinguishable bodies is the probability of finding one body at (\mathbf{x}, \mathbf{p}) and the other $N - 1$ bodies somewhere (anywhere!) else:

$$f_1(t, \mathbf{x}, \mathbf{p}) = N \int d^3 \mathbf{x}_2 \dots d^3 \mathbf{x}_N d^3 \mathbf{p}_2 \dots d^3 \mathbf{p}_N f_N(t, x, p). \quad (6.12)$$

In other words, we integrate over all possible states of $N - 1$ bodies, leaving just the probability of finding any single one at (\mathbf{x}, \mathbf{p}) . More generally, the s -particle distribution function is

$$f_s(t, \mathbf{x}_1, \dots, \mathbf{x}_s, \mathbf{p}_1, \dots, \mathbf{p}_s) = \frac{N!}{(N-s)!} \int d^3 \mathbf{x}_{s+1} \dots d^3 \mathbf{x}_N d^3 \mathbf{p}_{s+1} \dots d^3 \mathbf{p}_N f_N(t, x, p), \quad (6.13)$$

where $N!/(N-s)!$ is the number of equivalent ways to choose s coordinates $(\mathbf{x}_1, \dots, \mathbf{x}_s)$ out of a set of N .

The equation of motion for the f_s is given by

$$\frac{\partial f_s}{\partial t} = \frac{N!}{(N-s)!} \int d^3 \mathbf{x}_{s+1} \dots d^3 \mathbf{x}_N d^3 \mathbf{p}_{s+1} \dots d^3 \mathbf{p}_N \frac{f_N(t, x, p)}{\partial t}, \quad (6.14)$$

which, using Eq. (6.8), can be written as

$$\frac{\partial f_s}{\partial t} = -\frac{N!}{(N-s)!} \int d^3 \mathbf{x}_{s+1} \dots d^3 \mathbf{x}_N d^3 \mathbf{p}_{s+1} \dots d^3 \mathbf{p}_N \hat{h}_N f_N. \quad (6.15)$$

Splitting \hat{h}_N in the following manner

$$\hat{h}_N = \sum_{i=1}^s S_i + \sum_{i=s+1}^N S_i + \frac{1}{2} \sum_{i,j=1, i \neq j}^s P_{ij} + \frac{1}{2} \sum_{i,j=s+1, i \neq j}^N P_{ij} + \sum_{i=1}^s \sum_{j=s+1}^N P_{ij} \quad (6.16)$$

$$= \hat{h}_s(\mathbf{x}_1, \dots, \mathbf{x}_s, \mathbf{p}_1, \dots, \mathbf{p}_s) + \hat{h}_{N-s}(\mathbf{x}_{s+1}, \dots, \mathbf{x}_N, \mathbf{p}_{s+1}, \dots, \mathbf{p}_N) + \sum_{i=1}^s \sum_{j=s+1}^N P_{ij} \quad (6.17)$$

and substituting into Eq. (6.15) we arrive at

$$\begin{aligned}\frac{\partial f_s}{\partial t} &= -\frac{N!}{(N-s)!} \hat{h}_s \int d^3 \mathbf{x}_{s+1} \dots d^3 \mathbf{x}_N d^3 \mathbf{p}_{s+1} \dots d^3 \mathbf{p}_N f_N(t, x, p) \\ &- \frac{N!}{(N-s)!} \sum_{i=1}^s \sum_{j=s+1}^N \int d^3 \mathbf{x}_{s+1} \dots d^3 \mathbf{x}_N d^3 \mathbf{p}_{s+1} \dots d^3 \mathbf{p}_N P_{ij} f_N(t, x, p)\end{aligned}\quad (6.18)$$

$$= -\hat{h}_s f_s - \frac{N!}{(N-s)!} \sum_{i=1}^s \sum_{j=s+1}^N \int d^3 \mathbf{x}_{s+1} \dots d^3 \mathbf{x}_N d^3 \mathbf{p}_{s+1} \dots d^3 \mathbf{p}_N P_{ij} f_N(t, x, p) \quad (6.19)$$

$$= -\hat{h}_s f_s - \sum_{i=1}^s \int d^3 \mathbf{x}_{s+1} d^3 \mathbf{p}_{s+1} P_{i,s+1} f_{s+1}(t, x, p) \quad (6.20)$$

$$= -\hat{h}_s f_s - \sum_{i=1}^s \int d^3 \mathbf{x}_{s+1} d^3 \mathbf{p}_{s+1} \mathbf{K}_{i,s+1} \cdot \frac{\partial f_{s+1}}{\partial \mathbf{p}_i}. \quad (6.21)$$

To arrive at the above expression we have used the fact that \hat{h}_s is independent of $d^3 \mathbf{x}_{s+1} \dots d^3 \mathbf{x}_N d^3 \mathbf{p}_{s+1} \dots d^3 \mathbf{p}_N$, the sum over j gives $N-s$ identical terms,

$$\begin{aligned}&\int d^3 \mathbf{x}_{s+1} \dots d^3 \mathbf{x}_N d^3 \mathbf{p}_{s+1} \dots d^3 \mathbf{p}_N \hat{h}_{N-s} f_N(t, x, p) \\ &= \sum_{i=s+1}^N \int d^3 \mathbf{x}_{s+1} \dots d^3 \mathbf{x}_N d^3 \mathbf{p}_{s+1} \dots d^3 \mathbf{p}_N \left[\frac{\mathbf{p}_i}{m} \cdot \frac{\partial f_N}{\partial \mathbf{x}_i} - \frac{\partial U}{\partial \mathbf{x}_i} \cdot \frac{\partial f_N}{\partial \mathbf{p}_i} \right. \\ &\quad \left. - \sum \frac{\partial V(|\mathbf{x}_i - \mathbf{x}_j|)}{\partial \mathbf{x}_i} \cdot \left(\frac{\partial f_N}{\partial \mathbf{p}_i} - \frac{\partial f_N}{\partial \mathbf{p}_j} \right) \right]\end{aligned}\quad (6.22)$$

$$= \sum_{i=s+1}^N \frac{\mathbf{p}_i}{m} \Big|_{\text{bdry}} - \int d^3 \mathbf{x}_{s+1} \dots d^3 \mathbf{x}_N d^3 \mathbf{p}_{s+1} \dots d^3 \mathbf{p}_N \frac{\partial}{\partial \mathbf{x}_i} \cdot \frac{\mathbf{p}_i}{m} f_N + \text{similar terms} \quad (6.23)$$

$$= 0, \quad (6.24)$$

if f_N vanishes on the boundary (noting that \mathbf{x}_i and \mathbf{p}_i are independent). In deriving Eq. (6.21) we have also used the fact that the $\partial/\partial \mathbf{p}_j$ term in K_{ij} leads to a similar boundary term (which is zero) as above.

6.2 The Boltzmann equation

6.2.1 Lowest-order truncation of the BBGKY hierarchy

The most drastic truncation of the hierarchy we can make is to follow just the evolution of f_1 , the microscopic phase space density. The evolution involves f_2 through Eq. (6.21), so we need to keep the two lowest-order equations $s = 1, 2$:

$$\left(\frac{\partial}{\partial t} + \frac{\mathbf{p}_1}{m} \cdot \frac{\partial}{\partial \mathbf{x}_1} + \mathbf{F}_1 \cdot \frac{\partial}{\partial \mathbf{p}_1} \right) f_1(t, \mathbf{x}_1, \mathbf{p}_1) = - \int d^3 \mathbf{x}_2 d^3 \mathbf{p}_2 \mathbf{K}_{12} \cdot \frac{\partial}{\partial \mathbf{p}_1} f_2(t, \mathbf{x}_1, \mathbf{x}_2, \mathbf{p}_1, \mathbf{p}_2), \quad (6.25)$$

where \mathbf{F}_1 is the mean-field force ($\partial U / \partial \mathbf{x}_1$) acting on particle 1, *not* the inter-particle force, and

$$\begin{aligned} & \left(\frac{\partial}{\partial t} + \frac{\mathbf{p}_1}{m} \cdot \frac{\partial}{\partial \mathbf{x}_1} + \frac{\mathbf{p}_2}{m} \cdot \frac{\partial}{\partial \mathbf{x}_2} + \mathbf{F}_1 \cdot \frac{\partial}{\partial \mathbf{p}_1} + \mathbf{F}_2 \cdot \frac{\partial}{\partial \mathbf{p}_2} + \frac{1}{2} \mathbf{K}_{12} \cdot \left[\frac{\partial}{\partial \mathbf{p}_1} - \frac{\partial}{\partial \mathbf{p}_2} \right] \right) f_2(t, \mathbf{x}_1, \mathbf{x}_2, \mathbf{p}_1, \mathbf{p}_2) \\ &= - \int d^3 \mathbf{x}_3 d^3 \mathbf{p}_3 \left(\mathbf{K}_{13} \cdot \frac{\partial}{\partial \mathbf{p}_1} + \mathbf{K}_{23} \cdot \frac{\partial}{\partial \mathbf{p}_2} \right) f_3(t, \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3). \end{aligned} \quad (6.26)$$

To simplify the two BBGKY equations above we need to consider the relevant timescales (from shortest to longest):

- duration of a collision τ_c :

$$\left(\mathbf{K} \cdot \frac{\partial}{\partial \mathbf{p}} \right)^{-1} \approx \left(\frac{\text{inter-particle force}}{\Delta p} \right)^{-1} \quad (6.27)$$

- time to cross distance over which probability distribution varies significantly:

$$\left(\frac{\mathbf{p}}{m} \cdot \frac{\partial}{\partial \mathbf{x}} \right)^{-1} \approx \left(\frac{f}{|\nabla f| |\mathbf{v}|} \right)^{-1} \quad (6.28)$$

- time to cross distance over which the minefield varies significantly

$$\left(\mathbf{F} \cdot \frac{\partial}{\partial \mathbf{p}} \right)^{-1} \approx \left(\frac{\text{mean-field force}}{\Delta p} \right)^{-1}. \quad (6.29)$$

Note that the second and third time-scales are not the same. For example, in the Earths atmosphere, the length-scale over which the distribution f (or equivalently the gas density)

changes is the hydrostatic scale height (a few km), whereas the mean-field force (gravity) changes over a length-scale of order the Earth's radius (6×10^3 km).

This separation of time-scales allows us to simplify the two BBGKY equations. In Eq. (6.25), the LHS evolves at the slow time-scale for streaming, while the RHS drives the LHS at the fast time-scale $\tau_c n r_0^3$, where n is the typical number density and r_0 is the range of the inter-particle force. In Eq. (6.26), the LHS varies at the fast time-scale τ_c through the K_{12} term (2-body collisions), while the RHS is smaller by a factor $n r_0^3$, because the outsider particle must pass within r_0 of a particle pair in order to obtain a 3-body collision, limiting the integration over \mathbf{x}_3 to a small volume. Numerically:

- **dilute gas:** $r_0 \approx 10^{-10}\text{m}$, $n \approx 3 \times 10^{25}\text{m}^{-3} \rightarrow n r_0^3 \approx 10^{-5} \rightarrow \text{RHS (Eq. 6.26)} = 0$
- **water:** $r_0 \approx 10^{-10}\text{m}$, $n \approx 3 \times 10^{28}\text{m}^{-3} \rightarrow n r_0^3 \approx 10^{-2} \rightarrow \text{RHS (Eq. 6.26)} \neq 0$

Hence for the dilute gas case the hierarchy is closed:

$$\left(\frac{\partial}{\partial t} + \frac{\mathbf{p}_1}{m} \cdot \frac{\partial}{\partial \mathbf{x}_1} + \mathbf{F}_1 \cdot \frac{\partial}{\partial \mathbf{p}_1} \right) f_1(t, \mathbf{x}_1, \mathbf{p}_1) = - \int_{|\mathbf{x}_1 - \mathbf{x}_2| < r_0} d^3 \mathbf{x}_2 d^3 \mathbf{p}_2 \mathbf{K}_{12} \cdot \frac{\partial}{\partial \mathbf{p}_1} f_2(t, \mathbf{x}_1, \mathbf{x}_2, \mathbf{p}_1, \mathbf{p}_2), \quad (6.30)$$

$$\left(\frac{\partial}{\partial t} + \frac{\mathbf{p}_1}{m} \cdot \frac{\partial}{\partial \mathbf{x}_1} + \frac{\mathbf{p}_2}{m} \cdot \frac{\partial}{\partial \mathbf{x}_2} + \mathbf{F}_1 \cdot \frac{\partial}{\partial \mathbf{p}_1} + \mathbf{F}_2 \cdot \frac{\partial}{\partial \mathbf{p}_2} + \frac{1}{2} \mathbf{K}_{12} \cdot \left[\frac{\partial}{\partial \mathbf{p}_1} - \frac{\partial}{\partial \mathbf{p}_2} \right] \right) f_2(t, \mathbf{x}_1, \mathbf{x}_2, \mathbf{p}_1, \mathbf{p}_2) = 0 \quad (6.31)$$

6.3 Transport

6.3.1 Boltzmann collision integral in terms of scattering

We now try to understand the Boltzmann collision integral, RHS of Eq. (6.25), intuitively in terms of microscopic two-body scattering. Consider a unit flux of type 1 molecules incident on a single type 2 molecule, with relative velocity $\mathbf{V} = \mathbf{v}_1 - \mathbf{v}_2$. During collision (τ_c short), external forces have minimal time to do work, so the centre-of-mass velocity $\mathbf{u} = 1/2(\mathbf{v}_1 + \mathbf{v}_2)$ and kinetic energy $m/2(v_1^2 + v_2^2)$ are conserved, implying that during a collision external forces have no time to do external work and hence the collisions are

elastic, i.e.

$$|\mathbf{v}_1 - \mathbf{v}_2| = |\mathbf{v}'_1 - \mathbf{v}'_2|. \quad (6.32)$$

Consider molecules in the volume $d^3\mathbf{x}$ around \mathbf{x} and collisions in the time interval dt around t . Suppressing \mathbf{x} and t dependences in f to simplify notation we can define the number of molecules with velocities $(\mathbf{v}_1, \mathbf{v}_1 + d^3\mathbf{v}_1)$ *lost from* the volume $d^3\mathbf{x}$ in the time interval dt (by \mathbf{v}_1 scattering off \mathbf{v}_2 to \mathbf{v}'_1) as

$$\hat{D}_c^{(-)} f(\mathbf{v}_1) d^3\mathbf{x} d^3\mathbf{v}_1 dt = \int_{\mathbf{v}_2, \mathbf{v}'_1, \mathbf{v}'_2} A \times B \times C, \quad (6.33)$$

where A is the flux of particles with velocity \mathbf{v}_1 incident on molecules of type 2, with velocity \mathbf{v}_2 , B is fraction of \mathbf{v}_1 molecules scattered by a single type 2 molecule, i.e., no. of molecules/unit flux scattered and C is the number of targets (type 2 molecules) in volume $d^3\mathbf{x}$ and velocity range $(\mathbf{v}_2, \mathbf{v}_2 + d^3\mathbf{v}_2)$. Mathematically, Eq. (6.33) has the following form

$$\begin{aligned} \hat{D}_c^{(-)} f(\mathbf{v}_1) d^3\mathbf{x} d^3\mathbf{v}_1 dt &= \int |\mathbf{v}_1 - \mathbf{v}_2| f(\mathbf{v}_1) d^3\mathbf{v}_1 \\ &\times \sigma(\mathbf{v}_1, \mathbf{v}_2 \rightarrow \mathbf{v}'_1, \mathbf{v}'_2) dt d^3\mathbf{v}'_1 d^3\mathbf{v}'_2 \\ &\times f(\mathbf{v}_2) d^3\mathbf{x} d^3\mathbf{v}_2, \end{aligned} \quad (6.34)$$

where $\sigma(\mathbf{v}_1, \mathbf{v}_2 \rightarrow \mathbf{v}'_1, \mathbf{v}'_2)$ is the number of molecules per unit time that emerge after scattering with velocity ranges $\mathbf{v}'_1, \mathbf{v}'_1 + d^3\mathbf{v}'_1$ and $\mathbf{v}'_2, \mathbf{v}'_2 + d^3\mathbf{v}'_2$. Hence

$$\hat{D}_c^{(-)} f(\mathbf{v}_1) = \int d^3\mathbf{v}'_1 d^3\mathbf{v}'_2 d^3\mathbf{v}_2 |\mathbf{v}_1 - \mathbf{v}_2| f(\mathbf{v}_1) f(\mathbf{v}_2) \sigma(\mathbf{v}_1, \mathbf{v}_2 \rightarrow \mathbf{v}'_1, \mathbf{v}'_2). \quad (6.35)$$

In a similar manner we can define the number of molecules with velocities $(\mathbf{v}_1, \mathbf{v}_1 + d^3\mathbf{v}_1)$ *gained by* the volume $d^3\mathbf{x}$ in the time interval dt (by \mathbf{v}'_1 scattering off \mathbf{v}_2' to \mathbf{v}_1) as

$$\hat{D}_c^{(+)} f(\mathbf{v}_1) d^3\mathbf{x} d^3\mathbf{v}_1 dt = \int_{\mathbf{v}_2, \mathbf{v}'_1, \mathbf{v}'_2} A \times B \times C, \quad (6.36)$$

where A is the flux of particles with velocity \mathbf{v}'_1 incident on molecules of type 2, with velocity \mathbf{v}_2' , B is fraction of \mathbf{v}'_1 molecules scattered per incident flux and C is the number of targets (type 2 molecules) in volume $d^3\mathbf{x}$ and velocity range $(\mathbf{v}'_2, \mathbf{v}'_2 + d^3\mathbf{v}'_2)$. Mathematically,

Eq. (6.36) has the following form

$$\begin{aligned}\hat{D}_c^{(+)} f(\mathbf{v}_1) d^3 \mathbf{x} d^3 \mathbf{v}_1 dt &= \int |\mathbf{v}'_1 - \mathbf{v}'_2| f(\mathbf{v}'_1) d^3 \mathbf{v}'_1 \\ &\times \sigma(\mathbf{v}'_1, \mathbf{v}'_2 \rightarrow \mathbf{v}_1, \mathbf{v}_2) dt d^3 \mathbf{v}'_1 d^3 \mathbf{v}_2 \\ &\times f(\mathbf{v}'_2) d^3 \mathbf{x} d^3 \mathbf{v}'_2\end{aligned}\quad (6.37)$$

and hence

$$\hat{D}_c^{(+)} f(\mathbf{v}_1) = \int d^3 \mathbf{v}'_1 d^3 \mathbf{v}'_2 d^3 \mathbf{v}_2 |\mathbf{v}'_1 - \mathbf{v}'_2| f(\mathbf{v}'_1) f(\mathbf{v}'_2) \sigma(\mathbf{v}'_1, \mathbf{v}'_2 \rightarrow \mathbf{v}_1, \mathbf{v}_2). \quad (6.38)$$

Using Eq. (6.32) and the symmetry property:

$$\sigma(\mathbf{v}'_1, \mathbf{v}'_2 \rightarrow \mathbf{v}_1, \mathbf{v}_2) = \sigma(\mathbf{v}_1, \mathbf{v}_2 \rightarrow \mathbf{v}'_1, \mathbf{v}'_2) \quad (6.39)$$

results in a change in f due to collisions, RHS of Eq. (6.30) of the following form:

$$\frac{df}{dt} \Big|_{\text{coll}} = \hat{D}_c^{(+)} f(\mathbf{v}_1) - \hat{D}_c^{(-)} f(\mathbf{v}_1) \quad (6.40)$$

$$= \int d^3 \mathbf{v}'_1 d^3 \mathbf{v}'_2 d^3 \mathbf{v}_2 |\mathbf{v}_1 - \mathbf{v}_2| \sigma(\mathbf{v}_1, \mathbf{v}_2 \rightarrow \mathbf{v}'_1, \mathbf{v}'_2) (f(\mathbf{v}'_1) f(\mathbf{v}'_2) - f(\mathbf{v}_1) f(\mathbf{v}_2)). \quad (6.41)$$

As such, in the dilute limit a transport process is encapsulated by:

$$\begin{aligned}\frac{\partial f}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial f}{\partial \mathbf{x}_1} + \frac{\mathbf{F}_1}{m} \cdot \frac{\partial f}{\partial \mathbf{v}_1} &= \\ - \int d^3 \mathbf{v}'_1 d^3 \mathbf{v}'_2 d^3 \mathbf{v}_2 |\mathbf{v}_1 - \mathbf{v}_2| \sigma(\mathbf{v}_1, \mathbf{v}_2 \rightarrow \mathbf{v}'_1, \mathbf{v}'_2) (f(\mathbf{v}'_1) f(\mathbf{v}'_2) - f(\mathbf{v}_1) f(\mathbf{v}_2)).\end{aligned}\quad (6.42)$$

6.3.2 Relaxation time approximation

Assume the effect of collisions is to restore local equilibrium described by $f^{(0)}(\mathbf{r}, \mathbf{v}, t)$. Assume collisions restore f towards $f^{(0)}$ with a relaxation time τ , then, in the linear response limit, the Boltzmann equation can be written as (BGK approximation: P. L. Bhatnagar, E. P. Gross, and M. Krook, Phys. Rev. **94**, 511 (1954))

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = -\frac{f - f^{(0)}}{\tau} \quad (6.43)$$

6.3.3 Calculation of electrical conductivity

Consider a small electric field $\mathbf{E}^{(1)}$ applied to a uniform gas containing some ions (or electrons) of charge q (mass m). This causes a departure from equilibrium, i.e. an electrical current $\mathbf{J}^{(1)}$. The response is proportional to the perturbation: $J_i^{(1)} = \sigma_{ij} E_j^{(1)}$, where σ_{ij} is the electrical conductivity.

