LINEAR RESPONSE

As noted in class, we seek the change in the value $\langle A \rangle$ of some property described by the operator A due to an applied field. This applied field (F) must interact with property A so that it can respond. This leads to an interaction with the system that can be described by an "external" perturbation Hamiltonian.

$$\widehat{H}_{ext} = A \cdot F.$$

We want the dynamic response function $\chi(t)$ describing the response of $\langle A(t) \rangle$ to $F(t)$ in the form

$$\delta\langle A(t)\rangle = \int_{-\infty}^{t} dt' \chi(t-t')F(t').$$

Before the perturbation is applied, we assume the system is in equilibrium. The expectation value of the property A is,

$$\langle A \rangle_E = T_r\{\rho_E A\} = \sum_n \langle n \mid e^{-\beta H} A \mid n \rangle \frac{1}{Z}$$

$$Z = T_r\{\rho_E\} = \sum_n \langle n \mid e^{-\beta H} \mid n \rangle$$

We also assume that $H_{ext}(t)$ is zero at $t = -\infty$. It may be switched on "adiabatically" i.e. switched on slowly to its full value. e.g.

$$H_{ext}(t) = A(t) \cdot F(t) e^{\epsilon t} \qquad\qquad \epsilon \to +0$$

where ϵ is a small positive number. Here $H_{ext}(t) = 0$ at $t = -\infty$, $H_{ext}(t)$ is its full value at $t = 0$. Or, it could be switched on suddenly at some time $t = t_0$, e.g.

$$H_{ext}(t) = \Theta(t - t_0) A(t) \cdot F(t)$$

where $\Theta(t)$ is the Heaviside function. With the perturbation, the total Hamiltonian is,

$$H_T = H + H_{ext}(t)$$

and the density matrix is

$$\rho(t) = e^{-\beta H_T}$$

Due to $H_{ext}(t)$, the $\rho(t)$ changes with time and the property $\langle A(t) \rangle$ changes given by

$$\langle A(t) \rangle = T_r\{\rho(t) A\}$$

To calculate $\langle A(t) \rangle$ we need an equation of motion for $\rho(t)$. This is Liouville's Eqn,

$$i\frac{\delta\rho(t)}{\delta t} = [H_T, \rho] \qquad\qquad \hbar = 1$$

Where $\rho(t) = \rho_E$ at $t = -\infty$. We also assume that the perturbation is small so that the change in ρ is small, i.e.

$$\rho = \rho_E + \rho_1 \qquad\qquad \rho_1 = 0 \qquad t = -\infty$$

where ρ_1 is a small correction. This is where the linear assumption comes in – we keep first order changes in ρ only.

Evolution of ρ_1

Using Liouville's Eqn. we evaluate the evolution of ρ_1,

$$\begin{aligned} i\dot{\rho}_1 &= [H_T, \rho] = [H + H_{ext}(t), \rho_E + \rho_1(t)] \\ &= [H, \rho_1(t)] + [H_{ext}(t), \rho_E] \qquad \textit{– keep linear terms only.} \end{aligned} \tag{1}$$

assuming H_{ext}, ρ_1 are small and using $[H, \rho_E] = 0$. Recall that any operator, $\bar{O}(t)$, in the Heisenberg Rep. satisfies the Eqn. of notation,

$$\begin{aligned} \bar{O}(t) &\equiv e^{iHt} O e^{-iHt} \qquad \text{– Heinsberg Rep.} \\ \dot{\bar{O}}(t) &= [\bar{O}(t), \bar{H}(t)] = -[\bar{H}(t), \bar{O}(t)] \end{aligned} \tag{2}$$

This if we put $\dot{\rho_1}$ in the Heisenberg Rep., then the time dependence of $\dot{\bar{\rho}}_1$ will be just the second term in Eq.(1) – the first term in Eq.(1) will cancel with Eq.(2). To see this, define

$$\begin{aligned} \rho_2 &= e^{iHt} \rho_1 e^{-iHt} \qquad \text{– } \rho_1 \text{ in Heisenberg Rep.} \\ i\dot{\rho}_2 &= -H\bar{\rho_1} + \bar{\rho_1} H + e^{iHt} \dot{\rho}_1 e^{-iHt} \\ &= -[H, \bar{\rho_1}] + e^{iHt} i\dot{\rho}_1 e^{-iHt} \end{aligned}$$

And

$$e^{-iHt} i\dot{\rho}_2 e^{iHt} = -[H, \rho_1] + i\dot{\rho}_1 = [H_{ext}(t), \rho_E]$$

So that

$$\begin{aligned} i\dot{\rho}_2 &= [\bar{H}_{ext}, \rho_E] \qquad \bar{H}_{ext} \text{ – In Heisenberg Rep.} \\ \bar{H}_{ext} &= e^{iHt} H_{ext}(t) e^{-iHt} \end{aligned}$$

Integrating the equation, we have,

$$\begin{aligned} \rho_2(t) &= -i \int_{-\infty}^{t} dt' [\bar{H}_{ext}(t'), \rho_E] \\ \rho_1(t) &= -i \int_{-\infty}^{t} dt' e^{-iHt} [\bar{H}_{ext}(t'), \rho_E] e^{iHt} \end{aligned}$$

which gives the evolution of $\rho_1(t)$.

