561 Fall 2005 Lecture 5a

Continued from previous lecture

Linear Response Theory: Response Functions - Retarded Green's Functions and Fluctuations

5. General definition of response functions

The examples before can be written in general form of retarded Green's functions following notation in many texts (See Fetter, Mahan, Doniach.) We can also use the fact that all observable quantities depend only upon the time difference $t-t'$ to write the expressions with $t-t' \to t$. The retarded and advanced functions are (We will use either χ or G^R for retarded causal functions in the notes.)

$$G^R(t) = -i\Theta(t)\langle[\widehat{A}(t), \widehat{B}(0)]\rangle \quad (1)$$

$$G^A(t) = -i\Theta(-t)\langle[\widehat{A}(t), \widehat{B}(0)]\rangle \quad (2)$$

Thus

$$G^R(\omega) = \int_{-\infty}^{\infty} dt\, G^R(t)e^{i\omega t} = -i\int_0^{\infty}\langle[\widehat{A}(t), \widehat{B}(0)]\rangle e^{i\omega t}dt \quad (3)$$

is well defined for $Im\ \omega > 0$ in the upper half plane.

Time ordered functions ar a combination of G^R and G^A as is discussed later.

5a. Example - Phonons

The case of nuclear displacements serves as an example. This example applies to any case of coupled variables and it is exactly soluble for harmonic phonons.

An externally applied force causes an perturbation in the energy $-\sum_J F_J u_J = -\sum_k F_J u_k$., where k labels the normal modes. Thus to linear order the response of the nucleus I is

$$\langle u_I(t)\rangle = \int_{-\infty}^{t} G^R_{IJ}(t-t')[-F_J(t')]dt', \quad (4)$$

where

$$G^R_{IJ}(t) = -i\Theta(t)\langle[\widehat{u}_I(t), \widehat{u}_J(0)]\rangle_0. \quad (5)$$

6. Dissipation and causal response functions

The causal response expression $\chi(\omega)$ was defined in the previous lecture notes and it was shown the the real and imaginary parts obey the KK relations, and other conditions. Here we show that for real frequencies ω the imaginary part $Im\ \chi(\omega)$ of the response denotes energy loss. This is the same property that is used in many well-know examples in the dielectric function, mechanical loss, . . . The general point is that dissipation is the power lost to the environment. For a response Y due to a driving force W, the rate of energy loss is $dE/dt = \langle W dY/dt\rangle$. For example, for displacement of atoms due to forces is the familiar force times velocity, $dE/dt = \sum_I \langle F_I du_I/dt\rangle$. This is general and holds for classical or quantum problems.

The case of nuclear displacements serves as an example that can be extended to other cases. In terms of the response function χ, this becomes

$$\frac{dE}{dt} = \sum_I \langle \mathbf{F}_I du_I/dt\rangle = -\sum_{IJ} F_I(t)\int_{-\infty}^{\infty}\frac{d}{dt}G^R_{IJ}(t-t')F_J(t')dt'. \quad (6)$$

If F is a real force with frequency ω, $F(t) = Fcos(\omega t) = (F/2)(e^{i\omega t} + e^{-i\omega t})$, then

$$\frac{dE}{dt} = \sum_I \langle \mathbf{F}_I du_I/dt \rangle = -\frac{1}{4}\sum_{IJ} F_I \left[-i\omega G^R_{IJ}(\omega) + i\omega G^R_{IJ}(-\omega) \right] F_J. \tag{7}$$

Thus

$$\frac{dE}{dt} = -\frac{1}{2}\sum_{IJ} F_I \left[Im\ \omega G^R_{IJ}(\omega) \right] F_J. \tag{8}$$

It is straightforward to show that $Im\ G^R(\omega)$ is odd in ω and $-\omega Im\ G^R_{IJ}(\omega) > 0$ for all ω. (See P. C. Martin, p. 25-27 for nice discussion.)

7. Fluctuations in a quantum system

The causal response functions $G^r(t)$ or $\chi(t)$ are non-zero only for times $t > t'$. Here we define analogous expressions valid for all times; these are **dynamical correlation functions** and the spectrum defines the **Lehman representation**. Later we show the relation to **causal response functions** and we derive a form of the **fluctuation-dissipation (Nyquist) theorem**.

Using the fact that all observable quantities depend only upon the time difference $t - t'$, and considering Y and W as observables on an equal footing, we see that a closely related expression can be recognized as the correlation function of Y and W separated by time t. Defining the correlation function as S (the same notation as Phillips, Sec. 8.3.1) and writing out the expectation value, we find

$$S_{\widehat{Y}W}(t,0) = \langle | \widehat{Y}(t) W(0) | \rangle_0 = \frac{1}{Z}\sum_n \langle n | e^{-\beta H} e^{iHt} Y e^{-iHt} W | n \rangle, \tag{9}$$

where the sum over n is over a complete set of states, the partition function is $Z = \sum_n \langle n | e^{-\beta H} | n \rangle$, and we have used $\widehat{W}(0) = W$. (The expression appears to not be symmetric in Y and W; this is convenient and we show below that the expressions are in fact symmetric.)

