18.354J/3541 – Nonlinear Dynamics : Continuum Systems

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1 Math basics

1.1 Derivatives and differential equations

In this course, we will mostly deal with ordinary differential equations (ODEs) and partial differential equations (PDEs) real-valued scalar or vector fields. Usually, non-bold symbols will be reserved for scalar objects f (e.g., mass density) and bold font $\boldsymbol{f} = (f_1, f_2, \ldots)$ for vector-valued objects, such as time-dependent position vectors $\boldsymbol{x}(t)$ or velocity fields $\boldsymbol{v}(t, \boldsymbol{x}) = (v_1(t, \boldsymbol{x}), v_2(t, \boldsymbol{x}), \ldots)$.

ODEs are equations that contain derivatives of scalar or vector-valued or, more generally, tensor-valued functions $f(x)$ of a single variable x. Depending on context, we will denote derivatives of such functions by

$$\frac{d}{dx} f(x) = f' = f_x \tag{1}$$

For time derivatives, we will often use over-dots

$$\frac{d}{dt} g(t) = \dot{g} = g_t \tag{2}$$

PDEs are equations that contain derivatives of scalar or vector-valued functions $f(\boldsymbol{x}) = f(x_1, x_2, \ldots)$ of more than one variable. Depending on context, we will denote partial derivatives by

$$\frac{\partial f}{\partial x_i} = \partial_{x_i} f = \partial_i f = f_{x_i} = f_{,i} \tag{3}$$

In standard 3D Cartesian coordinates (x_1, x_2, x_3) defined with respect to some global orthonormal frame Σ, spanned by the basis vectors $(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$, the gradient-operator ∇ is defined by

$$\nabla = \partial_x \boldsymbol{e}_1 + \partial_y \boldsymbol{e}_2 + \partial_z \boldsymbol{e}_3 = \sum_{i=1}^{3} \partial_i \boldsymbol{e}_i \equiv \partial_i \boldsymbol{e}_i, \tag{4}$$

where we have introduced the Einstein summation convention on the rhs. Applying ∇ to a scalar function f gives a vector

$$\nabla f = (\partial_i f) \boldsymbol{e}_i = (\partial_1 f, \partial_2 f, \ldots) \tag{5}$$

whereas application of ∇ to a tensorial quantity depends on the choice of the product: For instance, in the case of a 3D vector field $\boldsymbol{v}(t, \boldsymbol{x})$, we can obtain a scalar field called *divergence*

$$\mathrm{div}\boldsymbol{v} = \nabla \cdot \boldsymbol{v} \equiv \partial_i v_i, \tag{6a}$$

another (pseudo-)vector field called *curl*

$$\mathrm{curl}\boldsymbol{v} = \nabla \wedge \boldsymbol{v} \equiv (\epsilon_{ijk} \partial_j v_k) \tag{6b}$$

and the *gradient* matrix

$$\nabla \boldsymbol{v} \equiv (\partial_i v_j) \tag{6c}$$

In particular, we have

$$\mathrm{tr}\nabla \boldsymbol{v} = \partial_i v_i = \mathrm{div}\boldsymbol{v} \tag{6d}$$

The (scalar) Laplacian operator $\triangle$ in Cartesian coordinates is defined by

$$\triangle \equiv \nabla^2 \equiv \sum_i \partial_i \partial_i = \partial_{ii}. \tag{7}$$

Please recall how these operators look in cylindrical and spherical coordinates.

1.2 Linear and nonlinear objects

A mathematical operator - or, more generally, some property – $\mathcal{P}$ defined on vectors or functions f, g, is said to be *linear*, if it satisfies

$$\mathcal{P}(\alpha f + \beta g) = \alpha \mathcal{P}(f) + \beta \mathcal{P}(g) \tag{8}$$

Important examples are derivatives, integrals and expectation values.

A famous linear ODE, is the simple harmonic oscillator equation

$$\ddot{x}(t) = -\omega^2 x(t) \tag{9}$$

which has fundamental sin- and cos-solutions, that can be used to construct more general solutions by superposition.

An important (homogeneous) linear PDE, is Laplace's equation

$$\nabla^2 f(\boldsymbol{x}) = 0. \tag{10}$$

Functions f satisfying this equation are called *harmonic*.

Later on, we will often try to approximate nonlinear PDEs through linear PDEs.

1.3 Linear stability analysis of fixed points for ODEs

Consider a particle moving in one-dimension with velocity $v(t)$, governed by the nonlinear ODE

$$\frac{d}{dt}v(t) = -(\alpha + \beta v^2)v =: f(v). \tag{11}$$

We assume that the parameter β is strictly positive, but allow α to be either positive or negative. The fixed points of Eq. (11) are, by definition, velocity values v_* that satisfy the condition $f(v_*) = 0$; that is, *fixed points are constant solutions.* For $\alpha > 0$, there exists only one fixed point $v_0 = 0$. For $\alpha < 0$, we find the three fixed points $v_0 = 0$ and $v_\pm = \pm\sqrt{-\alpha/\beta}$. This means the system undergoes *pitchfork bifurcation* at the critical parameter value $\alpha = 0$.

To evaluate the stability of a fixed points v_*, we can linearize the nonlinear equation (11) in the vicinity of the fixed points by considering small perturbations

$$v(t) = v_* + \epsilon(t). \tag{12}$$

Inserting this perturbation ansatz into (11) and keeping in mind that $f(v_*) = 0$ for fixed points, we can Taylor-expand the rhs. of (11) and find to leading order

$$f(v_* + \epsilon) \simeq f(v_*) + f'(v_*)\,\epsilon = f'(v_*)\,\epsilon, \tag{13}$$

The growth of the perturbation $\epsilon(t)$ is therefore governed by the linear ODE

$$\frac{d}{dt}\epsilon = f'(v_*)\,\epsilon, \tag{14a}$$

which has the solution

$$\epsilon(t) = \epsilon(0)\,e^{f'(v_*)t}. \tag{14b}$$

If $f'(v_*) > 0$, then the perturbation will grow and the fixed point is said to be linearly unstable, whereas for $f'(v_*) < 0$ the perturbation will decay implying that the fixed point is stable.

For our specific example, we find

$$f'(v_0) = -\alpha\,, \qquad f'(v_\pm) = -(\alpha + 3\beta v_\pm^2) = 2\alpha \tag{15}$$

This means that for $\alpha > 0$, the fixed point $v_0 = 0$ is stable, indicating that the particle will be damped to rest in this case. By contrast, for $\alpha < 0$, the fixed point v_0 becomes unstable and the new fixed points $v_\pm = \pm\sqrt{-\alpha/\beta}$ become stable; that is, for $\alpha < 0$ the particle will be driven to a non-vanishing stationary speed. Equation (11) with $\alpha < 0$ defines one of the simplest models of active particle motion.

1.4 Complex numbers and functions

Although we will mostly deal with real fields in this course, it is sometimes helpful to rewrite equations in terms of complex quantities, especially, when dealing with 2D hydrodynamic problems. Complex numbers are 2D extensions of real numbers,

$$z = x + iy \in \mathbb{C}\,, \qquad i^2 = -1 \tag{16}$$

with real part $\Re z = x \in \mathbb{R}$ and imaginary part $\Im z = y \in \mathbb{R}$. The complex conjugate of a real number is given by

$$\bar{z} = x - iy \tag{17}$$

and corresponds to a reflection at the real axis or, equivalently, at the line $\Im(z) = 0$.

Addition of complex numbers is linear

$$z = z_1 + z_2 = (x_1 + iy_1) + (x_2 + iy_2) = (x_1 + x_2) + i(y_1 + y_2) = x + iy \tag{18}$$

corresponding to the addition of the two 2D vectors (x_1, y_1) and (x_2, y_2). In contrast, complex multiplication mixes real and imaginary parts

$$z = z_1 z_2 = (x_1 + iy_1)(x_2 + iy_2) = (x_1 x_2 - y_1 y_2) + i(x_1 y_2 + y_1 x_2) = x + iy \tag{19}$$

A complex function is a map

$$f : \mathbb{C} \to \mathbb{C} , \qquad f(z) = u(x, y) + iv(x, y) \tag{20}$$

that can be interpreted as a map from $\mathbb{R}^2 \to \mathbb{R}^2$. We therefore sometimes also use the vector notation

$$f(z) = (u(x, y), v(x, y)) \tag{21}$$

A function f is said to be complex differentiable (or *analytic* or *holomorphic*) if it satisfies the Cauchy-Riemann equations

$$\partial_x u = \partial_y v , \qquad \partial_y u = -\partial_x v \tag{22a}$$

By differentiating again, we find

$$\partial_x^2 u = \partial_x \partial_y v = -\partial_y^2 u = 0 \qquad \Leftrightarrow \qquad (\partial_x^2 + \partial_y^2)u = 0 \tag{22b}$$

$$\partial_y^2 v = \partial_y \partial_x u = -\partial_x^2 v = 0 \qquad \Leftrightarrow \qquad (\partial_x^2 + \partial_y^2)v = 0 \tag{22c}$$

This means that analytic functions $f = (u, v)$ are harmonic, satisfying Laplace's equation

$$\nabla^2 f = 0 \tag{22d}$$

An analytic function that we will frequently encounter is the exponential function

$$\exp(z) = \sum_{k=0}^{\infty} \frac{z^n}{k!} = 1 + \frac{z}{1!} + \frac{z}{2!} + \dots \tag{23}$$

Euler's formula

$$e^{i\phi} = \cos\phi + i \sin\phi , \qquad \phi \in \mathbb{R} \tag{24}$$

relates exp to the trigonometric sin-and cos-functions.

When dealing with axisymmetric problems it is often advantageous to use the polar representation of a complex number

$$z = re^{i\phi} , \qquad r = |z| = \sqrt{z\bar{z}} \in \mathbb{R}_0^+ , \qquad \phi = \arctan 2(y, x) \in [0, 2\pi) \tag{25}$$

From the properties of the exp-function, it follows that the multiplication of complex numbers

$$z = z_1 z_2 = r_1 e^{i\phi_1} r_2 e^{i\phi_2} = r_1 r_2 e^{i(\phi_1 + \phi_2)} \tag{26}$$

corresponds to a combined rotation and dilatation.

1.5 Fourier transforms

A main advantage of Fourier transformations is that they translate linear (ordinary and partial) differential equations into simpler algebraic equations.

The Fourier transform of a function $f(t)$ is defined by

$$\hat{f}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt\, e^{-i\omega t}\, f(t), \tag{27a}$$

its the inverse is given by

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega\, e^{i\omega t}\, \hat{f}(\omega) \tag{27b}$$

In particular, for the Dirac delta-function $\delta(t)$

$$\hat{\delta}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt\, e^{-i\omega t}\, \delta(t) = \frac{1}{\sqrt{2\pi}}, \tag{28a}$$

yielding the useful Fourier representation

$$\delta(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega\, e^{i\omega t} \tag{28b}$$

These definitions and properties extend directly to higher dimensions.

Example Consider a Gaussian distribution centered about the point $x = 0$ with standard deviation σ,

$$n(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}}. \tag{29}$$

Note that in the limit where $\sigma \to 0$, this distribution corresponds to the Dirac delta-function $\delta(x)$, a function which is localized at zero.

The Fourier transform of the above distribution is

$$\hat{n}(k) = \frac{1}{\sqrt{2\pi\sigma^2}} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{-ikx - \frac{x^2}{2\sigma^2}} = \frac{1}{2\pi\sigma} \int_{-\infty}^{\infty} dx\, e^{-\left(\frac{x^2}{2\sigma^2} + ikx\right)} \tag{30}$$

Completing the square for the exponent

$$\frac{x^2}{2\sigma^2} + ikx = \frac{1}{2\sigma^2} \left(x^2 + 2\sigma^2 ikx\right) = \frac{1}{2\sigma^2} \left[\left(x + ik\sigma^2\right)^2 + k^2\sigma^4\right] \tag{31}$$

enables (30) to be rewritten as

$$\hat{n}(k) = \frac{e^{-\frac{k^2\sigma^2}{2}}}{2\pi\sigma} \int_{-\infty}^{\infty} dx\, e^{-\frac{(x+ik\sigma^2)^2}{2\sigma^2}} \tag{32}$$

To calculate the above integral, which involves a complex integrand, we use the Cauchy integral formula. It states that for a complex function $f(z) \in \mathbb{C}, z \in \mathbb{C}$, integration along a closed path in the complex plane is zero, provided that $f(z)$ has no poles inside the path:

$$\oint dz\, f(z) = 0 \tag{33}$$

Introducing the substitution $z = x + ik\sigma^2$, $dz = dx$, the integral (32) can be rewritten as

$$\hat{n}(k) = \frac{e^{-\frac{k^2\sigma^2}{2}}}{2\pi\sigma} \lim_{R\to\infty} \int_{-R+ik\sigma^2}^{R+ik\sigma^2} dz\, e^{-\frac{z^2}{2\sigma^2}} \tag{34}$$

Let's keep R finite for the moment. We can then think of the integral as one segment of a closed curve with rectangular shape:

$$\begin{aligned} 0 &= \oint dz\, e^{-\frac{z^2}{2\sigma^2}} \\ &= \int_{-R+ik\sigma^2}^{R+ik\sigma^2} dz\, e^{-\frac{z^2}{2\sigma^2}} + \int_{R+ik\sigma^2}^{R} dz\, e^{-\frac{z^2}{2\sigma^2}} + \int_{R}^{-R} dz\, e^{-\frac{z^2}{2\sigma^2}} + \int_{-R}^{-R+ik\sigma^2} dz\, e^{-\frac{z^2}{2\sigma^2}} \end{aligned} \tag{35}$$

In the limit $R \to \infty$, the second as well as the last integral vanish due to the exponential damping with large R, leading to

$$\lim_{R\to\infty} \int_{-R+ik\sigma^2}^{R+ik\sigma^2} dz\, e^{-\frac{z^2}{2\sigma^2}} = \lim_{R\to\infty} \int_{-R}^{R} dz\, e^{-\frac{z^2}{2\sigma^2}} \tag{36}$$

Inserting this into Eq. (34), we obtain

$$\hat{n}(k) = \frac{e^{-\frac{k^2\sigma^2}{2}}}{2\pi\sigma} \int_{-\infty}^{\infty} dx\, e^{-\frac{x^2}{2\sigma^2}} \tag{37}$$

This means that we can basically drop the imaginary part in the original integral, Eq. (32).