To calculate σ , need a perturbation $f^{(1)}$ to $f^{(0)}$. Taking the Boltzmann first order term and writing $f = f^{(0)} + f^{(1)}$ one has

$$\frac{\partial f^{(1)}}{\partial t} + \mathbf{v} \cdot \frac{\partial f^{(1)}}{\partial \mathbf{x}} + \frac{q\mathbf{E}^{(1)}}{m} \cdot \left(\frac{\partial f^{(0)}}{\partial \mathbf{v}} + \frac{\partial f^{(1)}}{\partial \mathbf{v}} \right) = -\frac{f^{(1)}}{\tau}. \quad (6.44)$$

In the above equation the term $\mathbf{E}^{(1)} \cdot (\partial f^{(1)})/(\partial \mathbf{v}) \approx 0$, since this is second order and we ave implicitly assumed that the perturbations away from equilibrium are small. Additionally, we assume $\mathbf{E}^{(1)}$ is uniform, hence $f^{(1)}$ is uniform implying $\partial f^{(1)}/\partial \mathbf{x} = 0$. Since the electric field perturbation is static $f^{(1)}$ must also be static implying $\partial f^{(1)}/\partial t = 0$. So

$$f^{(1)} = -\frac{q\mathbf{E}^{(1)}\tau}{m} \frac{\partial f^{(0)}}{\partial \mathbf{v}}. \quad (6.45)$$

Since the current density $\mathbf{J}^{(1)}$ is equal to the average velocity of the carriers multiplied by the charge density we have

$$\mathbf{J}^{(1)} = \int d^3 \mathbf{v} f^{(1)} \mathbf{v} q. \quad (6.46)$$

Assuming that the perturbation in the electric field is along z gives

$$J_z^{(1)} = -\frac{q^2 E_z^{(1)} \tau}{m} \int d^3 \mathbf{v} v_z \frac{\partial f^{(0)}}{\partial v_z}. \quad (6.47)$$

Integrating by parts and noting that $f^{(0)} \rightarrow 0$ as $|v_z| \rightarrow \infty$ we find

$$J_z^{(1)} = \frac{q^2 E_z^{(1)} \tau}{m} \int dv_x dv_y \int dv_z f^{(0)}, \quad (6.48)$$

where $\int dv_x dv_y \int dv_z f^{(0)}$ is just the number of particles per unit volume ($n^{(0)}$). As such we find

$$\sigma_{zz} = \frac{n^{(0)} q^2 \tau}{m} \quad (6.49)$$

6.3.4 Landau damping

Start from

$$\frac{\partial f^{(1)}}{\partial t} + \mathbf{v} \cdot \frac{\partial f^{(1)}}{\partial \mathbf{x}} - \frac{e\mathbf{E}^{(1)}}{m} \cdot \frac{\partial f^{(0)}}{\partial \mathbf{v}} = -\frac{f^{(1)}}{\tau}. \quad (6.50)$$

For simplicity we will assume that the plasma is collisionless and hence:

$$\frac{\partial f^{(1)}}{\partial t} + \mathbf{v} \cdot \frac{\partial f^{(1)}}{\partial \mathbf{x}} - \frac{e\mathbf{E}^{(1)}}{m} \cdot \frac{\partial f^{(0)}}{\partial \mathbf{v}} = 0. \quad (6.51)$$

Expressing (perturbation in z -direction)

$$f = f^{(0)} + f^{(1)} e^{ikz - i\omega t} \quad (6.52)$$

we find

$$f^{(1)} = \frac{ieE_z^{(1)}}{m} \left(\frac{1}{\omega - kv_z} \right) \frac{\partial f^{(0)}}{\partial v_z}, \quad (6.53)$$

so when the electron velocity \approx the phase velocity of the wave, i.e. $\omega - kv_z \approx 0$, $f^{(1)}$ gets big and the approximation breaks down. However, we also have to consider the self-consistency condition for the electric field:

$$\text{div}\mathbf{E}^{(1)} = -\frac{e}{\epsilon_0} \times \text{number density} = -\frac{e}{\epsilon_0} \int d^3\mathbf{v} f^{(1)}. \quad (6.54)$$

Combining Eqs. (6.53) and (6.54) results in the following dispersion relation:

$$0 = 1 - \frac{e^2}{\epsilon_0 m k^2} \int d^3\mathbf{v} \left(\frac{1}{\omega/k - v_z} \right) \frac{\partial f^{(0)}}{\partial v_z}. \quad (6.55)$$

Assuming a Maxwellian distribution for $f^{(0)}$:

$$f^{(0)}(v_z) = \frac{1}{n} \int dv_x \int dv_y f^{(0)}(\mathbf{v}) \quad (6.56)$$

Eq. (6.55) becomes

$$1 = \frac{\omega_p^2}{k^2} \int_{-\infty}^{\infty} dv_z \left(\frac{1}{\omega/k - v_z} \right) \frac{\partial f^{(0)}}{\partial v_z}, \quad (6.57)$$

where $\omega_p = ne^2/m\epsilon_0$. If we include collisions then the pole of the numerator is shifted off the real axis, i.e. $\omega/k - v_z \rightarrow \omega/k - v_z + i\epsilon$. Do the integral using Cauchy (Sokhotski-Plemelj theorem), in the limit $v_\phi = \omega/k \gg v_{\text{th}} = \sqrt{k_B T/m}$ then

$$\omega = \left[\omega_p^2 + \frac{3k^2 v_{\text{th}}^2}{2} \right]^{1/2} \left[1 - i \frac{\pi}{2} \frac{\omega_p^2}{k^2} \frac{\partial f^{(0)}}{\partial v_z} \Big|_{v_\phi} \right] \quad (6.58)$$

If $\partial f^{(0)} / \partial v_z$ is positive then damping occurs, if it is negative then wave growth occurs.

Physically, the above results say the following. Imagine a uniform electron plasma which is stationary and cold. Now displace a slab of the electrons to one side. They feel an electrostatic restoring force and slosh back and forth at frequency ω_p . If the plasma temperature is not zero, this standing wave turns into a compressional travelling wave. The wave propagates forever undamped if only fluid effects are considered. If we now also turn on the kinetic effects, we find that the travelling wave is damped (by Landau damping) at a rate given by the imaginary part of the dispersion relation above.

Now suppose the plasma bulk is a Maxwellian at the above temperature but a small fraction (say, 1%) of the electrons are travelling fast, at v_b . This is called a beam in velocity space, even though it is still uniform in real space in this example. Then $\partial f^{(0)} / \partial v_z < 0$ and Landau damping changes sign and becomes growth. The strongest growth is for waves satisfying the Landau resonance, i.e. with wave number $k = \omega_p/v_b$. They grow at a rate given by the imaginary part of the dispersion relation.

6.4 Problem(s)

1. Global clusters: An isolated, steady-state, spherically symmetric star cluster consists of N identical stars, each of mass m , orbiting in a self-consistent gravitational potential $\Phi(\mathbf{x})$. The stellar density is low enough for the orbits to be considered collisionless.

(a) Show that the stellar pdf $p(t, \mathbf{x}, \mathbf{v})$ identically satisfies the collisionless Boltzmann equation if it can be written wholly as a function $p(E)$ of the mechanical energy per unit mass of an arbitrary star, $E[t, \mathbf{x}(t), \mathbf{v}(t)]$.

(b) Show that the gravitational potential satisfies

$$\nabla^2 \Phi = 16\pi^2 G N m \int_0^\infty dv v^2 p \left[\frac{v^2}{2} + \Phi(\mathbf{x}) \right]. \quad (6.59)$$

(c) Show that the total mass of the cluster is infinite (another way of saying that

the pdf is not normalizable). Why does this happen, physically? How might we rescue the situation?

Chapter 7

Stability of uniform far-from-equilibrium systems

7.1 Systems of nonlinear ODEs

Consider an N -dimensional dynamical system, described by a state vector $\mathbf{x} = (x_1, \dots, x_N)$, whose evolution is governed by

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}[\mathbf{x}(t)]. \quad (7.1)$$

The system can be efficiently integrated numerically (e.g. using the 4th-order Runge-Kutta algorithm). If the system is non-autonomous, i.e. \mathbf{F} depends explicitly on t , it can be converted into an equivalent autonomous system by adding a new variable $x_{N+1}(t) = t$ supplemented by the initial condition $x_{N+1}(0) = 0$.

One or more equilibrium points of Eq. (7.1) may exist, satisfying $d\mathbf{x}/dt = 0$ at $\mathbf{x} = \mathbf{x}^{(0)}$:

$$\mathbf{F}[\mathbf{x}^{(0)}] = 0. \quad (7.2)$$

To examine the stability of $\mathbf{x}^{(0)}$, it is enough to linearise about it and solve for the fate of infinitesimal disturbances; the nonlinear dynamics are irrelevant to local (as opposed to global) stability in all situations where linearization does indeed lead to a linear system.

The fixed point at the origin of a system like $\dot{x} = x^2 - y^3$, $\dot{y} = x^3 - y^2$ is an obvious counterexample.

Linearising, we write

$$\mathbf{x}(t) = \mathbf{x}^{(0)} + \mathbf{x}^{(1)}(t), \quad (7.3)$$

where $\mathbf{x}^{(1)}(t)$ is a small perturbation. From Eq. (7.1), we get

$$\frac{dx_i^{(1)}}{dt} = F_i[\mathbf{x}^{(0)} + \mathbf{x}^{(1)}(t)]. \quad (7.4)$$

Taylor expanding the RHS of this equation (assuming the perturbation is small) results in

$$\frac{dx_i^{(1)}}{dt} \approx F_i[\mathbf{x}^{(0)}] + x_j^{(1)} \left. \frac{\partial F_i}{\partial x_j} \right|_{\mathbf{x}=\mathbf{x}^{(0)}}. \quad (7.5)$$

Let us write $A_{ij} = \partial F_i / \partial x_j |_{\mathbf{x}=\mathbf{x}^{(0)}}$ for the Jacobian at $\mathbf{x}^{(0)}$. Solutions of Eq. (7.5) are $\exp[\lambda_i t]$, where λ_i are the eigenvalues of the matrix A , i.e.

$$\det(A - \lambda I) = 0. \quad (7.6)$$

Hence a small displacement is bounded for all t as long as $\text{Re}(\lambda_i) \leq 0$ for all i , in which case the system is stable. Heuristically, think of a ball in a frictional bowl.

If all $\text{Re}(\lambda_i) = 0$, the system is still stable, but neutrally so. Small displacements do not die away with time, but nor do they grow. If the eigenvalues have imaginary parts, a small-amplitude oscillation occurs, whose amplitude is set by the initial conditions of the disturbance. Think of a ball on a flat table or a frictionless bowl.

If even one of the eigenvalues has positive real part, the system is unstable; the disturbance grows without bound locally. Think of a ball on an inverted bowl.

7.1.1 Worked example: Lotka-Volterra

Remember the predator-prey model from Sec. 5.1.1. In the limit of large N the population dynamics are given by the following coupled ODEs (Eq. (5.4)):

$$\frac{dX}{dT} = k_1 a X - k_2 X Y \quad (7.7)$$

$$\frac{dY}{dT} = k_2 X Y - k_3 Y. \quad (7.8)$$

Introducing dimensionless parameters, $x = (k_1/k_3)X$, $y = (k_1/k_3)Y$ and $t = k_3 T$ the above equations take the following dimensionless form:

$$\frac{dx}{dt} = \alpha x - \beta xy \quad (7.9)$$

$$\frac{dy}{dt} = \beta yx - y, \quad (7.10)$$

where $\alpha = ak_1/k_3$ and $\beta = k_2/k_1$.

Equilibrium is defined by

$$0 = x(\alpha - \beta y) \quad (7.11)$$

$$0 = y(\beta x - 1). \quad (7.12)$$

The two equilibria are $x = y = 0$ and $x = 1/\beta$, $y = \alpha/\beta$.

Stability of $x = y = 0$

Expanding around the equilibrium point $x = y = 0$ we have

$$x = x^{(0)} + x^{(1)}(t) = x^{(1)}(t) \quad (7.13)$$

$$y = y^{(0)} + y^{(1)}(t) = y^{(1)}(t). \quad (7.14)$$

Now linearise:

$$\frac{dx^{(1)}}{dt} = \alpha x^{(1)} \quad (7.15)$$

$$\frac{dy^{(1)}}{dt} = -y^{(1)}. \quad (7.16)$$

Hence, the equilibrium state $x = y = 0$ is stable if $\alpha < 0$ (unphysical) and unstable if $\alpha > 0$.

Stability of $x = 1/\beta$, $y = \alpha/\beta$

Expanding around the equilibrium point $x = 1/\beta$, $y = \alpha/\beta$ we have

$$x = x^{(0)} + x^{(1)}(t) = \frac{1}{\beta} + x^{(1)}(t) \quad (7.17)$$

$$y = y^{(0)} + y^{(1)}(t) = \frac{\alpha}{\beta} + y^{(1)}(t). \quad (7.18)$$

Hence linearising we find

$$\frac{dx^{(1)}}{dt} = -y^{(1)} \quad (7.19)$$

$$\frac{dy^{(1)}}{dt} = \alpha x^{(1)}, \quad (7.20)$$

which can be written in the following form:

$$\begin{pmatrix} -\lambda & -1 \\ \alpha & -\lambda \end{pmatrix} \begin{pmatrix} x^{(1)} \\ y^{(1)} \end{pmatrix} = 0. \quad (7.21)$$

Hence the eigenvalues are given by $\lambda^2 = -\alpha$ and the equilibrium state $x = 1/\beta$, $y = \alpha/\beta$ is unstable if $\alpha < 0$ (unphysical) and λ is purely imaginary if $\alpha > 0$: hence the system exhibits a limit cycle (period $2\pi/\sqrt{\alpha}$), see Sections 7.2 and 7.3.

✓ **Exercise:** Consider a Lotka-Volterra-type system comprising food fish x , predators (eg., sharks) y , and logistic competition between members of the same species:

$$\frac{dx}{dt} = ax - bxy - kx^2 \quad (7.22)$$

$$\frac{dy}{dt} = -cy + dxy - ey^2. \quad (7.23)$$

Explain why the food fish population declined when fishing decreased under war conditions. (Counterintuitive!)

7.1.2 Example: large trophic webs

Above we have considered a small trophic web, i.e. one predator and one prey. But one can ask the question *is a large ecosystem more or less stable than a small one?* Naively, one would expect that, in structurally complex systems, the myriad connections should cancel each other out and engender stability. This is false! For a review of this see the following articles: R.M. May 1973, Stability and complexity in model ecosystems, Princeton University Press (1973) and R.M. May, Nature **238**, 413 (1972).

Consider n predators P_i and n prey H_i , forming a trophic web with n^2 links:

$$\frac{dH_i}{dt} = H_i \left(a_i - \sum_{j=1}^n \alpha_{ij} P_j \right) \quad (7.24)$$

$$\frac{dP_i}{dt} = P_i \left(-b_i + \sum_{j=1}^n \beta_{ij} H_j \right). \quad (7.25)$$

The connection coefficients are arbitrary, except that the equilibrium (P_i^*, H_i^*) is non trivial. If we Taylor expand about the equilibrium value to test for stability we get a Jacobian of the following form:

$$A_{2n \times 2n} = \begin{pmatrix} 0_{n \times n} & -\alpha^* \\ \beta^* & 0_{n \times n} \end{pmatrix}. \quad (7.26)$$

If $\beta_{ij} = 0$ and α_{ij} is antisymmetric, the dynamics are purely oscillatory! But this choice is too special. In nature, α_{ij} and β_{ij} are random. The eigenvalues of the linearised system must then be found from the theory of random matrices. It turns out that the eigenvalues are distributed in a related way to the roots of Riemann zeta function, see C. E. Porter, *Statistical theories of spectra: fluctuations*, Academic Press (1965) and M.L. Mehta, *Random matrices* Academic Press (2004).

In this course I am not going to specifically cover random matrices, however, the key result is the following. The eigenvalues of a random matrix tend to repel each other in the complex plane, because the probability of coincident eigenvalues tends to zero as the matrix size $N \rightarrow \infty$. In fact, for matrices drawn from the Gaussian orthogonal ensemble, the distribution of the distances x between eigenvalues is $P_2(x) = \pi x / 2 \exp(-\pi x^2 / 4)$ (for a 2×2 matrix); i.e. zero spacings are improbable (cf. Poisson distribution). For a large- N matrix, the probability distribution of eigenvalues is obtained by integrating $P_N(x_1, x_2, \dots, x_N)$ over all eigenvalues except one, and we get Wigner's semicircle law $P(\lambda) = 2(N - \lambda)^{1/2} / (N\pi)$ for $\lambda < N^{1/2}$ and zero otherwise. Note that this is for a matrix ensemble with Gaussian statistics and dimensionless elements, with zero mean for off-diagonal elements and variance $1/4$, and zero mean for diagonal elements and variance $1/2$. If the off-diagonal variance is $a^2/4$, then λ needs to be multiplied by a .

May argued (Nature **238**, 413 (1972)) that you get similar results in large- N ecologies

even when the systems are not Hermitian and the random-matrix theory above does not apply directly. He found in his Nature paper that the ecology is stable for

$$\alpha < (NC)^{-1/2}, \quad (7.27)$$

where α is the rms of α_{ij} (zero mean), and C is the probability that any pair interacts (i.e. $\alpha_{ij} = 0$). Furthermore, he found the following features:

1. Rapid transition from stable to unstable as α or C are varied; the abruptness of the transition increases with N .
2. Unstable if the trophic web is too richly connected (C large) or the interaction between species is too strong (large α). Interestingly, this matches Nature, where one usually observes feeble interactions between many species, or strong interactions between few species. (Do humans fit this pattern?)
3. Block diagonal arrangements are preferred, e.g. a 12×12 trophic web with $\alpha = 1/\sqrt{3}$ and $C = 0.15$ is statistically unstable, whereas a trophic web split into three 4×4 blocks, with $C = 0.45$ within each block and α unchanged, is stable with probability of 35%.

The May results above are not completely general, as their author foreshadowed. You can find special classes of random matrices (possibly even some ecologically interesting ones) which don't satisfy the above results. For a fuller discussion, see Cohen and collaborators, *Annals of Probability* **12**, 283 (1984).

7.2 Phase plane

In this section we are going to consider phase plane analysis, i.e. what the trajectories look like, focusing on the two-dimensional case. Start by consider the following two-dimensional system:

$$\frac{dx}{dt} = f(x, y) \quad (7.28)$$

$$\frac{dy}{dt} = g(x, y). \quad (7.29)$$

What we want to obtain is how $x(t)$ and $y(t)$ evolve for perturbations around some equilibrium point. We can rewrite the two equations above as:

$$\frac{dx}{dy} = \frac{f(x, y)}{g(x, y)}. \quad (7.30)$$

If we consider some stationary state, at $(0, 0)$, then linearising about this point we have

$$\frac{dx}{dy} \approx \frac{ax + by}{cx + dy}, \quad (7.31)$$

which is equivalent to

$$\frac{dx}{dt} \approx ax + by \quad (7.32)$$

$$\frac{dy}{dt} \approx cx + dy. \quad (7.33)$$

Representing the expansion as a matrix we have

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} f_x & f_y \\ g_x & g_y \end{pmatrix}_{(0,0)}. \quad (7.34)$$

Evaluating

$$\begin{vmatrix} a - \lambda & b \\ c & d - \lambda \end{vmatrix} = 0 \quad (7.35)$$

provides the eigenvalues for the perturbation:

$$\lambda = \frac{(a+d) \pm \sqrt{(a+d)^2 - 4\det A}}{2}. \quad (7.36)$$

Thus the solutions for Eqs. (7.32,7.33) has the following form

$$\begin{pmatrix} x \\ y \end{pmatrix} = c_1 \mathbf{v}_1 e^{\lambda_1 t} + c_2 \mathbf{v}_2 e^{\lambda_2 t}, \quad (7.37)$$

noting that if the eigenvalues are degenerate $x = y = (c_1 + c_2) \exp(\lambda t)$. In the above c_1 and c_2 are arbitrary constants and \mathbf{v}_1 and \mathbf{v}_2 are the eigenvectors of A corresponding to λ_1 and λ_2 respectively.

