Lecture 4: Linear response theory-I (Derivation of response kernel)

As we have already argued in the first lecture, when dealing with a macroscopic system, *i.e.* a system whose volume V tends to infinity, $V \to \infty$, with the density ρ remaining a constant, it doesnt make sense for us to follow the tracks of each constituent particle (thinking classically, in regimes where quantum effects are not important), nor does it make sense for us to attempt to follow the unitary time evolution of the full many-particle wave function of the system as a whole.

As we reminded ourselves in the very first lecture, the standard solution to this difficulty is to adopt a *statistical approach*, and take recourse to the language of probabilities and *expected values* for physical observables. From this point on in my lectures, this is the point of view we adopt without further comment. In other words, everything from now on flows from the "master-formula"

$$Z \;=\; \sum_n e^{-\beta E_n} \equiv \mathrm{Tr}\; e^{-\beta \hat{H}} \tag{1}$$

Here, the idea is that

$$\frac{e^{-\beta E_n}}{Z}$$

is the probability with which the system is in a particular eigenstate n with energy E_n when it is in equilibrium.

This probability is to be used to make experimentally verifiable predictions for the expected value of any observable A. The self-evidently correct prescription for this is:

$$A_{\mathrm{measured}} \;=\; \frac{1}{Z}\sum_n \langle n|A|n\rangle e^{-\beta E_n} \equiv \frac{1}{Z}\mathrm{Tr}\;(\hat{A}e^{-\beta \hat{H}}). \tag{2}$$

From the usual analysis of the relative size of fluctuations in large systems, we expect that this gives an asymptotically exact prediction for the measured value of A in the $V \to \infty$ limit, as long as A is an *extensive* variable, *i.e.* a variable which gets additive contributions proportional to their volumes from different subsystems of the full system.

What we have just described is the so-called "canonical ensemble" of statistical mechanics in which the number of constituents and the volume are fixed (we are implicitly imagining a system of interacting particles in a "box", *i.e.* a gas or a liquid in a container). As we know from elementary courses on Statistical Physics, and as we reminded ourselves in the first lecture, there is another alternative we can use, if we need to obtain predictions for fluctuations in the number of particles, or for quantities like the compressibility. This is the "grand-canonical" approach. In this approach, we work in an extended hilbert space with varying numbers of particles

$$Z_{GC} = \sum_n e^{-\beta(E_n - \mu N_n)} \tag{3}$$

Again

$$\frac{e^{-\beta(E_n-\mu N_n)}}{Z_{GC}}$$

is probability to be in particular state with energy E_n and number N_n.

The *expected number* of particles, which will correspond to the result, N_{measured}, of a measurement of the number of particles present in the thermodynamic limit, is of course given as

$$N_{\text{measured}} = \langle N \rangle_{GC} = \frac{1}{Z_{GC}} \sum_n \langle n|\hat{N}|n\rangle e^{-\beta(E_n-\mu N_n)} = \frac{1}{Z_{GC}} \text{Tr}\left(\hat{N} e^{-\beta(\hat{H}-\mu/\hat{N})}\right) \tag{4}$$

At this point, it is important to quickly remind ourselves how the size of the system enters the discussion, *i.e.* just why is it that this statistical approach is expected to become asymptotically exact for *extensive* quantities in the *thermodynamic limit* of a large system size.

A measurement of an extensive quantity A gets contributions from all regions of the sample, with the contribution of a given region proportional to its size. In other words, we expect it to have a well-defined *density* a_x such that

$$A = \sum_x a_x$$

What is our expectation for the mean-square fluctuations of the actual, measured value of A from the expected value $\langle A \rangle$ computed by our statistical

prescription using the partition function? Clearly the answer is:

$$\begin{aligned}\langle (A - \langle A \rangle)^2 \rangle &= \langle \left(\sum_x a_x - \langle \sum_{x'} a_{x'} \rangle \right)^2 \rangle \\ &= \langle \sum_{xx'} a_x a_{x'} \rangle - \langle \sum_x a_x \rangle \langle \sum_{x'} a_{x'} \rangle \ . \end{aligned} \tag{5}$$

In the above $\langle \ldots \rangle$ denotes the expected value as computed from our statistical prescription.