From 18.01 we know that

$$\int_{-\infty}^{\infty} dx\, e^{-x^2} = \sqrt{\pi},$$

so by making a change of variable $y = x/\sqrt{2\sigma^2}$ we have that

$$\hat{n}(k) = \frac{1}{\sqrt{2\pi}} e^{-\frac{k^2\sigma^2}{2}}. \tag{38}$$

This result is worth keeping in mind: *The Fourier transform of a Gaussian is a Gaussian.*

2 Dimensional analysis

Before moving on to more 'sophisticated things', let us think a little about dimensional analysis and scaling. On the one hand these are trivial, and on the other they give a simple method for getting answers to problems that might otherwise be intractable. The idea behind dimensional analysis is very simple:

Any physical law must be expressible in any system of units that you use.

There are two consequences of this:

- One can often guess the answer just by thinking about what the dimensions of the answer should be, and then expressing the answer in terms of quantities that are known to have those dimensions[1].
- The scientifically interesting results are *always* expressible in terms of quantities that are *dimensionless*, not depending on the system of units that you are using.

One example of a dimensionless number relevant for fluid dynamics that we have already encountered in the introductory class is the *Reynolds number*, which quantifies the relative strength of viscous and inertial forces. Another example of dimensional analysis that we will study in detail is the solution to the diffusion equation for the spreading of a point source. The only relevant physical parameter is the diffusion constant D, which has dimensions of L^2/T. We denote this by writing

$$[D] = \frac{L^2}{T}$$

Therefore the characteristic scale over which the solution varies after time t must be $\sqrt{Dt}$. This might seem like a rather simple result, but it expresses the essence of solutions to the diffusion equation. Of course, we will be able to solve the diffusion equation exactly, so this argument wasn't really necessary. In practice, however, we will rarely find useful exact solutions to the Navier-Stokes equations, and so dimensional analysis will often give us insight before diving into the mathematics or numerical simulations. Before formalizing our approach, let us consider a few examples where simple dimensional arguments intuitively lead to interesting results.

2.1 The pendulum

This is a trivial problem that you know quite well. Consider a pendulum with length L and mass m, hanging in a gravitational field of strength g. What is the period of the pendulum? We need a way to construct a quantity with units of time involving these numbers. The only possible way to do this is with the combination $\sqrt{L/g}$. Therefore, we know immediately that

$$\tau = c\sqrt{L/g}. \tag{39}$$

This result might seem trivial to you, as you will probably remember (e.g., from a previous course) that $c = 2\pi$, if one solves the full dynamical problem for for small amplitude oscillations. However, the above formula works even for large amplitude oscillations.

[1] Be careful to distinguish between *dimensions* and *units*. For example mass (M), length (L) and time (T) are dimensions, and each of them can be measured in different units (e. g. length may be in feet or meters)

2.2 Pythagorean theorem

Now we try to prove the Pythagorean theorem by dimensional analysis. Suppose you are given a right triangle, with hypotenuse length L and smallest acute angle ϕ. The area of the triangle is clearly

$$A = A(L, \phi). \tag{40}$$

Since ϕ is dimensionless, it must be that

$$A = L^2 f(\phi), \tag{41}$$

where f is some function we don't know.

Now the triangle can be divided into two little right triangles by dropping a line from the right angle which is perpendicular to the hypotenuse. The two right triangles have hypotenuses that happen to be the other two sides of our original right triangle, let's call them a and b. So we know that the areas of the two smaller triangles are $a^2 f(\phi)$ and $b^2 f(\phi)$ (where elementary geometry shows that the acute angle ϕ is the same for the two little triangles as the big triangle). Moreover, since these are all right triangles, the function f is the same for each. Therefore, since the area of the big triangle is just the sum of the areas of the little ones, we have

$$L^2 f = a^2 f + b^2 f,$$

or

$$L^2 = a^2 + b^2. \tag{42}$$

2.3 The gravitational oscillation of a star

It is known that the sun, and many other stars undergo some mode of oscillation. The question we might ask is how does the frequency of oscillation ω depend on the properties of that star? The first step is to identify the physically relevant variables. These are the density ρ, the radius R and the gravitational constant G (as the oscillations are due to gravitational forces). So we have

$$\omega = \omega(\rho, R, G). \tag{43}$$

The dimensions of the variables are $[\omega] = T^{-1}$, $[\rho] = ML^{-3}$, $[R] = L$ and $[G] = M^{-1}L^3T^{-2}$. The only way we can combine these to give as a quantity with the dimensions of time, is through the relation

$$\omega = c\sqrt{G\rho}. \tag{44}$$

Thus, we see that the frequency of oscillation is proportional to the square root of the density and independent of the radius. The determination of c requires a real stellar observation, but we have already determined a lot of interesting details from dimensional analysis alone. For the sun, $\rho = 1.4 \times 10^3 \mathrm{kg/m}^3$, giving $\omega \sim 3 \times 10^{-4} \mathrm{s}^{-1}$. The period of oscillation is approximately 1 hour, which is reasonable. However, for a neutron star ($\rho = 7 \times 10^{11} \mathrm{kgm}^{-3}$) we predict $\omega \sim 7000 \mathrm{s}^{-1}$, corresponding to a period in the milli-second range.

2.4 The oscillation of a droplet

What happens if instead of considering a large body of fluid, such as a star, we consider a smaller body of fluid, such as a raindrop. Well, in this case we argue that surface tension γ provides the relevant restoring force and we can neglect gravity. γ has dimensions of energy/area, so that $[\gamma] = MT^{-2}$. The only quantity we can now make with the dimensions of T^{-1} using our physical variables is

$$\omega = c\sqrt{\frac{\gamma}{\rho R^3}}, \tag{45}$$

which is not independent of the radius. For water $\gamma = 0.07\text{Nm}^{-1}$ giving us a characteristic frequency of 3Hz for a raindrop.

One final question we might ask ourselves before moving on is how big does the droplet have to be for gravity to have an effect? We reason that the crossover will occur when the two models give the same frequency of oscillation. Thus, when

$$\sqrt{\rho G} = \sqrt{\frac{\gamma}{\rho R^3}} \tag{46}$$

we find that

$$R_c \sim \left(\frac{\gamma}{\rho^2 G}\right)^{\frac{1}{3}} \tag{47}$$

This gives a crossover radius of about 10m for water.

2.5 Water waves

This is a subject we will deal with in greater detail towards the end of the course, but for now we look to obtain a basic understanding of the motion of waves on the surface of water. For example, how does the frequency of the wave depend on the wavelength λ? This is called the *dispersion relation*.

If the wavelength is long, we expect gravity to provide the restoring force, and the relevant physical variables in determining the frequency would appear to be the mass density ρ, the gravitational acceleration g and the wave number $k = 2\pi/\lambda$. The dimensions of these quantities are $[\rho] = ML^{-3}$, $[g] = LT^{-2}$ and $[k] = L^{-1}$. We can construct a quantity with the dimensions of T^{-1} through the relation

$$\omega = c\sqrt{gk}. \tag{48}$$

We see that the frequency of water waves is proportional to the square root of the wavenumber, in contrast to light waves for which the frequency is proportional to the wavenumber.

As with a droplet, we might worry about the effects of surface tension when the wavelength gets small. In this case we replace g with γ in our list of physically relevant variables. Given that $[\gamma] = MT^{-2}$, the dispersion relation must be of the form

$$\omega = c\sqrt{\gamma k^3/\rho}, \tag{49}$$

which is very different to that for gravity waves. If we look for a crossover, we find that the frequencies of *gravity waves* and *capillary waves* are equal when

$$k \sim \sqrt{\rho g/\gamma}. \tag{50}$$

This gives a wavelength of 1cm for water waves.

3 Dimensionless groups

A formal justification of the dimensional analysis approach in the previous section comes from Buckingham's Pi Theorem. Consider a physical problem in which the dependent parameter is a function of $n-1$ independent parameters, so that we may express the relationship among the variables in functional form as

$$q_1 = g(q_2, q_3, ..., q_n), \tag{51a}$$

where q_1 is the dependent parameter, and $q_2, ..., q_n$ are the $n-1$ independent parameters. Mathematically, we can rewrite the functional relationship in the equivalent form

$$0 = f(q_1, q_2, ..., q_n). \tag{51b}$$

where $f = q_1 - g(q_2, q_3, ..., q_n)$. For example, for the period of a pendulum we wrote $\tau = \tau(l, g, m)$, but we could just as well have written $f(\tau, l, g, m) = 0$. The Buckingham Pi theorem states that given a relation of the form (51), the n parameters may be grouped into $n-d$ *independent dimensionless* ratios, or dimensionless groups Π_i, expressible in functional form by

$$\Pi_1 = G(\Pi_2, \Pi_3, ..., \Pi_{n-d}), \tag{52a}$$

or, equivalently,

$$0 = F(\Pi_1, \Pi_2, ..., \Pi_{n-d}), \tag{52b}$$

where d is the number of independent dimensions (mass, length, time...). The formal proof can be found in the book *Scaling, Self Similarity and Intermediate Asymptotics* by Barenblatt. The Pi theorem does not predict the functional form of F or G, and this must be determined experimentally. The $n-d$ dimensionless groups Π_i are independent. A dimensionless group Π_i is *not* independent if it can be formed from a product or quotient of other dimensionless groups in the problem.

3.1 The pendulum

To develop an understanding of how to use Buckingham's Pi theorem, let's first apply it to the problem of a swinging pendulum, which we considered in the previous lecture. We argued that the period of the pendulum τ depends on the length l and gravity g. It cannot depend on the mass m since we cannot form a dimensionless parameter including m in our list of physical variables. Thus

$$\tau = \tau(l, g), \tag{53a}$$

or alternatively

$$0 = f(\tau, l, g). \tag{53b}$$

We have $n = 3$ and $d = 2$, so the problem has one dimensionless group

$$\Pi_1 = \tau l^\alpha g^\beta. \tag{54}$$

The relevant dimensions are $[\tau] = T, [l] = L, [g] = LT^{-2}$, so for Π_1 to be dimensionless equate the exponents of the dimension to find

$$\begin{aligned} 1 - 2\beta &= 0, \\ \alpha + \beta &= 0, \end{aligned}$$

which are satisfied if $\alpha = -\frac{1}{2}$ and $\beta = \frac{1}{2}$. Thus

$$\Pi_1 = \tau\sqrt{g/l}. \tag{55}$$

We thus see Π_1 is just the constant of proportionality c from above. Thus we have

$$c = \tau\sqrt{g/l} \tag{56}$$

where c is a constant to be determined from an experiment.

3.2 Taylor's blast

This is a famous example, of some historical and fluid mechanical importance. The story goes something like this. In the early 1940's there appeared a picture of an atomic blast on the cover of Life magazine. GI Taylor, a fluid mechanician at Cambridge, wondered what the energy of the blast was. When he called his colleagues at Los Alamos and asked, they informed him that it was classified information, so he resorted to dimensional analysis. In a nuclear explosion there is an essentially instantaneous release of energy E in a small region of space. This produces a spherical shock wave, with the pressure inside the shock wave several thousands of times greater than the initial air pressure, that can be neglected. How does the radius R of this shock wave grow with time t? The relevant parameters are E, the density of air ρ and time t. Thus

$$R = R(E, \rho, t) \tag{57a}$$

or

$$0 = f(R, E, \rho, t). \tag{57b}$$

The dimensions of the physical variables are $[E] = ML^2T^{-2}, [t] = T, [R] = L$ and $[\rho] = ML^{-3}$. We have $n = 4$ physical variables and $d = 3$ dimensions, so the Pi theorem tells us there is one dimensionless group, Π_1. To form a dimensionless combination of parameters we assume

$$\Pi_1 = Et^\alpha \rho^\beta R^\gamma \tag{58}$$

and equating the exponents of dimensions in the problem requires that

$$\begin{aligned} 1 + \beta &= 0, \\ \alpha - 2 &= 0, \\ 2 - 3\beta + \gamma &= 0. \end{aligned}$$

It follows that $\alpha = 2, \beta = -1$ and $\gamma = -5$, giving

$$\Pi_1 = \frac{Et^2}{\rho R^5}. \tag{59}$$

Assuming that Π_1 is constant gives

$$R = c\left(\frac{E}{\rho}\right)^{\frac{1}{5}} t^{\frac{2}{5}}. \tag{60}$$

The relation shows that if one measures the radius of the shock wave at various instants in time, the slope of the line on a log-log plot should be 2/5. The intercept of the graph would provide information about the energy E released in the explosion, if the constant c could be determined. Since information about the development of blast with time was provided by the sequence of photos on the cover of Life magazine, Taylor was able to determine the energy of the blast to be 10^{14} Joules (he estimated c to be about 1 by solving a model shock-wave problem), causing much embarrassment.