Of course the above can be generalised to higher dimensions and the case where the expansion is not around $(0, 0)$. However, it gets complicated quickly, but in general for a two dimensional system the behaviour of the system can be characterised by the properties of λ_1 and λ_2 .

Catalogue of singularities in the phase plane: two dimensions

1. λ_1 and λ_2 are real and distinct:

(a) λ_1 and λ_2 have the same sign. Suppose $\lambda_1 < \lambda_2 < 0$, then for $c_2 = 0$, $c_1 \neq 0$

$$\begin{pmatrix} x \\ y \end{pmatrix} = c_1 \mathbf{v}_1 e^{\lambda_1 t} \quad (7.38)$$

so the solution in the phase space moves along \mathbf{v}_1 towards the origin as $t \rightarrow \infty$.

This is called a node (Type I) singularity. With $\lambda_1 \leq \lambda_2 \leq 0$ it is a stable node since all trajectories tend to $(0, 0)$ as $t \rightarrow \infty$. If $\lambda_1 \geq \lambda_2 \geq 0$ it is an unstable node: $(x, y) \rightarrow (0, 0)$ as $t \rightarrow -\infty$.

(b) λ_1 and λ_2 have different signs. Suppose $\lambda_1 < 0 < \lambda_2$ then $\mathbf{v}_1 \exp[\lambda_1 t] \rightarrow 0$ along \mathbf{v}_1 as $t \rightarrow \infty$ while $\mathbf{v}_2 \exp[\lambda_2 t] \rightarrow 0$ along \mathbf{v}_2 as $t \rightarrow -\infty$. There are therefore different directions on \mathbf{v}_1 and \mathbf{v}_2 .

2. λ_1, λ_2 complex: $\lambda_1, \lambda_2 = \alpha \pm i\beta$, $\beta \neq 0$. Solutions here involve $\exp[\alpha t] \exp[\pm i\beta t]$ which implies an oscillatory approach to $(0, 0)$.

- (a) $\alpha \neq 0$. Forms spiral singularity which is stable for $\alpha < 0$ and unstable for $\alpha > 0$.
- (b) $\alpha = 0$. The phase curves are ellipses, with a singularity called a centre. Centres are not stable in the usual sense; a small perturbation from one phase curve does not die out.

Summary of singularity

The singularity depends on a, b, c and d in the matrix A . Defining $\det A = f_x g_y - f_y g_x = ad - bc$, $\text{Tr}A = f_x + g_y = a + d$, where the partial derivatives are evaluated at the singularities, the solutions of $f(x, y) = g(x, y) = 0$ the following applies

- *Centre*: $\text{tr}A = 0$ and $\det A > 0$.
- *Unstable spiral*: $\text{Tr}A > 1/4\det A$ with $\text{Tr}A > 0$.

- *Unstable node*: $0 < \text{Tr}A < 1/4\det A$.
- *Stable spiral*: $1/4\det A < \text{Tr}A < 0$.
- *Stable node*: $\text{Tr}A < 1/4\det A$ with $\text{Tr}A < 0$.
- *Saddle point*: $\det A < 0$ and $\text{Tr}A$ is positive or negative.

7.3 Limit cycles: Hopf bifurcation theorem

A Hopf bifurcation occurs when a fixed point in a two-dimensional system controlled by a single parameter ν makes a transition from a stable spiral, to a limit cycle growing out of the origin, without becoming a centre as an intermediate stage.

Consider the nonlinear system:

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(\mathbf{x}, \nu), \quad (7.39)$$

where ν is a real parameter in the range $(-\nu_0, \nu_0)$. Suppose an equilibrium $\mathbf{x}^*(\nu)$ state exists for a particular ν :

$$\mathbf{F}(\mathbf{x}^*(\nu), \nu) = 0. \quad (7.40)$$

Let $A(\nu)$ be the Jacobian about the equilibrium point $\mathbf{x}^*(\nu)$:

$$A(\nu)_{ij} = \left. \frac{\partial F_i}{\partial x_j} \right|_{\mathbf{x}=\mathbf{x}^*(\nu)}. \quad (7.41)$$

Suppose A has pure imaginary eigenvalues eigenvalues $\pm i\omega$ for $\nu = 0$, i.e.

$$\text{Tr}A(0) = 0, \quad \det A(0) > 0.$$

If the matrix B , defined by

$$B(\nu) = \frac{A(\nu) - A(0)}{\nu} \quad (7.42)$$

satisfies

$$\text{Tr}B(0) \neq 0 \quad (7.43)$$

then the original system has a periodic solution for ν in some neighbourhood of $\nu = 0$ and \mathbf{x} near \mathbf{x}^* with period $\approx 2\pi/\omega$ for small ν .

7.3.1 Example 1

Consider a simple linear case (for instance, a damped SHO),

$$\frac{d\mathbf{x}}{dt} = \frac{d}{dt} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_2 \\ -x_1 + \nu x_2 \end{pmatrix} = \mathbf{F}(\mathbf{x}, \nu). \quad (7.44)$$

The only equilibrium point is $x_1 = 0 = x_2$. The single equation for x_1 is

$$\frac{d^2x_1}{dt^2} - \nu \frac{dx_1}{dt} + x_1 = 0, \quad (7.45)$$

and hence the solution for the system is

$$x_2 = \frac{dx_1}{dt} \quad (7.46)$$

$$x_1 = e^{\nu t/2} \left\{ A \cos \left[(1 - \nu^2/4)^{1/2} t \right] + B \sin \left[(1 - \nu^2/4)^{1/2} t \right] \right\}, \quad (7.47)$$

where A and B are constants with $\nu^2 < 4$. The value $\nu = 0$ is a bifurcation point, i.e., in the phase plane for Eq. (7.44) the singular point of

$$\frac{dx_2}{dx_1} = \frac{x_1 - \nu x_2}{x_2} \quad (7.48)$$

is a stable or unstable focus according to whether $\nu < 0$ and $\nu > 0$ but in either case $|\nu| < 2$.

For values of ν in the vicinity of the equilibrium point, the only periodic solutions from Eq. (7.44) are

$$\nu = 0 \quad (7.49)$$

$$x_1 = A \cos t + b \sin t \quad (7.50)$$

$$x_2 = \frac{dx_1}{dt}, \quad (7.51)$$

or if $\nu \neq 0$, $x_1 = x_2 = 0$, the trivial solution.

7.3.2 Example 2

Consider now the non-trivial nonlinear system

$$\frac{d\mathbf{x}}{dt} = \frac{d}{dt} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_2 \\ -x_1 + \nu x_2 - x_1^2 x_2 \end{pmatrix} = \mathbf{F}(\mathbf{x}, \nu). \quad (7.52)$$

Note by eliminating x_2 we have

$$\frac{d^2x_1}{dt^2} + (x_1^2 - \nu) \frac{dx_1}{dt} + x_1 = 0, \quad (7.53)$$

which is the Lienard equation. The equilibrium point is $x_1 = x_1^* = x_2 = x_2^* = 0$. To determine the matrix A (see Eq. (7.41)) one needs

$$A_{11} = \left. \frac{\partial F_1}{\partial x_1} \right|_{x_1=x_1^*, x_2=x_2^*} = \left. \frac{\partial x_2}{\partial x_1} \right|_{x_1=x_1^*, x_2=x_2^*} = 0 \quad (7.54)$$

$$A_{21} = \left. \frac{\partial F_2}{\partial x_1} \right|_{x_1=x_1^*, x_2=x_2^*} = \left. \frac{\partial -x_1 + \nu x_2 - x_1^2 x_2}{\partial x_1} \right|_{x_1=x_1^*, x_2=x_2^*} = -1 \quad (7.55)$$

$$A_{12} = \left. \frac{\partial F_1}{\partial x_2} \right|_{x_1=x_1^*, x_2=x_2^*} = \left. \frac{\partial x_2}{\partial x_2} \right|_{x_1=x_1^*, x_2=x_2^*} = 1 \quad (7.56)$$

$$A_{22} = \left. \frac{\partial F_2}{\partial x_2} \right|_{x_1=x_1^*, x_2=x_2^*} = \left. \frac{\partial -x_1 + \nu x_2 - x_1^2 x_2}{\partial x_2} \right|_{x_1=x_1^*, x_2=x_2^*} = \nu. \quad (7.57)$$

Hence

$$A = \begin{pmatrix} 0 & 1 \\ -1 & \nu \end{pmatrix}, \quad (7.58)$$

with eigenvalues given by $-\lambda(\nu - \lambda) + 1 = 0$. At $\nu = 0$ $\lambda = \pm i$, therefore oscillation period of limit cycle (if exists) is 2π .

Now consider $B(\nu)$ (see Eq. (7.42)) then for this case

$$B(\nu) = \frac{A(\nu) - A(0)}{\nu} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \quad (7.59)$$

Since $\text{Tr}B(0) \neq 0$ we have a Hopf bifurcation.

7.4 Nonlinear oscillators in nature

7.4.1 Field-Noyes model of cyclic chemical reactions: chemical clock

Consider the following chemical process:



where $A = \text{BrO}_3^-$, $Y = \text{Br}^-$, $X = \text{HBrO}_2$, $P = \text{HOBr}$ and $Z = \text{Ce}^{4+}$ and f is a stoichiometric factor. We can represent this via coupled ODEs:

$$\frac{dx}{dt} = k_1ay - k_2xy + k_3ax - k_4x^2 \quad (7.65)$$

$$\frac{dy}{dt} = -k_1ay - k_2xy + fk_5z \quad (7.66)$$

$$\frac{dz}{dt} = 2k_3ax - k_5z. \quad (7.67)$$

Do not always get oscillations. For example if $k_5 = 0$ the $Y \rightarrow 0$ and hence $\text{Br}^- \rightarrow 0$. So consider an intermediate range of concentrations and reformulate the above equations:

$$\epsilon \frac{dx}{dt} = qy - xy + x(1-x) \quad (7.68)$$

$$\delta \frac{dy}{dt} = -qy - xy + 2fz \quad (7.69)$$

$$\frac{dz}{dt} = x - z, \quad (7.70)$$

where $\epsilon \approx 5 \times 10^{-5}$, $\delta \approx 2 \times 10^{-4}$, $q \approx 8 \times 10^{-4}$ and $f = 1/2$. If ϵ and δ are small then either x, y, z are approximately constant or \dot{x} and \dot{y} are big \rightarrow rapid transition between states.

Examining Eqs. (7.68,7.69,7.70) there are two stable points: $(0, 0, 0)$ and $(x_s, 2fx_s/(q+x_s), x_s)$, where

$$2x_s = 1 - 2f - q + \sqrt{(1 - 2f - q)^2 + 4q(1 + 2f)}. \quad (7.71)$$

Linearising about each stable point and obtain the eigenvalues to determine the stability of the stationary states and the *motion* of excitations we find for $(0, 0, 0)$ that the eigenvalues are given by

$$\lambda^3 + \lambda^2 \left(1 + \frac{q}{\delta} - \frac{1}{\epsilon}\right) - \lambda \left[\frac{1}{\epsilon} \left(1 + \frac{q}{\delta}\right) - \frac{q}{\delta}\right] - \frac{q(1+2f)}{\epsilon\delta} = 0. \quad (7.72)$$

The above equation gives at least one positive root for λ and hence the stationary state $(0, 0, 0)$ is unstable.

For $(x_s, 2fx_s/(q+x_s), x_s)$, we obtain the following expression for the eigenvalues:

$$\lambda^3 + A\lambda^2 + B\lambda + C = 0, \quad (7.73)$$

where I leave it to you to determine A , B and C . The point to note is that for the special case $B = C/A$ we get a bifurcation, with solutions $\lambda = -A$ and $\lambda = \pm i\sqrt{C/A}$, hence oscillations are excited for $B < C/A$.

7.5 Parametric oscillators and resonance

7.5.1 General solution for a non-autonomous linear system

In general, the coefficients of a linear system of ODEs are themselves functions of time. An especially important sub-class are systems whose coefficients are periodic. An example is a pendulum whose length oscillates harmonically. Such systems exhibit a variety of interesting behaviours, e.g. *parametric instabilities*.

Consider a general, homogenous linear system in n dimensions:

$$\frac{dx_i(t)}{dt} = A_{ij}(t)x_j(t). \quad (7.74)$$

The dependence of A_{ij} on t makes the system non-autonomous. We state without proof that Eq. (7.74) has n linearly independent solutions, $\mathbf{u}^{(1)}(t), \dots, \mathbf{u}^{(n)}(t)$, which are also complete; any solution can be expressed as a linear combination of them. Let $\Phi_{ij} = [\mathbf{u}^{(j)}]_i$ be the matrix whose columns are the above independent solutions:

$$[\Phi_{ij}] = |\mathbf{u}^{(1)}(t)|, \dots, |\mathbf{u}^{(n)}(t)|. \quad (7.75)$$

The matrix $\Phi(t)$ is called the *fundamental matrix*.

- ✓ **Exercise:** Prove that any two fundamental matrices $\Phi_1(t)$ and $\Phi_2(t)$ are related by $\Phi_2(t) = \Phi_1(t)C$, where C is a matrix of constants.

We can now show that the solution of Eq. (7.74) that satisfies the initial condition $\mathbf{x}_0(t_0) = \mathbf{x}_0$ is given by

$$\mathbf{x}(t) = \Phi(t)\Phi^{-1}(t_0)\mathbf{x}_0, \quad (7.76)$$

where Φ is any fundamental matrix for Eq. (7.74).

- **Proof:** The general solution is $\mathbf{x}(t) = \Phi(t)C$, where Φ is a fundamental matrix. At $t = t_0$, we have $x_0 = \Phi(t_0)C$. But $\det\Phi(t) = 0$ for all t , as Φ is a fundamental matrix, so $\Phi(t_0)$ is invertible, giving $C = \Phi^{-1}(t_0)\mathbf{x}_0$.

For the inhomogenous (i.e. forced) system $\dot{\mathbf{x}}(t) = A(t)\mathbf{x}(t) + \mathbf{F}(t)$, the procedure is to find any one particular solution and add it to the complementary solution. Taking $\mathbf{x}(t) = \Phi(t)\Phi^{-1}(t_0)[\mathbf{x}_0 + \mathbf{u}(t)]$ without loss of generality, and substituting into Eq. (7.74), we find

$$\frac{d\mathbf{u}(t)}{dt} = \Phi(t_0)\Phi^{-1}(t)\mathbf{F}(t) \quad (7.77)$$

and hence

$$\mathbf{x}(t) = \Phi(t)\Phi^{-1}(t_0)\mathbf{x}(t_0) + \Phi(t_0) \int_{t_0}^t dt' \Phi^{-1}(t')\mathbf{F}(t'). \quad (7.78)$$

7.5.2 Periodic coefficients

Now consider the situation where A_{ij} is periodic, with minimum period T , i.e. $A_{ij}(t+T) = A_{ij}(t)$. Importantly, the solutions of the linear system, Eq. (7.74) are not necessarily periodic! For example, $\dot{x} = [1 + \sin t]x$ has the solutions $x = c \exp[t - \cos t]$.

- **Floquet's theorem:** The system Eq. (7.74) with $A_{ij}(t)$ periodic has at least one non-trivial solution $w(t)$ (known as a normal solution) such that $w(t+T) = \mu w(t)$, where μ is a constant.

In other words, at least one of the solutions is periodically self-similar (i.e., a magnified or shrunken copy of itself on the period T). For example, for $\dot{x} = (1 + \sin t)x$, we have $w = c \exp[t - \cos t]$ and hence $w(t+2\pi) = c \exp[t] \exp[2\pi] \exp[-\cos t] = \exp[2\pi]w(t)$. Clearly, even without knowing the form of $w(t)$, we see that the solution is unstable, i.e., $|w(t)|$ is unbounded, i.e., $|w(t)| \rightarrow \infty$ as $t \rightarrow \infty$.

Floquet's theorem is easy to prove. It relies on expressing the solutions at $t+T$ in terms of the solution at t . Let $\Phi(t)$ be a fundamental matrix of Eq. (7.74), i.e., $\dot{\Phi}(t) = A(t)\Phi(t)$. Then $\Phi(t+T)$ is also a fundamental matrix of Eq. (7.74), since $A(t+T) = A(t)$, and we can write $\Phi(t+T) = \Phi(t)C$ where C is a constant matrix with $\det C \neq 0$. Let μ be an eigenvalue of C with associated eigenvector \mathbf{u} . Define $\mathbf{w}(t) = \Phi(t)\mathbf{u}$. By construction, \mathbf{w} is a solution of Eq. (7.74). Moreover, we have

$$\mathbf{w}(t+T) = \Phi(t+T)\mathbf{u} = \Phi(t)C\mathbf{u} = \Phi(t)\mu\mathbf{u} = \mu\mathbf{w}(t). \quad (7.79)$$

The eigenvalues μ of C are called *characteristic numbers* of Eq. (7.74). They are independent of the choice of $\Phi(t)$. There are n of them in general (associated with n linearly independent solutions). If μ is an m^{th} complex root of unity, then $\mathbf{w}(t)$ is periodic with period mT .

Parametric instability

Consider a pendulum whose length oscillates harmonically, or an inverted pendulum with an oscillating point of suspension (or a double pendulum). Expressing time in units of the angular velocity, we obtain the following general equation of motion for the displacement $x(t)$:

$$\frac{d^2x}{dt^2} + (\alpha + \beta \cos t)x = 0, \quad (7.80)$$

where α is proportional to the natural frequency of the pendulum at its mean length, and β is proportional to the amplitude of the length oscillation. The above equation can be recast as coupled first order ODE's:

$$\frac{d}{dt} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\alpha - \beta \cos t & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = A \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \quad (7.81)$$

For this system the product of the characteristic numbers is $\mu_1\mu_2 = 1$, where μ_1 and μ_2 are eigenvalues of the characteristic matrix.. This comes from

$$\mu_1 \times \mu_2 \times \dots \times \mu_N = \exp \left[\int_{t_0}^t dt' \text{Tr} A_{ij} \right]. \quad (7.82)$$

We do not know $\mu_1 + \mu_2$ however we do know that it is only a function of α and β , so we can write

$$\mu^2 - \phi(\alpha, \beta)\mu + 1 = 0 \quad (7.83)$$

and hence

$$\mu = \frac{\phi(\alpha, \beta) \pm \sqrt{\phi(\alpha, \beta)^2 - 4}}{2}. \quad (7.84)$$

There are five possibilities:

1. $\phi > 2$: then both μ_1 and μ_2 are real and one exceeds unity, so $|\mathbf{w}(t + 2\pi)| > |\mathbf{w}(t)|$ and the solutions are unbounded.
2. $\phi = 2$: then $\mu_1 = \mu_2 = 1$ and only one solution has period 2π , the other is unbounded.
3. $-2 < \phi < 2$: then both μ_1 and $\mu_2 = \mu_1^*$ are complex. But $|\mu_1|\mu_2| = 1$, which implies $|\mu_1| = 1 = |\mu_2|$ and hence the solutions are of the form $\alpha \exp[\pm i\omega t]$. Hence the solutions are a mix of periods 2π and $2\pi/\omega$ and are stable (but not periodic, unless ω is an integer).
4. $\phi = -2$: then $\mu_1 = \mu_2 = -1$ and hence one solution has period 4π ; other is unbounded.
5. $\phi < -2$: then both μ_1 and μ_2 are real and negative and the solutions are unbounded: $|\mathbf{w}(t + 2\pi)| > |\mathbf{w}(t)|$.

Hence the curves $\phi(\alpha, \beta) = \pm 2$ (called transition curves) separate regions in the $\alpha - \beta$ plane where solutions are bounded and unbounded. Moreover, the periodic solutions (with periods 2π and 4π) only occur on these transition curves. So we seek periodic solutions in order to determine the transition curves.

