Lecture 5: Linear response theory-II (Properties of response kernel)

In the last lecture, we derived the formula for the linear response kernel that relates the response of an observable to the action of a perturbing field at previous times in a system initially in equilibrium. When is this linear response treatment valid? Unfortunately, there is no simple, general prescription for the validity of the linear approximation. All one can say is that if the perturbation is "weak enough", the leading behaviour is captured by the above linear response treatment. In any case, experimentalists usually have good ways of deciding via independent measurements whether they have perturbed the system beyond its linear regime, and are able to extract the linear response coefficients by careful measurements. It is such careful linear response measurements that the linear response formalism attempts to describe.

An important special case of all of the foregoing is when the perturbation couples to an operator A, which is the same as the observable being measured. For instance, one can imagine appling a spatially varying external potential and measuring the response of the density of the system. Or one can imagine applying an external magnetic field to a system of magnetic moments, and measuring the resulting change in the magnetization density of the system. In this special case, we have

$$R_{AA}(t-t') = -\frac{i\theta(t-t')}{Z}\mathrm{Tr}(e^{-\beta H}[A_H(t), A_H(t')]) \tag{1}$$

At this point, one must remember that this formula is deceptively simple looking—that this is the case becomes clear upon remembering that $A_H(t)$ does not commute with $A_H(t')$ unless A is a conserved quantity and itself commutes with the system Hamiltonian H.

Before we move on to discuss the properties of the linear response function in more detail, it is perhaps important to first highlight the following subtlety: When $B = A$ is a conserved quantity, the linear response is predicted to be zero by the foregoing formula, since the commutator is zero. However, we know that a uniform external field, that couples to the total magnetization (which is a conserved quantity), does change the magnetization of the system by an amount proportional to the field, *i.e.* within linear response. So what goes wrong with the formalism developed here? The answer has to do with the fact that we have assumed that the initial state of the system at time t_0

far in the past is drawn from an ensemble governed by the Gibbs probability for the system with Hamiltonian H. And since the quantity to which the external perturbation couples is conserved, there is no way for the system to change this "incorrect" probability distribution and replace it by a slightly perturbed probability distribution that takes into account the linear effect of the uniform field that couples to the conserved magnetization. This makes sense: If the magnetization were truly conserved on the time scale of the experiment, and if the external field was truly uniform, then it would indeed be impossible for the external field to change the magnetisation. A better description of the real experimental conditions is therefore to take a slightly non-uniform external field varying in time at some low frequency ω, and measure the linear response at the corresponding small wavevector q and frequency ω. Then, the linear response formalism developed here will give a sensible result, which should be extrapolated to the uniform d.c. limit by *first sending the frequency to zero keeping the wavevector non-zero, and then send q to zero.*

With that in mind, we turn to the focus of this lecture, namely the special case in which $A = B$. This is often the case of interest in experimentally relevant examples—for instance B could be the uniform magnetic field in the z direction, and A could be the z component of the total magnetization operator of the system. Another example that crops up often is the case when B is an external potential oscillating at wavevector q in space, and A is the component of the total density of the system at the same wavevector q.

As in the analysis of many other time-dependent phenomena in Physics, much insight can be gained by going over to frequency space and analyzing the properties of $R_{AA}(\omega)$. To this end, we define

$$R_{AA}(\omega) \;=\; \int_{-\infty}^{\infty} dt e^{i\omega t} R_{AA}(t) \tag{2}$$

Recalling the expression for $R_{AA}(t)$ in terms of a commutator of $A_H(t)$ with $A_H(0)$, and the definition of $A_H(t)$ as

$$A_H(t) \;\equiv\; \exp(iHt) A \exp(-iHt) \;, \tag{3}$$

we may expand this in terms of the exact eigenstates $|m\rangle$ of H and the corresponding eigenenergies E_m.

Indeed, if we recall the derivation in the previous lecture, it is from such an expansion that we had derived the compact expression for $R_{AA}(t)$ in terms of the commutator of $A_H(t)$ with $A_H(0)$, and by going back to the definition of $A_H(t)$ and expanding in terms of the complete set of states $|m\rangle$, we are merely going back to the corresponding intermediate step in our derivation of the result for $R_{AA}(t)$. This is nevertheless useful, since we can do the Fourier transform from $R_{AA}(t)$ to $R_{AA}(\omega)$ by doing the Fourier transform of *each term in this expansion.* In other words, we can write

$$R_{AA}(\omega) = -\frac{i}{Z}\int_{-\infty}^{\infty} dt\theta(t)e^{i\omega t}\sum_{m,n}|A_{nm}|^2 e^{-\beta E_n}(e^{-iE_{mn}t} - e^{iE_{mn}t}) , \quad (4)$$

and take the integral inside the summation sign to obtain:

$$R_{AA}(\omega) = -\frac{i}{Z}\sum_{m,n}|A_{nm}|^2 e^{-\beta E_n}\left[\int_{-\infty}^{\infty} dt\theta(t)e^{i(\omega - E_{mn})t} - \int_{-\infty}^{\infty} dt\theta(t)e^{i(\omega+E_{mn})t}\right] \quad (5)$$

Here and henceforth in this lecture, we are using the compact notation $E_{mn} = E_m - E_n$ and $E_{nm} = E_n - E_m$.