3.3 The drag on a sphere

Now what happens if you have two dimensionless groups in a problem? Let's consider the problem of the drag on a sphere. We reason that the drag force on a sphere D will depend on the relative velocity, U, the sphere radius, R, the fluid density ρ and the fluid viscosity μ, which has dimensions $M/(LT)$. Thus

$$D = D(U, R, \rho, \mu) \tag{61a}$$

or

$$0 = f(D, U, R, \rho, \mu). \tag{61b}$$

Since the physical variables are all expressible in terms of dimensions M, L and T, we have $n = 5$ and $d = 3$, so there are two dimensionless groups. There is now a certain amount of arbitrariness in determining these, however we look for combinations that make some physical sense. For our first dimensionless group, we choose the Reynolds number

$$\Pi_1 = \frac{\rho U R}{\mu}, \tag{62}$$

as we know that it arises naturally when you nondimensionalize the Navier-Stokes equations. For the second we choose the combination

$$\Pi_2 = D\rho^\alpha U^\beta R^\gamma, \tag{63}$$

which, if we replaced D with μ, would just give the Reynolds number. Equating the exponents of mass length and time gives, $\alpha = -1$, $\beta = -2$ and $\gamma = -2$. Thus

$$\Pi_2 = \frac{D}{\rho U^2 R^2}, \tag{64}$$

and this is called the dimensionless drag force. Buckingham's Pi theorem tells us that we must have the functional relationship

$$\Pi_2 = G(\Pi_1) \tag{65}$$

or alternatively

$$\frac{D}{\rho U^2 R^2} = G(\mathrm{Re}). \tag{66}$$

The functional dependence is determined by experiments. It is found that at high Reynolds numbers $G(\mathrm{Re}) = 1$, so that

$$D = \rho U^2 R^2. \tag{67}$$

This is known as *form drag*, in which resistance to motion is created by inertial forces on the sphere. At low Reynolds numbers $G(\mathrm{Re}) \propto 1/\mathrm{Re}$ so that

$$D \propto \mu U R. \tag{68}$$

This is *Stokes drag*, caused by the viscosity of the fluid.

The power of taking this approach can now be seen. Without dimensional analysis, to determine the functional dependence of the drag on the relevant physical variables would have required four sets of experiments to determine the functional dependence of D on velocity, radius, viscosity and density. Now we need only perform one set of experiments using our dimensionless parameters and we have all the information we need.

4 Hamiltonian dynamics and Liouville equation

Why do we study applied mathematics? Aside from the intellectual challenge, it is reasonable to argue that we do so to obtain an understanding of physical phenomena, and to be able to make predictions about them. Possibly the greatest example of this, and the origin of much of the mathematics we do, came from Newton's desire to understand the motion of the planets, which led to him formulate his *Newtonian dynamics*. Over the last two centuries, Newton's ODE-based approach has been generalized and reformulated to describe many classical mechanical (and other) systems. A particularly economical and fruitful reformulation is *Hamiltonian dynamics*, which played an essential role in paving the way for Schrödinger's theory of quantum mechanics.

In this section, we will briefly review Hamiltonian dynamics, and then use it as starting point to the derive the *Liouville equation*, which provides a linear PDE-based description of a nonlinear mechanical systems. The Liouville equation and its relatives shall become important later in class, when we will derive hydrodynamic equations for many-particle systems.

We first demonstrate the main ideas and concepts for a basic example, the harmonic oscillator; the generalization to more complex systems will then be straightforward.

4.1 Harmonic oscillator revisited

Newton's equation of motion for a one-dimensional harmonic oscillator (mass m, spring constant k) reads

$$m\ddot{X} = -kX, \tag{69}$$

where $X(t)$ is the oscillator position at time t. Defining the oscillator frequency

$$\omega = \sqrt{\frac{k}{m}} \tag{70}$$

we can rewrite (69) as

$$\ddot{X} = -\omega^2 X \tag{71a}$$

The solution to this linear second-order ODE with initial conditions

$$X(0) = x_0 \;, \qquad \dot{X}(0) = v_0 \tag{71b}$$

is given by

$$X(t; x_0, v_0) = x_0 \cos(\omega t) + \frac{v_0}{\omega} \sin(\omega t). \tag{72}$$

Hamiltonian formulation. An equivalent description of this system can be given within Hamiltonian dynamics. There one starts from the Hamiltonian

$$H(P, X) = T(P) + U(X) = \frac{P^2}{2m} + \frac{kX^2}{2} \tag{73a}$$

and the associated Hamilton equations of motion

$$\dot{X} = \frac{\partial H}{\partial P} \;, \qquad \dot{P} = \frac{\partial H}{\partial X} \tag{73b}$$

The pair (X, P) is called *phase space coordinates*, whereas X alone is often referred to as *comfiguration space coordinate*. In the case of the oscillator, the first-order ODE system for (X, P) is explicitly given by

$$\dot{X} = \frac{P}{m} \;, \qquad \dot{P} = -kX \tag{74}$$

which is of course equivalent to (69). The solution to this ODE system with initial conditions $X(0) = x_0$ and $P(0) = p_0$ is given by

$$\begin{aligned} X(t; x_0, p_0) &= x_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t) && \text{(75a)} \\ P(t; x_0, p_0) &= -m x_0 \omega \sin(\omega t) + p_0 \cos(\omega t) && \text{(75b)} \end{aligned}$$

The time-dependent vector $(X(t; x_0, p_0), P(t; x_0, p_0))$ describes a curve in phase space, called the *trajectory* of the system.

Energy conservation. The Hamiltonian H has a natural interpretation as the *energy* of the oscillator. Indeed it is conserved in time as can be seen by computing its total time derivative

$$\begin{aligned} \frac{dH}{dt} &= \frac{\partial H}{\partial P}\dot{P} + \frac{\partial H}{\partial X}\dot{X} \\ &= \frac{\partial H}{\partial P}\left(-\frac{\partial H}{\partial X}\right) + \frac{\partial H}{\partial X}\left(\frac{\partial H}{\partial P}\right) \equiv 0 \end{aligned} \tag{76}$$

That is, the energy value of the Hamiltonian is given by the initial condition

$$H(P,X) = H(p_0,x_0) = \frac{p_0^2}{2m} + \frac{kx_0^2}{2}. \tag{77}$$

So far, we have focussed on a particle-based description of the harmonic oscillator in terms of an ODE system; we now transition to a PDE-based description.

Phase space distribution. Each particle trajectory $(X(t;x_0,p_0), P(t;x_0,p_0))$ defines a fine-grained probability density function[2] (PDF)

$$\rho(t,x,p|x_0,p_0) = \delta\big(x - X(t;x_0,p_0)\big)\,\delta\big(p - P(t;x_0,p_0)\big) \tag{78}$$

This is a family of delta-distributions localized along the trajectory. Given an ensemble of initial conditions, described by another PDF $f_0(x_0,p_0)$, we can define the associated 'smeared-out' phase space PDF by integrating over the initial conditions

$$f(t,x,p) = \int dx_0 dp_0\; f_0(x_0,p_0)\,\rho(t,x,p|x_0,p_0) \tag{79a}$$

In particular, we then have

$$f(0,x,p) = f_0(x,p) \tag{79b}$$

Liouville equation. The Liouville equation is the PDE that describes the time-evolution of the phase space PDF $f(t,x,p)$. To derive this PDE, let's differentiate ρ using the Hamilton equations of motion

$$\begin{aligned}\partial_t\rho = \partial_t\left[\delta\big(x - X(t;x_0,p_0)\big)\,\delta\big(p - P(t;x_0,p_0)\big)\right] &= -\dot{X}\partial_x\rho - \dot{P}\partial_p\rho \\ &= -[\partial_p H(x,p)]\,\partial_x\rho + [\partial_x H(x,p)]\partial_p\rho\end{aligned}$$

This equation is linear in $\rho(t,x,p|x_0,p_0)$, so it also holds for $f(t,x,p)$. We thus have the Liouville equation

$$\partial_t f = [-(\partial_p H)\,\partial_x + (\partial_x H)\,\partial_p]\,f \equiv \mathcal{L}f \tag{80}$$

where the expression in square brackets defines the Liouville operator, which for the harmonic oscillator takes the explicit form

$$\mathcal{L} = -\frac{p}{m}\,\partial_x + kx\,\partial_p \tag{81}$$

Before we discuss solutions, let's emphasize an important conceptual point. In deriving the linear Liouville equation (80), we did not need to make specific assumptions about the Hamiltonian, except that it doesn't explicitly depend on time. i.e. does not contain time-varying parameters other than X and P. This means that the *Liouville equation will be linear even if the Hamiltonian particle dynamics is nonlinear.* As we will see soon, this remains true for higher dimensional problems.

[2] A PDF is a function that is non-negative everywhere and integrates to 1.

Stationary solutions. Although the Liouville equation (80) is linear, it is often difficult to construct exact time-dependent solutions. It is, however, easy to find stationary solutions $f_s(x,p)$, which by definition satisfy the time-independent Liouville equation

$$0 \;=\; [-(\partial_p H)\,\partial_x + (\partial_x H)\,\partial_p]\, f_s \tag{82}$$

In other words, stationary solutions $f_s(x,p)$ are eigenfunctions of the Liouville operator $\mathcal{L}$ with eigenvalues 0. Indeed, every non-negative function $f_s(x,p) = g(H)$ will do the job, since by chain rule

$$[-(\partial_p H)\,\partial_x + (\partial_x H)\,\partial_p]\, g(H) \;=\; [-(\partial_p H)\,(\partial_x H) + (\partial_x H)\,(\partial_p H)]\, g'(H) \;\equiv\; 0 \tag{83}$$

Particularly important stationary solutions are the microcanonical distribution at constant energy E,

$$g_E(H) = \frac{\delta(H-E)}{\omega(E)} \tag{84a}$$

and the canonical distribution at constant temperature T,

$$g_T(H) = \frac{e^{-E/(k_B T)}}{Z(T)}, \tag{84b}$$

where $\omega(E)$ and $Z(T)$ are normalization constants, and $k_B = 1.38 \times 10^{-23}\,\mathrm{J/K}$ is the Boltzmann constant.

4.2 Hamiltonian dynamics of many-body systems

In the remainder of this course, we will be interested in classical (non-quantum) systems that consist of $N \gg 1$ particles. The complete microscopic dynamics of such systems is encoded in their Hamiltonian

$$H = \sum_{n=1}^{N} \frac{\boldsymbol{p}_n^2}{2m_n} + U(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N), \tag{85a}$$

where m_n, $\boldsymbol{p}_n(t)$ and $\boldsymbol{x}_n(t)$ denote the mass, momentum and position of the nth particle. As in the oscillator example, the first contribution on the rhs. of Eq. (85a) is the kinetic energy, and U is the potential energy. For our purposes, it is sufficient to assume that we can decompose (85a) into a sum of pair interactions

$$U(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) = \frac{1}{2} \sum_{n,k:n\neq k} \Phi(\boldsymbol{x}_n, \boldsymbol{x}_k). \tag{85b}$$

Given H, Newton's equations can be compactly rewritten as

$$\dot{\boldsymbol{x}}_n = \nabla_{\boldsymbol{p}_n} H\,, \qquad \dot{\boldsymbol{p}}_n = -\nabla_{\boldsymbol{x}_n} H \tag{86}$$

That this higher-dimensional Hamiltonian dynamics is equivalent to Newton's laws of motion can be seen by direct insertion, which yields

$$\dot{\boldsymbol{x}}_n = \frac{\boldsymbol{p}_n}{m_n}\,, \qquad\qquad \dot{\boldsymbol{p}}_n = m_n \ddot{\boldsymbol{x}}_n = -\nabla_{\boldsymbol{x}_n} U \tag{87}$$

An important fact is that many physical systems obey certain conservation laws (to very good approximation). For instance, the Hamiltonian (85a) itself remains conserved under the time-evolution (86)

$$\begin{aligned}\frac{d}{dt}H &= \sum_n \left[(\nabla_{\boldsymbol{p}_n} H)\cdot\dot{\boldsymbol{p}}_n + (\nabla_{\boldsymbol{x}_n} H)\cdot\dot{\boldsymbol{x}}_n\right] \\ &= \sum_n \left[(\nabla_{\boldsymbol{p}_n} H)\cdot(-\nabla_{\boldsymbol{x}_n} H) + (\nabla_{\boldsymbol{x}_n} H)\cdot\nabla_{\boldsymbol{p}_n} H\right] \equiv 0 \end{aligned} \tag{88}$$

which is just the statement of energy conservation. Other important examples of conserved quantities are total linear momentum and angular momentum,

$$\boldsymbol{P} = \sum_n \boldsymbol{p}_n \ , \qquad \boldsymbol{L} = \sum_n \boldsymbol{x}_n \wedge \boldsymbol{p}_n \tag{89}$$

if the pair potentials Φ only depend on the distance between particles.

There exists a deep mathematical connection between such invariants and symmetries of the underlying Hamiltonian, known as Noether's theorem. For example, energy conservation is a consequence of the fact that the Hamiltonian (85a) is not explicitly time-dependent and, hence, invariant under time translations. Similarly, conservation of linear momentum is linked to spatial translation invariance and conservation of angular momentum to rotational invariance.