First we consider the period 2π solutions:

$$x(t) = \sum_{n=-\infty}^{\infty} c_n e^{-int}. \quad (7.85)$$

Substituting this into Eq. (7.80) results in the following:

$$0 = \sum_{n=-\infty}^{\infty} c_n e^{-int} \left[-n^2 + \alpha + \frac{\beta}{2} (e^{it} + e^{-it}) \right] \quad (7.86)$$

$$= \sum_{n=-\infty}^{\infty} e^{-int} \left[-n^2 c_n + \alpha c_n + \frac{\beta}{2} c_{n+1} + \frac{\beta}{2} c_{n-1} \right], \quad (7.87)$$

where we transform to the dummy variables $n' = n \pm 1$ in the 3rd and 4th terms and then relabel n' as n . Orthogonality implies

$$(-n^2 + \alpha) c_n + \frac{\beta}{2} c_{n+1} + \frac{\beta}{2} c_{n-1} = 0. \quad (7.88)$$

For the period 4π solutions we use

$$x(t) = \sum_{n=-\infty}^{\infty} d_n e^{-int/2} \quad (7.89)$$

to get

$$\left(-\frac{1}{4}n^2 + \alpha \right) d_n + \frac{\beta}{2} d_{n+2} + \frac{\beta}{2} d_{n-2} = 0. \quad (7.90)$$

The above equation is decoupled for n is odd and even. But the set with n even is equivalent to Eq. (7.88). So the set with odd n must expand to the 4π solutions.

Equation (7.88) has non-trivial solutions for

$$\det \begin{vmatrix} \ddots & & & \\ & \gamma_1 & 1 & \gamma_1 \\ & \gamma_0 & 1 & \gamma_0 \\ & \gamma_1 & 1 & \gamma_1 \\ & & & \ddots \end{vmatrix} = 0, \quad (7.91)$$

with $\gamma_n = \beta/[2(\alpha - n^2)]$. This infinite determinant is called a Hill determinant. Letting

$$D_n = \det \begin{vmatrix} 1 & \gamma_n & & & & \\ \gamma_{n-1} & 1 & \gamma_{n-1} & & & \\ & \gamma_{n-2} & 1 & \gamma_{n-2} & & \\ & \ddots & \ddots & \ddots & & \\ & & \gamma_0 & 1 & \gamma_0 & \\ & & & \ddots & \ddots & \ddots \\ & & & & \gamma_{n-2} & 1 & \gamma_{n-2} \\ & & & & \gamma_{n-1} & 1 & \gamma_{n-1} \\ & & & & \gamma_n & 1 & \end{vmatrix}, \quad (7.92)$$

you can prove by induction that

$$D_{n+2} = (1 - \gamma_{n+1}\gamma_{n+2}) D_{n+1} + \gamma_{n+1}\gamma_{n+2} (1 - \gamma_{n+1}\gamma_{n+2}) D_n + \gamma_n^2 \gamma_{n+1}^3 \gamma_{n+2} D_{n-1}. \quad (7.93)$$

But the γ 's are functions of α and β . So you can trace out the $\phi(\alpha, \beta) = \pm 2$ curves by picking α and running through β , and isolating the value of β for which $D_\infty = 0$ (calculated from the recurrence relation).

- ✓ **Exercise:** Plot the 2π period transition curves and compare with the result obtained from the 3×3 matrix, i.e. D_1
- ✓ **Exercise:** Redo for the 4π period transition curves. **Hint:** The recursion relation is the same but with $\gamma_n = \beta/[2(\alpha - (2n + 1)^2/4)]$.

7.5.3 Perturbation theory

Consider an open system whose Lagrangian depends on time through variations in the parameters. Energy can be added to, or subtracted from, the system in this way, the previous example of pendulum whose length changes with time falls into this category. Generally speaking, such a system exhibits an infinite response (if undamped) for a range of parameters, usually when the parameters oscillate at a simple fraction multiples of the natural frequency of the system.

For example consider the following example:

$$\frac{d^2x}{dt^2} + \omega_0 (1 + \epsilon \cos \omega t) x = 0. \quad (7.94)$$

Expect the strongest response to be at $2\omega_0$, so set $\omega = 2\omega_0 + \sigma$, where σ is small and look for solutions of the form

$$x(t) = A(\sigma t) \cos \left[\omega_0 + \frac{1}{2}\sigma \right] t + B(\sigma t) \sin \left[\omega_0 + \frac{1}{2}\sigma \right] t, \quad (7.95)$$

where $A(\sigma t)$ and $B(\sigma t)$ are slowly varying amplitudes, i.e. $dA(\sigma t)/dt \sim \sigma \ll \omega_0 \sim d \cos(\omega_0 + \sigma/2)t/dt$. Substituting this ansatz into Eq. (7.94) and ignoring terms which do not resonate with the natural oscillation frequency (ω_0) we find from the coefficients of cos and sin

$$2A' + B\sigma + \frac{1}{2}\epsilon\omega_0 B = 0 \quad (7.96)$$

$$2B' - A\sigma + \frac{1}{2}\epsilon\omega_0 A = 0, \quad (7.97)$$

where the primes denote derivatives with respect to σt . Non-trivial solutions arise, $\propto \exp \lambda t$ for

$$\det \begin{vmatrix} 2\lambda & \sigma + \frac{1}{2}\epsilon\omega_0 \\ -\sigma + \frac{1}{2}\epsilon\omega_0 & 2\lambda \end{vmatrix} = 0. \quad (7.98)$$

Resonant solutions (i.e. explicitly growing) arise for

$$0 \leq \lambda^2 = \frac{1}{4} \left[\frac{\epsilon^2 \omega_0^2}{4} - \sigma^2 \right], \quad (7.99)$$

i.e. $-\epsilon\omega_0/2 \leq \sigma \leq \epsilon\omega_0/2$.

7.6 Stability of forced nonlinear oscillators

7.6.1 Nonlinear responses

Consider an electronic amplifier, e.g., in a stereo system. The amplifier converts a voltage V_{in} at its input terminals into an output voltage V_{out} . If the system is linear then $V_{\text{out}}(t) = kV_{\text{in}}(t)$ (solid line in LHS of Fig. 7.1). If it is nonlinear then $V_{\text{out}}(t) = k[V_{\text{out}}(t) + \epsilon V_{\text{out}}(t)^2]$ ((dashed line in LHS of Fig. 7.1)).

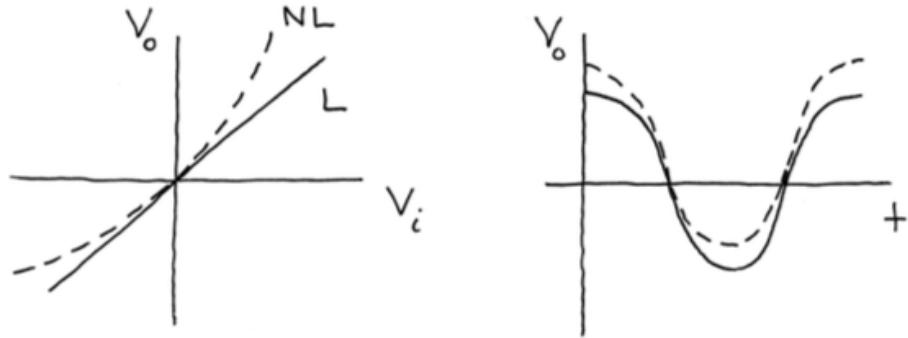


Figure 7.1. LHS: output voltage versus input voltage for a linear (solid line) and a nonlinear system (dashed line). RHS: output voltage versus time for a linear (solid line) and a nonlinear system (dashed line)

Suppose the input $V_{\text{in}}(t) = A \cos \omega t$ is a pure tone, then for a nonlinear system

$$V_{\text{out}}(t) = kA \cos \omega t + k\epsilon A^2 \cos^2 \omega t \quad (7.100)$$

$$= kA \cos \omega t + k\epsilon A^2 (1 + \cos^2 2\omega t), \quad (7.101)$$

hence the output is distorted (see LHS of Fig. 7.1):

- Anharmonic waveform
- Rectification (DC component)
- Harmonic generation (2ω component)

Now suppose the input $V_{\text{in}}(t) = A \cos \omega_1 t + B \cos \omega_2 t$ is a combination of two pure tones:

$$\begin{aligned} V_{\text{out}}(t) &= k(A \cos \omega_1 t + B \cos \omega_2 t) \\ &+ k\epsilon (A^2 \cos^2 \omega_1 t + 2AB \cos \omega_1 t \cos \omega_2 t + B^2 \cos^2 \omega_2 t) \end{aligned} \quad (7.102)$$

$$\begin{aligned} &= kA \cos \omega_1 t + \frac{1}{2}k\epsilon A^2 (1 + \cos 2\omega_1 t) \\ &+ kB \cos \omega_2 t + \frac{1}{2}k\epsilon B^2 (1 + \cos 2\omega_2 t) \\ &+ k\epsilon AB [\cos(\omega_1 + \omega_2)t + \cos(\omega_1 - \omega_2)t], \end{aligned} \quad (7.103)$$

hence the output is modulated (see Fig. 7.2):

- Principle of superposition *does not apply* in nonlinear system.

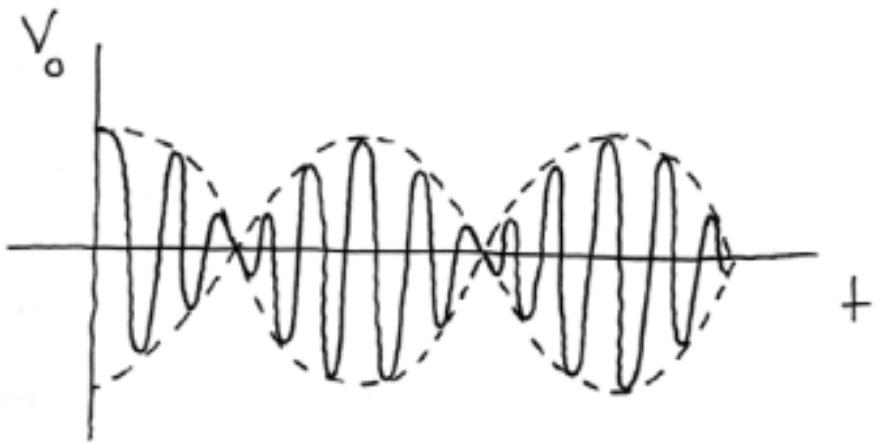


Figure 7.2. Output voltage versus time for a nonlinear system for an input of two pure tones.

- Generate sum and difference frequencies → beat notes, i.e. at frequencies $2\omega_1$, $2\omega_2$ and $\omega_1 \pm \omega_2$.
- If $\omega_1 \approx \omega_2$ then you get a *woo-woo-woo* effect.

Nonlinear effects ($\propto V^2$, V^3 , etc.) are stronger at larger amplitudes, e.g., human ear; loudspeaker driven to saturation; laser fusion experiments.

7.6.2 Damped, driven, simple harmonic oscillator

By definition a simple harmonic oscillator is linear:

$$\frac{d^2x}{dt^2} + \gamma \frac{dx}{dt} + \omega_0^2 x = F_0 \cos \omega t, \quad (7.104)$$

which can be thought of as a linear amplifier: if you drive it with a pure tone $F_0 \cos \omega t$ (input), you get back a pure tone (output) at the same frequency (but with different amplitude and phase, in general). Writing the output as $x(t) = \frac{1}{2}A \exp[-i\omega t] + \text{c.c}$ then the complex amplitude A of the output satisfies

$$(-\omega^2 - i\omega\gamma + \omega_0^2) \frac{1}{2}A e^{-i\omega t} + \text{c.c.} = \frac{1}{2}F_0 e^{-i\omega t} + \text{c.c.}, \quad (7.105)$$

i.e. (see Fig. 7.3)

$$A = \frac{F_0}{\omega_0^2 - \omega^2 - i\omega\gamma} = \frac{F_0}{\sqrt{(\omega_0^2 - \omega^2)^2 + \omega^2\gamma^2}} e^{i\theta} \quad (7.106)$$

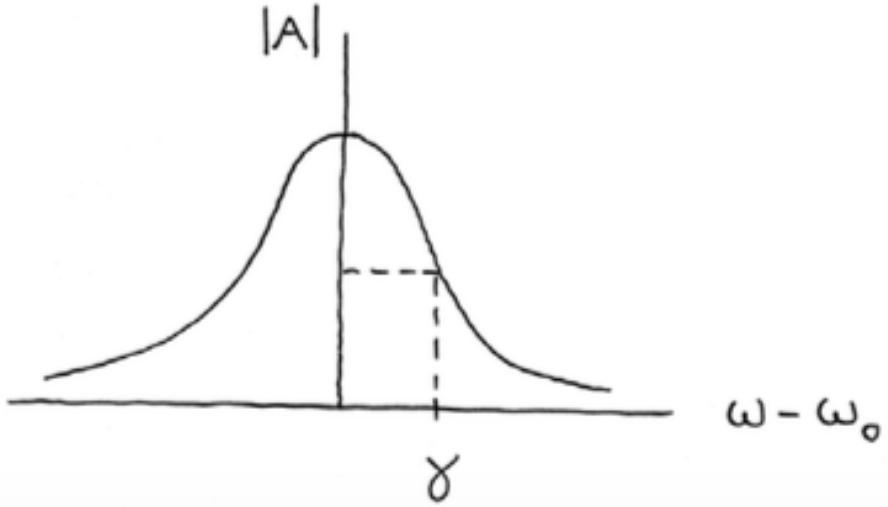


Figure 7.3. Driven damped simple harmonic oscillator amplitude versus driving frequency.

with $\tan \theta = \omega \gamma / (\omega_0^2 - \omega^2)$. Damping causes a phase shift; the output *leads or lags* the driving force

7.6.3 Period-amplitude relation

Now consider an undriven, undamped oscillator with (say) a cubic nonlinearity. An example is a pendulum with a moderate swing angle θ , which obeys the equation $0 = \ddot{\theta} + (g/l) \sin \theta \approx \ddot{\theta} + (g/l)(\theta - \theta^3/6 + \dots)$. In general:

$$\frac{d^2x}{dt^2} + \omega_0^2 x = -\epsilon x^3. \quad (7.107)$$

Below we consider ϵ to be small so that the system is approximately a simple harmonic oscillator.

Clearly, if we start with a pure tone $x(t) = \frac{1}{2}A \exp[i\omega t] + \text{c.c.}$, the nonlinear term will generate new harmonics $\propto (A \exp[i\omega t] + A^* \exp[-i\omega t])^3 = A^3 \exp[3i\omega t] + 3A^2 A^* \exp[i\omega t] + 3A(A^*)^2 \exp[-i\omega t] + (A^*)^3 \exp[-3i\omega t]$ (see Section 7.6.1). If $\omega = \omega_0$ (the only possibility, as the system is undriven), the $\exp[\pm i\omega t]$ terms on the right-hand side of Eq. (7.107) cause big trouble; they act as internal drivers of the undamped linear oscillation $\ddot{x} + \omega_0^2 x = 0$ and hence produce an infinite resonant response. This is impossible, as it violates conservation

of energy, so the amplitude A must take a special value that kills the $\exp[\pm i\omega t]$ terms. This special value satisfies the condition

$$(-\omega^2 + \omega_0^2) \frac{1}{2} A e^{i\omega t} + \text{c.c.} = -\frac{3\epsilon}{8} A^2 A^* e^{i\omega t} + \text{c.c.}, \quad (7.108)$$

obtained by substituting the pure tone into Eq. (7.107) and equating the coefficients of the $\exp i\omega t$ terms to make them disappear. Upon rearranging and noting that $\omega_0^2 - \omega^2 = (\omega_0 - \omega)(\omega_0 + \omega) \approx 2\omega_0(\omega_0 - \omega)$ for ω very close to ω_0 (again, the only possibility, as the system is undriven), we obtain

$$\omega = \omega_0 + \frac{3\epsilon}{8\omega_0} |A|^2. \quad (7.109)$$

This result tells us that, when a nonlinear spring oscillates stably, its oscillation frequency ω is shifted slightly away from its natural frequency ω_0 . For a cubic nonlinearity, the shift (also called the detuning) is proportional to the square of the oscillation amplitude $|A|^2$. This is an important general result with many practical applications. It is called the period-amplitude relation. For a pendulum with amplitude θ_{\max} , we have $\epsilon = \omega_0^2/6$ and hence $\omega \approx \omega_0(1 - \theta_{\max}^2/16)$.

The $\exp[\pm 3i\omega t]$ terms remain and beat together with the natural oscillation at ω_0 to generate responses at $3\omega \pm \omega_0$, which are then fed back into the nonlinear term to generate even more harmonics. And so on.

7.6.4 Bistability in a driven, damped anharmonic oscillator

Now suppose that the driven, damped SHO is also generalised to include a small ($\epsilon \ll 1$) nonlinear (cubic, say) term in the restoring force, in the spirit of the previous section:

$$\frac{d^2x}{dt^2} + \gamma \frac{dx}{dt} + \omega_0^2 x = -\epsilon x^3 + F_0 \cos \omega t. \quad (7.110)$$

From Section 7.6.2 the amplitude response of a driven, damped simple harmonic oscillator is

$$|A|^2 = \frac{F_0^2}{(\omega_0^2 - \omega^2)^2 + \omega^2 \gamma^2}, \quad (7.111)$$

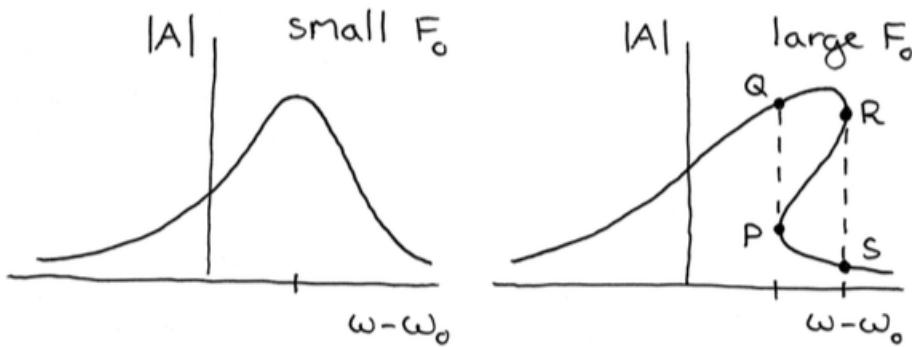


Figure 7.4. Driven, damped, nonlinear simple harmonic oscillator amplitude versus driving frequency. LHS: weak driving force. RHS: strong driving force, with bistable solutions.

whilst the period amplitude relation (see Section 7.6.3) for a undriven, undamped simple harmonic oscillator with a cubic nonlinearity is

$$\omega = \omega_0 + \frac{3\epsilon}{8\omega_0} |A|^2. \quad (7.112)$$

Combining these two results and keeping terms up to order ϵ^2 in the denominator, we find

$$|A|^2 = \frac{F_0^2}{\gamma^2 \omega_0^2 + \frac{3\epsilon\gamma^2}{4} |A|^2 + \frac{9\epsilon^2}{16} \left(1 + \frac{\gamma^2}{4\omega_0^2}\right) |A|^4}. \quad (7.113)$$

The above is cubic in $|A|^2$ and can be bistable (see Fig. 7.4). Specifically, there are two stable states Q-R and P-S available for a range of detunings $\omega - \omega_0$, provided that F_0 is large enough, see RHS of Fig. 7.4. (The central state P-R is unstable.) The history of the system determines which state is occupied. For example, if you approach the bistable region by sweeping ω starting from $\omega \ll \omega_0$ (i.e. $\omega - \omega_0$ very negative), you end up in the state Q-R. In contrast, if you start from $\omega \gg \omega_0$, you end up in P-S.

7.6.5 Multiple scale analysis

One annoying aspect of nonlinear oscillators is that different approximation techniques sometimes give different answers unless applied extremely carefully. For the most part, however, there is one approach which is more robust than the rest in the hands of mere

non-mathematicians: the method of multiple scales. We illustrate the method by applying it to the driven nonlinear oscillator in the previous section.

When applied to ODEs, the method of multiple scales handles systems where there exists a separation of time-scales. For example, if an oscillator comprises a small nonlinearity $\propto \epsilon \ll 1$, the solution may well turn out to be an approximately harmonic oscillation at frequency ω_0 , whose amplitude and phase vary slowly on the time-scale $\epsilon^{-1}\omega_0^{-1}$.

In general the solution can be written as

$$x(t) = x_0(T_0, T_1, \dots) + x_1(T_0, T_1, \dots) + \dots, \quad (7.114)$$

where quantities with subscript 0, 1, and so on are of order 0, 1, and so on respectively; e.g. we have $T_n = \epsilon^n t$. Time derivatives now separate into several terms by the chain rule:

$$\frac{d}{dt} = \frac{dT_0}{dt} D_0 + \frac{dT_1}{dt} D_1 + \frac{dT_2}{dt} D_2 + \dots \quad (7.115)$$

$$= D_0 + \epsilon D_1 + \epsilon^2 D_2 \dots \quad (7.116)$$

$$\frac{d^2}{dt^2} = \left(\frac{dT_0}{dt} D_0 + \frac{dT_1}{dt} D_1 + \frac{dT_2}{dt} D_2 + \dots \right) \left(\frac{dT_0}{dt} D_0 + \frac{dT_1}{dt} D_1 + \frac{dT_2}{dt} D_2 + \dots \right) \quad (7.117)$$

$$= D_0^2 + 2\epsilon D_1 D_0 + \epsilon^2 (2D_2 D_0 + D_1^2) + \dots, \quad (7.118)$$

where $D_n = d/dT_n$.

