

Lecture 6: Fluctuation-Dissipation theorem and introduction to systems of interest

In the last lecture, we have discussed how one can describe the response of a well-equilibrated macroscopic system to some external probe, and how this response encodes information about the excitations of the system. To do this, we developed the spectral representation (in terms of exact eigenstates of the system). We also saw how such formal spectral representations can lead to considerable insight, for instance, an appreciation of the Kramers Kronig relations that relate the real and imaginary part of the frequency dependent response functions to each other. One thing we did not emphasize in the previous lecture in this connection is the following: The real part of the response function measures the *in-phase* part of the response to a sinusoidal external field, while the imaginary part of the response function measures the *out-of-phase* part of the response function.

Now, we consider the question of energy dissipation. Intuitively, it is clear that some energy is dissipated into the macroscopic system if we drive it with an external field (think for instance of Joule heating in response to a current being driven in a system by an external potential). It is clearly interesting to ask: What aspect of the response determines the amount of energy dissipated into the system?

To answer this, we first demonstrate that the energy dissipated is intimately connected with the imaginary part $R''_{AA}(\omega)$ of the response function if an external field that couples to \hat{A} drives the system. Why is this the case? Well, let us start by recalling that the full time-dependent Hamiltonian of the system in the presence of the driving field is

$$H' = \hat{H} + b(t)\hat{A} \quad (1)$$

and the energy in the system at time t is therefore

$$E(t) = \langle \psi(t) | H' | \psi(t) \rangle_n \quad (2)$$

if the system was initially in energy eigenstate $|n\rangle$ of the system Hamiltonian H —here, $|\psi(t)\rangle_n$ denotes the state of the system at time t assuming it was in eigenstate $|n\rangle$ when the driving field was turned on, and, as usual, we will finally sum over initial states with the statistical Gibbs weight $\exp(-\beta E_n)/Z$. Next, we note that the rate of increase of $E(t)$ may be written as

$$\frac{dE(t)}{dt} = \langle \psi(t) | \frac{db(t)}{dt} \hat{A} | \psi(t) \rangle_n$$

$$= \langle \hat{A} \rangle_n(t) \frac{db(t)}{dt}. \quad (3)$$

In other words, the only contribution to the time derivative comes from the explicit dependence of $b(t)$ on t , since the contributions from the time dependences of the bra and the ket cancel each other. We now average over initial states $|n\rangle$ with the Gibbs distribution to get

$$\frac{dE(t)}{dt} = \langle \hat{A} \rangle_T(t) \frac{db(t)}{dt}. \quad (4)$$

where the subscript now reminds us that $\langle \hat{A} \rangle_T(t)$ denotes the response at time t of a system that was initially in equilibrium at temperature T . This response can now be represented in terms of the response function R_{AA} :

$$\langle A \rangle_T(t) = \int_{-\infty}^{\infty} dt' R_{AA}(t-t') b(t') \quad (5)$$

(here, we are assuming without loss of generality that $\langle A \rangle_T = 0$ in equilibrium—if this were not the case, one could simply redefine A to subtract out the corresponding constant piece).

Therefore, we have

$$\frac{dE(t)}{dt} = \int_{-\infty}^{\infty} dt' \frac{db(t)}{dt} R_{AA}(t-t') b(t'). \quad (6)$$

Integrating this, we obtain the total increase ΔE in the system energy:

$$\begin{aligned} \Delta E &= \int dt \frac{dE(t)}{dt} \\ &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} R_{AA}(\omega) \left(\int_{-\infty}^{\infty} dt \frac{db(t)}{dt} e^{-i\omega t} \right) \left(\int_{-\infty}^{\infty} dt' b(t') e^{i\omega t'} \right) \\ &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} i\omega R_{AA}(\omega) |b(\omega)|^2 \end{aligned} \quad (7)$$

Now, we note that

$$R'_{AA}(\omega) = R'_{AA}(-\omega), \quad (8)$$

i.e the real part of $R_{AA}(\omega)$ is an even function of the frequency. Therefore it does not contribute to the integral in the last line above. On the other hand, the imaginary part obeys

$$R''_{AA}(\omega) = -R''_{AA}(-\omega) , \quad (9)$$

i.e, the imaginary part of the response function is an odd function of the frequency, and therefore contributes to the integral that gives the total energy dissipated in the system.