For the remainder of this course, it will be important to keep in mind that *microscopic symmetries and conservation laws must be preserved in coarse-grained macroscopic continuum descriptions.*

Writing $(x_\alpha, p_\beta) = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N, \boldsymbol{p}_1, \ldots, \boldsymbol{p}_N)$ and using Einstein's summation convention, the Liouville equation for the N-particle phase space density $f(t, x_\alpha, p_\beta)$ takes the form

$$\partial_t f = \left[-(\partial_{p_\alpha} H)\,\partial_{x_\alpha} + (\partial_{x_\beta} H)\,\partial_{p_\beta}\right] f, \tag{90}$$

with functions $f_s = g(H)$ being stationary solutions.

4.3 Practical limitations

The critical number of ODEs for complicated ('chaotic') things to happen is typically three, and yet any relevant problem in the world contains many more than three degrees of freedom. Indeed a physical problem typically contains 10^{23} interacting particles (Avogadro's number), which is so great a number that it is unclear if the mathematical techniques described above are of any use. The central aim of this course is to make theoretical progress towards understanding systems with many degrees of freedom. To do so we shall invoke the "continuum hypothesis", imagining that the discrete variable (e.g. the velocity of a particular molecule of fluid) can be replaced with a continuum (e.g. the velocity field $\boldsymbol{v}(\boldsymbol{x}, t)$). There are many subtleties that arise in trying to implement this idea, among them;

(i) How does one write down macroscopic descriptions in a systematic way? It would be terrible to have to solve 10^{23} coupled differential equations!

(ii) Forces and effects that *a priori* appear to be small are not always negligible. This turns out to be of fundamental importance, but was not recognised universally until the 1920's.

(iii) The mathematics of how to solve 'macroscopic equations', which are nonlinear partial differential equations, is non-trivial. We will need to introduce many new ideas.

In tackling these problems we will spend some time doing fluid mechanics, the reason being that it is by far the most developed field for the study of these questions. Experiments are readily available and the equations of motion are very well known (and not really debated!). Furthermore, fluid dynamics is an important subject in its own right, being relevant to many different scientific disciplines (e.g. aerospace engineering, meteorology, coffee cups). We will also introduce other examples (e.g. elasticity) to show the generality of the ideas.

5 Random walkers and diffusion

The most important (and obvious) problem when introducing the continuum hypothesis is to figure out how to treat Avogadro's number of particles obeying Schrödinger's equation or Newton's laws. This a little ambitious for us to start with, so we begin by trying to understand how the simplest microscopic model for the motion of particles can lead to macroscopic laws. We will see that the simplest model, that of a randomly moving particle, leads to a nice derivation of the diffusion equation, whose properties will be investigated in the next lecture.

Consider the motion of particles along one axis. The particles start at time $t = 0$ at position $x = 0$ and execute a random walk according to the following rules:

(i) Each particle steps to the right or the left once every τ seconds, moving a distance $dx_i = \pm\delta$.

(ii) The probability of going to the right at each step is $1/2$, and the probability of going to the left is $1/2$, independently of the previous history.

(iii) Each particle moves independently of all the other particles, i.e. the particles do not interact with one another.

There are two striking consequences of these rules. Let N be the total number of particles and $x_i(n)$ be the position of the ith particle after n steps, and denote the average position of all particles by

$$X(n) = \frac{1}{N}\sum_{i=1}^{N} x_i(n). \tag{91}$$

The mean displacement of the particles after n steps is

$$\begin{aligned}
\langle X(n)\rangle &= \frac{1}{N}\sum_{i=1}^{N}\langle x_i(n)\rangle \\
&= \frac{1}{N}\sum_{i=1}^{N}\left[\langle x_i(n-1)\rangle + \langle dx_i\rangle\right] \\
&= \frac{1}{N}\sum_{i=1}^{N}\left[\langle x_i(n-1)\rangle + \delta\cdot\frac{1}{2} + (-\delta)\cdot\frac{1}{2}\right] \\
&= \frac{1}{N}\sum_{i=1}^{N}\langle x_i(n-1)\rangle \\
&= \langle X(n-1)\rangle. \qquad (92)
\end{aligned}$$

Thus particles go nowhere on average.

Secondly, assuming that the all particles start at $x_i(0) = 0$, the root-mean-square displacement of the particles, which is a good measure of spreading, is obtained as follows:

$$\begin{aligned}
\langle [X(n) - X(0)]^2\rangle &= \langle X(n)^2\rangle \\
&= \left\langle \left[\frac{1}{N}\sum_{i=1}^{N} x_i(n)\right]\left[\frac{1}{N}\sum_{k=1}^{N} x_k(n)\right]\right\rangle \\
&= \frac{1}{N^2}\sum_{i=1}^{N}\sum_{k=1}^{N}\langle x_i(n)x_k(n)\rangle \\
&= \frac{1}{N^2}\sum_{i=1}^{N}\langle x_i(n)^2\rangle, \qquad (93)
\end{aligned}$$

where we have used that, by virtue of assumption (iii),

$$\langle x_i(n)x_k(n)\rangle = \langle x_i(n)\rangle\langle x_k(n)\rangle = 0 \qquad \text{for } i \neq k.$$

The mean-square displacement per particle can be calculated from

$$\begin{aligned}
\langle x_i(n)^2\rangle &= \langle [x_i(n-1) + dx_i]^2\rangle \\
&= \langle x_i(n-1)^2\rangle + 2\langle x_{i-1}(n)\, dx_i\rangle + \langle dx_i^2\rangle \\
&= \langle x_i(n-1)^2\rangle + 2\langle x_{i-1}(n)\rangle\langle dx_i\rangle + \delta^2 \\
&= \langle x_i(n-1)^2\rangle + \delta^2. \qquad (94)
\end{aligned}$$

Repeating this procedure n times and recalling that $x_i(0) = 0$, we find

$$\langle x_i(n)^2\rangle = \langle x_i(0)^2\rangle + n\delta^2 = n\delta^2 \qquad (95)$$

and, hence, for the mean square displacement of the cloud's mean value

$$\langle X(n)^2\rangle = \frac{1}{N^2}\sum_{i=1}^{N} n\delta^2 = \frac{\delta^2}{N}\, n. \qquad (96)$$

If we write n in terms of time such that $t = n\tau$, where τ is the time in between each step, then

$$\sqrt{\langle x_i(n)^2 \rangle} = \left(\frac{t}{\tau}\right)^{\frac{1}{2}} \delta = \left(\frac{\delta^2 t}{\tau}\right)^{\frac{1}{2}} = \left(\frac{\delta^2}{\tau}\right)^{\frac{1}{2}} \sqrt{t}. \tag{97}$$

The root-mean-square displacement of each particle is proportional to the square-root of the time.

We now seek to derive a theory to predict the distribution of a cloud of random walkers at some time t given the distribution at $t = 0$. There are two ways to do so, one using particle fluxes and the other adopting a probabilistic approach.

5.1 Derivation of the diffusion equation using particle fluxes

Consider two neighbouring points on a line. At time t there are $N(x,t)$ particles at x and $N(x+\delta,t)$ particles at position $x+\delta$. At time $t+\tau$ half the particles at x will have stepped across the dashed line from left to right and half of the particles at $x+\delta$ will have stepped across the dashed line from right to left. The net number of particles crossing to the right is therefore

$$-\frac{1}{2}\left[N(x+\delta,t) - N(x,t)\right]. \tag{98}$$

To obtain the net flux, we divide by the area normal to the x-axis, A, and by the time interval τ,

$$J_x = -\frac{[N(x+\delta,t) - N(x,t)]}{2A\tau}. \tag{99}$$

Multiplying by δ^2/δ^2 gives

$$J_x = -\frac{\delta^2}{2\tau}\frac{1}{\delta}\left[\frac{N(x+\delta,t) - N(x,t)}{A\delta}\right] = -D\frac{n(x+\delta,t) - n(x,t)}{\delta} \tag{100}$$

where $D = \delta^2/2\tau$ is the diffusion coefficient and

$$n(x,t) = \frac{N(x,t)}{A\delta}$$

is the particle density (i.e., the number of particles per unit volume at position x at time t). If δ is assumed to be very small, then in the limit $\delta \to 0$, the flux becomes

$$J_x = -D\frac{\partial n}{\partial x}, \tag{101}$$

where we have ignored higher-order derivatives in making the approximation.

Now consider a single box with boundaries at $x-\delta/2$ and $x+\delta/2$. In a single time step, $J_x(x-\delta/2,t)A\tau$ particles will enter from the left and $J_x(x+\delta/2,t)A\tau$ particles will leave through the right boundary. The number of particles in the box changes as follows,

$$N(x,t+\tau) - N(x,t) \quad = \quad \left[J_x(x-\delta/2,t) - J_x(x+\delta/2,t)\right] A\tau.$$

By dividing both sides by $A\delta\tau$ the number of particles per unit volume in the box $n(x,t)$ is seen to increase at the rate[3]

$$\frac{n(x,t+\tau)-n(x,t)}{\tau} = -\frac{[J_x(x+\delta/2,t)-J_x(x-\delta/2,t)]}{\delta} \tag{102}$$

In the limit $\tau \to 0$ and $\delta \to 0$, this becomes

$$\frac{\partial n}{\partial t} = -\frac{\partial J_x}{\partial x} = D\frac{\partial^2 n}{\partial x^2} \tag{103}$$

which is Fick's law. This is commonly known as the *diffusion equation*. It tells us how a cloud of particles will redistribute itself in time. If we know the initial distribution and the boundary conditions, we can figure out all later distributions. It can be used to model many things, such as the spreading of dye in water, the transport of heat in solids, and the motion of bacteria.

5.2 Derivation using probabilities

Before going on to solve the diffusion equation, let us derive the diffusion equation using a different approach, involving probabilities. Assuming non-interacting particles, the number of particles in the interval $[x-\delta/2, x+\delta/2]$ at any given time is

$$N(x,t) = N_0 P(x,t) = N_0 p(x,t)\delta, \tag{104}$$

where N_0 is the total number of particles in the sample. $P(x,t) = p(x,t)\delta$ the probability of finding the particle at time t in $[x-\delta/2, x+\delta/2]$ and $p(x,t)$ the associated probability density. If we consider discrete changes in position and time, then for particles that move to the left or right with equal probability

$$P(x,t+\tau) = \frac{1}{2}\left[P(x+\delta,t) + P(x-\delta,t)\right] \tag{105}$$

where the size of the time step is τ and the spatial separation is δ. Upon dividing by δ, we can rewrite (105) in terms of the associated probability density

$$p(x,t+\tau) = \frac{1}{2}\left[p(x+\delta,t) + p(x-\delta,t)\right]. \tag{106}$$

Performing a Taylor expansion about the position x and time t in the limit $\delta, \tau \to 0$,

$$p(x,t) + \frac{\partial p}{\partial t}\tau \approx \frac{1}{2}\left[p(x,t) + \frac{\partial p}{\partial x}\,\delta + \frac{\partial^2 p}{\partial x^2}\frac{\delta^2}{2} + p(x,t) - \frac{\partial p}{\partial x}\delta + \frac{\partial^2 p}{\partial x^2}\,\frac{\delta^2}{2}\right]. \tag{107}$$

which simplifies to the diffusion equation for the probability density

$$\frac{\partial p}{\partial t} \approx D\frac{\partial^2 p}{\partial x^2}, \qquad D = \frac{\delta^2}{2\tau}. \tag{108}$$

To recover Eq. (103), we note that the number density of particles is given by $n = N_0 p$, and our derivation is complete.

[3]For strictly one-dimensional systems, the boundary area is just a point and, hence, $A = 1$ in this case.

Note that we have ignored higher-order terms in the Taylor expansion. Additional terms would give us

$$\frac{\partial p}{\partial t} + \frac{\tau}{2}\frac{\partial^2 p}{\partial t^2} \approx \frac{\delta^2}{2\tau}\frac{\partial^2 p}{\partial x^2} - \frac{\delta^4}{4!\tau}\frac{\partial^4 p}{\partial x^4}. \tag{109}$$

Are we allowed to ignore these extra terms? To see if we are, compare the ratio of the neglected terms on the right hand side

$$\frac{\delta^4}{\tau}\frac{\partial^4 p}{\partial x^4} \Big/ \frac{\delta^2}{\tau}\frac{\partial^2 p}{\partial x^2}. \tag{110}$$

Now $\partial p/\partial x$ is essentially $\Delta p/\Delta x$, where Δp is a characteristic change in the value of p and Δx is the characteristic length over which it changes. Let $\Delta p = P$ and $\Delta x = L$; the ratio of the two terms is

$$\frac{\delta^4}{\tau}\frac{P}{L^4} \Big/ \frac{\delta^2}{\tau}\frac{P}{L^2} \sim O\left(\frac{\delta}{L}\right)^2, \tag{111}$$

which is typically very small. This is an example of a scaling argument, which in this case implies that we are justified in neglecting the extra terms provided L is much greater than δ. You must be careful however, as this estimate is not correct everywhere. For example, in the tails of the distribution the characteristic lengthscale over which there is a change in p may become important. The argument of neglecting terms is therefore not always valid, and we shall discuss this point more when we encounter *singular perturbations* later in the course. The discovery of this issue and its resolution was probably the greatest achievement of applied mathematics in the twentieth century.

5.3 Suggestions

For an excellent read on random walkers and the diffusion equation, and their applications in biology, have a look at *Random Walks in Biology by Howard C. Berg* (a professor over at Harvard). In this book, the ideas we have discussed are applied to a number of biological phenomena, including the motion of bacteria (which would make a good course project).