Principal resonance

Consider the following

$$\frac{d^2x}{dt^2} + 2\epsilon\mu \frac{dx}{dt} + \omega_0^2 x + \epsilon\alpha x^3 = \epsilon K \cos \Omega t. \quad (7.119)$$

Let us focus first on the principal resonance $\Omega = \omega_0$. Near the principal resonance, we expect the solution to be large, i.e. $x \sim \mathcal{O}(\epsilon^{(0)})$ to leading order. But the nonlinearity is small. As we are working near resonance, we know that a moderate excitation ϵK produces a huge response; for a driven linear SHO. This is why the forcing must be of order, ϵ , i.e. $\epsilon K \cos \omega t$, so that the peak response at $\omega = \omega_0$ is something sensible. Similarly, we should

be within $\mathcal{O}\epsilon^1$ of resonance so that the first term in the denominator is of the same order as the second term, i.e. $\omega = \omega_0 + \epsilon\sigma$.

Collecting terms of order ϵ^0 :

$$\frac{d^2x^{(0)}}{dT_0^2} + \omega_0^2 x^{(0)} = 0, \quad (7.120)$$

where

$$x^{(0)} = A(T_1, T_2, \dots) e^{-i\omega_0 T_0} + \text{c.c.} \quad (7.121)$$

Now collect terms of order ϵ^1 :

$$\begin{aligned} \frac{d^2x^{(1)}}{dT_0^2} + \omega_0^2 x^{(1)} &= 2i\omega_0 \frac{dA(T_1, T_2, \dots)}{dT_1} e^{-i\omega_0 T_0} + 2\mu i\omega_0 A e^{-i\omega_0 T_0} \\ &\quad - \alpha (A^3 e^{-3\omega_0 T_0} + 3A^2 A^* e^{-i\omega_0 T_0}) + \frac{K}{2} e^{-i\omega_0 T_0} e^{-i\sigma T_1} + \text{c.c.}, \end{aligned} \quad (7.122)$$

where the LHS is an undamped simple harmonic oscillator with natural frequency ω_0 . So terms on the RHS going as $\exp(-i\omega_0 T_0)$ must sum to zero to avoid an infinite response: $x^{(1)} \rightarrow \infty$. Hence,

$$2i\omega_0 \frac{dA}{dT_1} + 2\mu i\omega_0 A - 3A^2 A^* + \frac{K}{2} e^{-i\sigma T_1} = 0. \quad (7.123)$$

To solve for A , write it in terms of an amplitude and phase, i.e. $A(T_1) = a(T_1) \exp(-i\theta(T_1))/2$ with a , θ real. (We dont need to go farther and consider T_2 dependences.):

$$i\omega_0 (a' e^{-i\theta} - i\theta' a e^{-i\theta}) + i\omega_0 \mu a e^{-i\theta} - \frac{3}{8} \alpha a^3 e^{-i\theta} + \frac{K}{2} e^{-i\sigma T_1} = 0, \quad (7.124)$$

where $a' = da/dT_1$ and $\theta' = d\theta/dT_1$. Multiplying through by $\exp(i\theta)$ and take real and imaginary parts we have two coupled equations:

$$\omega_0 \theta' a - \frac{3}{8} \alpha a^3 + \frac{K}{2} \cos(\theta - \sigma T_1) = 0 \quad (7.125)$$

$$\omega_0 a' + \omega_0 \mu a - \frac{K}{2} \sin(\theta - \sigma T_1) = 0. \quad (7.126)$$

Now change variables from $\theta(T_1)$ to $\gamma(T_1) = \theta(T_1) - \sigma T_1$ such that $\theta' = \gamma' + \sigma$. Hence

$$\omega_0 \gamma' a + \omega_0 \sigma a - \frac{3}{8} \alpha a^3 + \frac{K}{2} \cos(\gamma) = 0 \quad (7.127)$$

$$\omega_0 a' + \omega_0 \mu a - \frac{K}{2} \sin(\gamma) = 0. \quad (7.128)$$

If the oscillations are steady, i.e., the amplitude and phase of $A(T_1)$ (which are slowly varying anyway) in fact do not vary at all, then $a' = \gamma' = 0$:

$$-\omega_0\sigma a + \frac{3}{8}\alpha a^3 = \frac{K}{2} \cos(\gamma) \quad (7.129)$$

$$\omega_0\mu a = \frac{K}{2} \sin(\gamma). \quad (7.130)$$

Squaring and adding the two above equations gives

$$\frac{K^2}{4a^2\omega_0^2} = \left(\frac{3\alpha a^2}{8\omega_0} - \sigma \right)^2 + \mu^2. \quad (7.131)$$

This is the amplitude-frequency relation (also known as the frequency response curve). To plot a as a function of σ , it is easier to do the reverse and plot $\sigma(a)$:

$$\sigma = \frac{3\alpha a^2}{8\omega_0} \pm \sqrt{\frac{K^2}{4a^2\omega_0^2} - \mu^2}. \quad (7.132)$$

This is the same result as in section 7.6.4 and reproduces Fig. 7.4.

Subharmonics

Even a linear oscillator can oscillate at a frequency which differs from the forcing frequency and is related to it by a simple rational ratio. For example, a linear undamped oscillator contains responses at the natural frequency ω_0 and the driving frequency ω . If $\omega = n\omega_0$, where n is an integer, the response is said to contain a subharmonic of order $1/n$.

Of course, in a linear oscillator, the subharmonic disappears in the face of even a tiny bit of damping. In a nonlinear oscillator, the subharmonic is regenerated continuously by the nonlinear terms through the beat phenomenon. Not all of the possible beats contribute, though. As we show below, the cubic oscillator only has a subharmonic of order $1/3$ when μ and α are both small, i.e., $\mathcal{O}(\epsilon)$, as in the previous sections.

When the driving frequency is far away from ω_0 , the response is very small unless the driver is hard, with $K = \mathcal{O}(1)$. The equation of motion then reads

$$\frac{d^2x}{dt^2} + 2\epsilon\mu\frac{dx}{dt} + \omega_0^2x + \epsilon\alpha x^3 = K \cos \Omega t. \quad (7.133)$$

Collecting terms of order ϵ^0 , we get

$$D_0^2 x^{(0)} + \omega_0^2 x^{(0)} = K \cos \Omega T_0, \quad (7.134)$$

which has the solution

$$x^{(0)} = A(T_1, T_2, \dots) e^{-i\omega_0 t} + \Lambda e^{-i\Omega T_0} + \text{c.c.}, \quad (7.135)$$

where

$$\Lambda = \frac{K}{2(\omega_0^2 - \Omega^2)}. \quad (7.136)$$

Now collect terms of order ϵ^1 :

$$\begin{aligned} D_0^2 x^{(1)} + \omega_0^2 x^{(1)} &= -[-2i\omega_0 (A' + \mu A) + 6\alpha\Lambda^2 A + 3\alpha A^2 A^*] e^{-i\omega_0 T_0} \\ &\quad - \Lambda (-2i\mu\Omega + 3\alpha\Lambda^2 + 6\alpha A A^*) e^{-i\Omega T_0} \\ &\quad - \alpha A^3 e^{-3i\omega_0 T_0} - \alpha\Lambda^3 e^{-3i\Omega T_0} \\ &\quad - 3\alpha\Lambda A^2 e^{-i(2\omega_0 + \Omega)T_0} - 3\alpha\Lambda (A^*)^2 e^{-i(-2\omega_0 + \Omega)T_0} \\ &\quad - 3\alpha\Lambda^2 A e^{-i(\omega_0 + 2\Omega)T_0} - 3\alpha\Lambda^2 A e^{-i(\omega_0 - 2\Omega)T_0}. \end{aligned} \quad (7.137)$$

If Ω is very small (slow, secular driver), we get a special behaviour driven by the $\exp(-i\Omega T_0)$ term on the T_1 time-scale, which we do not discuss further here (it damps out slowly $\propto \exp(-\mu T_1)$). If Ω is away from the principal resonance and all subharmonic or superharmonic (see below) resonances, the free oscillation again damps out $\propto \exp(-\mu T_1)$, with an amplitude-dependent frequency as it decays. Neither of these cases is *interesting*.

Now let us consider the subharmonic case $\Omega \approx 3\omega_0$. In this case, the terms proportional to $\exp(-i\omega_0 T_0)$ and $\exp(-i(-2\omega_0 + \Omega)T_0)$ both oscillate near the natural frequency Ω and resonantly excite the left-hand side of the equation of motion for $x^{(1)}$. Hence their coefficients must sum to zero to prevent divergent motion:

$$0 = 2i\omega_0 (A' + \mu A) - 6\alpha\Lambda^2 A - 3\alpha A^2 A^* - 3\alpha\Lambda (A^*)^2 e^{-i\sigma T_1}, \quad (7.138)$$

where we put $\Omega = 3\omega_0 + \epsilon\sigma$ and $A' = dA/dT_1$. As before, to solve for A , write it in terms of an amplitude and phase, i.e. $A(T_1) = a(T_1) \exp(-i\theta(T_1))/2$ with a, θ real. Separating the real and imaginary parts leads to

$$a' = -\mu a + \frac{3\alpha\Lambda a^2}{4\omega_0} \sin(\sigma T_1 + 3\theta) \quad (7.139)$$

$$a\theta' = -\frac{3\alpha}{\omega_0} \left(\Lambda^2 + \frac{a^2}{8} \right) a - \frac{3\alpha\Lambda a^2}{4\omega_0} \sin(\sigma T_1 + 3\theta). \quad (7.140)$$

Changing variables from $\theta(T_1)$ to $\gamma(T_1) = \sigma T_1 + \theta(T_1)$, we find that the solution to order $\mathcal{O}(\epsilon^0)$ is given by

$$x^{(0)} = a \cos[(\Omega t - \gamma)/3] + 2\Lambda \cos(\Omega t). \quad (7.141)$$

In the steady state ($D_1 = 0$), we arrive at the following frequency-amplitude equation

$$\left[9\mu^2 + \left(\sigma - \frac{9\alpha\Lambda^2}{\omega_0} - \frac{9\alpha a^2}{8\omega_0} \right)^2 \right] a^2 = \frac{81\alpha^2\Lambda^2 a^4}{16\omega_0^2}, \quad (7.142)$$

which has the trivial solution $a = 0$ (which it turns out is a saddle point and therefore unstable) and a nontrivial solution (which turns out to be stable; prove as an exercise) which only exists for

$$\Lambda^2 < \frac{4\omega_0\sigma}{27\alpha} \quad (7.143)$$

and

$$\frac{\alpha\Lambda^2}{\omega_0} \left(\sigma - \frac{63\alpha\Lambda^2}{8\omega_0} \right) - 2\mu^2 \geq 0. \quad (7.144)$$

Hence α and σ must have the same sign and the driver amplitude and detuning must satisfy

$$\left[\frac{63\alpha\Lambda^2}{4\omega_0\mu} - \frac{\sigma}{\mu} \right] \leq \left(\frac{\sigma^2}{\mu^2} - 63 \right)^{1/2}. \quad (7.145)$$

In contrast with the linear solution, if the driver parameters satisfy the foregoing relation, the free oscillation does not decay; it is continually regenerated by the nonlinear terms and the free oscillation is locked to one third of the driver frequency. This is a subharmonic resonance. These sorts of resonances between propeller-driven wing vibrations and secondary rudder vibrations can rip an aeroplane apart.

Superharmonics

Now suppose instead that we have $\Omega \approx \omega_0/3$. In the above equation for $x^{(1)}$, we see that the driving terms proportional to $\exp(-i\omega_0 T_0)$ and $\exp(-3i\Omega T_0)$ (the latter occurring when the driven zeroth-order response is fed back into the system through the cubic nonlinearity) resonate with the natural frequency of the system and must therefore vanish to avoid divergent behaviour:

$$0 = 2i\omega_0(A' + \mu A) - 6\alpha\Lambda^2 A - 3\alpha A^2 A^* - 3\alpha\Lambda^3 e^{-i\sigma T_1}, \quad (7.146)$$

where we put $3\Omega = \omega_0 + \epsilon\sigma$. As before, to solve for A , write it in terms of an amplitude and phase, i.e. $A(T_1) = a(T_1) \exp(-i\theta(T_1))/2$ with a, θ real. Separating the real and imaginary parts leads to

$$a' = -\mu a + \frac{\Lambda^3}{\omega_0} \sin(\gamma) \quad (7.147)$$

$$a\gamma' = \left(\sigma + \frac{3\alpha\Lambda^2}{\omega_0} \right) + \frac{3\alpha a^3}{8\omega_0} + \frac{\alpha\Lambda^3}{\omega_0} \cos \gamma. \quad (7.148)$$

In the steady state ($D_1 = 0$), we arrive at the following frequency-amplitude equation

$$\left[\mu^2 + \left(\sigma + \frac{3\alpha\Lambda^2}{\omega_0} + \frac{3\alpha a^2}{8\omega_0} \right)^2 \right] a^2 = \frac{\alpha^2 \Lambda^6}{\omega_0^2}. \quad (7.149)$$

Curves of a versus σ show the characteristic bistable shape (of a breaking wave viewed side-on), with the curvature of the tongue increasing as α (nonlinearity) and Λ (driver strength) increase.

Again, the superharmonic resonance means that the free-oscillation part of the response does not damp away but is constantly regenerated (and locked to the natural frequency).

✓ **Exercise:** Show that the peak amplitude of the free oscillation depends on the strength of the nonlinearity, unlike for the primary resonance. What is the peak amplitude? At what detuning does it occur? [Answers: $\alpha\Lambda^2/(\mu\omega_0)$ and $3\alpha\Lambda^2/\omega_0 + 3\alpha^3\Lambda^6/(8\mu^2\omega_0^3)$]

7.7 Synchronisation of coupled nonlinear oscillators

References: P.C. Matthews, R.E. Mirollo and S.H. Strogatz, Physica D **52**, 293 (1991); S. Chaturvedi and V. Srinivasan, Physical Review A **43**, 4054 (1991); I. Waller and R. Kapral, Physical Review A **30**, 2047 (1984). In this section, we follow closely the discussions in S.H. Strogatz and R.E. Morillo, Journal of Statistical Physics **63**, 613 (1991) and J.A. Acebron *et al.*, Reviews of Modern Physics **77**, 137 (2005).

Synchronisation of coupled oscillators is a widespread phenomenon in Nature. It is responsible for the synchronous flashing observed in swarms of fireflies, the chirping of

crickets in unison. In every case, the phenomenon is collective. Moreover, each individual must oscillate nonlinearly, with a globally attracting limit cycle; the phenomenon does not occur for linear oscillators. When the coupling is weak, the individuals oscillate incoherently at their natural frequencies, which are randomly distributed. When the coupling exceeds a critical threshold, the oscillators synchronise collectively, converging to a unique frequency. The great theoretical biologist A. T. Winfree (1942-2002) discovered this phenomenon in the late 1960s.

In physics, an important example of synchronisation is observed in networks of superconducting Josephson junctions, when the junctions are connected in series through a load. (In contrast, if the junctions are connected in parallel, they experience diffusive coupling and support soliton solutions.) Synchronisation is also observed in chemical oscillators like the BZ reaction (e.g. in separate tank reactors which exchange molecules through a perforated membrane) and in arrays of solid-state or semiconductor lasers (described by the Lang-Kobayashi equations).

You can see videos of synchronised fireflies on the World Wide Web. Dramatic performances take place annually in the jungle near Kuala Selangor, Malaysia and near Elkmont, in the Great Smoky Mountains of Tennessee!

7.7.1 Kuramoto's model

Kuramotos synchronisation model stipulates that the phase $\theta_i(t)$ of the i^{th} oscillator (out of N in total) satisfies the equation of motion

$$\frac{d\theta_i}{dt} = \omega_i + \frac{K}{N} \sum_{j=1}^N \sin(\theta_j - \theta_i) \quad (7.150)$$

where ω_i is its natural frequency, chosen randomly from a probability distribution $g(\omega)$, and the coupling K between all oscillator pairs is equal.

Let

$$r(t)e^{i\psi(t)} = \frac{1}{N} \sum_{j=1}^N e^{i\theta_j(t)} \quad (7.151)$$

be the average phasor of the oscillator ensemble. Multiplying by $\exp(-i\theta_i)$ and taking the imaginary part, we obtain

$$\dot{\theta}_i = \omega_i + Kr \sin(\psi - \theta_i). \quad (7.152)$$

Now the oscillators are coupled implicitly through their interaction with the common (mean) field described by r and ψ , not explicitly as before. We have $\dot{\theta}_i < 0$ for $\theta_i > \psi$ and $\dot{\theta}_i > 0$ for $\theta_i < \psi$, so that θ_i tends towards ψ if K is large, although the ω_i oscillation tends to push it away. In the special case $\omega_i = \omega_0$ for all i , the previous two equations have the obvious (and obviously stable) solution $\theta_i = \psi = \omega_0 t$ for all i (with $r = 1$).

Now let N tend to infinity. Clearly, there exists an incoherent solution, where all the oscillators oscillate at their natural frequencies ($\theta_i = \omega_i t$), and one has $r = 0$, because the average on the righthand side of Eq. (7.151) obviously reduces to zero, if the oscillators end up distributed uniformly on $[-\pi, \pi]$ at every instant t and are infinitely numerous. There also exists a second family of partially coherent solutions for

$$K > K_c = \frac{2}{\pi g(0)}. \quad (7.153)$$

In these, the oscillators split into a synchronized group near the centre of the frequency distribution with $|\omega_i| \leq Kr$ and a wandering group near the fringe of the frequency distribution with $|\omega_i| > Kr$. How can we prove this?

In the limit $N \rightarrow \infty$, we can convert the sum in (Eq. (7.151)) into an integral. Let $p(\theta, \omega, t | \omega) d\theta$ be the fraction of oscillators with phase in the range $[\theta, \theta + d\theta]$ and natural frequency ω . Then Eq. (7.151) converts to

$$r(t)e^{i\psi(t)} = \int_{-\pi}^{\pi} d\theta \int_{-\infty}^{\infty} d\omega \exp[i\theta] p(\theta, t | \omega) g(\omega). \quad (7.154)$$

Normalisation requires

$$1 = \int_{-\pi}^{\pi} d\theta p(\theta, t | \omega). \quad (7.155)$$

In the absence of noise, we can write a Liouville equation for the evolution of the pdf

describing conservation of phase-space volume:

$$\frac{\partial p(\theta, t|\omega)}{\partial t} = -\frac{\partial}{\partial \theta} \left[\left\langle \frac{\Delta \theta}{\Delta t} \right\rangle p(\theta, t|\omega) \right] \quad (7.156)$$

$$= -\frac{\partial}{\partial \theta} \{ [\omega + Kr \sin(\psi - \theta)] p(\theta, t|\omega) \}. \quad (7.157)$$

This is the first term (the A_i term) in a noise-free Fokker-Planck equation, where there is no diffusion.

