Thermodynamics and noise

Thermodynamics and statistical mechanics,
Equipartition theorem, Fluctuation-dissipation theorem

Thermal fluctuations and noise are intimately related. We will briefly review macroscopic thermodynamics and its origin in microscopic statistical mechanics, and then we will look at the **Equipartition Theorem** (relation between temperature to the average energy stored in a system's degree of freedom) and the **Fluctuation-Dissipation Theorem** (relation between fluctuations to the dissipation in a system).

Thermodynamics and Statistical Mechanics

- a thermodynamics system can be described by a ***temperature T****, an* ***internal energy E****,* and an ***entropy S****;*

  the **internal energy** is the sum off all of the energy stored in all of the degree of freedom of the system;

  the **entropy** provides a relationship between heat and temperature: if the system is kept at a constant temperature, and a heat δQ flows into or out of the system, the change in entropy is

  $$\delta Q = T\, dS;$$

  (δQ rather than dQ because energy that flows in and increases the entropy of a system cannot reversibly recovered to do work)
  In any spontaneous process the entropy cannot decrease $\mathbf{dS \geq 0}$
  This is the II° law of thermodynamics, with equality holding for reversible process(the firs law is conservation law).

Because of the second law, all of the internal energy in a system is not available to do work on another system, only that part that was not associated with an entropy increase.

Integrating equation $\delta Q = T\,dS$ shows that the total energy in a system is $Q = T\,S$. Therefore the ***free energy, A***, defined to be

$$A = E - T\,S$$

is the difference between the internal energy and the heat energy. It measures the energy in the system that is available to do work. We will see that a system seeks to minimize its free energy, by both reducing the internal energy and incresing the entropy.

Entropy was originally introduced in the early 1800s as a phenomenological quantity to help to explain the efficiency of heat engines; one of the greatest problems in modern science has been explaining its microscopic origin.

All systems are quantized so that they are restricted to a discrete set of possible states even though the spacing between the states may be so small that macroscopically they appear continuous.

The microscopic definition of the entropy:

$$S = -k\sum_{i=1}^{\Omega} p_i \log p_i$$

where:

i = index the possible states of a system;

Ω total states;

p_i probability to be in the *i*-th state

k is Boltzmann's constant.

If all of the states are equally likely ($p_i = 1/\Omega$) then

$$S = -k \log \Omega \;.$$

This equation was so important to Boltzmann that it appears on his grave!

According to the postulates of statistical mechanics, if there are Ω microscopic configurations of a system compatible with a *given* macroscopic state, then the probability *p* of seeing that macroscopic state is proportional to the number of states Ω:

$$p \propto e^{S/k}$$

The system is equally likely to be in any of the available microscopic states.

If the total energy is fixed, then the probability to be in any state with that energy is the same. This is called ***microcanonical ensemble***

In the real world it is much more common to be able to determine the ***average energy*** rather than the exact energy. That case is called a ***canonical ensemble***.

To work out its properties we need one more postulate from statistical mechanics: the system chooses the distribution of probabilities that maximizes its entropy, subject to the constraints that we impose. Justifying this is essentially experimental fact is the subject of end ess mathemathical if not mystical discussion; Boltzmann's H-Theorem provides a derivation in the context of scattering in a diluite gas.

For the canonical ensemble there are two constraints: the probability distribution must be normalized

$$\sum_{i=1}^{\Omega} p_i = 1$$

and the average energy must be constant

$$\sum_{i=1}^{\Omega} E_i p_i = E$$

To do a constrained maximization we will use the method of Lagrange multipliers.

Define a quantity I to be the entropy plus Lagrange multipliers times the constraint equations

$$I = -k\sum_{i=1}^{\Omega} p_i \log p_i + \lambda_1 \sum_{i=1}^{\Omega} p_i + \lambda_2 \sum_{i=1}^{\Omega} E_i p_i$$

we want to find the values for the p_i that make this extremal: $\dfrac{\partial I}{\partial p_i} = 0$

we can do this because the two terms that we have added are just constants!

We just need to choose the values of the Lagrange multipliers to make sure that they have the right values.