Evolution of $\langle \mathbf{A(t)} \rangle$

The thermal expectation value of A is,

$$\begin{aligned}\langle A(t)\rangle &= T_r\{\rho A\} = T_r\{\rho_E A\} + T_r\{\rho_1 A\} \\ &= \langle A\rangle_E - i\int_{-\infty}^{t} dt^{'} T_r\{e^{-iHt}[\bar{H}_{ext}(t^{'}), \rho_E]e^{iHt}A\} \\ &= \langle A\rangle_E - i\int_{-\infty}^{t} dt^{'} \langle[\bar{A}(t), \bar{H}_{ext}(t^{'})]\rangle\end{aligned}$$

Here we have used cyclic permutation under the trace, i.e.

$$\begin{aligned}T_r\{ABC\} &= \sum_n \langle n \mid ABC \mid n\rangle \\ &= \sum_n \langle n \mid CAB \mid n\rangle = \sum_n \langle n \mid BCA \mid n\rangle \\ & etc.\end{aligned}$$

to write the commutation relation in this form. This is the basic result we seek,

$$\langle A(t)\rangle - \langle A\rangle_E = -i\int_{-\infty}^{t} dt^{'} \langle[\bar{A}(t), \bar{H}_{ext}(t^{'})]\rangle$$

the change $\delta\langle A(t)\rangle = \langle A(t)\rangle - \langle A(t)\rangle_E$ in the property A is related the commutation of $\bar{A}(t)$ and $\bar{H}_{ext}(t^{'})$ averaged over the ρ_E of the original system in equilibrium.

Define the dynamic susceptibility or retarded Green function as

$$\chi_{AB}(t-t^{'}) = -i\Theta(t-t^{'})\langle[A(t), B(t^{'})]\rangle$$

involving two properties A and B. Substituting the $H_{ext} = A \cdot F$ into $\delta\langle A(t)\rangle = \langle A(t)\rangle - \langle A(t)\rangle_E$, we have,

$$\delta\langle A(t)\rangle = -i\int_{-\infty}^{t} dt^{'} \langle[\bar{A}(t), \bar{A}(t^{'})]\rangle F(t^{'})$$

$$\delta\langle A(t)\rangle = \int_{-\infty}^{\infty} dt^{'} \chi_{AA}(t-t^{'})F(t^{'}) \qquad (A)$$

where

$$\chi_{AA}(t-t^{'}) = -i\Theta(t-t^{'})\langle[\bar{A}(t), \bar{A}(t^{'})]\rangle$$

We obtain the change $\langle\delta A(t)\rangle$ of A due to the external field F interacting with A via $H_{ext} = A(t) \cdot F(t)$ in terms of the time dependent susceptibility χ_{AA}. This is a very general and powerful result which we will use in many examples; screening, light scattering. We may also use Green function techniques to evaluate $\chi_{AA}(t-t^{'})$. The Fourier transform is,

$$\delta\langle A(t)\rangle = \int \frac{d\omega}{2\pi} e^{-i\omega t}\delta\langle A(\omega)\rangle = \int_{-\infty}^{\infty} dt^{'} \chi_{AA}(t-t^{'})F(t^{'})$$

$$= \int_{-\infty}^{\infty} dt^{'} \int \frac{d\omega}{2\pi} e^{-i\omega(t-t^{'})}\chi_{AA}(\omega) \int \frac{d\omega^{'}}{2\pi} e^{-i\omega^{'}t^{'}} F(\omega^{'})$$

using,

$$\int_{-\infty}^{\infty} dt^{'} e^{i(\omega-\omega^{'})t^{'}} = 2\pi\delta(\omega-\omega^{'})$$

we have

$$\delta\langle A(t)\rangle = \int \frac{d\omega}{2\pi} e^{-i\omega t}\chi(\omega)F(\omega) =$$

Thus

$$\delta\langle A(\omega)\rangle = \chi_{AA}(\omega)F(\omega)$$

In summary, if there is an external applied force (field or potential) $F(q,t)$ that interacts with a property $A(q,t)$ of a system and the interaction Hamiltonian is given by,

$$H_{ext}(q,t) = A(q,t)F(q,t)$$

then the response or change of $A(q,t)$ to $F(q,t)$ (linear response) is

$$\langle\delta A(q,\omega)\rangle = \chi_{AA}(q,\omega)F(q,\omega)$$

or

$$\langle\delta A(q,t)\rangle = \int_{-\infty}^{\infty} dt^{'} \chi_{AA}(t-t^{'})F(t^{'})$$

where

$$\chi_{AA}(t-t^{'}) = -i\Theta(t-t^{'})\langle\Big[\bar{A}(t), \bar{A}(t^{'})\Big]\rangle$$

and $\bar{A}(t)$ is in the Heisenberg representation.