Therefore, we obtain

$$\Delta E = - \int_0^\infty \frac{d\omega}{\pi} \omega R''_{AA}(\omega) |b(\omega)|^2 . \quad (10)$$

We can now recall spectral representation of R''_{AA} and use this to check that ΔE , as obtained from the above expression, will always be positive.

Indeed, from the spectral representation, it is quite easy to give a Fermi's Golden Rule type interpretation for this formula that we have derived. By inspection of the spectral representation derived in the last-but-one lecture, we see that $-R''(\omega)/\pi$ for positive ω gives the Fermi's Golden Rule probability for making a transition in which the energy of the system increases by ω due to the action of the perturbation. Multiplying this by the amount of energy gained, which is ω in our present units in which \hbar is set to 1, we immediately see how the formula derived above is indeed the correct result for ΔE , the energy dissipated in the system.

So $R''(\omega)$ tells us about dissipation in the system in response to a probe at frequency ω . Now, a system in equilibrium has fluctuations even in the absence of any external drive. These equilibrium fluctuations have a spectrum, and it is natural to ask if there is any simple and general connection between the spectrum of fluctuations and the dissipative part of the response—the intuition behind seeking such a connection is the idea that the external field must be driving those fluctuations whose natural frequencies are in resonance with the frequency of the external field.

To make this connection precise, we need to quantify what we mean by the spectrum of fluctuations. This is done by defining the time-dependent correlation function

$$\begin{aligned} S(t) &\equiv \langle A(t)A(0) \rangle_T \\ &= \frac{1}{Z} \text{Tr}(e^{-\beta H} e^{iHt} A e^{-iHt} A) \end{aligned} \quad (11)$$

The rationale for this definition is that it keeps track of the correlations between the Heisenberg operator $A_H(t)$ at different times. Such correlation functions play a key role in our theoretical description and understanding of collective behaviour of many-body systems both in and out of equilibrium, and much of the machinery of statistical mechanics and many-body theory is geared towards efficient and reliable calculations of such correlation functions.

However, experimental measurements always measure the response of the system to some field that is turned on by the experimentalist, and we have no “embedded observers” who can look inside the system and keep track of correlations. Therefore, it is of great interest to relate such time dependent correlations, at least in equilibrium, to the response of the same equilibrium system to some perturbing field. This is the main motivation for the result we are about to derive.

In any case, the next step is to write the trace as a sum over all exact eigenstates, and introduce a resolution of identity between the two occurrences of A . In this manner, we can rewrite the expression for $S(t)$ as

$$S(t) = \frac{1}{Z} \sum_{nm} e^{-\beta E_n} e^{i(E_n - E_m)t} |A_{nm}|^2 \quad (12)$$

Now, we may Fourier transform to define the frequency space density $S(\omega)$, which is usually referred to as the “dynamic structure factor”. In this manner, we obtain the following spectral representation for $S(\omega)$

$$\begin{aligned} S(\omega) &\equiv \int dt e^{i\omega t} \langle A(t) A(0) \rangle_T \\ &= \frac{2\pi}{Z} \sum_{nm} e^{-\beta E_n} |A_{nm}|^2 \delta(\omega - E_{mn}) \end{aligned} \quad (13)$$

Now, the idea is to compare this expression with that for the imaginary part of the corresponding response function:

$$R''_{AA}(\omega) = -\frac{\pi}{Z} \sum_{mn} |A_{nm}|^2 e^{-\beta E_n} (\delta(\omega - E_{mn}) - \delta(\omega + E_{mn})) \quad (14)$$