Now suppose that a state of partial coherence exists. (We need to verify its existence and stability a posteriori.) From the viewpoint of an individual oscillator with natural frequency ω , its phase does not wander if it is shifted with respect to the phase of the mean phasor (not the same as the mean phase $N^{-1} \sum_i \theta_i$) according to $\theta = \psi + \arcsin(\omega/Kr)$. Clearly, this is only possible for natural frequencies satisfying $|\omega| \leq Kr$; otherwise, the phase is destined to wander. For the moment, we treat r as known and constant, although it is actually an output of the dynamics and varies with t in general (except in the stationary states we are searching for). Then, for $|\omega| \leq Kr$ and hence $|\psi - \theta| \leq \pi/2$, we have

$$p(\theta, t|\omega) = \delta[\theta - \psi - \arcsin(\omega/Kr)]. \quad (7.158)$$

This pdf automatically satisfies the Liouville equation: it does not depend explicitly on t (LHS vanishes) and, together with the single-oscillator equation of motion, it implies $\langle \Delta \theta / \Delta t \rangle = 0$ (RHS vanishes). On the other hand, for $|\omega| > Kr$, we have $\partial p / \partial t = 0$ (stationary state comprising wandering phases) and hence $p(\theta, t|\omega) = \text{constant}/|\omega + Kr \sin(\psi - \theta)|$ from Liouville's equation above. Evaluating the constant from the normalisation condition at fixed ω (see above), we obtain

$$p(\theta, t|\omega) = \frac{\sqrt{\omega^2 - K^2 r^2}}{2\pi |\omega + Kr \sin(\psi - \theta)|}. \quad (7.159)$$

The two sub-populations are completely distinct, so they enter as two terms when evaluating the mean phasor:

$$r = \int_{-\pi/2}^{\pi/2} d(\theta - \psi) \int_{|\omega| \leq Kr} d\omega e^{i(\theta - \psi)} \delta[\theta - \psi - \arcsin(\omega/Kr)] g(\omega) \quad (7.160)$$

$$+ \int_{-\pi}^{\pi} d(\theta - \psi) \int_{|\omega| > Kr} d\omega e^{i(\theta - \psi)} \frac{\sqrt{\omega^2 - K^2 r^2}}{2\pi |\omega + Kr \sin(\psi - \theta)|} g(\omega). \quad (7.161)$$

If $g(\omega) = g(-\omega)$ is an even function, then the second term is zero and we are left with

$$r = \int_{|\omega| \leq Kr} d\omega g(\omega) \cos [\arcsin(\omega/Kr)] \quad (7.162)$$

$$= Kr \int_{-\pi/2}^{\pi/2} d\phi g(Kr \sin \phi) \cos^2 \phi. \quad (7.163)$$

This equation has the trivial incoherent solution $r = 0$ for all K , corresponding to uniform pdf $p(\theta, t|\omega) = 1/2\pi$, and the non-trivial, partially coherent solution

$$1 = K \int_{-\pi/2}^{\pi/2} d\phi g(Kr \sin \phi) \cos^2 \phi, \quad (7.164)$$

which becomes available for $r \geq 0$ and hence $K \geq K_c = 2/[\pi g(0)]$.

To get an explicit expression for r as a function of K , we evaluate Eq. (7.164) for specific forms of $g(\omega)$. If $g(\omega)$ is a Cauchy (i.e. Lorentzian) distribution, one finds $r = \sqrt{1 - K_c/K}$. The square-root scaling is universal for all frequency distributions with $g''(0) = 0$ in this mean-field ($N \rightarrow \infty$) analysis. Hence synchronization behaves like a second-order phase transition.

✓ **Exercise:** Write a simple computer program to plot the probability distribution function of the oscillator frequencies. Does the distribution change abruptly at the critical coupling strength K_c ? Plot the standard deviation of the distribution as a function of $|K - K_c|$. Does it approach zero as a power of $|K - K_c|$, like a second-order phase transition in thermodynamics?

Hint: For typical solutions see Fig. 7.5

Kuramoto's model with noise

Noise enters the synchronisation problem in two ways: (i) environmental perturbations always exist to perturb the oscillators; (ii) when N is large but finite, there are fluctuations in the phases due to finite-size effects, and these fluctuations can occasionally be of order unity, even when $g(\omega)$ is uniform and/or $K = 0$, due to Poincare recurrence. With noise added, the stability of the incoherent and partially coherent states becomes an important issue.

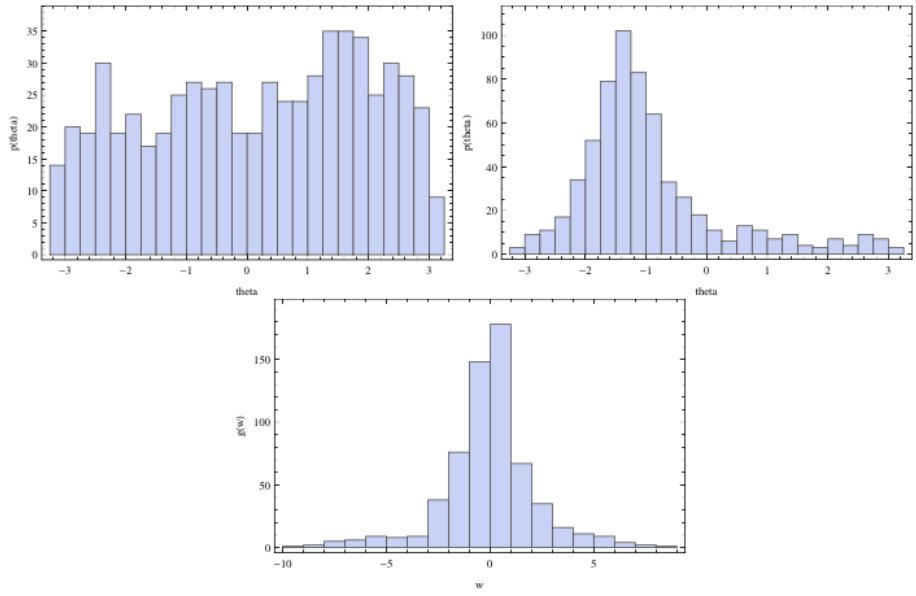


Figure 7.5. Simulations of Kuramotos model without noise for 625 oscillators whose natural frequencies are drawn from a Cauchy distribution $p(w) = (a/\pi)(a^2 + \omega^2)^{-1}$ with $a = 1$ (truncated at $|\omega| \leq 10a$ to avoid numerical problems) and whose initial phases are drawn uniformly from $[-\pi, \pi]$. (Top left.) Histogram of the phase distribution $p(\theta)$ at $t = 10$ for coupling below the critical threshold $2a$ ($K = 1$). (Top right.) Histogram of the phase distribution $p(\theta)$ at $t = 10$ for coupling above the critical threshold $2a$ ($K = 3$). (Bottom.) Histogram of the natural frequency distribution $g(\omega)$.

Let us add white noise $\xi_i(t)$ to Kuramotos equations of motion, Eq. (7.150). The equations convert into a system of Langevin equations, with

$\langle \xi_i(t) \rangle = 0$ and $\langle \xi_i(t) \xi_j(t') \rangle = 2D\delta_{ij}\delta(t - t')$. The Liouville equation now acquires a second-order term describing diffusion in the usual Fokker-Planck manner:

$$\frac{\partial p(\theta, t|\omega)}{\partial t} = -\frac{\partial}{\partial \theta} \{ [\omega + Kr \sin(\psi - \theta)] p(\theta, t|\omega) \} + D \frac{\partial^2 p(\theta, t|\omega)}{\partial \theta^2}. \quad (7.165)$$

The incoherent solution $p^{(0)}(\theta, t|\omega) = 1/2\pi$ satisfies Eq. (7.165) identically, if we note that it implies $r = 0$ from Eq. (7.154). Now add a small disturbance $p^{(1)}(\theta, t|\omega)$ to the incoherent solution; how does $p^{(1)}$ evolve with time? Substituting into Eq. (7.154), we find that $r(t)$ is of the same order as $p^{(1)}$, because it vanishes for the incoherent solution, i.e.

$$r^{(1)}(t) = \int_{-\pi}^{\pi} d\theta \int_{-\infty}^{\infty} d\omega \exp[i(\theta - \psi)] p^{(1)}(\theta, t|\omega) g(\omega). \quad (7.166)$$

Substituting into Eq. (7.165), we find (to first order)

$$\frac{\partial p^{(1)}}{\partial t} = -\omega \frac{\partial p^{(1)}}{\partial \theta} + \frac{K}{2\pi} r^{(1)}(t) \cos(\psi - \theta) + D \frac{\partial^2 p^{(1)}}{\partial \theta^2}, \quad (7.167)$$

with

$$0 = \int_{-\pi}^{\pi} d\theta p^{(1)}(\theta, t|\omega) \quad (7.168)$$

by normalisation.

The linearised FPE has two kinds of modes: (i) those that oscillate at ω , which are affected by the coupling term proportional to K ($\propto \exp(i\theta)$, not $\exp(2i\theta)$ et cetera); and (ii) those that oscillate at harmonics of ω , which are unaffected by the coupling term for the same reason. Noting that $p(\theta, t|\omega)$ is 2π -periodic in θ , we expand in a Fourier series, as follows:

$$p^{(1)}(\theta, t|\omega) = c(t, \omega) e^{i\theta} + c^*(t, \omega) e^{-i\theta} + \eta(\theta, t, \omega). \quad (7.169)$$

Now substituting into Eq. (7.154). As $\eta(\theta, t, \omega)$ contains harmonics of $\exp(i\theta)$ (like $\exp(2i\theta)$), the term it contributes to the $r^{(1)}$ integral vanishes by orthogonality, leaving

$$r^{(1)}(t) = 2\pi \exp[-i\psi] \int_{-\infty}^{\infty} d\omega' c^*(t, \omega') g(\omega'). \quad (7.170)$$

Substituting into Eq. (7.165) and extracting factors proportional to $\exp(i\theta)$, we find

$$\frac{\partial c}{\partial t} = -(D + i\omega)c + \frac{K}{2} \int_{-\infty}^{\infty} d\omega' c(t, \omega')g(\omega'). \quad (7.171)$$

By inspection, we see that the stability of an oscillator with natural frequency ω depends on all the other oscillators, but in a way which is independent of ω (because the couplings are through the common mean field $r \exp i\psi$); the rightmost term is just a number. Since the above equation is linear in c , it must have solutions $\propto \exp(\lambda t)$, where λ is the eigenvalue determining stability. Writing $c(t, \omega) = c(\omega) \exp(\lambda t)$, we obtain

$$(\lambda + D + i\omega)c(\omega) = \frac{K}{2} \int_{-\infty}^{\infty} d\omega' c(\omega')g(\omega'). \quad (7.172)$$

Multiplying by $(\lambda + D + i\omega)^{-1}g(\omega)$ and integrating over all ω , we get

$$\int_{-\infty}^{\infty} d\omega c(\omega)g(\omega) = \frac{K}{2} \int_{-\infty}^{\infty} d\omega' c(\omega')g(\omega') \int_{-\infty}^{\infty} d\omega \frac{g(\omega)}{\lambda + D + i\omega}, \quad (7.173)$$

i.e.

$$1 = \frac{K}{2} \int_{-\infty}^{\infty} d\omega \frac{g(\omega)}{\lambda + D + i\omega}. \quad (7.174)$$

If $g(\omega)$ is even and decreases monotonically from a peak at $\omega = 0$, one can show (*leap of faith*) that the solution for λ is purely real. Taking the real part of the above equation, we find

$$1 = \frac{K}{2} \int_{-\infty}^{\infty} d\omega \frac{(\lambda + D)g(\omega)}{(\lambda + D)^2 + \omega^2}. \quad (7.175)$$

What does this dispersion relation tell us? First of all, the pdf $g(\omega)$ is positive everywhere, as is the left-hand side. So we must have $\lambda + D > 0$. This immediately implies $\lambda > 0$ if $D = 0$, i.e. the incoherent state is unstable if there is no noise! If there is noise, then the boundary between stability and instability occurs at $\lambda = 0$ and hence sets the critical coupling to be

$$K_c = \frac{2}{D} \left[\int_{-\infty}^{\infty} d\omega \frac{g(\omega)}{D^2 + \omega^2} \right]^{-1}. \quad (7.176)$$

As $D \rightarrow 0$ and $\lambda \rightarrow 0$, the kernel $(\lambda + D)[(\lambda + D)^2 + \omega^2]^{-1}$ approaches $\pi\delta(\omega)$ and we recover the minimum coupling required for synchronisation, $K_{c,\min} = 2/[\pi g(0)]$.

✓ **Exercise:** Show that the linear growth rate of the instability for $g(\omega) = (a/\pi)(a^2 + \omega^2)^{-1}$ is given by $\lambda = -D + (K - K_{c,\min})/2$.

The above eigenvalue constitutes the discrete spectrum of the problem. There is also a continuous spectrum, which we do not discuss further; see the papers by Strogatz referenced above for details.

The stability of the higher harmonics contained in $\eta(\theta, t, \omega)$ can also be calculated for completeness. But they are of academic interest, as they do not contribute to $r(t)$ (at leading order in the perturbation analysis; in principle, they do affect the saturation of the instability) and hence do not contribute to the degree of synchronisation.

✓ **Exercise:** Show that one has

$$\frac{\partial \eta}{\partial t} = -\omega \frac{\partial \eta}{\partial \theta} + D \frac{\partial^2 \eta}{\partial \theta^2}. \quad (7.177)$$

By expanding in a Fourier series in θ , show that

$$\eta(\theta, t, \omega) = \sum_{|k| \geq 2} a_k(0, \omega) \exp[-k^2 Dt] \exp[ik(\theta - \omega t)]. \quad (7.178)$$

Hence the higher harmonics are all stable for $D \neq 0$ and quickly disappear from the system. By contrast, for $D = 0$, the higher harmonics do not dissipate away; they form a rotating wave in the pdf $p(\theta, t | \omega)$, which does not contribute to the synchronisation parameter r and therefore corresponds to all the oscillators rotating around the circle independently at frequency ω without mutually interacting.

If you are interested in the many variations on Kuramotos model, e.g. introducing delays, disorder, different coupling strengths between different oscillator pairs, et cetera, please consult the comprehensive review by Acebron (2005) referenced above. The stability diagram of the system becomes quite intricate, once all these features are incorporated.

7.8 Problems

1. **Large, richly connected Lotka-Volterra ecologies:** Consider a hierarchical

Lotka-Volterra system,

$$\frac{dx_i}{dt} = k_i x_i + \sum_{j=1}^N a_{ij} x_i x_j, \quad (7.179)$$

where each species i eats all its successors $j > i$, and is eaten by all its predecessors $j < i$, but there is no cannibalism ($a_{ii} = 0$ for all $i = j$). Suppose furthermore that there is a nontrivial equilibrium solution $x_i^{(0)}$ and that the connection coefficients are related to this equilibrium solution by

$$a_{ij} = \sqrt{x_i^{(0)} x_j^{(0)}}. \quad (7.180)$$

- (a) Linearise about the equilibrium solution. Show that the perturbations $x_i^{(1)}$ satisfy

$$\frac{dx_i^{(1)}}{dt} = \sum_{j=1}^N c_{ij} x_j^{(1)}, \quad (7.181)$$

with $c_{ij} = 0$ for $i = j$, $c_{ij} = 1$ for $i < j$ and $c_{ij} = -1$ for $i > j$.

- (b) Prove that the eigenvalues of the linearised system are pure imaginary:

$$\lambda_k = i \cot[\pi(k + 1/2)/N] \quad (7.182)$$

and the associated eigenvectors are given by

$$(\mathbf{u}_k)_j = \frac{1}{N} \exp[2\pi i(k + 1/2)j/N]. \quad (7.183)$$

- (c) Show that, in the limit $N \rightarrow \infty$, the entries of the fundamental matrix of the system are given by

$$\Phi_{jk}(t) = \frac{1}{\pi} \int_0^\pi d\phi \exp[2i(j-k)\phi + it \cot \phi]. \quad (7.184)$$

- (d) How is it possible that an irreversible damping appears even though all the normal modes are oscillatory?

- (e) Show that, for the i^{th} species, we have

$$\frac{dx_i^{(1)}}{dt} = -x_i^{(1)}(t) + \xi_i(t), \quad (7.185)$$

where

$$\xi_i(t) = \sum_{j \neq i} [\Phi_{ij}(t) + \dot{\Phi}_{ij}] x_j^{(1)}(0). \quad (7.186)$$

- (f) Explain physically why $\xi_i(t)$ can be viewed as a Langevin force in the limit $N \rightarrow \infty$.
- (g) Assume the species are initially in thermal equilibrium at temperature T , i.e. their population perturbations $x_i^{(1)}$ are distributed according to the Boltzmann law

$$\text{probability} \propto \exp \left[-\frac{1}{2T} \sum_{i=1}^N (x_i^{(1)})^2 \right]. \quad (7.187)$$

Show explicitly that the ensemble-averaged auto-correlation function reduces to the white-noise form

$$\langle \xi_i(t) \xi_j(t') \rangle = 2T \delta_{ij} \delta(t - t'). \quad (7.188)$$

- (h) What does this imply physically about the interaction between the species? Do you expect this to remain true irrespective of the form of a_{ij} ?

- 2. Bird populations:** The male and female populations $M(t)$ and $F(t)$ of a bird community have constant, equal death rates k and periodic, equal birth rates $\mu(t)$ (with period T).

- (a) If the birth rates are seasonal, with duty cycle ϵT , so that $\mu(t) = \delta$ for $0 < t \leq \epsilon$ and $\mu(t) = 0$ for $\epsilon < t \leq T$ prove, using Floquet theory or otherwise, that the populations socialite with period T if $kT = \epsilon\delta$.
- (b) What is the range of $kT/\delta\epsilon$ that allows oscillatory populations of any period?
- (c) Does this conclusion change qualitatively if the death rates are unequal? What about the birth rates?

Chapter 8

Nonuniform far-from-equilibrium systems: pattern formation

8.1 Introduction

In the previous chapter we primarily focused on systems which are uniform, i.e. the spatial variation is not included. In this Chapter we focus on systems where spatial variations in the *density* play a significant role in defining the how the system reacts to perturbations.

We will start by in general considering the formation of patterns and quantify their stability. We will then address two examples, (i) pattern formation in mammalian coats and how a rotating Bose-Einstein admits a vortex, due to dynamical instabilities in the rotating solution.

8.2 Pattern formation: reaction diffusion

The ultimate aim of this section is to answer the question: Why does a tiger have stripes, but a leopard have spots?

Start by considering the variable $c(\mathbf{x}, t)$, which defines the concentration of some species. Then $\mathbf{J}(\mathbf{x}, t)$ is defined as being the species flux and $f(\mathbf{x}, t)$ is defined as being the source

or sink. Conservation implies

$$\frac{\partial c}{\partial t} = \operatorname{div} \mathbf{J} = f. \quad (8.1)$$

Expressing $\mathbf{J} = \pm D\nabla c$ we then have two possibilities: (i) *Fick diffusion* $\mathbf{J} = -D\nabla c$ (flux moves down concentration gradients) and (ii) *Chemotaxis* $\mathbf{J} = +D\nabla c$ (flux moves up concentration gradients). For chemotaxis a positive feedback mechanism is required, for example if a signalling chemical is emitted by some species and members of that species diffuse **towards** the place of high concentration (e.g. slime mould: *Dicryostelium Discoideurm*).

For slime mould consider n to be the concentration of cells and a to be the concentration of cAMP (secretion signal). Then

$$\frac{\partial n}{\partial t} = Kn(n - 1) - D_n \operatorname{div}(n \nabla a), \quad (8.2)$$

where the first term (RHS) denotes the growth of cells and the second term characterises chemotaxis. In addition we have to consider the evolution of a :

$$\frac{\partial a}{\partial t} = hn - h'a + D_a \nabla^2 a, \quad (8.3)$$

where the first term (RHS) characterises the production of cAMP, the second term accounts for evaporation of cAMP and the third term is Fick diffusion. For such a reaction diffusion system we have two questions: (i) When do patterns form and (ii) once they form how do they spread?

Starting with question (ii): a pattern forming instability starts at a point and spreads *as a wave* (non-linear). Why *as a wave* and not as a diffusion front? If the pattern spreads by diffusion we find that the patterns do not persist for long enough and the spreading of the pattern is too slow.

In general for reaction-diffusion system there may be some perturbation which is linear unstable, i.e. there may exist some wavenumber \mathbf{k} for which solutions $\exp(\lambda(\mathbf{k})t)$ have real eigenvalues: $\operatorname{Re}(\lambda(\mathbf{k})) > 0$. If this is the case can have three options: (i) \mathbf{k} is preserved; (ii) new \mathbf{k} 's for through non-linear terms and (iii) get *every* \mathbf{k} , i.e. turbulence.

8.3 Non-linear waves

Consider a one-dimensional logistic population, with Fick diffusion:

$$\frac{\partial u}{\partial t} = u(u - 1) + \nabla^2 u. \quad (8.4)$$

then the steady states are $u = 0$ (unstable) and $u = 1$ (stable). Assume you start with some $u(x, t)$ and evolve, with $\nabla^2 \neq 0$ (non-uniform). Look for a travelling wave solution: $u(x, t) = u(x - ct)$ hence

$$-cu' = u(u - 1) + u'', \quad (8.5)$$

where the ' denotes $\partial/\partial\xi$, with $\xi = x - ct$. Letting $v = u'$ we have

$$v' = -cv - u(1 - u). \quad (8.6)$$

Now linearising about the fixed points $(u, v) = (0, 0)$ and $(1, 0)$ we have the following Jacobian

$$\begin{pmatrix} 0 & 1 \\ -1 + 2u & -c \end{pmatrix}, \quad (8.7)$$

with the corresponding eigenvalues

$$\lambda = \frac{c \pm \sqrt{c^2 - 4(1 - 2u)}}{2}. \quad (8.8)$$

For $(u, v) = (0, 0)$ if $|c| > 2$ the eigenvalues are real and less than zero, i.e. the wave decays (stable node), if $|c| < 2$ the eigenvalues are complex, with the real part less than zero, i.e. the wave decays and oscillates (stable spiral). For $(u, v) = (1, 0)$ the eigenvalues are real, with one less than zero (the wave decays) and one greater than zero (wave grows).

