561 Fall 2005 Lecture 5 - modified 9/15/05 to correct small errors and typos
Linear Response Theory: Response Functions - Retarded Green's Functions

References: P. C. Martin; Mahan 2.9 and 3.3; Fetter 5; Doniach; nice short summary of quantum formulation in Phillips, Ch. 8.

1. Classical Oscillator with thermal damping force

Consider an oscillator driven by external force (Following P. C. Martin, Ch. 1),

$$m\ddot{x}(t) + m\omega_0^2 x(t) = F^{int}(t) + F^{ext}(t), \tag{1}$$

where F^{int} represents internal forces from parts of the system not explicitly taken into account - random forces that act to bring the oscillator into equilibrium. The oscillator is driven from equilibrium by $F^{ext}(t)$ leading to $\langle F^{int}(t)\rangle \neq 0$. The forces always tend to restore equilibrium on the average and an approximate form is a friction term $\langle F^{int}(t)\rangle = -m\gamma\dot{x}(t)$ with $\gamma > 0$. Then the time evolution of the average of x is given by

$$m\left[\frac{d^2}{dt^2} + \omega_0^2 + \gamma\frac{d}{dt}\right]\langle x\rangle(t) = F^{ext}(t). \tag{2}$$

A Green's function for this system is defined by the response to a delta function source (We will use the same symbol χ for both the in time and in frequency, with the arguments shown ($\chi(t)$ or $\chi(\omega)$ when we need to differentiate the functions.)

$$m\left[\frac{d^2}{dt^2} + \omega_0^2 + \gamma\frac{d}{dt}\right]\chi(t-t') = \delta(t-t'), \tag{3}$$

and

$$\langle x\rangle(t) = \int_{-\infty}^{\infty} dt'\, \chi(t-t')F^{ext}(t') \tag{4}$$

Eq. 3 does not uniquely specify the Green's function; depending on boundary conditions, one can specify the different Green's functions:

- Retarded - Needed for causal response functions - $\chi^A(t-t') = 0$ for $t - t' < 0$
- Advanced - $\chi(t-t') = 0$ for $t - t' > 0$
- Time-ordered - Useful for treating particle interactions in perturbation expansions (more on this later)

The response to a single frequency driving force $F^{ext}(t) = F^{ext}(0)exp(i\omega t)$ is given by the Fourier transform

$$\chi(\omega) = \int_{-\infty}^{\infty} dt\, \chi(t)e^{i\omega t}; \quad \chi(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\chi(\omega)e^{-i\omega t} \tag{5}$$

For the damped oscillator example,

$$\chi(\omega) = \frac{1}{m}\left[\frac{-1}{\omega^2 - \omega_0^2 + i\gamma\omega}\right] \tag{6}$$

We show below that this is an example of a causal retarded function.

2. Retarded Causal Green's Functions (Response Functions) - complex analysis

(Note: Complex analysis holds for both classical and quantum response functions. The description of the classical oscillator follows P. C. Martin, Ch. 1; it gives a useful physical picture but is not essential to derive the quantum expressions.)

Consider $\chi(z)$ as a complex function of a complex frequency z. A retarded function satisfies $\chi(t-t') = 0$ for $t - t' < 0$,

$$\chi(\omega) = \int_{-\infty}^{\infty} dt\ \chi(t) e^{i\omega t}. \tag{7}$$

This equation can be considered the definition of $\chi(\omega)$ for complex ω, which we sometimes write as $\chi(z)$ to avoid confusion with teh cases where ω is a real frequency. The integral is well-defined for $Im\omega > 0$, since we only need to consider $t > 0$ and the exponential factor converges for large $Im\omega > 0$. Thus a physical, causal response function is analytic in the upper plane ($Im\omega > 0$).

- There are poles in $\chi(\omega)$ *only* in lower half of complex plane ($Im\ \omega < 0$) no matter how complicated the system and the functional form of $\chi(\omega)$. For example, the response function Eq. 6 for the damped oscillator can readily be shown to have two poles at $\pm\omega_0 - i\eta$ where $Im\eta > 0$. Show they this is related to the causal assumptions in the formulation of the damping. in be worked out easily

- Using Cauchy Relations and closing the contour in upper plane (where χ is analytic) leads to

$$\chi(z) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega\ \frac{\chi(\omega)}{\omega - z}, \quad Imz > 0, \tag{8}$$

  where the integral is for ω on the real axis (i.e., involves the physically measurable $\chi(\omega)$ for real frequencies ω. The analytic continuation of Eq. 7 to $Imz < 0$ gives $\chi(z) = 0$ since z is outside the contour which is closed in the upper plane.