6 Solving the diffusion equation

We have shown, through two different arguments, that the density of random walkers on a one dimensional lattice obeys the diffusion equation,

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2}. \tag{112}$$

This description is valid whenever examining the dynamics of large quantities of random walkers on scales much larger than the lattice spacing. As the next step, it is important to understand how to solve this equation, as the same mathematical problem will arise later on in our studies of fluid motion. For instance we would like to know the solution to the above equation, subject to the initial condition $n(x, t = 0) = n_0(x)$ and the boundary conditions that n vanishes at $\pm\infty$.

There exits different techniques for solving PDEs of the type (112), each of which relies on a different method for representing the solution. In all cases, however, the central idea

is that since the equation is *linear*, it is possible to "break down" any initial state into a linear combination of simpler problems. By solving the simpler problems explicitly it is then possible to reconstruct the general solution.

6.1 Separation of variables and normal modes

To illustrate the first method, let's assume diffusion is confined to the interval $[0, L]$ and that no particle can escape. Mathematically, this corresponds to solving

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2} \tag{113a}$$

$$\frac{\partial}{\partial_x} n(0,t) = 0\ , \qquad \frac{\partial}{\partial_x} n(L,t) = 0 \quad \text{for} \quad t \geq 0 \tag{113b}$$

$$n(x,0) = n_0(x) \quad \text{for} \quad x \in (0,L), \tag{113c}$$

where $n_0(x)$ is a given initial density profile. We now use an important technique called *separation of variables.* Forgetting about the initial condition $n(x,0) = n_0(x)$ for now, we look for nonzero solutions of the form

$$n(x,t) = v(x)\, w(t)$$

Substituting into the PDE gives

$$\dot{w}(t)v(x) = Dv''(x)w(t) \tag{114a}$$

$$\Leftrightarrow \qquad \frac{\dot{w}(t)}{w(t)} = D\frac{v''(x)}{v(x)} \tag{114b}$$

at least where $w(t)$ and $v(x)$ are nonzero. Whenever a function of x is equal to a function of t there is a constant λ such that

$$D\frac{v''(x)}{v(x)} = \lambda \quad \text{and} \quad \frac{\dot{w}(t)}{w(t)} = \lambda,$$

or in other words,

$$Dv''(x) = \lambda\, v(x) \quad \text{and} \quad \dot{w}(t) = \lambda\, w(t).$$

Substituting $n(x,t) = w(t)v(x)$ into the first boundary condition $\partial_x n(0,t) = 0$ gives $w(t)v'(0) = 0$ for all t, but $w(t)$ is not the zero function, so this translates into $v'(0) = 0$. Similarly, the second boundary condition $\partial_x n(L,t) = 0$ translates into $v'(L) = 0$. So we have to solve

$$Dv''(x) = \lambda\, v(x)\ , \qquad v'(0) = 0, \qquad v'(L) = 0 \tag{115a}$$

Nonzero solutions $v(x)$ exist only if

$$\lambda_k = -\frac{D\pi^2}{L^2}k^2 \tag{115b}$$

for some non-negative integer k, and in that case

$$v_k(x) = A_k \cos\left(k\frac{\pi x}{L}\right) \tag{115c}$$

Since

$$\dot{w} = \lambda w = -\frac{D\pi^2}{L^2}k^2 w \tag{115d}$$

we find

$$w_k(t) = e^{-\frac{D\pi^2}{L^2}k^2 t} \tag{115e}$$

and therefore

$$n_k(x,t) = a_k e^{-\frac{D\pi^2}{L^2}k^2 t}\cos\left(k\frac{\pi x}{L}\right), \qquad k \geq 0 \tag{116}$$

Each such solution n_k is called a *normal mode*. The full solution is then given by the superposition

$$n(x,t) = \sum_{k=0}^{\infty} a_k e^{-\frac{D\pi^2}{L^2}k^2 t}\cos\left(k\frac{\pi x}{L}\right). \tag{117}$$

The one thing we haven't used so far is the initial condition $n_0(x) = n(x,0)$. This condition determines the coefficients a_k, as we we can see by setting $t = 0$ in the solution formula, which gives

$$n(x,0) = \sum_{n=0}^{\infty} a_k \cos\left(k\frac{\pi x}{L}\right) = n_0(x). \tag{118}$$

That is, the coefficients a_k are simply the coefficients of the Fourier-cosine series of $n_0(x)$, and we know how determine those from the scalar product of $n_0(x)$ and the basis functions $\cos(k\pi x/L)$.

6.2 Fourier method

We now consider diffusion on an unbounded domain. The Fourier solution method relies on the fact that it is possible to express $n(x,t)$ in a basis of plane waves[4], i.e.

$$n(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\, e^{ikx}\hat{n}(k,t) \tag{119a}$$

As a complement to (119a), the *Fourier coefficients* for a given distribution are found using the *Fourier transform*

$$\hat{n}(k,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{-ikx} n(x,t) \tag{119b}$$

and we define $\hat{n}_0(k)$ to be the Fourier coefficients of the initial condition $n_0(x)$.

[4]An intuitive way of thinking is to note that a plane wave can be written as $e^{ikx} = \cos(kx) + i\sin(kx)$. The Fourier transform thus can be interpreted as expressing a (complex) function as a superposition of real and complex sinusoidal waves. The Fourier coefficient $\hat{n}(k,t)$ describes how large the contribution of a wave with wave vector $k \propto 1/\lambda$, with λ the wavelength, is in this superposition.

The strength of this approach is that it is simple to solve the diffusion equation for a single plane wave. For example, integrating the diffusion equation in the following manner

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, \frac{\partial n}{\partial t} e^{-ikx} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, D\frac{\partial^2 n}{\partial x^2} e^{-ikx} \tag{120}$$

gives

$$\frac{\partial \hat{n}(k,t)}{\partial t} = (ik)^2 D\hat{n}(k,t) = -k^2 D\hat{n}(k,t). \tag{121}$$

Given the initial condition $n_0(x) \to \hat{n}_0(k)$ the solution of (121) is

$$\hat{n}(k,t) = \hat{n}_0(k)e^{-Dk^2 t}. \tag{122}$$

The solution of the original problem is therefore

$$n(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\, \hat{n}_0(k) e^{ikx - Dk^2 t} \tag{123}$$

We note that the high-wavenumber components (which correspond to sharp gradients) are rapidly damped, emphasizing the smoothing property of diffusion.

As an example, consider a distribution that is initially Gaussian (normal) about the point $x = 0$ at time $t = 0$, with standard deviation σ,

$$n(x,0) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}} \tag{124}$$

In the limit where $\sigma \to 0$, this distribution corresponds to the Dirac delta-function $\delta(x)$, a function which is localized at zero. We showed earlier in Sec. 1.5 that the Fourier transform of the above initial distribution is

$$\hat{n}_0(k) = \frac{1}{\sqrt{2\pi}} e^{-\frac{k^2\sigma^2}{2}} \tag{125}$$

To obtain the full solution of the diffusion equation in real space, we have to insert $\hat{n}_0(k)$ into (123),

$$n(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ikx - Dk^2 t - k^2\sigma^2/2} \tag{126}$$

We can do a bit of rearranging to get

$$n(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ikx - k^2\left(Dt + \sigma^2/2\right)} \tag{127}$$

As before we complete the square for the exponent,

$$k^2\left(Dt + \frac{\sigma^2}{2}\right) - ikx = \left(Dt + \frac{\sigma^2}{2}\right)\left\{\left[k - \frac{ix}{2(Dt + \sigma^2/2)}\right]^2 + \frac{x^2}{4\left(Dt + \sigma^2/2\right)^2}\right\}, \tag{128}$$

so that the integral becomes

$$n(x,t) = \frac{e^{-\frac{x^2}{4(Dt+\sigma^2/2)}}}{2\pi}\int_{-\infty}^{\infty} dk\, e^{-(Dt+\sigma^2/2)\left[k - \frac{ix}{2(Dt+\sigma^2/2)}\right]^2} \tag{129}$$

This is essentially the same integral that we had before in Sec. 1.5, so we drop the imaginary part and change the integration variable, giving the result

$$n(x,t) = \frac{e^{-\frac{x^2}{2(2Dt+\sigma^2)}}}{\sqrt{2\pi(2Dt+\sigma^2)}}. \tag{130}$$

This is the solution of the diffusion equation starting from a Gaussian distribution at time $t = 0$.

Note:

- Introducing $\tilde{\sigma}^2 = 2(Dt+\sigma^2/2)$, the solution is a Gaussian with a standard deviation $\tilde{\sigma}$, i.e. the width of the solution grows like $\sqrt{Dt}$ in time. Similarly, the amplitude decreases like $\frac{1}{\sqrt{Dt}}$.
- Let us substitute $t_d = \sigma^2/(2D)$. The solution then can be written as

$$n(x,t) = \frac{e^{-\frac{x^2}{4D(t+t_d)}}}{\sqrt{4\pi D(t+t_d)}}. \tag{131}$$

  Remember that in the limit $t_d = \frac{\sigma^2}{2D} \to 0$ the initial condition (124) corresponds to a Dirac delta function. Thus an initially Gaussian distribution of particles that is diffusing may be viewed as having originated from a delta function a time t_d ago. Indeed, it can be shown that diffusion will cause any form of particle distribution initially localized about zero to eventually look like a Gaussian.

6.3 Green's function method

This method relies on another trick for representing the solution, that is somewhat more intuitive. Now, instead of representing n in a basis of plane wave states, we will express it as a basis of states which are localised in *position*. This is done by using the Dirac delta function, denoted $\delta(x - x_0)$. You should think of this of a large spike of unit area that is centered exactly at the position x_0. The definition of δ is that given any function[5] $f(x)$,

$$\int_{-\infty}^{\infty} dx'\, f(x')\, \delta(x - x') = f(x). \tag{132}$$

[5]Intuitively, one can obtain the Dirac δ-function from the normalized Gaussian (124) by letting $\sigma \to 0$. Derivatives of order n of the δ-function, denoted by $\delta^{(n)}$, can be defined by partial integration

$$\int_{-\infty}^{\infty} dx'\, f(x')\, \delta^{(n)}(x - x') = (-1)^n \int_{-\infty}^{\infty} dx'\, f^{(n)}(x')\, \delta(x - x')$$

The Fourier transformation of the δ-function is given by

$$\hat{\delta}(k) = \int_{-\infty}^{\infty} dx\, e^{-ikx} \delta(x) = 1.$$

Applying the inverse transformation yields a useful integral representation of the Dirac δ-function

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ikx} \hat{\delta}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ikx}$$

We can represent the initial distribution of particles $n(x,0) = n_0(x)$ as a superposition of δ-functions

$$n_0(x) = \int_{-\infty}^{\infty} dx'\, n_0(x')\, \delta(x - x') \tag{133}$$

This formula decomposes n_0 into a continuous series of "spikes". The idea is to then understand how each spike individually evolves and then superimpose the evolution of each spike to find the final density distribution. We define the Green's function $G(x - x', t)$ so that $G(x - x', 0) = \delta(x - x')$, and

$$n(x,t) = \int_{-\infty}^{\infty} G(x - x', t)\; n_0(x')\, dx'. \tag{134}$$

Plugging this into the diffusion equation we see that

$$\int_{-\infty}^{\infty} dx'\, n_0(x')\, \frac{\partial G(x - x', t)}{\partial t} = D \int_{-\infty}^{\infty} dx'\, n_0(x')\, \frac{\partial^2 G(x - x', t)}{\partial x^2} \tag{135}$$

Thus $G(x - x', t)$ *obeys the diffusion equation* and we have reduced the problem to the mathematics of solving the diffusion equation for the localised initial condition $\delta(x - x')$.