We now note that this can be written as a linear combination of the Fourier transform of the Heaveside step function at two different frequencies:

$$R_{AA}(\omega) = -\frac{i}{Z}\sum_{m,n}|A_{nm}|^2 e^{-\beta E_n}\left(\hat{\theta}(\omega - E_{mn}) - \hat{\theta}(\omega + E_{mn})\right)$$

Thus, we need to only ask:

What is $\hat{\theta}(\omega)$?

and the answer will lead us to the expression for $R_{AA}(\omega)$.

To answer this question, we make a guess, and then check that it is correct. The guess is

$$\hat{\theta}(\omega) = \lim_{\eta\to 0^+}\frac{i}{\omega + i\eta} \quad (6)$$

To check this, we compute the inverse Fourier transform

$$\lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{i}{\omega + i\eta}e^{-i\omega t} \quad (7)$$

by contour integration as follows: The initial contour is an open contour from $-\infty$ to $+\infty$ along the real axis in the ω plane, and because η is a small

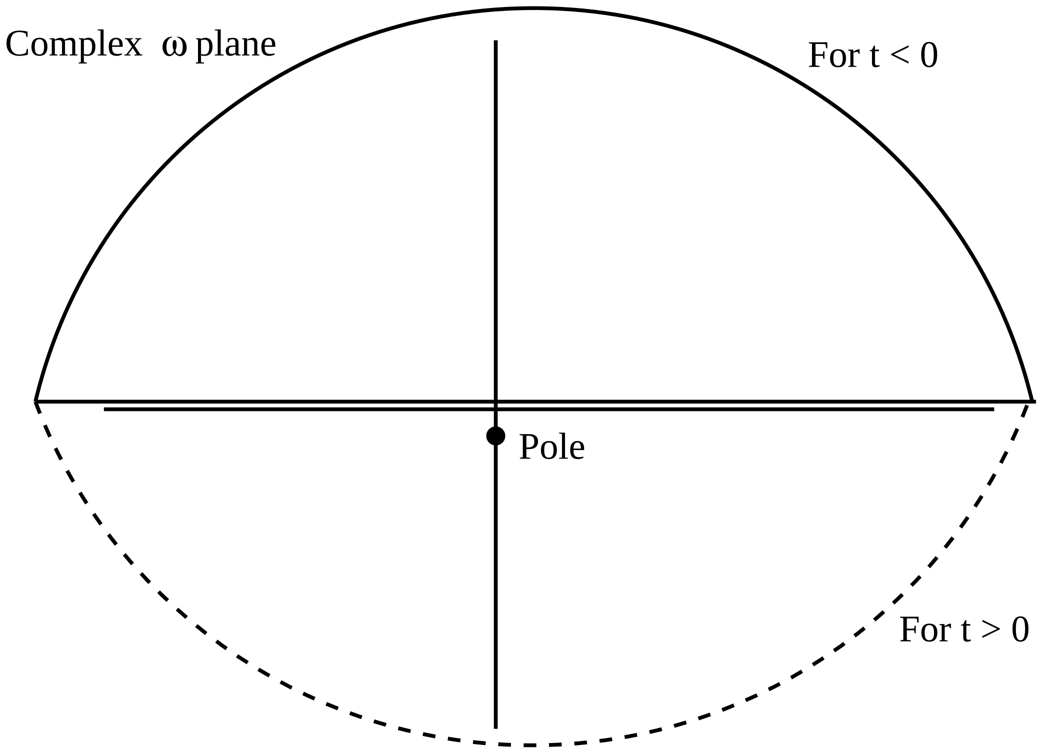

Figure 1: Completing the contour to calcuate the inverse Fourier transform of $i/(\omega + i\eta)$

positive real number that is sent to zero at the end of the calculation, we are allowed to close this contour by adding a large semicircle "at infinity" so long as it gives a zero contribution to the contour integral. For $t > 0$, this is guaranteed if the semicircle at infinity is in the lower half-plane. The closed contour then encloses the pole at $\omega_{\rm pole} = -i\eta$, and the integral then equals $+1$ (see Fig 1). On the other hand, for $t < 0$, the semicircle at infinity must be in the upper half-plane if it is to not contribute, and therefore the contour gets closed in the upper half-plane without enclosing any pole. As a result, the original integral is 0. Thus we have

$$\lim_{\eta \to 0^+} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{i}{\omega + i\eta} e^{-i\omega t} \quad = \quad \theta(t) \tag{8}$$

which proves that our guess was correct.