- The fact that $\chi(z) = 0$ for z approaching the real axis from below is one of the ways to derive the famous Kramers-Kronig relations for real frequency ω valid for all causal response functions (see many texts for details)

$$Re\chi(\omega) = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega'\ \frac{Im\chi(\omega')}{\omega - \omega'}, \quad Im\chi(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega'\ \frac{Re\chi(\omega')}{\omega - \omega'}. \tag{9}$$

- Interpretation of the complex response for $\chi(\omega)$ for real ω:
  - $Re\chi(\omega)$ is the real response to a perturbation - in-phase - no energy loss
  - $Im\chi(\omega)$ is the imaginary response to a perturbation - out-of-phase - represents energy loss

- Sum rules: Since particles always act as free particles at high enough frequency, it follows that $\chi(z) \to -\frac{1}{mz^2}$. Using the first KK relation for $Re\chi$ it follows that (straightforward to show by expanding energy denominator in KK integrand)

$$\frac{1}{m} = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega' \; Im\chi(\omega')\omega'. \tag{10}$$

- Static Response Function: for a static perturbation $\langle x \rangle = \chi(\omega = 0)F^{ext}$ to linear order. Using the KK relation we find

$$\chi(\omega = 0) = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega' \; \frac{Im\chi(\omega')}{\omega'}. \tag{11}$$

3. Quantum Theory for Retarded Causal Green's Functions

(Following Phillips Sec 8.3; more details are given in Fetter, Ch. 5, sect 13, Mahan 2.9 and 3.3)

Consider a system described by a hamiltonian $H = H_0 + W(t)$ where $W(t)$ is an external perturbation turned on at some time. In the Schrodinger representation, the operators are independent of time and the wavefunction $\Psi(t)$ evolves. For ensembles one can work with the density matrix $\rho(t)$ and the expectation value of an observable Y is given by

$$\langle Y \rangle(t) = Tr(\rho(t)Y), \tag{12}$$

with ρ the density matrix in the Schrodinger representation, which satisfies the equation

$$i\hbar\frac{d\rho(t)}{dt} = [H, \rho(t)] = [H_0 + W(t), \rho(t)], \tag{13}$$

where $[A, B] = AB - BA$ is the commutator.

It is easiest to work in the interaction representation in which an operator $\widehat{O}(t)$ is defined by

$$\widehat{O}(t) = e^{\frac{+iH_0 t}{\hbar}} O e^{\frac{-iH_0 t}{\hbar}}, \tag{14}$$

where O is a time-independent operator in the Schrodinger picture. Then

$$\langle \widehat{Y}(t) \rangle = Tr(\widehat{\rho}(t)\, \widehat{Y}(t)), \tag{15}$$

where the evolution is given by

$$i\hbar\frac{d\widehat{\rho}(t)}{dt} = [\widehat{W}(t), \widehat{\rho}(t)] \tag{16}$$

or the formal solution

$$\widehat{\rho}(t) = T\exp\left(-\frac{i}{\hbar}\int_{-\infty}^{t} [\widehat{W}(t'), \widehat{\rho}(t')]dt'\right). \tag{17}$$

The time ordering operator T specifies how the exponential is to be interpreted. (See Mahan, Fetter and other references for a careful exposition.) To lowest order it is simply

$$\widehat{\rho}(t) = \widehat{\rho}_0(t) - \frac{i}{\hbar}\int_{-\infty}^{t} [\widehat{W}(t'), \widehat{\rho}_0(t')]dt'. \tag{18}$$

The expectation value is given by

$$\langle \widehat{Y}(t) \rangle = \langle \widehat{Y}(t) \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^{t} Tr(\widehat{Y}(t)[\widehat{W}(t'), \widehat{\rho}_0(t')]dt' + \ldots . \tag{19}$$

Cyclic permutation leads to the desired result:

$$\delta\langle \widehat{Y}(t) \rangle = \langle \widehat{Y}(t) \rangle - \langle \widehat{Y}(t) \rangle_0 = \int_{-\infty}^{t} \chi_{YW}(t, t')dt', \tag{20}$$

where the response function for Y due to W is given by

$$\chi_{YW}(t, t') = -\frac{i}{\hbar} \langle [\widehat{Y}(t), \widehat{W}(t')] \rangle_0. \tag{21}$$

(Note: Phillips defines χ without the factor $-\frac{i}{\hbar}$, but it is only with the factor that that χ has the expected properties, e.g., that $Im\ \chi(\omega)$ is the energy loss function.) Here $\langle \ldots \rangle_0$ denotes expectation value with the unperturbed $\widehat{\rho}_0$, and the response function is a commutator of the response $\widehat{Y}(t)$ and the perturbation $\widehat{W}(t')$ in the interaction representation.

4. Example: density-density response function

Consider the problem of charged particles in an external potential

$$W(t) = \int d^3r \hat{n}(r) e \phi^{ext}(r, t), \tag{22}$$

where $\hat{n}(r)$ is the density operator, e the charge, and $\phi^{ext}(r, t)$ the perturbing potential that is explicitly time-dependent.

To linear order the response of the ground state to the perturbation is

$$\delta\langle \widehat{n}(r, t) \rangle = -\frac{i}{\hbar} \int_{-\infty}^{t} dt' \int d^3r' e \phi^{ext}(r', t') \langle [\widehat{n}(r', t'), \widehat{n}(r, t)] \rangle_0. \tag{23}$$

If the density-density response function is defined by (here Θ is the step function)

$$\chi_{nn}(rt, r't') == -\frac{i}{\hbar} \Theta(t - t') \langle [\widehat{n}(r', t'), \widehat{n}(r, t)] \rangle_0, \tag{24}$$

then the response of the system to linear order is

$$\delta\langle \widehat{n}(r, t) \rangle = -\frac{i}{\hbar} \int_{-\infty}^{\infty} dt' \int d^3r'\ \chi_{nn}(rt, r't') e \phi^{ext}(r', t'). \tag{25}$$

We will return to the density-density correlation function in the analysis of the dielectric function.

Linear Response Theory - continued next time:

Example of phonons - also see Homework 2
General properties of Green's functions
Fluctuation-dissipation theorem
Scattering spectra and experiments