Turbulence

At high Reynolds number, the static solutions of viscous hydrodynamics are no longer physically relevant; real systems show rapidly varying flow configurations across many length and time scales. The problem of “fully developed turbulence” for open systems (i.e., work is supplied to the system externally and dissipated by viscosity) is still not completely understood, but many simpler examples of the transition from static solutions to chaotic time-dependent solutions have been understood in the last 20-30 years. Turbulent flow is probably the most physically important example of a chaotic “steady state” in an open nonlinear system: here “steady state” means that even though the system is rapidly fluctuating, it is meaningful to define time averages for quantities like the mean fluid velocity.

Now we briefly review one phenomenological law about fully developed turbulence. Weakly turbulent systems (i.e., when the Reynolds number is just above the limit for turbulent flow) have been studied in great detail with a variety of sophisticated techniques, and are connected to some major developments in chaos theory such as the notion of period doubling (cf. Berkeley physics course on nonlinear dynamics). Here we focus on statistical physics: we find a statistical scaling law in the limit of highly turbulent flows, when the intermittent variation in the velocity $v_{\lambda}$ at the smallest scales is comparable to the mean velocity $u$.

\textit{Big whorls have little whorls}
\textit{That feed on their velocity,}
\textit{And little whorls have lesser whorls}
\textit{And so on to viscosity.}

Lewis Richardson

Let’s start with an estimate of the energy dissipation due to viscosity in a system. How much energy per time per mass is dissipated? Recall that

$$R = \frac{\rho v l}{\mu} = \frac{v l}{\nu},$$

(1)

where $\nu \equiv \frac{\mu}{\rho}$ is the so-called “kinematic” viscosity. In fully developed turbulence, energy is transferred from large eddies/whorls down to eddies of smaller and smaller size, until it is eventually dissipated in the smallest eddies. Since all the energy passes through large eddies, which know nothing about the viscosity, it should be possible to express the energy dissipation without using the viscosity. We define $L$ as the typical size of a large eddy where energy is put in, and $\lambda$ as the smaller length scale where viscosity becomes significant.

The units of energy dissipation $\epsilon$ are energy per time per mass; to make a fluid quantity with these units, without using viscosity, we need $-3$ powers of time, so we guess

$$\epsilon = \frac{(\delta u)^3}{l},$$

(2)
Here $l$ is the size of an eddy and $\delta u$ is the variation in the velocity for that eddy. This is an estimate of the order of magnitude of the energy dissipation based on observing eddies of size $l$. We can use this assumption to derive a simple picture of turbulence: assume that the above formula is correct for eddies of all different sizes, so that all the estimates of energy dissipation are consistent: by looking either at the large-scale flow or at a different scale, we want to get the same answer. Then

$$\delta u = (l \epsilon)^{1/3}. \quad (3)$$

Here $\delta u$ for smaller and smaller eddies becomes dominated by the turbulent velocity variation, and this law (“Kolmogorov’s law”) predicts that the velocity variation goes as the cube root of the eddy size. Hence it decreases only very slowly as the eddy size decreases.

We can finally ask about the length scale of the smallest eddies, where energy is rapidly dissipated. The effective Reynolds number for a small eddy is

$$R_\lambda = \frac{v_\lambda \rho}{\mu} \sim \frac{\lambda^{4/3} \epsilon^{1/3} \rho}{\mu}. \quad (4)$$

Let the Reynolds number for the flow as a whole be

$$R = \frac{L(\delta u) \rho}{\mu} = \frac{\epsilon^{1/3} L^{4/3} \rho}{\mu}. \quad (5)$$

Then defining $\lambda_0$ as the scale where $R_\lambda = 1$, we have

$$\lambda_0^{4/3} = \frac{L^{4/3}}{R}, \quad (6)$$

or $\lambda_0 = L/R^{3/4}$. This sets the eddy size below which dissipation dominates. The “cascade”, where scaling laws like we have derived are valid, is on length scales between $\lambda_0$ and $L$.

One problem with our hydrodynamical equations is that they don’t seem to fully describe thermal equilibrium, as there are no thermal fluctuations of $n, u$, and the other macroscopic averages. For fluids this is quite a good approximation, as the large number of particles mean that the relative fluctuation of quantities summed over the particles are small. For other systems, however, such as the Brownian particle discussed in a moment, we need to understand how to write dynamical equations that include fluctuations. Before doing so, we start with some general considerations of how dynamics respecting equilibrium should work.