Now , a_x and $a_{x'}$ will not "know about" each other if $|x - x^{'}| \gg \xi$ where ξ is the so-called "correlation length". Since the notion of a correlation length is crucial in some of our later discussion, this is perhaps a good time for a brief digression: As we know from studies of Brownian motion and associated phenomena, equilibrium systems are not *static* systems. In fact, there exist fluctuations about the mean in all equilibrium systems. These fluctuations are cooperative in nature, in the sense that regions of order the correlation volume ξ^d fluctuate in tandem (here d is the spatial dimension). A good strategy to get a handle on the correlation length ξ is to measure some quantity whose value depends on the so-called "connected correlation function"

$$G(x - x^{'}) = \langle a_x a_{x'} \rangle_c \equiv \langle a_x a_{x'} \rangle - \langle a_x \rangle \langle a_{x'} \rangle \tag{6}$$

For $|x - x^{'}| \gg \xi$, we expect

$$\langle a_x a_{x'} \rangle = \langle a_x \rangle \langle a_x^{'} \rangle$$

and the connected correlation function vanishes.

It is this correlation length ξ that determines how quickly fluctuations become unimportant (compared to the mean values computed from our statistical prescription). To see this, we begin by noting that

$$G(r) \sim \frac{1}{\xi^{d-2+\eta}} F(r/\xi) \tag{7}$$

with $F(r/\xi) \sim \exp(-r/\xi)$ for $r \gg \xi$ and $F(r/\xi) \sim (\xi/r)^{d-2+\eta}$ for $a \ll r \ll \xi$ (where a is a microscopic length scale like the lattice spacing), provides a good description of the long-distance properties of the connected correlation function both in a phase and at a phase transition between two phases. In

a phase, ξ is finite, while at a second-order phase transition, ξ diverges, reducing the above form to a power-law with power parameterized in terms of the dimensionality d and "anomalous exponent" η (we will be studying such critical exponents in some detail later in this course). Now, the expected mean-square fluctuations in a sample of size L^d can be estimated as

$$\langle (A - \langle A \rangle)^2 \rangle \;\; = \;\; \int_{L^d} \int_{L^d} d^d x d^d x^{'} G(x - x^{'}) \tag{8}$$

As a result, the *relative* strength of fluctuations, *i.e* the ratio of the root-mean-square fluctuations and the average value, scales as

$$\frac{\sqrt{\langle (A - \langle A \rangle)^2 \rangle}}{\langle A \rangle} \;\; = \;\; \frac{1}{L^{d/2}} \tag{9}$$

as long as ξ is finite (ξ enters this formula in the prefactor, which is not displayed explicitly). Thus, our statistical prescription $\langle A \rangle$ for the measured value $A_{\rm measured}$ becomes asymptotically exact in the $L \to \infty$ thermodynamic limit. What happens at a critical point, when ξ diverges? Revisiting the above analysis, it is easy to see that the $\langle A \rangle$ continues to become asymptotically exact in the $L \to \infty$—however, flucutations are more important than in a phase, since

$$\frac{\sqrt{\langle (A - \langle A \rangle)^2 \rangle}}{\langle A \rangle} \;\; = \;\; \frac{1}{L^{(d-2+\eta)/2}} \tag{10}$$

With this digression out of the way, let us move on by noting that fluctuations in every globally conserved quantity can be studied by using a generalized ensemble in which that quantity is allowed to fluctuate, but a "conjugate" Lagrange multiplier variable is held fixed—we have already seen an example of this in our review in the first lecture. This Lagrange multiplier variable plays the same role as the chemical potential. For example, later in this course we will have occasion to study the cooperative behaviour of magnetic moments in an insulating solid. In this case, it is not natural to work in an ensemble in which the total magnetization is held fixed, since conventional experimental protocols do not allow one to establish such conditions in the laboratory. The conjugate chemical potential-like variable in this case is the external magnetic field. And it is therefore much more natural to work in an ensemble in which the external magnetic field is held fixed—this is indeed what we will do later in this course.