8.3.1 Conditions for pattern formation

Consider two fields:

$$\frac{\partial u}{\partial t} = \gamma f(u, v) + D_1 \nabla^2 u \quad (8.9)$$

$$\frac{\partial v}{\partial t} = \gamma g(u, v) + D_2 \nabla^2 v. \quad (8.10)$$

Want to ask the following, general question, if (u_0, v_0) is a stable *uniform* equilibrium state when does it go unstable (i.e. pattern formation) when diffusion is included?

If we are at a stable node then $f(u_0, v_0) = g(u_0, v_0) = 0$ and the eigenvalues of the Jacobian must be real and negative, i.e. $\text{Tr}(A) < 0, \det(A) > 0$ where

$$A = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}_{(u_0, v_0)}, \quad (8.11)$$

Now introduce a perturbation of the general form:

$$W = \begin{pmatrix} u - u_0 \\ v - v_0 \end{pmatrix}. \quad (8.12)$$

Linearizing Eqs. (8.9,8.10) we have

$$\frac{d\mathbf{W}}{dt} = \gamma A \mathbf{W} + \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix} \nabla^2 \mathbf{W}, \quad (8.13)$$

where $d = D_2/D_1$. Assume time dependence $\propto \exp \lambda t$. Expand the spatial part in a complete set of eigenfunctions of ∇^2 which satisfy given boundary conditions:

$$\nabla^2 W_{\mathbf{k}}(x) = k^2 W_{\mathbf{k}}(x), \quad (8.14)$$

substitute

$$\mathbf{W} \propto \sum_{\mathbf{k}} e^{\lambda t} W_{\mathbf{k}}(x) \quad (8.15)$$

and use orthogonality

$$\lambda \mathbf{W}_{\mathbf{k}} = \gamma A \mathbf{W}_{\mathbf{k}} + \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix} k^2 \mathbf{W}_{\mathbf{k}}. \quad (8.16)$$

The above equations have non-trivial solutions when:

$$\det \left(\lambda I - \gamma A - \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix} k^2 \right) = 0. \quad (8.17)$$

A *bit* of maths leads to

$$0 = \lambda^2 + \lambda [k^2(1+d) - \gamma(f_u + g_v)] + dk^4 - \gamma(df_u + g_v)k^2 + \gamma^2(f_u g_v - f_v g_u), \quad (8.18)$$

where instability requires $\text{Re}(\lambda) > 0$ for at least one value of \mathbf{k} . The above equation is critical when $\lambda = 0$. So setting $\lambda = 0$ and looking for the criteria that k is real defines the regime for which patterns form. Using this criteria we have

$$(df_u + g_v)^2 \geq 4d(f_u g_v - f_v g_u). \quad (8.19)$$

The critical d_c is defined by $(d_c f_u + g_v)^2 = 4d_c(f_u g_v - f_v g_u)$, i.e.

$$d_c^2 f_u^2 + 2d_c(f_v g_u - f_u g_v) + g_v^2 = 0. \quad (8.20)$$

Can define a critical wave vector by setting λ to zero in Eq. (8.18), such that

$$dk^4 - \gamma k^2(df_u + g_v) + \gamma^2(f_u g_v - f_v g_u) = 0 \quad (8.21)$$

and using the criteria that k is real (Eq. (8.19)), i.e. $(d_c f_u + g_v) = 2\sqrt{d_c(f_u g_v - f_v g_u)}$ to replace $(df_u + g_v)$ in the above equation, such that

$$d_c k_c^4 - 2\gamma k_c^2 \sqrt{d_c(f_u g_v - f_v g_u)} + \gamma^2(f_u g_v - f_v g_u) = 0. \quad (8.22)$$

Thus

$$k_c^2 = \gamma \sqrt{\frac{f_u g_v - f_v g_u}{d_c}}. \quad (8.23)$$

If we now consider a system with boundary conditions then there is a minimum k which can be supported by the system, i.e. for a one dimensional box, of length L , $k_{\min} = \pi/L$. If $k_c > k_{\min}$ then a pattern will form.

8.3.2 Mammalian coats

From the previous section can we understand why a tiger has stripes and leopard has spots? The pre-pattern is set up in the embryo, i.e. small.

Consider the eigenfunctions for the tail of the tiger/leopard (for a theorist view of a tail see Fig. 8.1). At the end of the tail ($z = 0$) we have a zero-flux boundary condition and the eigenfunctions have the following form:

$$\mathbf{W}_k \propto \cos(n\theta) \cos\left(\frac{m\pi z}{s}\right), \quad (8.24)$$

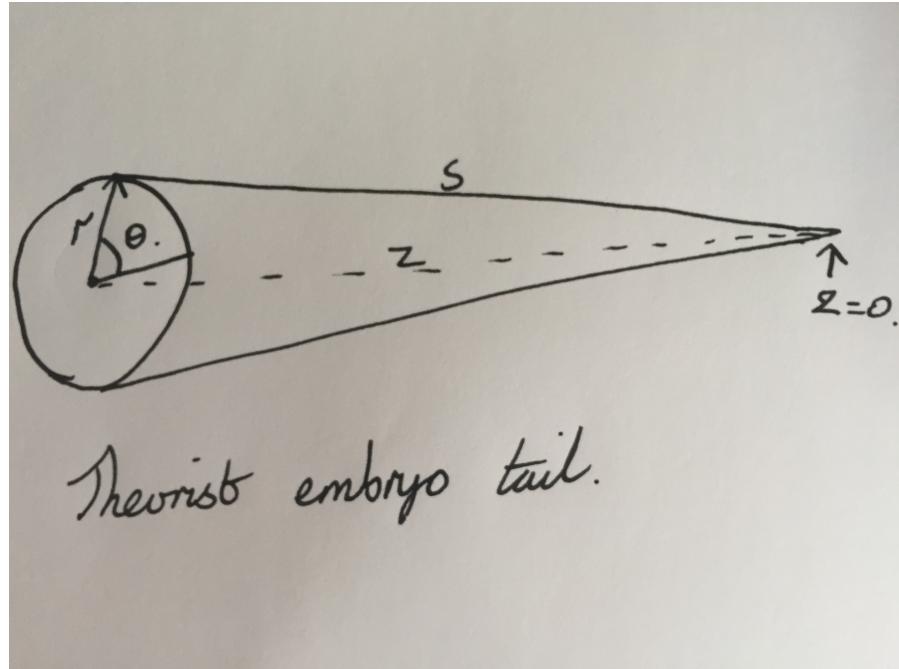


Figure 8.1. Schematic of an idealised embryo tail.

with

$$k^2 = \frac{n^2}{r^2} + \frac{m^2\pi^2}{s^2}, \quad (8.25)$$

Hence the condition for pattern formation can be characterised in the following manner:
 $k_{\min} < k < k_{\max}$.

Consider the thin end of the tail then r is effectively to small and falls outside the range $k_{\min} < k < k_{\max}$ unless $n = 0$. Hence in his case the tail pattern will have rings, independent of θ , see Eq. (8.24). If the tail is thicker then can also have $n = 1, 2, 3..n_{\max}$, i.e. $\cos \theta, \cos 2\theta, \dots$ leading to spots.

8.4 Stability of rotating Bose-Einstein condensate

This section closely follows the work of N.G. Parker *et al.*, Physical Review A **73**, 061603(R) (2006).

Vortex lattices are a striking manifestation of superfluidity in rotating systems, which have been generated in atomic Bose-Einstein condensates BECs via rotation in an elliptical

harmonic trap. Vortex lattices form for trap rotation frequencies $\Omega \sim 0.7\omega_{\perp}$, where ω_{\perp} is the mean harmonic trap frequency in the rotating plane. Although a vortex lattice is thermodynamically favourable for much lower rotation frequencies, the instabilities necessary to seed lattice formation are only present in this region. Such instabilities have been predicted by hydrodynamic studies of condensate solutions in the rotating frame and the dynamical perturbations of these states.

In this section we present an investigation of the instabilities leading to vortex lattice formation in elliptical traps. We consider the adiabatic introduction of trap ellipticity or rotation frequency. In order to probe the condensate instabilities we consider the classical hydrodynamic solutions in the rotating frame and their response to dynamical perturbations. Furthermore, we perform time-dependent simulations to test these results and probe the fate of the unstable condensate.

In experiments the harmonic confining trap is transformed radially into an ellipse and rotated about the z -axis. In the limit of zero temperature, the condensate can be approximated by a mean-field wave function," which can be expressed as $\psi = \sqrt{\rho} \exp i\phi$, where ρ and ϕ are the condensate density and phase. In the frame rotating at Ω , the density ρ and fluid velocity $\mathbf{v} = (\hbar/m)\nabla\phi$ satisfy the hydrodynamic equations

$$\frac{\partial\rho}{\partial t} + \nabla \cdot [\rho(\mathbf{v} - \boldsymbol{\Omega} \times \mathbf{r})] = 0 \quad (8.26)$$

$$m\frac{\partial\mathbf{v}}{\partial t} + \nabla \left(\frac{1}{2}m\mathbf{v} \cdot \mathbf{v} + \frac{1}{2}m(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2) + \rho g - \frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}} - m\mathbf{v} \cdot [\boldsymbol{\Omega} \times \mathbf{r}] \right) = 0. \quad (8.27)$$

Here m is the atomic mass, g is the interaction coefficient and $\omega_x, \omega_y, \omega_z$ are the harmonic trap frequencies. When the trap is elliptical we can write $\omega_x = \omega_{\perp}\sqrt{1-\epsilon}$ and $\omega_y = \omega_{\perp}\sqrt{1+\epsilon}$ where ϵ characterizes the trap ellipticity, and $\omega_{\perp}^2 = (\omega_x^2 + \omega_y^2)/2$.

We employ the Thomas-Fermi approximation by neglecting the $\nabla^2\sqrt{\rho}/\sqrt{\rho}$ term in Eq. (8.27), and assuming an irrotational quadrupolar velocity field,

$$\mathbf{v} = \alpha\nabla(xy), \quad (8.28)$$

where α is the velocity field amplitude. Substituting this into Eq. (8.27) and setting $\partial\rho/\partial t =$

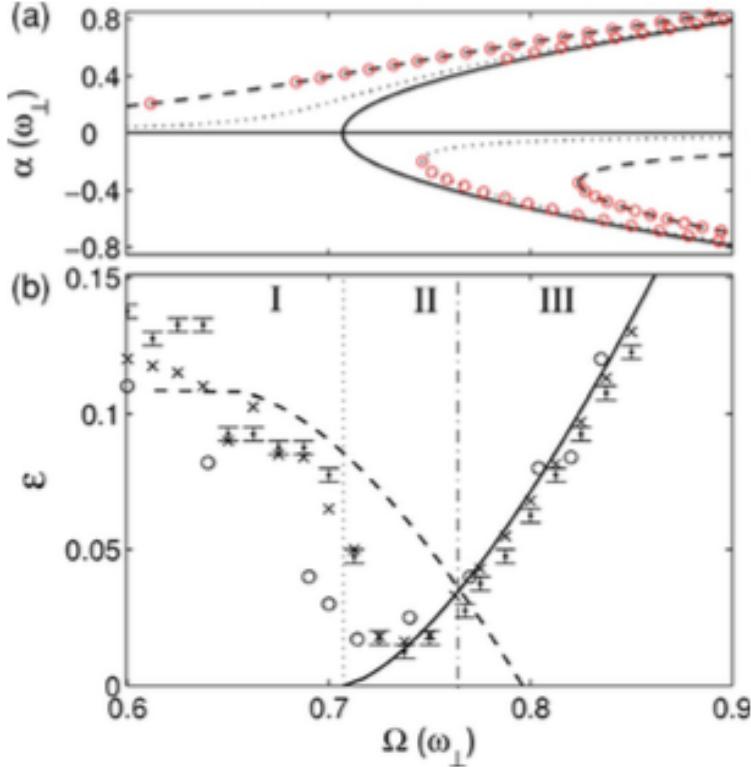


Figure 8.2. (a) Velocity field amplitude α of the stationary solutions of Eq. (8.30) versus rotation frequency Ω for $\epsilon = 0$ (solid line), 0.02 (dotted line), and 0.1 (dashed line). Regions of dynamical instability for $\epsilon = 0.02$ and 0.1 are shown (circles). (b) Phase diagram of ϵ versus Ω . Plotted are the bifurcation point $\Omega_{\text{bif}}(\epsilon)$ (solid line) from Eq. (8.30), the onset of dynamical instability $\Omega_{\text{ins}}(\epsilon)$ from Eq. (8.31) (dashed line), and experimental data of Hodby *et al* (Physical Review Letters **88**, 010405 (2001)) (circles). Simulations of Eqs. (8.26) and (8.27) show the critical ellipticities beyond which the condensate deviates from an elliptical shape $\epsilon_{\text{cr}}^{\text{dev}}$ (crosses) and beyond which lattice formation ultimately occurs $\epsilon_{\text{cr}}^{\text{ins}}$ (points with error bars). The bifurcation point for $\epsilon = 0$ (dotted line) and the crossing frequency Ω_X (dot-dashed line) at which $\Omega_{\text{bif}}(\epsilon) = \Omega_{\text{ins}}(\epsilon)$ are indicated.

$\partial\mathbf{v}/\partial t = 0$, we obtain stationary density solutions of the form

$$\rho^{(0)} = \frac{1}{g} \left(\mu - \frac{1}{2} m (\tilde{\omega}_x^2 x^2 + \tilde{\omega}_y^2 y^2 + \omega_z^2 z^2) \right), \quad (8.29)$$

in the region where the chemical potential $\mu \geq m (\tilde{\omega}_x^2 x^2 + \tilde{\omega}_y^2 y^2 + \omega_z^2 z^2) / 2$, and $\rho^{(0)} = 0$ elsewhere. The rotation induces effective trap frequencies $\tilde{\omega}_x^2 = [(1 - \epsilon) + \alpha^2 - 2\alpha\Omega]\omega_\perp^2$ and $\tilde{\omega}_y^2 = [(1 + \epsilon) + \alpha^2 + 2\alpha\Omega]\omega_\perp^2$ where α determines the ellipticity of the Bose-Einstein condensate density. Plugging Eq. (8.29) into Eq. (8.26) we obtain the following condition for the rotating Thomas-Fermi solutions

$$\tilde{\omega}_x^2(\alpha + \Omega) + \tilde{\omega}_y^2(\alpha - \Omega) = 0. \quad (8.30)$$

Figure 8.2(a) shows the stationary solutions in $\Omega - \alpha$ space for various values of trap ellipticity. In the limit $\epsilon = 0$ solid line a non-rotating $\alpha = 0$ solution occurs for all Ω , with two additional solutions bifurcating from the $\alpha = 0$ axis at $\Omega_{\text{bif}}^0 = \omega_\perp/\sqrt{2}$. For finite ϵ dotted and dashed lines, the $\alpha = 0$ solution disappears and the plot consists of two distinct branches. The upper branch positive α is single valued and exists for all Ω , while the lower branch negative is double valued and exists only when Ω is greater than the bifurcation frequency $\Omega_{\text{bif}}(\epsilon)$. As ϵ is increased from zero, the branches move away from the $\alpha = 0$ axis [Fig. 8.2(a)]. Furthermore the bifurcation point of the lower branch $\Omega_{\text{bif}}(\epsilon)$ shifts to higher Ω , as shown in Fig. 8.2(b) (solid line). The branch diagrams are key to understanding the response of the system to the adiabatic introduction of trap ellipticity (ϵ) or rotation frequency (Ω). Before any rotation and ellipticity is applied the BEC has $\alpha = 0$. When Ω is increased adiabatically for fixed ϵ , the BEC follows the upper branch, with increasing α . When ϵ is introduced adiabatically for fixed Ω , the BEC can follow two routes, depending on the value of Ω relative to the bifurcation point Ω_{bif}^0 [dotted line in Fig. 8.2(b)]. For $\Omega < \Omega_{\text{bif}}^0$ the lower branch is nonexistent and the BEC follows the upper branch to increasing values of α . For $\Omega > \Omega_{\text{bif}}^0$, the BEC follows the lower branch from $\alpha = 0$ to negative α . However, as Ω is increased, the edge of the lower branch $\Omega_{\text{bif}}(\epsilon)$ shifts to higher frequencies, and when $\Omega_{\text{bif}}(\epsilon) > \Omega$ the lower branch no longer exists. In this manner, the evolution of the branches can induce instability, and has been linked to lattice formation.

The stationary solutions of Eq. (8.30) are not necessarily stable solutions. To investigate

their stability we consider small perturbations $\rho^{(1)}$ and $\phi^{(1)}$ of stationary solutions of density $\rho^{(0)}$ and phase $\phi^{(0)}$:

$$-\begin{pmatrix} \mathbf{v}_c \cdot \nabla & g/m \\ \nabla \cdot (\rho^{(0)} \nabla) & \mathbf{v}_c \cdot \nabla \end{pmatrix} \begin{pmatrix} \phi^{(1)} \\ \rho^{(1)} \end{pmatrix} = \frac{d}{dt} \begin{pmatrix} \phi^{(1)} \\ \rho^{(1)} \end{pmatrix}, \quad (8.31)$$

where $\mathbf{v}_c = \mathbf{v} - \boldsymbol{\Omega} \times \mathbf{r}$ is the velocity field in the rotating frame. The eigenfunctions of Eq. (8.31) grow in time as $\exp[\lambda t]$, where λ is the eigenvalue. Solutions are unstable when one or more eigenvalues contain a positive real part, and are thought to seed vortex lattice formation.

Using a polynomial ansatz for the perturbations, this predicts dynamical instability when Ω exceeds a critical value Ω_{ins} , [circles in Fig. 8.2(a)]. In the limit of $\epsilon = 0$, $\Omega_{\text{ins}} = 0.78\omega_{\perp}$. As ϵ is increased, Ω_{ins} is reduced [dashed line in Fig. 8.2(b)]. The outlying point in Fig. 8.2(a) for $\epsilon \approx 0.1$ dashed line at $\Omega \approx 0.61\omega_{\perp}$ is not considered to be in the unstable region due to its narrow width and small eigenvalues. Note that the lower-branch solution closest to the $\alpha = 0$ axis is not dynamically unstable. A key rotation frequency is Ω_X , which is the crossing point of $\Omega_{\text{bif}}(\epsilon)$ and $\Omega_{\text{ins}}(\epsilon)$, and has the value $\Omega_X = 0.765$ [dot-dashed-line in Fig. 8.2(b)].

From the solutions of Eq. (8.30) and the dynamical instability of Eq. (8.31) we can predict the BEC stability following the adiabatic introduction of Ω or ϵ . However, to determine how the instability manifests itself and if it leads to lattice formation numerical simulations of Eqs. (8.26) and (8.27) need to be performed. Noting that the solutions of Eq. (8.30) and Eq. (8.31) are independent of z , we consider a two-dimensional system. In real time, either ϵ is ramped up linearly at a rate $d\epsilon/dt = 10^{-4}$ for fixed Ω , or Ω is ramped up linearly at a rate $d\Omega/dt = 10^{-2}$ for fixed ϵ .

We first consider the adiabatic increase of trap ellipticity ϵ for fixed Ω . We discriminate three cases of instability as indicated in Fig. 8.2(b): I ripple, II interbranch, and III catastrophic instabilities.

- (I) *Ripple instability* $\Omega < \omega_{\perp}/\sqrt{2}$. The case for $\Omega = 0.7\omega_{\perp}$ is shown in Fig. 8.3(a)I.