**Basic ideas of statistical dynamics: detailed balance**

Except for Liouville’s theorem, our focus in the last few lectures has been on the specific case of a dilute classical gas. While this case is the model for similar approaches to some other systems, it is a good idea to step back a moment and think about dynamics in general. We will start talking in the next lecture about linear-response theory and dynamics in systems slightly perturbed from equilibrium, but first let us try to come up with a few general ideas about dynamics in statistical mechanics.

To make this problem more specific, note the following distinction between Hamiltonian systems (including quantum systems) and non-Hamiltonian systems, such as the Ising model of a ferromagnet in zero magnetic field:

$$E = -J \sum_{\langle ij \rangle} s_i s_j, \quad s_i = \pm 1. \quad (7)$$
A Hamiltonian system has both an energy function and a dynamics: a fundamental property of quantum mechanics is that the Hamiltonian determines both the energy levels that appear in the Boltzmann factor $\exp(-\beta E)$ and the dynamics (through the Schrödinger equation). However, it is not at all obvious what dynamics should be put on the Ising model (7).

In fact there is no unique answer. One can impose different dynamics on the Ising model for different physical situations, as we will discuss explicitly later in the course. However, one restriction that we would be tempted to impose on the dynamics near equilibrium is the following: if we are modeling the dynamics at a temperature $T$, then the probability distribution over states that corresponds to thermal equilibrium should be an equilibrium of the dynamics we choose. Our two goals in the remainder of this lecture are to show that a simple requirement (the “principle of detailed balance”) will guarantee that thermal equilibrium is a dynamical equilibrium, and to discuss a key application of this principle to numerical studies of equilibrium systems.

To be more precise about the above, let us say that given some states of a system $i = 1, \ldots, N$, giving the dynamics corresponds to giving rates $r_{i \to j}$ such that if a system starts in state $i$ at time 0, its probability to be in a different state $j$ at time $dt$ is given by $P_j = r_{i \to j} dt$. More precisely, taking derivatives we have

\[ \frac{dP_j}{dt} \bigg|_{t=0} = r_{i \to j}, \quad j \neq i, \tag{8} \]

if the initial state of the system was in state $i$. The key assumption we are making here is that the immediate future of a system depends on its past history only through its current state: such random processes are known as Markov chains. For an initial condition that is not a specific state but an assignment of probabilities $P_i(t)$, it is then natural to define

\[ \frac{dP_j}{dt} = \sum_i \left[ r_{i \to j} P_i - r_{j \to i} P_j \right], \tag{9} \]

where now we are assuming that the rates are time-independent so that the above holds for all times. The second term arose because conservation of probability requires that we take into account systems leaving state $j$ just as we did states coming into state $i$. (Does this remind you of the collision term in the Boltzmann equation?) Mathematically we just have a first-order matrix differential equation with constant coefficients. Note that here we are choosing to work with a discrete set of states, as in the Ising model, and in continuous time, but there are appropriate generalizations of what we’ll find to other cases.

There are several requirements we might want to impose on the rates $r_{i \to j}$, depending on the microscopics of our system, but let us focus on obtaining an equilibrium that corresponds to thermal equilibrium at some temperature $T$:

\[ P_i^{eq} = \frac{e^{-E_i/k_BT}}{Z}. \tag{10} \]

We are going to show that the following condition, known as the principle of detailed balance, is sufficient to guarantee that $P^{eq}$ is an equilibrium:

\[ \frac{r_{i \to j}}{r_{j \to i}} = \frac{e^{(E_i-E_j)/k_BT}}. \tag{11} \]

Now substitute $P^{eq}$ into the evolution equations (9) and apply the above condition. Each individual term in the sum over $i$ vanishes, so the whole sum vanishes and the probabilities do not evolve in
time, which is what we wanted to show. The detailed balance rule, in words, is that the rate to go
to a state higher in energy should be slower than the rate of the inverse process by a factor related
to the temperature.

This argument proves that detailed balance is sufficient to guarantee that thermal equilibrium
is an equilibrium of the dynamics; it is left to the reader to find an example showing that the
converse is not true. That is, there can be choices of dynamics that give an equilibrium but do not
satisfy the detailed balance criterion: this is just saying that the sum over \( i \) may turn out to vanish
even if individual terms do not all vanish but instead cancel each other. It is also a useful exercise
to consider the stability of the thermal equilibrium configuration of such a dynamics.