Now, the total magnetization M or the total number of particles N are what one usually calls "thermodynamic quantitites" or "static observables". However, experimental measurements are of course not restricted to such static properties. Many of the most useful experiments involve "dynamical" measurements. A typical measurement of this type can be modeled as follows: A system initially in equilibrium is weakly disturbed with an external "field" which is turned on at some time. This field is left on (possibly with some oscillatory behaviour) for some time, taking care that its strength remains low enough that the perturbation felt by the system remains within the realm of linear behaviour. A probe measures the response of the system by monitoring the value of some physical observable.

How are such dynamical measurements to be thought about within the framework of Statistical Physics? This is somehow not as well known as it should be, since it "falls in the crack" between a conventional Classical or Qauntum Mechanics course, and a conventional Statistical Physics course. Since it plays a key role in connecting theoretical insights of Statistical Physics to the results of experimental measurements, we will summarize here the so-called "linear-response formalism" for dynamical measurements.

Such a description is quite straightforward to set up: One starts with a system initially in equilibrium, *i.e.* in an initial eigenstate $|n\rangle$ with probability $e^{-\beta E_n}/Z$. The subsequent time evolution is described by the Schrodinger equation of motion (we will not bother to put in factors of $\hbar$ unless we want to emphasize dimensional aspects of our final answer) for the state of the system:

$$i\frac{d|\psi\rangle}{dt} = (H + b(t)B)|\psi\rangle \tag{11}$$

Here, H is the Hamiltonian of the system of interest, and $b(t)B$ is the external perturbation (B is the operator to which the external classical field $b(t)$ couples).

Next, we write this equation in terms of $\psi_m = \langle m|\psi\rangle$

$$i\frac{d\psi_m(t)}{dt} = E_m\psi_m + b(t)\sum_{m'} B_{mm'}\psi_{m'}(t) \tag{12}$$

where $B_{mm'} = \langle m|B|m'\rangle$. Now, it is useful to "factor out" the time-evolution that would anyway occur in the absense of the external perturbation $b(t)B$.

To this end, we write $\psi_m(t) = e^{-iE_m t}\tilde{\psi}_m(t)$, and in terms of $\tilde{\psi}_m(t)$, we have

$$\begin{aligned} & i\frac{d\tilde{\psi}_m(t)}{dt}e^{-iE_m t} + E_m e^{-iE_m t}\tilde{\psi}_m(t) = \\ & E_m e^{-iE_m t}\tilde{\psi}_m(t) + b(t)\sum_{m'} B_{mm'}e^{-iE_{m'}t}\tilde{\psi}_{m'}(t). \end{aligned} \tag{13}$$

i.e.

$$i\frac{d\tilde{\psi}_m(t)}{dt} = b(t)\sum_{m'} B_{mm'}e^{i(E_m - E_{m'})t}\tilde{\psi}_{m'}(t). \tag{14}$$

As expected

$$i\frac{d\tilde{\psi}_m(t)}{dt} = 0$$

when $b = 0$, *i.e.* $\tilde{\psi}_m(t) = \tilde{\psi}_m(t_0)$, the state of the system at time t_0 in the distant past.

The evolution equation is now in a form that allows for a straightforward iterative solution. We need to carry this out only to linear order in b. To this order, we can write

$$\tilde{\psi}_m(t) = \tilde{\psi}_m(t_0) - i\sum_{m'}\int_{t_0}^{t} dt' b(t') B_{mm'}e^{i(E_m - E_{m'})t'}\tilde{\psi}_{m'}(t_0). \tag{15}$$

Now, let us choose $\tilde{\psi}_m(t_0) \equiv \delta_{mn}$, *i.e.* choose the initial state to be $|n\rangle$. let us call this solution $\tilde{a}_{mn}(t)$. For this solution, we have

$$\tilde{a}_{mn}(t) = \delta_{mn} - i\int_{t_0}^{t} dt' b(t') B_{mn}e^{i(E_m - E_n)t'} \tag{16}$$

From this, we can calculate $|\psi(t)\rangle$ to first order by noting that

$$\begin{aligned} |\psi(t)\rangle &= \sum_m a_{mn}(t)|m\rangle \\ &= \sum_m e^{-iE_m t}\tilde{a}_{mn}(t)|m\rangle \end{aligned} \tag{17}$$