There are many ways of solving this problem. The one in most textbooks is to actually use the Fourier decomposition of $\delta(x - x')$ and solve the equation in Fourier space, and then transform back into real space. This is an advisable procedure as the Fourier transform of δ is very simple[6]. We will advocate another procedure however, that is more elegant and uses an idea that we will return to later in our studies of fluids. The idea is to use dimensional analysis to determine the solution. If we look at the diffusion equation

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2} \tag{136}$$

we see that roughly '$\partial/\partial t$' $\sim$ '$\partial^2/\partial x^2$'. (I've written this in quotes because there is a sense in which this equality is meaningless.) What I mean by it is that if you have a function n which obeys a diffusion equation, taking a single time derivative of the function gives a number of about the same size as when you take two spatial derivatives. This means that the characteristic length scale over which n varies is of order $\sqrt{t}$. Now, since the initial distribution δ is perfectly localised, we expect that at time t, $G(x - x', t)$ will have a characteristic width $\sqrt{t}$. Thus, we guess a (so-called) similarity solution

$$G(x - x', t) = A(t)\; F\left(\frac{x - x'}{\sqrt{t}}\right). \tag{137}$$

The time dependence of $A(t)$ is determined by the conservation of particles. Since

$$\int_{-\infty}^{\infty} dx\; G = \int_{-\infty}^{\infty} dx\; A(t)\; F\left(\frac{x}{\sqrt{t}}\right) = A(t)\sqrt{t} \int_{-\infty}^{\infty} dy\, F(y) \tag{138}$$

[6]Note that in the limit $t_d = \sigma^2/(2D) \to 0$ the initial condition (124) approaches a Dirac delta function, so we have already 'solved'the problem: equation (131) tells us that an initially Gaussian distribution of particles that is diffusing may be viewed as having originated from a delta function a time t_d ago.

must be constant in time (we have changed variables from x to $y = x/\sqrt{t}$), we see that

$$A(t) = \frac{A_0}{\sqrt{t}} \tag{139}$$

for some constant A_0. Now let's just plug in

$$G(x,t) = \frac{A_0}{\sqrt{t}} F(x/\sqrt{t})$$

into the diffusion equation. Using $y = x/\sqrt{t}$ and the chain rule gives

$$\begin{aligned} \partial_t G &= \partial_t \left(\frac{A_0}{\sqrt{t}}\right) F(y) + \frac{A_0}{\sqrt{t}}\, \partial_t F(y) \\ &= -\frac{1}{2}\frac{A_0}{t^{3/2}} F(y) + F'(y)\partial_t y \\ &= \frac{A_0}{2t^{3/2}} \left[-F(y) - F'(y) y\right] = -\frac{A_0}{2t^{3/2}} (Fy)' \end{aligned} \tag{140a}$$

and

$$\partial_{xx} G = \frac{A_0}{t^{\frac{3}{2}}} F'' \tag{140b}$$

which leads to the following ordinary differential equation for $F(y)$

$$\frac{1}{t^{\frac{3}{2}}} \left(-\frac{1}{2} F - \frac{1}{2} y F'\right) = \frac{1}{t^{\frac{3}{2}}} D F''. \tag{141}$$

Cancelling out the time factors and integrating this equation once gives[7]

$$-\frac{1}{2} F y = D F'. \tag{142}$$

This equation can be immediately integrated to give $F(y) = F_0 e^{-y^2/4D}$, and thus

$$G(x - x', t) = \frac{F_0}{\sqrt{t}} e^{-\frac{(x-x')^2}{4Dt}}, \tag{143}$$

where the constant $F_0 = 1/\sqrt{4\pi D}$ is determined by requiring that $\int dx\, G = 1$.

Mean square displacement We would like to determine $\langle x(t)^2 \rangle$ for a collection of particles starting at $x_0 = 0$. Since $G(x - x_0, t)$ is the solution of the diffusion equation with initial condition $\delta(x - x_0)$, we can compute the mean square displacement from

$$\begin{aligned} \left\langle x(t)^2 \right\rangle &= \int_{-\infty}^{\infty} dx\; x^2\, G(x,t) \\ &= \int_{-\infty}^{\infty} dx\; \frac{x^2}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}} \\ &= \frac{\sqrt{\alpha}}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx\; x^2 e^{-\alpha x^2} \end{aligned} \tag{144}$$

[7]The additional constant of integration must be zero if we assume that density and flux vanish at $y \pm \infty$.

where $\alpha = 1/(4Dt)$. To evaluate the integral, note that

$$\int_{-\infty}^{\infty} dx\; x^2 e^{-\alpha x^2} = -\frac{d}{d\alpha}\int_{-\infty}^{\infty} dx\; e^{-\alpha x^2} = -\frac{d}{d\alpha}\sqrt{\frac{\pi}{\alpha}} = \frac{\pi}{2\alpha^{3/2}}. \tag{145}$$

which then gives

$$\left\langle x(t)^2 \right\rangle = \frac{1}{2\alpha} = 2Dt. \tag{146}$$

We have thus recovered the fundamental result that the mean square displacement of Brownian particles grows linearly in time.

7 Langevin & Fokker-Planck equation

Often, Brownian particles are not just freely diffusing but do also feel the effects of an external field. Important examples are the sedimentation of particles in river and oceans, the Brownian dynamics of charges particles in electric fields, or the motion of bacteria in chemical gradient fields. These situations can be modeled using diffusion equations with an extra flux (or drift) term or, called a Fokker-Planck equations, or by adopting an equivalent particle dynamics picture. In this part, we will briefly look at both.

7.1 Sedimentation

7.1.1 Langevin equation

Consider a spherical Brownian particle (mass m, radius a) sedimenting under the influence of a constant gravitational force in a quiescent fluid. Denoting the particle's vertical position measured relative to the bottom by by $X(t) \geq 0$, it's dynamics can be described by Newton's equation

$$m\ddot{X} = -\gamma\dot{X} - m_* g + F_B(t) \tag{147}$$

where $\gamma = 6\pi\eta a$ is the Stokes friction coefficient, m_* the buoyant mass[8] , g is the gravitational acceleration, and $F_s(t)$ is a random force representing the collisions with the fluid molecules. Considering the *over-damped limit* by assuming that the force on the rhs. balance, $m\ddot{X} \approx 0$, Eq. (147) simplifies to a first-order ODE

$$\dot{X} = u + u_B(t) \tag{148}$$

where

$$u = -\frac{m_* g}{\gamma} = -\frac{m_* g}{6\pi\eta a} \tag{149}$$

is the sedimentation velocity. The random Brownian velocity component

$$u_B(t) = \frac{F_B(t)}{\gamma} \tag{150}$$

[8]The buoyant mass m_* is defined as the difference between the particle mass and the mass of the liquid that is displaced by the particle. Particles heavier than water have $m_* > 0$ whereas $m_* < 0$ for gas bubbles.

has zero mean and is delta-correlated

$$\langle u_B(t)\rangle = 0\,, \qquad \langle u_B(t)u_B(t')\rangle = 2D\delta(t-t') \tag{151}$$

A quick check of dimensions shows that the parameter D, which determines the strength of the correlations, has dimensions $[D] = L^2/T$ and hence must be a diffusion constant.

We can formally integrate equation (148) with initial condition $X(0) = X_0$ to get

$$X(t) - X_0 = ut + \int_0^t ds\, u_B(s). \tag{152}$$

Using the first property in (151), we obtain for the average

$$\langle X(t) - X_0\rangle = \left\langle ut + \int_0^t ds\, u_B(s)\right\rangle = ut + \int_0^t ds\, \langle u_B(s)\rangle = ut \tag{153}$$

That is, on average, a sinking Brownian particle moves with the sedimentation speed. Let's also compute the mean squared displacement (MSD)

$$\begin{aligned}
\langle [X(t)-X_0]^2\rangle &= \langle [X(t)-X_0][X(t)-X_0]\rangle \\
&= \left\langle \left[ut + \int_0^t ds\, u_B(s)\right]\left[ut + \int_0^t ds'\, u_B(s')\right]\right\rangle \\
&= (ut)^2 + 2ut\int_0^t ds\,\langle u_B(s)\rangle + \left\langle \int_0^t ds\, u_B(s)\int_0^t ds'\, u_B(s')\right\rangle \\
&= (ut)^2 + \int_0^t ds\int_0^t ds'\,\left\langle u_B(s)u_B(s')\right\rangle \\
&= (ut)^2 + 2D\int_0^t ds\int_0^t ds'\,\delta(s-s') \\
&= (ut)^2 + 2D\int_0^t ds\, 1 \\
&= (ut)^2 + 2Dt
\end{aligned} \tag{154}$$

The first part $\propto t^2$ is the *super-diffusive ballistic* contribution to the MSD due to the external force, and the second part $\propto t$ is diffusive contribution. In particular, for a density-matched particle with $m_* = 0$ corresponding to $u = 0$, we recover our earlier result (146) for a freely diffusing particle.

As a final remark, for computer simulations, one can rewrite Eq. (148) in the differential form

$$dX(t) = -u\, dt + \sqrt{2Ddt}\, Z(t) \tag{155}$$

where $dX(t) = X(t+dt) - X(t)$ is the position increment, and the $Z(t)$ are independently drawn Gaussian number with mean zero $\mu = 0$ and variance $\sigma^2 = 1$. That is, at each time step, one has to draw a new random number $Z(t)$ from a standard normal distribution.

7.1.2 Fokker-Planck equation & zero-flux solution

We now want describe the sedimentation problem using a continuum model. As in the preceding part, consider spherical particles diffusing under the effect of a constant drift velocity

$$u = \frac{-gm_*}{6\pi\eta a}$$

If no particles are lost or added, then their concentration is described by the conservation law

$$\partial_t n = -\partial_x J_x \tag{156}$$

with current

$$J_x = un - D\partial_x n. \tag{157}$$

Inserting the current into the mass conservation equation gives the Fokker-Planck equation

$$\partial_t n = -u\partial_x n + D\partial_{xx} n \tag{158}$$

This is a linear PDE and we could find the general solution by applying one of the techniques from the previous sections.

Instead of doing this, let's focus on the stationary (time-independent) solution, which is of direct practical importance in many sedimentation problems. If there is no external particle influx or outflux, then the stationary solution must have zero-current,

$$J_x = un - D\partial_x n = 0 \tag{159}$$

We can integrate this equation and obtain an exponentially decaying density profile

$$n(x) = n_0 e^{-x/\lambda} \tag{160}$$

with characteristic sedimentation length

$$\lambda = \frac{D}{|u|} = \frac{6\pi\eta a D}{gm_*} > 0. \tag{161}$$

Sutherland and Einstein showed in 1905 that the diffusion constant D of a small particle moving in a fluid is given by

$$D = \frac{kT}{6\pi\eta a}, \tag{162}$$

where k is the Boltzmann's constant and T the temperature (measured on a Kelvin scale), implying that

$$\lambda = \frac{kT}{gm_*}. \tag{163}$$

Note that particle shape (and mass density) enter through the buoyant mass m_*.

7.2 Escape problem

Langevin and Fokker-Planck equations are extremely useful for modeling escape problems, which are ubiquitous in biological, biophysical and biochemical processes. Prominent examples include, but are not restricted to,

- unbinding of molecules from receptors,
- chemical reactions,
- transfer of ion through through pores,
- evolutionary transitions between different fitness optima.

Their mathematical treatment typically involves models that are structurally very similar to the one-dimensional examples discussed in this section[9].

7.2.1 Generic minimal model

Consider the over-damped Langevin equation

$$\dot{X}(t) = -U'(X(t)) + u_B(t). \tag{164a}$$

with a confining effective[10] potential $U(x)$

$$\lim_{x\to\pm\infty} U(x) \to \infty \tag{164b}$$

that has two (or more) minima and maxima. A typical example is the bistable quartic double-well

$$U(x) = -\frac{a}{2}x^2 + \frac{b}{4}x^4\ , \qquad a, b > 0 \tag{164c}$$

with minima at $\pm\sqrt{a/b}$.

Generally, we are interested in characterizing the transitions between neighboring minima in terms of a rate k (units of time^{-1}) or, equivalently, by the typical time required for escaping from one of the minima. To this end, we shall first discuss the general structure of the time-dependent solution of the FPE[11] for the corresponding PDF $p(t, x)$, which reads

$$\partial_t p = -\partial_x j\ , \qquad j(t, x) = -[(\partial_x U)p + D\partial_x p], \tag{164d}$$

and has the stationary zero-current ($j \equiv 0$) solution

$$p_s(x) = \frac{e^{-U(x)/D}}{Z}\ , \qquad Z = \int_{-\infty}^{+\infty} dx\ e^{-U(x)/D}. \tag{165}$$

[9] Although things usually get more complicated in higher-dimensions.

[10] The effective potential U appearing (164a) is simply the potential of the force in Newton's equation divided by the friction coefficient; see the sedimentation problem

[11] FPEs for over-damped processes are sometimes referred to as Smoluchowski equations.

To find the time-dependent solution, we can make the ansatz

$$p(t,x) = \varrho(t,x)\, e^{-U(x)/(2D)}, \tag{166}$$

which leads to the new PDE

$$-\partial_t \varrho = \left[-D\partial_x^2 + W(x)\right] \varrho =: \mathcal{H}\varrho, \tag{167a}$$

with a transformed effective potential

$$W(x) = \frac{1}{4D}(\partial_x U)^2 - \frac{1}{2}\partial_x^2 U. \tag{167b}$$

The advantage of the transformation (166) is that Eq. (167) looks like a (imaginary-time) Schrödinger equation, for which numerous solution techniques have been developed by physicists and applied mathematicians over the last century.

Using separation of variables and assuming that the linear operator $\mathcal{H}$ has a discrete non-degenerate spectrum $\lambda_0 < \lambda_1 < \ldots$, the general solution $p(t,x)$ may be written as

$$p(t,x) = e^{-U(x)/(2D)} \sum_{n=0}^{\infty} c_n\, \phi_n(x)\, e^{-\lambda_n t}, \tag{168a}$$

where the eigenfunctions ϕ_n of $\mathcal{H}$ satisfy

$$\mathcal{H}\phi_n = \lambda_n \phi_n\ , \qquad\qquad \int dx\ \phi_n^*(x)\, \phi_m(x) = \delta_{nm}, \tag{168b}$$

and the constants c_n are determined by the initial conditions

$$c_n = \int dx\ \phi_n^*(x)\, e^{U(x)/(2D)}\ p(0,x). \tag{168c}$$

At large times, $t \to \infty$, the solution (168a) must approach the stationary solution (165), implying that

$$\lambda_0 = 0\ , \qquad c_0 = \frac{1}{\sqrt{Z}}\ , \qquad \phi_0(x) = \frac{e^{-U(x)/(2D)}}{\sqrt{Z}}. \tag{169}$$

Note that $\lambda_0 = 0$ in particular means that the first non-zero eigenvalue $\lambda_1 > 0$ dominates the relaxation dynamics at large times and, therefore,

$$\tau_* = 1/\lambda_1 \tag{170}$$

is a natural measure of the escape time. In practice, the eigenvalue λ_1 can be computed by various standard methods (WKB approximation, Ritz method, techniques exploiting supersymmetry, etc.) depending on the specifics of the effective potential W.