The meaning of this expression can be appreciated by cyclically permuting the operators so that W is on the left; inserting a complete set of states we find

$$S_{\widehat{Y}W}(t,0) = \frac{1}{Z}\sum_{nm} \langle n | W e^{-\beta H} | m \rangle \langle m | e^{iHt} Y e^{-iHt} | n \rangle, \tag{10}$$

and if we consider the exact eigenstates of the hamiltonian

$$S_{\widehat{Y}W}(t,0) = \frac{1}{Z}\sum_{nm} e^{-\beta E_m} \langle n | W | m \rangle \langle m | Y | n \rangle e^{i(E_m - E_n)t}. \tag{11}$$

Finally, the Fourier transform shows that $S_{\widehat{Y}W}(\omega)$ is the spectrum of excitations (the exact spectrum in principle if H is the exact hamiltonian) weighted by thermal probability factors and matrix elements,

$$S_{\widehat{Y}W}(\omega) = \int_{-\infty}^{\infty} dt S_{\widehat{Y}W}(t,0) e^{i\omega t} = 2\pi \frac{1}{Z}\sum_{nm} e^{-\beta E_m} \langle n | W | m \rangle \langle m | Y | n \rangle \delta(E_m - E_n + \omega). \tag{12}$$

If we consider $S_{W\widehat{Y}}(0,t) = \langle W\widehat{Y}(t)\rangle_0$ with $\widehat{Y}(t)$ and W interchanged, similar steps lead to the same expression as 12 except that $e^{-\beta E_m} \to e^{-\beta E_n}$. Using the fact that the delta function is non-zero only if $E-n = E_m + \omega$, we find

$$S_{W\widehat{Y}}(0,t) = e^{-\beta\omega} S_{\widehat{Y}W}(\omega). \tag{13}$$

7a. Lehman representation

The Lehman representation specifies the excitation spectrum in a way that can be used to compute all the correlation functions and Green's functions. There is not a standard notation because each case involves the matrix elements of the specific operators.

The form given in 12 shows the basic point: except for the matrix elements all factors in the equation are positive, and $S_{\widehat{Y}W}(\omega)$ represents the spectrum of excitations. For example, if we let the temperature go to zero, we find

$$\frac{1}{2\pi} S_{\widehat{Y}W}(\omega) \to \sum_n \langle 0|Y|n\rangle\langle n|W|0\rangle \delta(E_0 - E_n + \omega), \tag{14}$$

which is the weighted density of states of the *exact* spectrum of excitations.

7b. Relation of dynamical correlation functions and causal response functions

The relation to the causal response function can now be written simply. Using the definition the the function is non-zero only for times $t > t'$, we can rewrite the expressions from the previous lecture as (here the $1/\hbar$ factor is not written explicitly)

$$\chi_{YW}(t,0) = -i\Theta(t)\langle[\widehat{Y}(t), \widehat{W}(0)]\rangle_0, \tag{15}$$

and

$$\chi_{YW}(\omega) = \frac{-i}{Z}\sum_{nm}\langle n|W|m\rangle\langle m|Y|n\rangle \left[e^{-\beta E_m} - e^{-\beta E_n}\right] \int_0^\infty dt e^{i(E_m - E_n + \omega)t} \tag{16}$$

$$= \frac{1}{Z}\sum_{nm}\langle n|W|m\rangle\langle m|Y|n\rangle \frac{e^{-\beta E_m} - e^{-\beta E_n}}{E_m - E_n + \omega}, \tag{17}$$

which is well-defined for $Im\ \omega > 0$. Note that this expression his has a nice physical interpretation!

In terms of the correlation functions (simply related to the Lehman representation), It is straightforward to show that

$$Im\ \chi_{YW}(\omega) = \frac{-1}{2}(1 - e^{-\beta\omega}) S_{\widehat{Y}W}(\omega), \tag{18}$$

for ω on the real axis.

7c. Fluctuation-dissipation theorem (Nyquist theorem)

The results above establish the fluctuation-dissipation (Nyquist) theorem in a general form. We have shown that the imaginary part of the response function measures dissipation and the correlation function function measures fluctuations. Thus 18 is the fluctuation-dissipation (Nyquist) theorem. The expression is the same as Phillips Eq. 8.48 except that Phillips does not carefully specify the real and imaginary parts.

8. Scattering experiments and Green's functions

A very important experimental approach in studying physical systems is scattering of particles in all fields of physics. In condensed matter the most important are neutron scattering, Raman scattering of photons, electron scattering, ...

The relations follow from the analysis given above. Consider the expression given in Eqs. 12, 14, and 17. Each of these is in fact a "golden rule" expression for a scattering cross section; in these cases the operators Y and W are the same and we will omit them. Examples will be given in class.

A general feature can be derived from the expressions. The cross section always has the form (see Eq. 18)

$$S(\omega) = \frac{-2}{1 - e^{-\beta\omega}} Im\ \chi(\omega), \tag{19}$$

which leads to

$$S(\omega) = [n(\omega) + 1](-2Im\ \chi(\omega)), \quad \omega > 0, \tag{20}$$

and

$$S(\omega) = n(|\omega|)(-2Im\ \chi(|\omega|)), \quad \omega < 0, \tag{21}$$

where

$$n(\omega) = \frac{1}{e^{\beta\omega} - 1} \tag{22}$$

Thus one finds the "Bose factors" for Stokes and anti-Stokes scattering without assuming bosons!

Conclusions

- Causal response describe physical response to perturbations
  - Described by retarded Green's functions
  - Behavior in complex frequency plane
  - K-K relations; Sum rules
  - Note: we will use related *time ordered Green's function* later. They do *not* have same analytic form.
- Relations to correlation functions
  - Lehman representation - spectra in terms of exact excitations of many-body system
  - Scattering spectra
  - Fluctuation-dissipation theorem