Solving:

$$\frac{\partial I}{\partial p_i} = 0 \qquad \Rightarrow \; -k \log p_i - k + \lambda_1 + \lambda_2 E_i = 0$$

$$\Rightarrow \; p_i = e^{(\lambda_1 / k) + (\lambda_2 E_i / k) - 1}$$

if we sum over i

$$\sum_{i=1}^{\Omega} p_i = 1 = e^{\lambda_1 / k - 1} \sum_{i=1}^{\Omega} e^{\lambda_2 E_i / k}$$

this can be rearranged to define the partition function:

$$z = e^{1 - \lambda_1 / k} = \sum_{i=1}^{\Omega} e^{\lambda_2 E_i / k}$$

Another equation follows from multiplying equation $\dfrac{\partial I}{\partial p_i} = 0$

$$-k \log p_i - k + \lambda_1 + \lambda_2 E_i = 0$$

by pi and summing

$$\sum_{i=1}^{\Omega} p_i \frac{\partial I}{\partial t} = S - k + \lambda_1 + \lambda_2 E = 0$$

Since $z = e^{1-\lambda_1/k}$ then $k \log z = k - \lambda_1$

and the equation $S - k + \lambda_1 + \lambda_2 E = 0$ can be written as

$$S - k \log z + \lambda_2 E = 0$$

Comparing this with the definition of the free energy $A = E - T S$

we can identify: $k \log z = -A/T$, $\lambda_2 = -1/T$

This provides a connection between macroscopic thermodynamic quantities and the microscopic statistical mechanical ones.

Putting the value of λ_2 into the previous equation, shows that the partition function is given by:

$$z = \sum_{i=1}^{\Omega} e^{-E_i/kT} = \sum_{i=1}^{\Omega} e^{-\beta E_i}$$ and $$\boxed{p_i = e^{(\lambda_1/k)+(\lambda_2 E_i/k)-1} = \frac{e^{-E_i/kT}}{z}}$$

The expected value of a function f_i that depends on the state of the system is :

$$\boxed{\langle f \rangle = \sum_{i=1}^{\Omega} f_i p_i = \frac{\sum_{i=1}^{\Omega} f_i e^{-E_i/kT}}{z}}$$

Equipartition theorem

The Equipartition theorem is a simple, broadly applicable result that can give the magnitude of the thermal fluctuations associated with the energy storage in independent degrees of freedom of a system.

Assume that the state of a system is specified by variables: $x_0, x_1, \ldots, x_n$; and that the internal energy of the system is given in terms of them by

$$E = E(x_0, x_1, \ldots, x_n)$$

Now consider the case where one of the degrees of freedom splits off additively in the energy:

$$E = E_0(x_0) + E_1(x_1, \ldots, x_n)$$

E might be the energy in a circuit, and $E_0 = \frac{1}{2}CV_0^2$ the energy in a particular capacitor in terms of the voltage V_0 across it, or $E_0 = \frac{1}{2}mv_0^2$ the kinetic energy of one particle in terms of its velocity v_0.

If we now assume that the overall system is in equilibrium at a temperature T, the expectation value for E_0 is given by the canonical statistical mechanics distribution: (β = kT)

$$\left\langle E_0 \right\rangle = \frac{\int_{-\infty}^{+\infty} e^{-\beta E(x_0,\dots,x_n)} E_0(x_0) dx_0 \cdots dx_n}{\int_{-\infty}^{+\infty} e^{-\beta E(x_0,\dots,x_n)} (x_0) dx_0 \cdots dx_n} =$$

$$= \frac{\int_{-\infty}^{+\infty} e^{-\beta [E_0(x_0)+E_1(x_1,\dots,x_n)]} E_0(x_0) dx_0 \cdots dx_n}{\int_{-\infty}^{+\infty} e^{-\beta [E_0(x_0)+E_1(x_1,\dots,x_n)]} dx_0 \cdots dx_n} =$$

$$= \frac{\int_{-\infty}^{+\infty} e^{-\beta E_0(x_0)} E_0(x_0) dx_0 \int_{-\infty}^{+\infty} e^{-\beta E_1(x_1,\dots,x_n)} dx_1 \cdots dx_n}{\int_{-\infty}^{+\infty} e^{-\beta E_0(x_0)} dx_0 \int_{-\infty}^{+\infty} e^{-\beta E_1(x_1,\dots,x_n)} dx_1 \cdots dx_n} =$$

$$= \frac{\int_{-\infty}^{+\infty} e^{-\beta E_0(x_0)} E_0(x_0) dx_0}{\int_{-\infty}^{+\infty} e^{-\beta E_0(x_0)} dx_0} = -\frac{\partial}{\partial \beta} \ln \int_{-\infty}^{+\infty} e^{-\beta E_0(x_0)} dx_0$$

if $E_0 = ax_0^2$, for some constant a, we can simplify the integral further:

($y^2 = \beta x_0^2$)

$$\langle E_0 \rangle = -\frac{\partial}{\partial \beta} \ln \int_{-\infty}^{+\infty} e^{-\beta E_0(x_0)} dx_0 = -\frac{\partial}{\partial \beta} \ln \int_{-\infty}^{+\infty} e^{-\beta a x_0^2} dx_0 =$$

$$= -\frac{\partial}{\partial \beta} \ln \left[\frac{1}{\sqrt{\beta}} \int_{-\infty}^{+\infty} e^{-ay^2} dy \right] = -\frac{\partial}{\partial \beta} \left[-\frac{1}{2} \ln \beta + \ln \int_{-\infty}^{+\infty} e^{-ay^2} dy \right] =$$

$$= \frac{1}{2} kT = a \langle x_0^2 \rangle$$

Each independent thermalized quadratic degree of freedom has an average energy of kT/2 due to fluctuations.

Fluctuation-Dissipation Theorem

The Equipartition Theorem relates the size of thermal fluctuations to the energy stored in independent degres of freedom of a system; the Fluctuations-Dissipation Theorem relattes the thermal fluctuations to the amount of dissipation. We will start with a simple example and then discuss the more general theory.

Consider an ideal inductor L connected in parallel with a resistor R. Because of thermal fluctuations there will be a voltage across the resistor; model that by a fluctuating voltage source V in series with a noiseless resistor.

The energy stored in an inductor is $L\,I^2/2$. Since the inductor is the only energy storage element, from the equipartition theorem we know what the current across it due to the thermal fluctuations must be:

$$\left\langle \frac{1}{2} L I^2 \right\rangle = \frac{1}{2} kT$$

Ohm's law still applies, so this current must also be equal to the fluctuating thermal voltage divided by the total impedance Z of the circuit.

$$I(\omega) = \frac{V(\omega)}{Z(\omega)} = \frac{V(\omega)}{R + j\omega L}$$

Writing the equipartition result in terms of frequency components,

$$\frac{1}{2}kT = \left\langle \frac{1}{2}LI^2 \right\rangle = \frac{1}{2}L\left\langle I^2 \right\rangle = \frac{1}{2}L\int_0^{+\infty}\left\langle \left|I(\omega)\right|^2 \right\rangle d\omega = \frac{1}{2}L\int_0^{+\infty}\left\langle \frac{\left|V(\omega)\right|^2}{\left|Z(\omega)\right|^2} \right\rangle d\omega =$$

$$= \frac{1}{2}L\int_0^{+\infty}\frac{\left\langle \left|V(\omega)\right|^2 \right\rangle}{R^2 + \omega^2 L^2} d\omega$$

since this is assumed to be an ideal resistor with no time constant from an inductive or capacitive component, it's reasonable assumption to take the fluctuating voltage V to have a delta function autocorrelation.

And since that implies that the power spectrum of the fluctuations is flat, V does not depend on *w* and come out of the integral:

$$\frac{1}{2}kT = \frac{1}{2}L\left\langle \left|V(\omega)\right|^2 \right\rangle \int_0^{+\infty} \frac{1}{R^2 + \omega^2 L^2} d\omega = \frac{\pi}{2}\frac{\left\langle \left|V(\omega)\right|^2 \right\rangle}{R}$$

therefore $\left\langle \left|V(f)\right|^2 \right\rangle = 4kTR$

This is the familiar Johnson noise formula.

Johnson noise is a simple example of a much more general relationship between the fluctuations in a system and the dissipation in the system: more dissipation implies smaller fluctuations.

