12.7: Relation to Spectra

Suppose that $F_e(t)$ is a monochromatic field

$$F_e(t) = F_\omega e^{i\omega t} e^{\epsilon t}$$

where the parameter ϵ insures that field goes to 0 at $t = -\infty$. We will take $\epsilon \rightarrow 0^+$ at the end of the calculation. The expectation value of B then becomes

$$\begin{aligned} \langle B(t)\rangle &= \langle B\rangle_0 + \int_{-\infty}^{t} ds\ \Phi_{BB}(t-s) F_\omega e^{i\omega s} e^{\epsilon s} \\ &= \langle B\rangle_0 + F_\omega e^{(i\omega+\epsilon)t} \int_0^\infty d\tau \Phi_{BB}(\tau) e^{-i(\omega - i\epsilon)\tau} \end{aligned}$$

where the change of integration variables $\tau = t - s$ has been made.

Define a frequency-dependent susceptibility by

$$\chi_{BB}(\omega - i\epsilon) = \int_0^\infty d\tau \Phi_{BB}(\tau) e^{-i(\omega - i\epsilon)\tau}$$

then

$$\langle B(t)\rangle = \langle B\rangle_0 + F_\omega e^{i\omega t} e^{\epsilon t} \chi_{BB}(\omega - i\epsilon)$$

If we let $z = \omega - i\epsilon$, then we see immediately that

$$\chi_{BB}(z) = \int_0^\infty d\tau\ \Phi_{BB}(\tau) e^{-iz\tau}$$

i.e., the susceptibility is just the Laplace transform of the after effect function or the time correlation function.

Recall that

$$\begin{aligned} \Phi_{AB}(t) &= \frac{i}{\hbar} \langle [A(t), B(0)]\rangle_0 \\ &= \frac{i}{\hbar} \langle [e^{iH_0 t/\hbar} A e^{-iH_0 t\hbar}, B]\rangle_0 \end{aligned}$$

Under time reversal, we have

$$\begin{aligned} \Phi_{AB}(-t) &= \frac{i}{\hbar} \langle \left[e^{-iH_0 t/\hbar} A e^{iH_0 t/\hbar}, B \right] \rangle_0 \\ &= \frac{i}{\hbar} \langle \left(e^{-iH_0 t/\hbar} A e^{iH_0 t/\hbar} B - B e^{-iH_0 t/\hbar} A e^{iH_0 t/\hbar} \right) \rangle_0 \\ &= \frac{i}{\hbar} \langle \left(A e^{iH_0 t/\hbar} B e^{-iH_0 t/\hbar} - e^{iH_0 t/\hbar} B e^{-iH_0 t/\hbar} A \right) \rangle_0 \\ &= \frac{i}{\hbar} \langle (AB(t) - B(t)A)\rangle_0 \\ &= -\frac{i}{\hbar} \langle [B(t), A]\rangle \\ &= -\Phi_{BA}(t) \end{aligned}$$

Thus,

$$\Phi_{AB}(-t) = -\Phi_{BA}(t)$$

and if $A = B$, then

$$\Phi_{BB}(-t) = -\Phi_{BB}(t)$$

Therefore

$$\begin{aligned}\chi_{BB}(\omega) &= \lim_{\epsilon\to 0^+}\int_0^\infty dt\; e^{-i(\omega - i\epsilon t)}\,\Phi_{BB}(t) \\ &= \lim_{\epsilon\to 0^+}\int_0^\infty dt\; e^{-\epsilon t}\left[\Phi_{BB}(t)\cos\omega t - i\Phi_{BB}(t)\sin\omega t\right] \\ &= \mathrm{Re}(\chi_{BB}(\omega)) - i\mathrm{Im}(\chi_{BB}(\omega))\end{aligned}$$

From the properties of $\Phi_{BB}(t)$ it follows that

$$\begin{aligned}\mathrm{Re}(\chi_{BB}(\omega) &= \mathrm{Re}(\chi_{BB}(-\omega) \\ \mathrm{Im}(\chi_{BB}(\omega) &= -\mathrm{Im}(\chi_{BB}(-\omega)\end{aligned}$$

so that $\mathrm{Im}(\chi_{BB}(\omega))$ is positive for $\omega > 0$ and negative for $\omega < 0$. It is a straightforward matter, now, to show that the energy difference $Q(\omega)$ derived in the lecture from the Fermi golden rule is related to the susceptibility by

$$Q(\omega) = 2\omega|F_\omega|^2\mathrm{Im}(\chi_{BB}(\omega))$$