In this manner, we obtain

$$|\psi(t)\rangle \;=\; e^{-iE_nt}|n\rangle - i\sum_m \int_{t_0}^{t} dt' b(t') B_{mn} e^{-iE_mt} e^{i(E_m-E_n)t'} |m\rangle \quad (18)$$

Now, we can use this to compute $\langle A\rangle_n$, the value of A at time t when the initial state was $|n\rangle$ at time t_0 far in the past:

$$\begin{aligned}\langle\psi(t)|A|\psi(t)\rangle_n \;&=\; A_{nn} - i\int dt' b(t') \sum_m e^{i(En-E_m)(t-t')} A_{nm}B_{mn} \\ &\quad +i\int dt' b(t') \sum_m e^{-i(E_n-E_m)(t-t')} B^{\star}_{mn}A_{mn}\end{aligned} \quad (19)$$

In the absence of the perturbation, a system that was in state $|n\rangle$ at time t_0 far in the past would have remained in that state and had a value A_{nn} for the observable A at all future times t. Therefore, $\delta\langle A\rangle$, the change in A due to the action of the perturbation, can be computed by subtracting out this part and averaging over all initial states $|n\rangle$ with the Gibbs probability distribution $\exp(-\beta E_n)/Z$:

$$\begin{aligned}\delta\langle A\rangle(t) \;&=\; \frac{i}{Z}\sum_{m,n}\int_{t_0}^{t} dt' b(t') e^{-\beta E_n} B_{nm}A_{mn} e^{-i(E_n-E_m)(t-t')} \\ &\quad -\frac{i}{Z}\sum_{m,n}\int_{t_0}^{t} dt' b(t') e^{-\beta E_n} B_{mn}A_{nm} e^{+i(E_n-E_m)(t-t')} \\ &=\; -\frac{i}{Z}\int_{t_0}^{t} dt' b(t') \sum_n e^{-\beta E_n}\langle n|[e^{iHt}Ae^{-iHt}, e^{iHt'}Be^{-iHt'}]|n\rangle\end{aligned} \quad (20)$$

This can be written in a more compact and basis independent way in the following way:

$$\begin{aligned}\delta\langle A\rangle(t) \;&=\; -\frac{i}{Z}\int_{-\infty}^{t} dt' b(t') \mathrm{Tr}(e^{-\beta H}[A_H(t), B_H(t')]) \\ &=\; -\frac{i}{Z}\int_{-\infty}^{\infty} dt' b(t') \theta(t-t') \mathrm{Tr}(e^{-\beta H}[A_H(t), B_H(t')])\ .\end{aligned} \quad (21)$$

This is conventionally represented by defining a response function, $R_{AB}(t-t')$ which, by definition, gives $\delta\langle A\rangle(t)$ via the relation

$$\delta\langle A\rangle(t) = \int_{-\infty}^{\infty} dt^{'} R_{AB}(t-t^{'})b(t^{'}) \ , \tag{22}$$

This response function clearly has the compact formula

$$R_{AB}(t-t^{'}) \ = \ -\frac{i\theta(t-t')}{Z}\mathrm{Tr}(e^{-\beta H}[A_H(t), B_H(t')]) \tag{23}$$

Here, the Heaveside step function $\theta(t-t')$ has been included to ensure the proper limits of integration, which make sure that the external field at time $t^{'}$ can only affect values of A at *later times*, as is of course required by causality, and as is clear already from the expression we have derived above.

In Fourier (frequency) space, we can write this expression more compactly as

$$\delta\langle A\rangle(\omega) \ = \ \int_{-\infty}^{\infty} d\omega R_{AB}(\omega)b(\omega) \ , \tag{24}$$

where $R_{AB}(\omega)$ is the Fourier transform of $R_{AB}(t)$. Not surprisingly, within the present *linear* approximation, an external perturbation at frequency ω produces a response at the same frequency ω. Higher order nonlinear terms would also involve components at higher harmonics of ω.

In the next lecture, we will discuss the validity of this linear response treatment, and analyze the properties of the response function $R(\omega)$ in frequency space, and see what one can learn from the real and imaginary parts of this function.