Let's start by assuming that the microscvopic state of a system is indexed by a single degree of freedom x.
This mean that the entropy is a function of this variable, S(x).
In equilibrium, the system will be in the state that maximizes the entropy.
Taking for convenience this to be at $x = 0$.
the entropy can be approximed by a Taylor series around its maximum:

$$S = S_0 - \frac{1}{2} k\alpha x^2$$

(remember that there is no linear term around a maximum !!!)
The constant α determines how sharply peaked the entropy is.
The probability to see a state away from the maximun is then

$$p(x) \alpha \; e^{S(x)/k} \; \alpha \; e^{-\alpha \; x^2 / 2}$$

where x is a random variable.

$$p(x) \propto e^{S(x)/k} \propto e^{-\alpha x^2/2}$$

we see that it has a Gaussian distribution with a variance

$$\sigma^2 = \langle x^2 \rangle = \int x^2 p(x) dx = \frac{1}{\alpha}$$

- we see now why fluctuations such as Johnson noise so often have Gaussian distribution.

As α grows larger the entropy becomes more harply peaked $\Rightarrow$ the distribution becomes narrower.

If the state of the system is away from equilibrium there will be an effective restoring force that moves it back

This restoring force will depend on how the entropy varies with the state; the simplest assumption good for small deviations takes the time rate of change of the state to be proportional to the slope of the entropy.

$$R\frac{dx}{dt} = \frac{dS}{dx}$$

There are familiar examples of this kind of linear restoring force, such as Ohm's law IR=V, for which the flux dx/dt is the current I, the slope of the entropy dS/dx is the driving force V, and the damping constant R is the resistance.

Plugging into the quadratic expression of the entropy we get a stochastic differential equation for the relaxation of x

$$R\frac{dx}{dt} = -k\alpha\, x$$

Langevin equation

Squaring both sides and averaging over the times:

$$R^2 \left\langle \left(\frac{dx}{dt} \right)^2 \right\rangle = k^2 \alpha^2 \left\langle x^2 \right\rangle$$

The right side is just the variance, the size of the fluctuations;
To understand the left hand side we need to return to the restoring force:

$$P = \left(\frac{dS}{dx} \right)\left(\frac{dx}{dt} \right) = \left(R\frac{dx}{dt} \right)\left(\frac{dx}{dt} \right) = R\left(\frac{dx}{dt} \right)^2$$

the *power dissipated in time dt* is the energy; the restoring force (dS/dx), multiplied by the displacement dx, divided by dt;

therefore $P = \dfrac{k^2 \alpha^2 \left\langle x^2 \right\rangle}{R} = k^2 \dfrac{\alpha}{R}$ (remember $\sigma^2 = \left\langle x^2 \right\rangle = \dfrac{1}{\alpha}$)

Again: if the entropy is sharply peaked (α >> R), then the fluctuations will be small but the dissipation will be large.

Viceversa, if the entropy is flatter (α small), the fluctuations will be large but the dissipation will be small.

A related equation is found by multiplying both sides of equation by x and averaging:

$$R\,x\frac{dx}{dt} = -k\alpha\;x^2$$

$$R\frac{1}{2}\frac{dx^2}{dt} = -k\alpha\;x^2$$

$$\frac{d\left\langle x^2\right\rangle}{dt} = -2k\frac{\alpha}{R}\left\langle x^2\right\rangle$$

If the system is perturbed, the variance also relaxes at a rate proportional to α/R; It doesn't go to zero, of course, because we have left off the noise source term in the Langevin equation that drives the fluctuations

The equation $P = \frac{k^2\alpha^2\langle x^2\rangle}{R} = k^2\frac{\alpha}{R}$ is a simple example of the Fluctuation-Dissipation Theorem. In higher dimension the relaxation constant R becomes a matrix.....

The fluctuation dissipation theorem can be understood by remembering that a change in entropy is associated with a heat current $\delta Q = T\,dS$;
if the entropy is sharply peaked then the fluctuations lead a larger changes in entropy.

This is an essential tradeoff in the design of any system: the faster and more accurately you want it to do something, the more powerit will require.
For example, one of the most important lessons in the design of low-power electronics is to make sure tat the system does not produce results any faster than they are needed.
This also shows why, without knowing anything else about electronics, low-noise amplifiers require more power than noisy ones