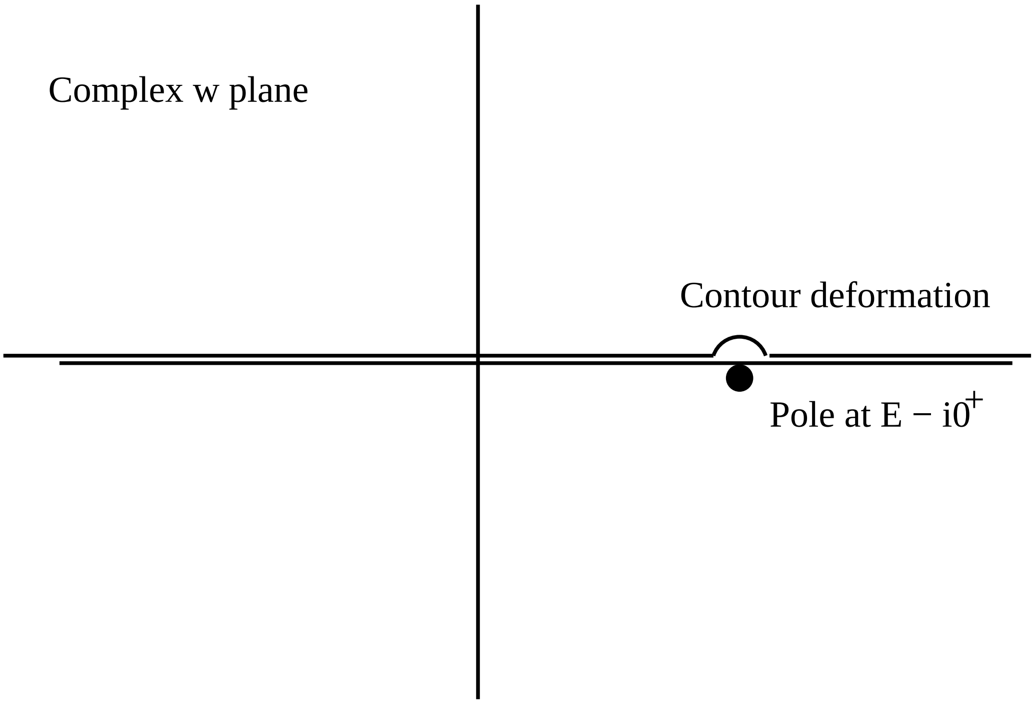

Figure 2: Contour deforms in response to the pole $E - i\eta$ being "pushed up" to the real axis

So we have

$$R_{AA}(\omega) = \frac{1}{Z}\sum_{m,n} |A_{nm}|^2 e^{-\beta E_n}\left(\frac{1}{\omega - E_{mn} + i\eta} - \frac{1}{\omega + E_{mn} + i\eta}\right) \quad (9)$$

Here, the limit $\lim_{\eta\to 0^+}$ is implicit. To explicitly take this limit, we need to remember the following fact from our Complex Analysis or Mathematical Methods course:

$$\lim_{\eta\to 0^+} \frac{1}{\omega - E + i\eta} = \mathrm{Pr}\,\frac{1}{\omega - E} - i\pi\delta(\omega - E) \quad (10)$$

In case you haven't seen this before, let me give you a quick way to understand this formula: Consider doing the integral

$$\int_{-\infty}^{\infty} d\omega \frac{f(\omega)}{\omega - E + i\eta} \quad (11)$$

where again the limit $\lim_{\eta \to 0^+}$ is implicit, and will be taken at the end, and f is any "good" real-valued function of the real frequency ω, *i.e.* smooth enough and falling off rapidly enough at infinity. To do this integral, we may again use the method of contour integration: The initial contour is an open contour along the real ω axis from $-\infty$ to $+\infty$. To evaluate this integral, we note the following: As η is sent to 0^+, we can deform the contour continuously so that it develops a little semicircular bump above the real axis, centered at E (see Fig 2).

The full integral can thus be obtained as a sum of two contributions. The first contribution is a sum of two parts: The first part is the integral along the real axis from $-\infty$ to $E - \eta$, and the second part is the integral along the real axis from $E + \eta$ to $+\infty$. This is a purely real contribution, and the limit $\eta \to 0^+$ of this first contribution is precisely what we mean by the Cauchy principal value Pr in the mathematics of singular integrals. The second is the contribution of the little semicircle in the upper half-plane of radius η centered at E. This give a purely imaginary contribution equal to half the residue from the pole of the integrand at $E - i0^+$.