7.2.2 Two-state approximation

We next illustrate a commonly used simplified description of escape problems, which can be related to (170). As a specific example, we can again consider the escape of a particle from the left well of a symmetric quartic double well-potential

$$U(x) = -\frac{a}{2}x^2 + \frac{b}{4}x^4 \,, \qquad p(0,x) = \delta(x - x_-) \tag{171a}$$

where

$$x_- = -\sqrt{a/b} \tag{171b}$$

is the location of the left minimum, but the general approach is applicable to other types of potentials as well.

The basic idea of the two-state approximation is to project the full FPE dynamics onto simpler set of master equations by considering the probabilities $P_\pm(t)$ of the coarse-grained particle-states 'left well' $(-)$ and 'right well' $(+)$, defined by

$$P_-(t) \;=\; \int_{-\infty}^{0} dx\, p(t,x), \tag{172a}$$

$$P_+(t) \;=\; \int_{0}^{\infty} dx\, p(t,x). \tag{172b}$$

If all particles start in the left well, then

$$P_-(0) = 1 \,, \qquad P_+(0) = 0. \tag{173}$$

Whilst the exact dynamics of $P_\pm(t)$ is governed by the FPE (164d), the two-state approximation assumes that this dynamics can be approximated by the set of master equations[12]

$$\dot{P}_- = -k_+\, P_- + k_-\, P_+ \,, \qquad \dot{P}_+ = k_+\, P_- - k_-\, P_+. \tag{174}$$

For a symmetric potential, $U(x) = U(-x)$, forward and backward rates are equal, $k_+ = k_- = k$, and in this case, the solution of Eq. (174) is given by

$$P_\pm(t) = \frac{1}{2} \mp \frac{1}{2}\, e^{-2k\,t}. \tag{175}$$

For comparison, from the FPE solution (168a), we find in the long-time limit

$$p(t,x) \simeq p_s(x) + c_1 e^{-U(x)/2D} \phi_1(x)\; e^{-\lambda_1 t}, \tag{176}$$

Due to the symmetry of $p_s(x)$, we then have

$$P_-(t) \simeq \frac{1}{2} + C_1\, e^{-\lambda_1 t} \tag{177a}$$

where

$$C_1 = c_1 \int_{-\infty}^{0} e^{-U(x)/2D} \phi_1(x) \,, \qquad c_1 = \phi_1^*(x_-)\, e^{U(x_-)/(2D)}. \tag{177b}$$

[12]Note that Eqs. (174) conserve the total probability, $P_-(t) + P_-(t) = 1$.

Since Eq. (177a) neglects higher-order eigenfunctions, C_1 is in general not exactly equal but usually close to 1/2. But, by comparing the time-dependence of (177a) and (175), it is natural to identify

$$k \simeq \frac{\lambda_1}{2} = \frac{1}{2\tau_*}. \tag{178}$$

We next discuss, by considering in a slightly different setting, how one can obtain an explicit result for the rate k in terms of the parameters of the potential U.

7.2.3 Constant-current solution

Consider a bistable potential as in Eq. (171), but now with a particle source at $x_0 < x_- < 0$ and a sink[13] at $x_1 > x_b = 0$. Assuming that particles are injected at x_0 at constant flux $j(t,x) \equiv J = const$, the escape rate can be defined by

$$k := \frac{J}{P_-}, \tag{179}$$

with P_- denoting the probability of being in the left well, as defined in Eq. (172a) above. To compute the rate from Eq. (179), we need to find a stationary constant flux solution $p_J(x)$ of Eq. (164d), satisfying $p_J(x_1) = 0$ and

$$J = -(\partial_x U)p_J - D\partial_x p_J \tag{180}$$

for some constant J. This solution is given by

$$p_J(x) = \frac{J}{D} e^{-U(x)/D} \int_x^{x_1} dy\, e^{U(y)/D}, \tag{181}$$

as one can verify by differentiation

$$\begin{aligned} -(\partial_x U)p_J - D\partial_x p_J &= -(\partial_x U)p_J - D\partial_x \left[\frac{J}{D} e^{-U(x)/D} \int_x^{x_1} dy\, e^{U(y)/D}\right] \\ &= -(\partial_x U)p_J - J\left[-\frac{(\partial_x U)}{D} e^{-U(x)/D} \int_x^{x_1} dy\, e^{U(y)/D} - 1\right] \\ &= J. \end{aligned} \tag{182}$$

Therefore, the inverse rate k^{-1} from Eq. (179) can be formally expressed as

$$k^{-1} = \frac{P_-}{J} = \frac{1}{D} \int_{-\infty}^{x_1} dx\, e^{-U(x)/D} \int_x^{x_1} dy\, e^{U(y)/D}, \tag{183}$$

and a partial integration yields the equivalent representation

$$k^{-1} = \frac{1}{D} \int_{-\infty}^{x_1} dx\, e^{U(x)/D} \int_{-\infty}^{x} dy\, e^{-U(y)/D}. \tag{184}$$

[13] The source could be a protein production site and the barrier could present a semi-permeable membrane.

Assuming a sufficiently steep barrier, the integrals in Eq. (184) may be evaluated by adopting steepest descent approximations near the potential minimum at x_- and near the maximum at the barrier position x_b. More precisely, taking into account that $U'(x_-) = U'(x_b) = 0$, one can replace the potentials in the exponents by the harmonic approximations

$$U(x) \simeq U(x_b) - \frac{1}{2\tau_b}(x - x_b)^2, \tag{185a}$$

$$U(y) \simeq U(x_-) + \frac{1}{2\tau_-}(y - x_-)^2, \tag{185b}$$

where $\tau_{b,-}$ defined by

$$\tau_-^{-1} = U''(x_-) > 0\,, \qquad \tau_b^{-1} = -U''(x_b) > 0 \tag{186}$$

carry units of time. Inserting (185) into (184) and replacing the upper integral boundaries by $+\infty$, one thus obtains the so-called Kramers rate

$$k \simeq \frac{e^{-\Delta U/D}}{2\pi\sqrt{\tau_-\tau_b}} =: k_{\mathrm{K}}\,, \qquad \Delta U = U(x_b) - U(x_-). \tag{187}$$

This result agrees with the well-known empirical Arrhenius law. Note that, because typically $D \propto k_B T$ for thermal noise, binding/unbinding rates depend sensitively on temperature – this is one of the reasons why many organisms tend to function properly only within a limited temperature range.

8 Stochastic resonance

Noise typically impairs signal transduction, but under certain conditions an optimal dose of randomness may actually help to enhance weak signals [GHJM98]. This remarkable phenomenon is known as stochastic resonance (SR). Whilst SR was originally proposed as a possible explanation for periodically recurring climate cycles [NN81, BPSV83], experiments suggest [FSGB$^+$02] that some organisms like juvenile paddle-fish might exploit SR to enhance signal detection while foraging for food.

The occurrence of SR requires three main 'ingredients'

1. a nonlinear measurement device[14],
2. a periodic signal weaker than the threshold of measurement device,
3. additional input noise, uncorrelated with the signal of interest.

To provide some intuition, assume that a weak periodic signal (frequency Ω) is detected by a particle that can move move in the bistable double well-potential (171). For weak noise, the particle will remain trapped in one of the minima and we will be unable to infer the signal from the particle's motion. Similarly, not much information about the underlying signal can be gained if the noise is too strong, for in this case the particle will jump randomly

[14] That is, the input-output relationship between the input signal and the observable must be nonlinear

back and forth between the minima. If, however, the noise strength is tuned such that the Kramers escape rate (187) is of the order of the driving frequency,

$$k_{\rm K} \sim \Omega, \tag{188}$$

then it is plausible to expect that the particle's escape dynamics will be closely correlated with the driving frequency, thus exhibiting SR.

8.1 Generic model

To illustrate SR more quantitatively, consider the periodically driven SDE

$$\dot{X}(t) = -\partial_x U + A\cos(\Omega t) + u_B(t), \tag{189a}$$

where A is the signal amplitude and

$$U(x) = -\frac{a}{2}x^2 + \frac{b}{4}x^4 \tag{189b}$$

a symmetric double-well potential with minima at $\pm x_* = \pm\sqrt{a/b}$ and barrier height $\Delta U = a^2/(4b)$. The Brownian velocity component satisfies

$$\langle u_B(t)\rangle = 0\ , \qquad \langle u_B(t)u_B(t')\rangle = 2D\delta(t-t')$$

Introducing rescaled variables

$$x' = x/x_*\ , \qquad t' = at\ , \qquad A' = A/(ax_*)\ , \qquad D' = D/(ax_*^2)\ , \qquad \Omega' = \Omega/a$$

and dropping primes, we can rewrite (189a) in the dimensionless form

$$\dot{X}(t) = (x - x^3) + A\cos(\Omega t) + u_B(t), \tag{189c}$$

with a rescaled barrier height $\Delta U = 1/4$. The associated FPE reads

$$\partial_t p \;\; = \;\; -\partial_x\{[-(\partial_x U) + A\cos(\Omega t)]p - D\partial_x p\}. \tag{190}$$

For our subsequent discussion, it is useful to rearrange terms on the rhs. as

$$\partial_t p = \partial_x[(\partial_x U)p + D\partial_x p] - A\cos(\Omega t)\partial_x p. \tag{191}$$

To solve Eq. (191) perturbatively, we insert the series ansatz

$$p(t,x) = \sum_{n=0}^{\infty} A^n p_n(t,x), \tag{192}$$

which gives

$$\sum_{n=0}^{\infty} A^n \partial_t p_n = \sum_{n=0}^{\infty} \left\{A^n \partial_x[(\partial_x U)p_n + D\partial_x p_n] - A^{n+1}\cos(\Omega t)\partial_x p_n\right\} \tag{193}$$

Focussing on the liner response regime, corresponding to powers A^0 and A^1, we find

$$\partial_t p_0 = \partial_x[(\partial_x U)p_0 + D\partial_x p_0] \tag{194a}$$
$$\partial_t p_1 = \partial_x[(\partial_x U)p_1 + D\partial_x p_1] - \cos(\Omega t)\partial_x p_0 \tag{194b}$$

Equation (194a) is just an ordinary time-independent FPE, and we know its stationary solution is just the Boltzmann distribution

$$p_0(x) = \frac{e^{-U(x)/D}}{Z_0}\,, \qquad Z_0 = \int dx\, e^{-U(x)/D} \tag{195}$$

To obtain a formal solution to Eq. (194b), we make use of the following ansatz

$$p_1(t,x) = e^{-U(x)/(2D)} \sum_{m=1}^{\infty} a_{1m}(t)\,\phi_m(x), \tag{196}$$

where $\phi_m(x)$ are the eigenfunctions of the unperturbed effective Hamiltonian, cf. Eq. (167),

$$\mathcal{H}_0 = -D\partial_x^2 + \frac{1}{4D}(\partial_x U)^2 - \frac{1}{2}\partial_x^2 U. \tag{197}$$

Inserting (196) into Eq. (194b) gives

$$\sum_{m=1}^{\infty} \dot{a}_{1m}\phi_m = -\sum_{m=1}^{\infty} \lambda_m a_{1m}\,\phi_m - \cos(\Omega t)\; e^{U(x)/(2D)}\; \partial_x p_0. \tag{198}$$

Multiplying this equation by $\phi_n(x)$, and integrating from $-\infty$ to $+\infty$ while exploiting the orthonormality of the system $\{\phi_m\}$, we obtain the ODEs

$$\dot{a}_{1m} = -\lambda_m a_{1m} - M_{m0}\cos(\Omega t), \tag{199}$$

with 'transition matrix' elements

$$M_{m0} = \int dx\; \phi_m\, e^{U(x)/(2D)} \partial_x p_0. \tag{200}$$

The asymptotic solution of Eq. (199) reads

$$a_{1m}(t) = -M_{m0}\left[\frac{\Omega}{\lambda_m^2+\Omega^2}\sin(\Omega t) + \frac{\lambda_m}{\lambda_m^2+\Omega^2}\cos(\Omega t)\right]. \tag{201}$$

Note that, because $\partial_x p_0$ is an antisymmetric function, the matrix elements M_{m0} vanish[15] for even values $m = 0, 2, 4, \ldots$, so that only the contributions from odd values $m = 1, 3, 5\ldots$ are asymptotically relevant.

[15]The potential $U(x)$ is symmetric and, therefore, the effective Hamiltonian commutes with parity operator, implying that the eigenfunctions ϕ_{2k} are symmetric under $x \mapsto -x$, whereas eigenfunctions ϕ_{2k+1} are antisymmetric under this map.