We are now going to explain how the detailed balance rule justifies what is probably the most
famous computer algorithm in physics. The challenge is to calculate the thermodynamic average
of some quantity \( \hat{O} \) in the canonical ensemble at temperature \( T \):

\[
\langle \hat{O} \rangle \equiv \sum_k \hat{O}(k)e^{-\beta E_k}/Z. \tag{12}
\]

Here \( \hat{O}(k) \) is the value of \( \hat{O} \) in state \( k \). Now suppose we have a system of \( N \) Ising spins, for which
there are \( 2^N \) possible states. Even for quite small \( N \), it is impossible to simply sum over all these
states. Instead one would like to try a probabilistic or “Monte Carlo” strategy of summing over
some randomly chosen configurations; as more and more configurations are included in the sum,
this will indeed converge to the correct answer. This brute-force Monte Carlo approach would
work as follows: generate a random configuration of \( N \) spins and calculate the value of \( \hat{O} \) in that
configuration. After this has been done many times, use the Boltzmann weights to average over
the random configurations that were generated. Simple arguments from statistics can be used to
determine the convergence of this Monte Carlo approach as the number of sampled configurations
increases.

However, this brute-force algorithm works in principle but is practically impossible to use,
especially at low temperatures. The reason is that at low temperatures many of the configurations
sampled will have such a small Boltzmann weight that they contribute essentially nothing to the
average, while the low-energy configurations that dominate are practically never sampled. We need
an algorithm that generates configurations in a way as to include the Boltzmann weight already:
the Metropolis algorithm is a simple but very clever way to do this that has survived for half a
century.

Instead of randomly picking independent configurations of the system, let us come up with a
random process that evolves one configuration to another one that may depend on the previous
state. (Note that on a computer it is convenient to implement discrete-time rather than continuous-
time Markov chains.) We label the possible steps that go from one state to another as “moves”:
for example, flipping a single spin of the Ising model is a perfectly fine move. One can argue that
if this dynamics satisfies the detailed-balance criterion and is “ergodic” (will eventually explore all
the allowed configurations), then the time-average of any operator over the Metropolis dynamics
will converge to the static average over the thermal ensemble.

An example will make this much more concrete. Take the Ising model in 1D: we have a chain
of spins \( s_i = \pm 1 \) coupled by an interaction that favors configurations in which spins are aligned.
At each step, we randomly choose a spin \( i \) and decide whether to flip it. The detailed balance rule
says that the rate to flip spin $i$ from up to down and the rate to flip it from down to up, with all other spins remaining the same, should be related by the energy difference between the two states:

$$\frac{r^i_{\uparrow\rightarrow\downarrow}}{r^i_{\downarrow\rightarrow\uparrow}} = e^{(E_{\uparrow} - E_{\downarrow})/kT}.$$  \hspace{1cm} (13)

A simple way to satisfy this is as follows: if flipping spin $i$ would lower the energy, do it; if flipping the spin $i$ would raise the energy by $\Delta E$, then flip it with probability $e^{-\Delta E/k_B T}$. Then this process satisfies detailed balance, and it is also ergodic: if we wait long enough, every state can be reached from any initial state by enough single-spin flips. One can argue based on these properties that averages over time in the evolution process will eventually reproduce the desired equilibrium average.

Since the Ising model has only nearest-neighbor interactions on the chain, the probability to flip a spin depends just on its two neighbors. You can apply the above rules to find out that a chosen spin $i$ will flip automatically unless both its neighbors have the same value as $s_i$, in which case the probability to flip is $\exp(-4J/kT)$. As the Metropolis algorithm walks through configurations, all a program has to do is keep track of $\hat{O}$ in each time-step, add up these values at the end, and divide by the number of time-steps. Think about why this works: all the weights $e^{-\beta E}$ are included through their effect on the amount of time the system spends in different states. It is amazing how much better this simple Metropolis Monte Carlo algorithm (choosing an unphysical dynamics to evaluate rapidly equilibrium expectation values) is than the brute-force Monte Carlo approach, and variants of the Metropolis approach are still widely used in physics and chemistry.