Clearly, the first term in the quoted formula yields the Cauchy principal value contribution, while the secod term that involves a delta function is precisely what is needed to give the second residue contribution which is purely imaginary.

With this in mind, we see that we can now write

$$\begin{aligned} R_{AA}(\omega) &= \frac{1}{Z}\sum_{m,n}|A_{nm}|^2 e^{-\beta E_n}\left(\mathrm{Pr}\,\frac{1}{\omega - E_{mn}} - \mathrm{Pr}\,\frac{1}{\omega + E_{mn}}\right) \\ &\quad -\frac{i\pi}{Z}\sum_{m,n}|A_{nm}|^2 e^{-\beta E_n}\left(\delta(\omega - E_{mn}) - \delta(\omega + E_{mn})\right) \end{aligned}$$

Writing $R_{AA}(\omega) = R'(\omega) + iR''(\omega)$ and comparing with the above, we thus obtain formal spectral representations for the real and the imaginary parts of R.

With this in hand, we now establish a very general, and at first sight somewhat surprising connection between the real and the imaginary parts of $R_{AA}(\omega)$. This connection is usually referred to as the "Kramers-Kronig" relations.

One half of this connection—the part that expresses R' in terms of an integral over R'' can be established by inspection and reads

$$R'_{AA}(\omega) \;=\; \mathrm{Pr}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{R''_{AA}(\omega')}{\omega' - \omega} \tag{12}$$

To see that this is true, simply plug in the spectral representation of R''_{AA} on the right hand side, and do the ω' integral (which is straightforward since the integrand contains a delta function).

Let me now pose a question: Can you find inverse relation, *i.e* a formula that expresses R''_{AA} as an integral over R'_{AA} times something? The answer to this question is considerably less obvious, at least at first sight.

One way to see how it goes is to begin by noting that $R_{AA}(\omega)$, analytically continued to complex frequency plane, *i.e.* defined by replacing $\omega + i\eta$ in the spectral representation for R_{AA} by the complex number z, has no poles in the upper half plane—this is clear from the spectral representation of $R_{AA}(z)$, and is actually a consequence of *causality*, *i.e* the fact that any perturbation can only affect the behaviour of the system at later times and not before it is applied. Therefore, the contour integral

$$\oint_C dz \frac{R_{AA}(z)}{z - \omega + i\eta} \tag{13}$$

taken over a contour C, that travels from $-\infty$ to $+\infty$ along the real z axis and then return along a semicircular path in the upper half-plane, must give zero by the residue theorem, since it encloses no poles either of $R(z)$ or of $1/(z - \omega + i\eta)$, where η is a positive real number, and ω is a real frequency (again, the $\eta \to 0^+$ limit is implicit, and will be taken at the end).

Thus we have the equation

$$\oint_C dz \frac{R_{AA}(z)}{z - \omega + i\eta} \;=\; 0 \tag{14}$$

Now, on physical grounds, namely, the fact that a system cannot respond to an arbitrarily high-frequency perturbation because the response time cannot be arbitrarily short, we expect $R_{AA}(z)$ to decay rapidly at large $|z|$ in the complex plane. Therefore, the contribution of the semicircle at infinity in the upper half plane must be zero. Therefore, we obtain the equation

$$\int_{-\infty}^{\infty} d\omega' \frac{R_{AA}(\omega')}{\omega' - \omega + i\eta} \;=\; 0 \tag{15}$$

We may now take the real and the imaginary parts of this complex equation (complex because R_{AA} is complex even for real arguments, and because the $\eta \to 0^+$ limit of the denominator yields both a real and an imaginary part, as seen earlier).

The imaginary part of this equation gives back the first Kramers-Kronig relation that relates the real part of R_{AA} to an integral over the imaginary part of R_{AA}. But now, we have an additional relation, obtained by taking the *real* part of this equation. This gives the required representation of the imaginary part of R_{AA} in terms of an integral over the real part of R_{AA}:

$$R''_{AA}(\omega) = -\,\mathrm{Pr}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{R'_{AA}(\omega')}{\omega' - \omega} \tag{16}$$

These are the Kramers-Kronig relations. They are very useful if one has limited experimental data, and wants to draw some conclusions about parts of the response that have not been measured. In the next lecture, we will explore another aspect of the frequency dependent response by understanding just how the imaginary part of the response function signals dissipation of energy into the system from the source of the external field applied to the system, and how the amount of energy dissipated is intimately connected with the frequency spectrum of equilibrium fluctuations in the system.