Focussing on the leading order contribution, $m = 1$, and noting that $p_0(x) = p_0(-x)$, we can estimate the position mean value

$$\langle X(t)\rangle = \int dx\, p(t,x)\, x \tag{202}$$

from

$$\begin{aligned}
\langle X(t)\rangle &\simeq A \int dx\, p_1(t,x)\, x \\
&\simeq A \int dx\, e^{-U(x)/(2D)}\, a_{11}(t)\, \phi_1(x)\, x \\
&= -AM_{10} \left[\frac{\Omega}{\lambda_1^2 + \Omega^2} \sin(\Omega t) + \frac{\lambda_1}{\lambda_1^2 + \Omega^2} \cos(\Omega t) \right] \int dx\, e^{-U(x)/(2D)}\, \phi_1(x)\, x
\end{aligned}$$

Using $\lambda_1 = 2k_{\rm K}$, where $k_{\rm K}$ is the Kramers rate from Eq. (187), we can rewrite this more compactly as

$$\langle X(t)\rangle = \overline{X} \cos(\Omega t - \overline{\varphi}) \tag{203a}$$

with phase shift

$$\overline{\varphi} = \arctan\left(\frac{\Omega}{2k_{\rm K}} \right) \tag{203b}$$

and amplitude

$$\overline{X} = -A \frac{M_{10}}{(4k_{\rm K}^2 + \Omega^2)^{1/2}} \int dx\, e^{-U(x)/(2D)}\, \phi_1(x)\, x. \tag{203c}$$

The amplitude $\overline{X}$ depends on the noise strength D through $k_{\rm K}$, through the integral factor and also through the matrix element

$$M_{10} = \int dx\ \phi_1\, e^{U(x)/(2D)} \partial_x p_0. \tag{204}$$

To compute $\overline{X}$, one first needs to determine the eigenfunction ϕ_1 of $\mathcal{H}_0$ as defined in Eq. (197). For the quartic double-well potential (189b), this cannot be done analytically but there exist standard techniques (e.g., Ritz method) for approximating ϕ_1 by functions that are orthogonal to $\phi_0 = \sqrt{p_0/Z_0}$. Depending on the method employed, analytical estimates for $\overline{X}$ may vary quantitatively but always show a non-monotonic dependence on the noise strength D for fixed potential parameters (a, b). As discussed in [GHJM98], a reasonably accurate estimate for $\overline{X}$ is given by

$$\overline{X} \simeq \frac{Aa}{Db} \left(\frac{4k_{\rm K}^2}{4k_{\rm K}^2 + \Omega^2} \right)^{1/2}, \tag{205}$$

which exhibits a maximum for a critical value D_* determined by

$$4k_{\rm K}^2 = \Omega^2 \left(\frac{\Delta U}{D_*} - 1 \right). \tag{206}$$

That is, the value D_* corresponds to the optimal noise strength, for which the mean value $\langle X(t)\rangle$ shows maximal response to the underlying periodic signal – hence the name 'stochastic resonance' (SR).

8.2 Master equation approach

Similar to the case of the escape problem, one can obtain an alternative description of SR by projecting the full FPE dynamics onto a simpler set of master equations for the probabilities $P_\pm(t)$ of the coarse-grained particle-states 'left well' $(-)$ and 'right well' $(+)$, as defined by Eq. (172). This approach leads to the following two-state master equations with time-dependent rates

$$\begin{aligned} \dot{P}_-(t) &= -k_+(t)\,P_- + k_-(t)\,P_+, && \text{(207a)} \\ \dot{P}_+(t) &= k_+(t)\,P_- - k_-(t)\,P_+. && \text{(207b)} \end{aligned}$$

The general solution of this pair of ODEs is given by

$$P_\pm(t) = g(t)\left[P_\pm(t_0) + \int_{t_0}^{t} ds\,\frac{k_\pm(s)}{g(s)}\right] \tag{208a}$$

where

$$g(t) = \exp\!\left\{-\int_{t_0}^{t} ds\,[k_+(s)+k_-(s)]\right\}. \tag{208b}$$

To discuss SR within this framework, it is plausible to postulate time-dependent Arrhenius-type rates,

$$k_\pm(t) = k_{\rm K}\exp\!\left[\pm\frac{Ax_*}{D}\cos(\Omega t)\right] \tag{209}$$

with $k_{\rm K}$ denoting Kramers rate as defined in Eq. (187).

Considering the asymptotic limit $t_0 \to -\infty$, one can Taylor-expand the rates for $Ax_* \ll D$ to obtain

$$k_\pm(t) = k_{\rm K}\left[1 \pm \frac{Ax_*}{D}\cos(\Omega t) + \left(\frac{Ax_*}{D}\right)^2\cos^2(\Omega t) \pm \ldots\right]$$

These approximations are valid for slow driving (adiabatic regime), and they allow us to compute expectation values to leading order in Ax_*/D. To first order, one then finds for the conditional probability

$$\begin{aligned} P_+(t|x_0,t_0) &= 1 - P_-(t|x_0,t_0) \\ &= \frac{1}{2}\left\{e^{-2k_{\rm K}(t-t_0)}\,[2\delta_{x_0,x_*} - 1 - \kappa(t_0)] + 1 + \kappa(t)\right\} && \text{(210a)} \end{aligned}$$

where

$$\kappa(t) = \frac{Ax_*}{D}\,\cos(\Omega t - \overline{\varphi})\,\left(\frac{4k_{\rm K}^2}{4k_{\rm K}^2+\Omega^2}\right)^{1/2}, \qquad \overline{\varphi} = \arctan\!\left(\frac{2\Omega}{k_{\rm K}}\right). \tag{210b}$$

Note that the conditional probability $P_+(t|x_0,t_0)$ satisfies the initial condition

$$P_+(t_0|x_0,t_0) = \delta_{x_0,x_*} = \begin{cases} 1, & x_0 = x_* \\ 0, & \text{otherwise} \end{cases}, \tag{211}$$

where $x_* = x_\pm$ depending on whether the particle starts in the left or right well. Furthermore, one then finds for the mean position the asymptotic linear response result

$$\langle X(t)\rangle = \overline{X}\cos(\Omega t - \overline{\varphi}) \tag{212a}$$

where

$$\overline{X} = \frac{Ax_*^2}{D}\left(\frac{4k_{\rm K}^2}{4k_{\rm K}^2+\Omega^2}\right)^{1/2}, \qquad \overline{\varphi} = \arctan\left(\frac{\Omega}{2k_{\rm K}}\right). \tag{212b}$$

Note that Eqs. (212) are consistent with our earlier result (203).

9 Quantum mechanics

The examples of linear PDEs we have discussed so far involved real-valued fields such as the concentration profile of a collection of non-interacting Brownian particles or the phase-space density in the Liouville equation. There exist, however, important classes of physical systems that have natural descriptions in terms of complex-valued fields. The arguably most import ones are quantum-mechanical systems, whose behavior can be modeled using a complex wavefunction $\psi(t,x)$ that is governed by a linear PDE called Schrödinger's equation. There are many subtleties and some controversies associated with the interpretation of quantum mechanics, but the mathematical description is well-defined and pretty straightforward. For our (and many other) purposes, it will be sufficient to consider quantum mechanics as continuum model that describes the energy states and dynamics of microscopic systems in terms of a complex field.

Historically, several phenomena observed in experiments at the end of the 19th and beginning of the 20th century demanded a departure from a purely particle-based description of microscopic matter; these included

- the stability and the discrete spectral lines of atoms and molecules, and
- the wave-like defraction and interference of single electrons in double slit experiments,

Conversely, other experiments suggested that certain systems that were long thought to be purely wave-like also carry some inherently discrete properties, as exemplified by

- the shape of the blackbody spectrum, or
- the photo-electric effect.

In essence, what was needed to reconcile these observations was a continuum theory that provides discrete energy levels.

9.1 Bohr' model

The first semi-quantum-mechanical model to explain the discrete spectral lines of the hydrogen atom was introduced by Niels Bohr in 1913, who postulated that the electron's trajectory around the nucleus forms a standing wave-pattern, i.e.

$$2\pi r = n\lambda\,, \qquad n = 1, 2, \ldots \tag{213}$$

Combining this with de Broglie's hypothesis that a particle of momentum p has an associated wave-length

$$\lambda = \frac{h}{p}, \tag{214}$$

where $h = 6.6260701510^{-34}$Js is Planck's quantum of action, Bohr concluded that the electron's angular momentum must be quantized

$$\ell = rp = \frac{h}{2\pi} n = \hbar n \ , \qquad n = 1, 2, \ldots \tag{215}$$

i.e., take integer multiples of $\hbar = h/(2\pi)$.

This allowed him to explain the experimentally observed discrete energy spectra of hydrogen and hydrogen-like ions as follows. The classical energy of an electron on a spherical orbit is given by

$$E = \frac{mv^2}{2} - \frac{kZe^2}{r} \tag{216}$$

where $k = 1/(4\pi\epsilon_0)$ is Coulomb's constant, and Z denotes the proton number of the nucleus. Equating centripetal and Coulomb force gives

$$\frac{mv^2}{r} = \frac{kZe^2}{r^2} \tag{217}$$

so that one can rewrite the energy as

$$E = -\frac{kZe^2}{2r} \tag{218}$$

Furthermore, multiplying (217) by mr^3 and using the quantization condition (215), one finds

$$m^2v^2r^2 = kmZe^2r = \hbar^2 n^2 \ , \qquad n = 1, 2, \ldots \tag{219}$$

implying discrete radii

$$r_n = \frac{\hbar^2 n^2}{kmZe^2} \ , \qquad n = 1, 2, \ldots \tag{220}$$

Finally inserting into (218), we get the discrete energy levels

$$E_n = -Z^2 \frac{E_R}{n^2} = -Z^2 \frac{13.6}{n^2}\,\text{eV} \ , \qquad E_R = \frac{m(ke^2)^2}{2\hbar^2} \tag{221}$$

which explains the key features of the spectra of the hydrogen atom ($Z = 1$) and hydrogen-like ions ($Z > 1$). $E_R = 13.6\,\text{eV}$ is called the Rydberg energy.

Bohr's model was not yet a satisfactory theory but nevertheless provided essential guidance for the development of modern quantum mechanics.

9.2 Schrödinger's equation

In 1921, Erwin Schrödinger succeeded in constructing a linear PDE that produced the spectrum (221). The essential steps underlying the construction of Schrödinger's wave equation can be summarized as follows:

1. Start from a classical Hamiltonian system whose dynamics conserves the energy

$$E = H(\boldsymbol{p}, \boldsymbol{x}) = \frac{\boldsymbol{p}^2}{2m} + U(\boldsymbol{x}) \tag{222a}$$

2. Reinterpret E and $\boldsymbol{p}$ as operators,

$$E \to i\hbar\partial_t \ , \qquad \boldsymbol{p} \to -i\hbar\nabla \tag{222b}$$

   acting on a complex wave function $\psi(t, \boldsymbol{x})$.

3. Substitute the operators into the Hamiltonian $H(\boldsymbol{p}, \boldsymbol{q})$ to obtain the wave equation

$$i\hbar\partial_t\psi = \left[-\frac{\hbar^2\nabla^2}{2m} + U(\boldsymbol{x})\right]\psi \equiv \mathcal{H}\psi \tag{222c}$$

4. Interpret

$$\rho(t, \boldsymbol{x}) = |\psi(t, \boldsymbol{x})|^2 \tag{222d}$$

   as probability density of finding the quantum particle at time t at position $\boldsymbol{x}$.

The linear PDE (222c) is called the *time-dependent Schrödinger equation*. Note that the linear differential operator $\mathcal{H}$ on the rhs. of (222c) has exactly the same structure as the one derived from the Fokker-Planck equation in Eq. (167). However, the factor i on the lhs. of (222c) makes things very different: Solutions to the Fokker-Planck equation are damped whereas solutions to the Schrödinger equation are oscillatory in time. Despite this difference, we can solve both equations with similar methods.

The interpretation of $|\psi(t, \boldsymbol{x})|^2$ as probability density is due to Max Born and nowadays widely accepted. This interpretation requires that

$$\int d\boldsymbol{x}\ |\psi(t, \boldsymbol{x})|^2 = 1 \tag{223}$$

That is, the complex wave function must decay sufficiently fast at infinity. This boundary condition implies a discrete spectrum of the Hamilton operator $\mathcal{H}$. Indeed separation of variables

$$\psi(t, \boldsymbol{x}) = h(t)\phi(\boldsymbol{x})$$

and subsequent superposition yields a general solution of the form[16]

$$\psi(t, \boldsymbol{x}) = \sum_{n=1}^{\infty} c_n e^{-i\lambda_n t/\hbar}\phi_n(\boldsymbol{x}) \tag{224a}$$

[16] We assume here that the eigenvalues are non-degenerate $\lambda_1 < \lambda_2 < \lambda_2 < \ldots$

where λ_n and $\phi_n(\boldsymbol{x})$ are the eigenvalues and eigenfunctions of the Hamilton operator

$$\mathcal{H}\phi_n(\boldsymbol{x}) = \left[-\frac{\hbar^2\nabla^2}{2m} + U(\boldsymbol{x})\right]\phi_n(\boldsymbol{x}) = \lambda_n\phi_n(\boldsymbol{x}) \tag{224b}$$

One typically refers to this eigenvalue problem as the *time-independent* Schrödinger equation. For confining potentials, the eigenfunctions can be chosen orthonormal

$$\int d\boldsymbol{x}\, \phi_m^*(\boldsymbol{x})\phi_n(\boldsymbol{x}) = \delta_{nm} \tag{224c}$$

The *complex* coefficients c_n are then determined by the initial condition

$$c_m = \int d\boldsymbol{x}\, \phi_m^*(\boldsymbol{x})\, \psi(0,\boldsymbol{x}) \tag{224d}$$

This can be seen by considering the solution (224a) at time $t = 0$, multiplying by ϕ_m^* and integrating over space using (224c). In particular, when inserting the Coulomb potential

$$U(\boldsymbol{x}) = -\frac{kZe^2}{|\boldsymbol{x}|} \tag{225}$$

into (222c), one finds[17] that the spectrum of the corresponding Hamilton operator is given by the Bohr formula (221).

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[17] This somewhat lengthy calculation, which uses separation of variables in spherical spherical coordinates, can be found in any textbook on quantum mechanics.