The velocity field amplitude α (dots) follows the upper branch of Eq. (8.30) solid

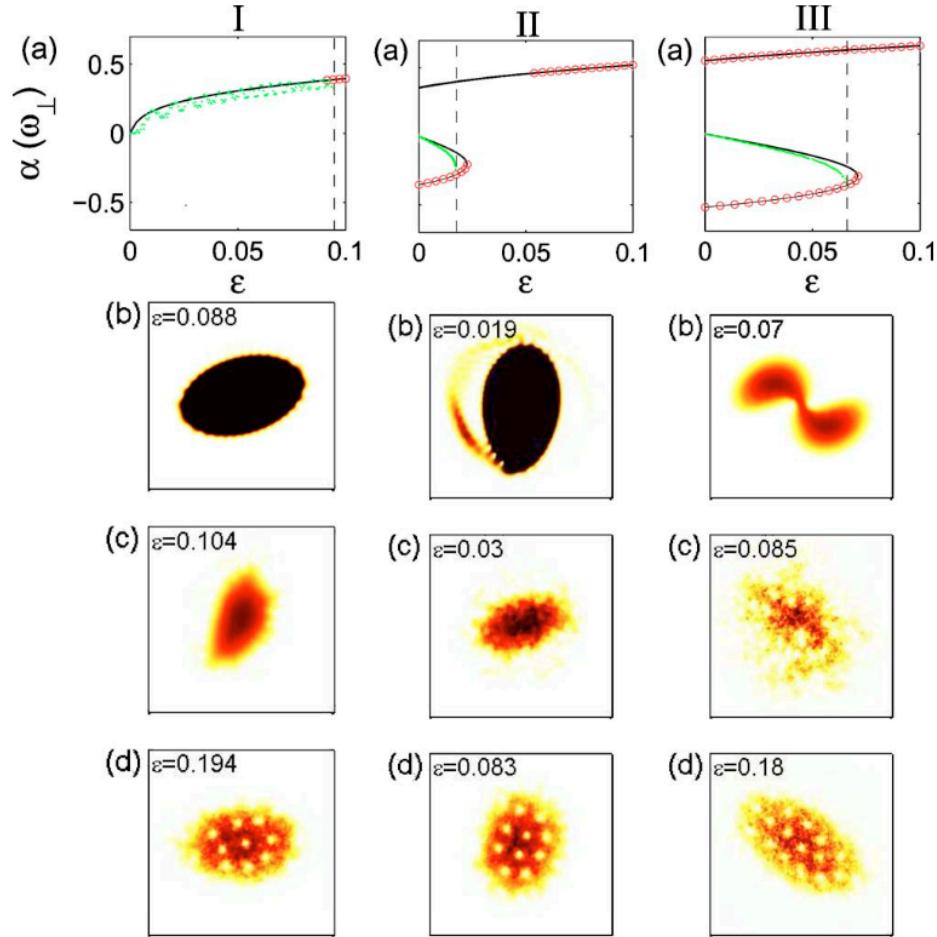


Figure 8.3. Dynamics under a continuous increase of ϵ for I ripple instability ($\Omega/\omega_{\perp} = 0.7$), II interbranch instability ($\Omega/\omega_{\perp} = 0.75$), and III catastrophic instability ($\Omega/\omega_{\perp} = 0.8$). (a) Velocity field amplitude α versus ϵ according to Eq. (8.30) (black solid lines) and numerical simulations of Eqs. (8.26) and (8.27) (green dots). To the right of the dashed line, Eq. (8.28) is no longer a valid fit to the simulated velocity field (the standard deviation of the fit becomes of the order of α). The regions of dynamical instability are indicated [(red) circles]. Density snap shots showing the (b) onset of instability, (c) disrupted state seeded by instability, and (d) vortex lattice. Dark/light regions represent high/low density.

line. Here the BEC and trap axes rotate in phase. As ϵ is increased, the BEC moves along the branch to higher α , and when ϵ exceeds a critical value, corresponding to when $\Omega > \Omega_{\text{ins}}$, the solution becomes dynamically unstable, according to Eq. (8.31). This occurs for $\epsilon \approx 0.09$ in Fig. 8.3(a)I (dashed line). Subsequently α (dots) deviates from the upper branch (solid lines) consistent with the onset of dynamical instability. For low ϵ , α (dots) oscillates slightly due to the center-of-mass motion caused by the initial offset of the BEC.

At a critical ellipticity $\epsilon_{\text{cr}}^{\text{dev}}$ low-density ripples form on the BEC edge [Fig. 8.3(b)I] and grow in amplitude as ϵ is increased. If ϵ becomes fixed when the ripples have very low amplitude, they do not grow over the time scales considered. However, once ϵ exceeds a second critical value $\epsilon_{\text{cr}}^{\text{ins}}$ corresponding to when the ripple amplitude is of order of 10% $\rho^{90)}$ the dynamical instability of Eq. (8.31) is triggered by the ripples. This instability generates large-scale shape oscillations [Fig. 8.3(c)I] disrupting the BEC, and enabling ghost vortices to nucleate, which slowly crystallize into a lattice [Fig. 8.3(d)I]. Once $\epsilon_{\text{cr}}^{\text{ins}}$ is reached, lattice formation occurs independently of whether ϵ is fixed or continuously increased. Since the ripples originate in the non-Thomas-Fermi tails of the BEC, they cannot be explained by the Thomas-Fermi analytics of Eqs. (8.28)-(8.31).

- (II) *Interbranch instability* $\omega_{\perp} < \Omega < \Omega_X$. The case for $\Omega = 0.75\omega_{\perp}$ is shown in Fig. 8.3(a)II. Since $\Omega > \omega_{\text{perp}}/2$, α (dots) initially follows the lower-branch solutions, where we observe that the BEC and trap axes are $\pi/2$ out of phase. As ϵ is increased, a point is reached when $\Omega < \Omega_{\text{bif}}(\epsilon)$. Here the lower branch is no longer a solution of Eq. (8.30). In Fig. 8.3(a)II, this occurs for $\epsilon \approx 0.02$ (dashed line). Due to the non-Thomas-Fermi nature of the numerical solutions of Eqs. (8.26) and (8.27) α does not perfectly fit the branch solutions of Eq. (8.30).

When α (dots) reaches the cusp of the lower branch it deviates non-adiabatically. Since $\Omega < \Omega_X$ the upper branch is dynamically stable at this ϵ . The BEC tries to transform to the upper branch, but without dissipation α (dots) is forced to oscillate between positive and negative values, with the density oscillating between a circular and highly

elliptical shape. If ϵ is fixed close to this critical ellipticity, the shape oscillations are stable. However, if ϵ is increased further, the shape oscillations destabilize, with the BEC shedding low-density material at its extrema in a spiral pattern [Fig. 8.3(b)II]. This situation is closely analogous to when Ω is suddenly turned on, with the fate of the BEC being qualitatively similar. The growth of the ejected material gradually destabilizes the BEC [Fig. 8.3(c)II] leading to vortex nucleation and ultimately a lattice [Fig. 8.3(d)II].

- (III) *Catastrophic instability* $\Omega > \Omega_X$. The case for $\Omega = 0.8\omega_\perp$ is shown in Fig. 8.3(a)III. Again α (dotted line) follows the lower branch, which ceases to be a solution at some critical ϵ (dashed line). However, since $\Omega > \Omega_X$ the upper branch is dynamically unstable and no stable solutions exist. The BEC undergoes a quick and catastrophic instability, with α (dots) deviating rapidly from the rotating solutions of Eq. (8.30). The BEC density becomes strongly contorted into a spiral shape [Fig. 8.3(b)III]. The arms of the spiral collapse inward and trap phase singularities to form vortices. Energy and angular momentum are very rapidly injected into the BEC in contrast to the ripple and interbranch instabilities. The BEC becomes highly excited and turbulent [Fig. 8.3(c)III], with structure on length scales less than the healing length. Although we observe this state to ultimately settle into a lattice [Fig. 8.3(d)III], one may question the validity of our zero temperature simulations for such a heated state.

In the simulations we have measured two distinct critical ellipticites: $\epsilon_{\text{cr}}^{\text{dev}}$ [crosses in Fig. 8.2(b)] is when, for a continuously increasing ϵ , we observe the density to deviate from a smooth ellipse (on the level of $0.1\%\rho^{(0)}$); $\epsilon_{\text{cr}}^{\text{ins}}$ [points with error bars in Fig. 8.2(b)] is when, for ϵ ramped up to some final value, instability and lattice formation ultimately occur. In regime I, typically $\epsilon_{\text{cr}}^{\text{dev}} \leq \epsilon_{\text{cr}}^{\text{ins}}$ since surface ripples are generated that are stable for a narrow range of ϵ , above which they induce instability and lattice formation. In regimes II and III, $\epsilon_{\text{cr}}^{\text{dev}} \approx \epsilon_{\text{cr}}^{\text{ins}}$, indicating the relatively sudden onset of this instability once the density deviates from a smooth ellipse.

According to the simulations, the region above the points in Fig. 8.2(b) is unstable, leading to lattice formation. The prediction of Eq. (8.31) (dashed line) gives reasonable agreement with the simulation results in region I, while Eq. (8.30) gives excellent agreement in region III. Also plotted in Fig. 8.2(b) are the experimental results of Hodby *et al.* (Physical Review Letters **88**, 010405 (2001)) (circles). The numerical results give good agreement with the experimental data throughout, with the agreement being particularly good in region III.

So far we have considered the adiabatic introduction of ϵ for fixed Ω . However, Fig. 8.2(b) also applies to the case when Ω is introduced adiabatically for fixed ϵ . Here the BEC follows the upper branch until it becomes dynamically unstable to the ripple instability. According to Eq. (8.31) dynamical instability occurs when $\Omega > \Omega_{\text{ins}}(\epsilon)$ [dashed line in Fig. 8.2(b)].

8.5 Problems

1. Consider a predator-prey model with diffusion:

$$\frac{\partial u}{\partial t} = u(1 - u - v)a + D_1 \nabla^2 u \quad (8.32)$$

$$\frac{\partial v}{\partial t} = v(u - b)a + D_2 \nabla^2 v \quad (8.33)$$

- (a) Show that the uniform stationary solutions are given by $(u, v) = (0, 0)$, $(1, 0)$ and $(b, 1 - b)$.
- (b) Consider wave solutions and find four first order ODE's describing their motion.
- (c) Consider the case that the prey diffuses slowly ($D_1 \approx 0$) and find the conditions for pattern formation.

2. To zeroth order the ground-state wavefunction of Bose-Einstein condensate, in a parabolic trap, can be modelled by the Gross-Pitaevskii equation:

$$i\hbar \frac{\partial}{\partial t} \Psi_0 = \left(-\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) + g |\Psi_0|^2 \right) \Psi_0, \quad (8.34)$$

where m is the mass of the atoms in the condensate, g (typically ≥ 0) characterises the strength of the interactions between the particles in the Bose-Einstein condensate and ω_x , ω_y and ω_z are the trapping frequencies in the x , y and z directions respectively.

- (a) By expressing $\Psi_0 = \sqrt{\rho} \exp i\phi$ and starting from the Gross-Pitaevskii equation, in the rotating frame (where the rotation is about the z -axis):

$$i\hbar \frac{\partial}{\partial t} \Psi_0 = \left(-\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) + g |\Psi_0|^2 + i\hbar \Omega \mathbf{r} \times \nabla \right) \Psi_0 \quad (8.35)$$

derive Eqs. (8.26) and (8.27).

- (b) Employing the Thomas Fermi approximation and expressing $\omega_x = \omega_{\perp} \sqrt{1 - \epsilon}$ and $\omega_y = \omega_{\perp} \sqrt{1 + \epsilon}$, show that for an irrotational velocity field of the form in Eq. (8.28) that the stationary solutions are constrained by Eqs. (8.29) and (8.30). Show that the solutions for α are consistent with the lines in Fig. 8.3(a).
- (c) By considering small perturbation in the density and phase, show that their dynamics are governed by Eq. (8.31).
- (d) By considering perturbations of the density and phase of the form $x^n y^k z^j$, where n, k, j run from zero to sum maximum defined by $n + k + j = M$ show that the regions of instability are consistent with the red circles shown in Fig. 8.3(a).

[Numerical]

Chapter 9

Practice exam

Below is a practice exam. The final exam will be of the same format but, obviously, with different questions.

The University of Melbourne

School of Physics

**PHYC90010
Statistical Mechanics: Practice Exam**

Reading time: **15 minutes**

Exam Duration: **4 hours**

This paper has: **7 pages**

Authorised Materials: This is an open book exam

Instructions to Invigilators: **This examination paper is to remain in the examination room. Students may not retain any part of this exam.**

Instructions to students: Attempt ALL questions. The total number of marks is 80.
This examination paper is to remain in the examination room. Students may not retain any part of this exam.

Paper may NOT be held by the Baillieu Library.

Question 1(a)**10 marks**

An isolated, steady-state, spherically symmetric star cluster consists of N identical stars, each of mass m , orbiting in a self-consistent gravitational potential $\Phi(\mathbf{x})$. The stellar density is low enough for the orbits to be considered collisionless.

- Show that the stellar pdf $p(t, \mathbf{x}, \mathbf{v})$ identically satisfies the collisionless Boltzmann equation if it can be written wholly as a function $p(E)$ of the mechanical energy per unit mass of an arbitrary star, $E[t, \mathbf{x}(t), \mathbf{v}(t)]$.
- Show that the gravitational potential satisfies

$$\nabla^2 \Phi = 16\pi^2 G N m \int_0^\infty dv v^2 p \left[\frac{v^2}{2} + \Phi(\mathbf{x}) \right]. \quad (1(a).1)$$

- Consider the thermodynamically inspired choice $p(E) = A \exp(-E/\sigma^2)$, where A is a normalisation constant to be determined and σ is the stellar velocity dispersion. Alas, in this special example, such an approach causes problems; see below. By trialling a solution of the form $\Phi(r) \propto \ln(r)$, show that the associated density profile takes the form

$$\rho(r) = \frac{\sigma^2}{2\pi G r^2}. \quad (1(a).2)$$

- Show that the total mass of the cluster is infinite (another way of saying that the pdf is not normalizable). Why does this happen, physically? How might we rescue the situation?

Question 1(b)**10 marks**

Consider a two level quantum system, with energies E_1 and E_2 , with transition rates t_{12} and t_{21} .

- Write down the master equation for $p(E,t)$.
- Compute $\langle E \rangle$ in the limit $t \rightarrow \infty$.
- Calculate the autocorrelation function and comment on the *noise*.

Question 2**30 marks**

It is never too soon to plan your superannuation strategy! Some respected economists predict that asset prices will decline steadily in real terms (i.e. after inflation) over the next few decades, as the world's population hits environmental capacity constraints and stabilises for the first time since the Industrial Revolution. At the same time, higher volatility is expected to become the norm in investment markets, as the financial industry grows its share of the economy. In this environment, what should you do to ensure that you maintain access to the essentials — fine wine, say, and adventure holidays — as you live to a ripe old age? Below we show that the answer to this question is *be lucky*.

Let $x(t)$ be a random variable denoting the dollar balance of your retirement fund as a function of time, t , measured in years. Every year, you deposit a fixed sum $\lambda > 0$ into the fund. The fund is invested in a mix of stocks and bonds. It earns *interest* at a fluctuating rate $\alpha + \eta(t)$ per annum, where α is the steady, underlying rate of return (which can be

positive or negative), and $\eta(t)$ is a stochastic variable of Langevin type which obeys stationary Gaussian statistics with $\langle \eta(t) \rangle = 0$, $\langle \eta(t)\eta(t') \rangle = 2D\delta(t-t')$, with $D > 0$.

- (a) Justify the following Langevin equation describing the evolution of $x(t)$:

$$\frac{\partial x(t)}{\partial t} = x(t) [\alpha + \eta(t)] + \lambda$$

- (b) By introducing an integrating factor, or otherwise, explicitly solve Langevin equation to obtain (for a fund starting with zero balance)

$$x(t) = \lambda \exp \left[\int_0^t dt' (\alpha + \eta(t')) \right] \int_0^t dt'' \exp \left[- \int_0^{t''} dt' (\alpha + \eta(t')) \right]. \quad (1)$$

- (c) By Taylor expanding, or otherwise, prove the result

$$\left\langle \exp \left[\int_{t_1}^{t_2} dt' f(t') \eta(t') \right] \right\rangle = \exp \left[D \int_{t_1}^{t_2} dt' f(t')^2 \right] \quad (2)$$

for any deterministic (i.e. non-stochastic) function of time $f(t)$.

- (d) From (1) and (2), show that the mean balance is given by

$$\langle x(t) \rangle = \frac{\lambda}{\alpha + D} \{ \exp [(\alpha + D)t] - 1 \}. \quad (3)$$

Note that the system must self-regulate, such that $\langle x(t) \rangle$ (and hence the total money in the system after inflation) does not diverge in the long term ($t \rightarrow \infty$). This requires $\alpha + D < 0$.

- (e) Let $q(u,t)$ be the probability distribution function of the logarithmic balances $u = \ln(x)$ of an ensemble of retirement funds. Write down the Langevin equation for u and thereby show that the associated Fokker-Planck equation takes the form

$$\frac{\partial q(u,t)}{\partial t} = -\frac{\partial}{\partial u} \{ [\lambda \exp(-u) + \alpha] q(u,t) \} + D \frac{\partial^2 q(u,t)}{\partial u^2}. \quad (4)$$

- (f) Explain why the system self-imposes a reflecting boundary at $x = 0$.

- (g) Use the boundary condition from part (f) to solve for the steady-state distribution

$$q_s(u) = C \exp \left[\frac{\lambda \exp(-u) + \alpha u}{D} \right], \quad (5)$$

where C is a normalization constant¹.

¹You **do not** need to evaluate C . However, the condition $\alpha + D < 0$ from part (d) makes $q_s(u)$ normalizable. The normalization constant takes the value $C = ((D/\lambda)^{\alpha/D})/\Gamma(-\alpha/D)$, where Γ denotes the gamma function.

(h)

- i. Relate $p_s(x)$, the steady-state probability distribution function of x , to $q_s(u)$.
- ii. Sketch $p_s(x)$ and comment on its properties.
- iii. If the system self-regulates to be marginally stable, i.e. $\alpha + D$ adjusts to be slightly negative, what happens to the dispersion, $\text{var}(x)$, as $t \rightarrow \infty$?
- iv. Comment briefly on what all this means in practice for policy makers seeking to design a viable superannuation system.

Question 3

30 marks

The amoebae of the slime mould *Dictyostelium discoideum* aggregate to form patterns when starved of nutrients. They do so by emitting a chemical, called cyclic AMP, which attracts nearby amoebae. The patterns are seen experimentally as light and dark bands under dark-field illumination. Commonly, the patterns begin as spirals (irrespective of the shape of the habitat) and evolve into irregular ‘domains’ (partly determined by the shape of the habitat).

In one idealised model of *Dictyostelium discoideum*, the amoeba number density $n(\mathbf{x}, t)$ and cyclic AMP concentration $c(\mathbf{x}, t)$ evolve according to the coupled reaction-diffusion equations

$$\frac{\partial n}{\partial t} = D\nabla^2 n - \alpha\nabla \cdot (n\nabla c) + srn(N - n), \quad (3.1)$$

$$\frac{\partial c}{\partial t} = \nabla^2 c + \frac{sn}{1+n} - sc. \quad (3.2)$$

Equations (3.1) and (3.2) are written in dimensionless form. The constants D , α , s , r , and N are all positive.

- (a) Carefully explain in words the physical origin of each term (and its sign) on the right-hand sides of (3.1) and (3.2).
- (b) Find the nontrivial uniform equilibrium state (n_0, c_0) .
- (c) Show that (n_0, c_0) is a stable node if diffusion is (artificially) switched off.
- (d) By linearising (3.1) and (3.2) about (n_0, c_0) , show that perturbations proportional to $\exp(i\mathbf{k} \cdot \mathbf{x} + \lambda t)$ satisfy the dispersion relation

$$\lambda^2 + [(D+1)k^2 + s(1+rN)]\lambda + (k^2 + s)(Dk^2 + srN) - \frac{\alpha s N k^2}{(1+N)^2} = 0. \quad (3.3)$$

- (e) Hence argue that the uniform equilibrium state is *unstable in the presence of diffusion* if and only if there exists a wavenumber k for which

$$Dk^4 + \left[srN + sD - \frac{\alpha s N}{(1+N)^2} \right] k^2 + rNs^2 < 0. \quad (3.4)$$

- (f) In the remaining parts of this question, we restrict attention to the special case $\alpha = (2r + DN^{-1})(1 + N)^2$, in order to ease the calculational burden². For this special case, show that the slime mould develops patterns if

$$4D < rN, \quad (3.5)$$

for wavenumbers in the range

$$\left| \frac{2Dk^2}{srN} - 1 \right| < \left(1 - \frac{4D}{rN} \right)^{1/2}. \quad (3.6)$$

- (g) A film of slime mould is grown in a sealed, rectangular Petri dish. The dimensions of the dish are L_x and L_y , measured in units of $(2D/srN)^{1/2}$. Sketch carefully (using light and dark shading) the patterns of slime mould concentration that develop for $4D/rN = 3/4$ and
- i. $(L_x, L_y) = (1, 1)$;
 - ii. $(L_x, L_y) = (1, 3)$;
 - iii. $(L_x, L_y) = (4, 4)$.
- (h) Equations (3.1) and (3.2) can also be used to describe pattern formation on snake skins, if n is taken to be the number density of chromatophores (pigment cell precursors in the embryo) and c is the concentration of chemoattractant. Explain very briefly how you would modify the calculation in part (g) to model snake skin patterns. [Hint. Boundary conditions; geometry.]

² The fine-tuned relation is not satisfied by real slime moulds in general, but it may be satisfied at a particular temperature.