The above expression has the inconvenient (for our purposes below) feature that the two terms have two different delta functions. However, it is easy to transform this into an expression made up of two terms, both of which have the same delta function but different coefficients in front of the delta

function. This is achieved by interchanging the dummy indices m and n in the second summation to obtain:

$$\begin{aligned}
R''_{AA} &= -\frac{\pi}{Z} \sum_{mn} |A_{nm}|^2 (e^{-\beta E_n} - e^{-\beta E_m}) \delta(\omega - E_{mn}) \\
&= -\frac{\pi}{Z} \sum_{mn} |A_{nm}|^2 e^{-\beta E_n} (1 - e^{-\beta E_{mn}}) \delta(\omega - E_{mn}) \\
&= -\frac{\pi}{Z} \sum_{mn} |A_{nm}|^2 e^{-\beta E_n} (1 - e^{-\beta \omega}) \delta(\omega - E_{mn}) , \tag{15}
\end{aligned}$$

where the last line is obtained by noting that E_{mn} can be replaced by ω in the prefactor to $\delta(\omega - E_{mn})$.

This is now in a form that allows direct comparison with the spectral representation of $S(\omega)$. And thus, we obtain the well-known *fluctuation-dissipation theorem* of linear response theory:

$$R''_{AA}(\omega) = -\frac{1}{2}(1 - e^{-\beta \omega})S(\omega) \tag{16}$$

or

$$S(\omega) = \frac{-2}{1 - e^{-\beta \omega}} R''_{AA}(\omega) \tag{17}$$

With all of this in hand, we now move on to a brief overview of the physical systems of interest to us. Typically, statistical physics is used to describe the behaviour of classical and quantum condensed matter systems. The former are composed of atoms or molecules that interact weakly through Lennard-Jones type potentials, and are typically classical because the temperature at which they are studied is relatively large, and the fermionic or bosonic statistics of the constituent particles plays little or no role in determining the macroscopic properties. In contrast, electrons in a solid at very low temperature, or Helium-3 and Helium-4 at very low temperature, constitute a quantum fluid because the temperatures are low enough that the quantum statistics of the constituents plays an important role in determining the macroscopic properties.

For instance, the behavior of ultra-cold bosonic atoms in atom-trap experiments at very low temperature is determined to a reasonably large extent by Bose-Einstein distribution function which determines the probabilities with which the atoms occupy various plane-wave states. Similarly, electrons in a

metallic solid at very low temperature form a degenerate “fermi-liquid” whose behaviour is largely controlled by the Fermi-Dirac statistics of the electrons. Roughly speaking, the physics is determined by the spectrum of itinerant (traveling) electron waves and the occupation of these traveling wave states according to the Fermi-Dirac distribution.

This is however not the case when electron-electron interactions cause the electrons to localize on to individual ions of an ionic insulator. In such cases, the traveling wave picture of electronic states is not valid, and a much better description is a local one whereby one imagines a lattice of ions, each with an optimal charge on it. Movement of electrons is forbidden by the fact that such motion involves transferring charge from one ion to another and is energetically very “expensive” due to the large charging energy of these little “ionic capacitors”. Such insulators are called “Mott insulators” after Sir Neville Mott who first described the mechanism that forces the electron fluid to make a transition to an insulating state.

In such Mott insulators, the charge of an electron is no longer an active participant in the low temperature physics since it is “frozen out” by the requirement that each ion have an optimal energetically favourable charge configuration that minimizes the Coulomb repulsion energy between electrons. However, in many such Mott insulators, the optimal number of electrons on some ions can be odd. In such cases, the ion has a spin degree of freedom (we are imagining that the orbital angular quantum number is quenched by crystal field effects familiar from solid state physics). These spins are typically coupled antiferromagnetically to each other (we will see exactly how in more detail later), and the low energy physics is thus determined by the behaviour of a system of interacting quantum mechanical spins.

Thus, the principal players in our story are itinerant fermions and bosons, and quantum mechanical spins which may be thought of as electrons that have lost the ability to hop from ion to ion. Starting with the next lecture we will introduce a very convenient path-integral formalism for working with the partition function for bosons, fermions or spins, and computing various properties of such systems in equilibrium. Then we will take up an example and examine in more detail the issues of symmetry breaking and stability associated with phases that develop long-range order when the equilibrium state breaks some global symmetry of the underlying Hamiltonian.