8.512 Recitation 9

Today: 1) Spectral representation of response function
2) Kramers – Kronig relations
3) Fluctuation – Dissipation theorem
4) Sum rules

- Consider a system H_0 subject to a perturbation

$$H_1(t) = -\sum_i O_i A_i(t)$$

Hermitian ops. → real fields/potential

Ex: $H_1(t) = -\vec{M}\cdot\vec{B}(t)$

- To linear order, the effect of perturbation is

$$\langle O_i(t)\rangle = \int_{-\infty}^{\infty} dt'\, \chi_{ij}(t-t')\, A_j(t')$$

response function

- Kubo formula:

$$\chi_{ij}(t-t') = \frac{i}{\hbar}\langle [O_i(t), O_j(t')]\rangle \Theta(t-t')$$

$$= \frac{i}{\hbar}\langle [O_i(t-t'), O_j(0)]\rangle \Theta(t-t')$$

causality!

1) Let H_0 have eigenstates $H_0|n\rangle = \hbar\omega_n|n\rangle = E_n|n\rangle$

$$\Rightarrow \chi_{ij}(\omega) = \frac{i}{\hbar}\int_0^{\infty} dt\, e^{i\omega t}\langle [O_i(t), O_j(0)]\rangle$$

$$= \frac{i}{\hbar}\int_0^{\infty} dt\, e^{i\omega t}\,\frac{1}{Z}\sum_{m,n} e^{-\beta\hbar\omega_m}\Big[\langle m|O_i|n\rangle\langle n|O_j|m\rangle e^{i(\omega_m-\omega_n)t} - \langle m|O_j|n\rangle\langle n|O_i|m\rangle e^{i(\omega_n-\omega_m)t}\Big]$$

Regularize the integral at $t\to\infty$ with $e^{-\epsilon t}$, $\epsilon\to 0^+$

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$$\int_0^\infty dt\ e^{i(\omega - \Omega + i\varepsilon)t} = \frac{i}{\omega - \Omega + i\varepsilon}$$

$$\Rightarrow \chi_{ij}(\omega) = \frac{1}{\hbar Z} \sum_{m,n} e^{-\beta\hbar\omega_m} \left[\frac{\langle m|O_j|n\rangle\langle n|O_i|m\rangle}{\omega - \omega_m + \omega_n + i\varepsilon} - \frac{\langle m|O_i|n\rangle\langle n|O_j|m\rangle}{\omega + \omega_m - \omega_n + i\varepsilon} \right]$$

relabel $m \leftrightarrow n$

$$= \frac{1}{\hbar Z} \sum_{m,n} \langle m|O_j|n\rangle\langle n|O_i|m\rangle \frac{e^{-\beta\hbar\omega_m} - e^{-\beta\hbar\omega_n}}{\omega - (\omega_m - \omega_n) + i\varepsilon}$$

2) Notice that $\chi_{ij}^*(t) = \chi_{ij}(t)$ is real

$$\Rightarrow \quad \chi_{ij}(\omega)^* = \chi_{ij}(-\omega)$$

Separate $\chi_{ij}(\omega)$ into real and imaginary parts

$$\chi_{ij}(\omega) = \chi_{ij}'(\omega) + i\,\chi_{ij}''(\omega)$$

$$\chi_{ij}''(\omega) = -\frac{i}{2}\left(\chi_{ij}(\omega) - \chi_{ij}^*(\omega)\right) = -\frac{i}{2}\int_{-\infty}^{\infty} dt\, e^{i\omega t}\left(\chi_{ij}(t) - \chi_{ij}(-t)\right) = -\chi_{ij}''(-\omega)$$

$\Rightarrow$ Imag. part is not invariant under time-reversal $t \to -t$

$\Rightarrow \chi''$ knows about the arrow of time and corresponds to dissipation

$$\chi_{ij}'(\omega) = \frac{1}{2}\int_{-\infty}^{\infty} dt\ e^{i\omega t}\left(\chi_{ij}(t) + \chi_{ij}(-t)\right) = \chi_{ij}'(-\omega)$$

$\Rightarrow$ Real part is invariant under $t \to -t$

χ' is the reactive part

- Analytically continue $\chi_{ij}(\omega)$ to complex frequency z, as long as $\chi_{ij}(z)$ does not diverge exponentially at $|z| \to \infty$

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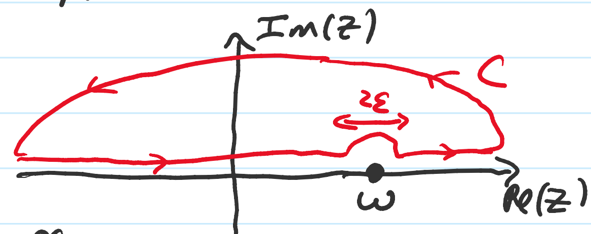
$$\chi_{ij}(t) = \oint \frac{dz}{2\pi} e^{-izt} \chi_{ij}(z)$$

where the contour is in the upper (lower) half plane for $t<0$ ($t>0$). Since $\chi_{ij}(t<0)=0$ we have

$\chi_{ij}(z)$ is analytic (has no poles) in the upper half plane

$$\Rightarrow \quad \oint_C dz \frac{\chi_{ij}(z)}{\omega - z} = 0$$



$$\Leftrightarrow \left(\int_{-\infty}^{\omega-\varepsilon} + \int_{\omega+\varepsilon}^{\infty}\right) d\omega' \frac{\chi_{ij}(\omega')}{\omega-\omega'} + \oint_{\substack{z=\omega+\varepsilon e^{i\theta} \\ \theta\in[\pi,0]}} dz \frac{\chi_{ij}(z)}{\omega - z} = 0$$

$$\Leftrightarrow \mathcal{P}\int_{-\infty}^{\infty} d\omega' \frac{\chi_{ij}(\omega')}{\omega-\omega'} - i\int_{\pi}^{0} d\theta\, \chi_{ij}(\omega+\varepsilon e^{i\theta}) = 0$$

Take $\varepsilon\to 0$ $\quad \mathcal{P}\int_{-\infty}^{\infty} d\omega' \frac{\chi_{ij}(\omega')}{\omega-\omega'} + i\pi \chi_{ij}(\omega) = 0$

Principal value of an integral

$$\Rightarrow \quad \boxed{\begin{aligned} \chi'(\omega) &= \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''(\omega')}{\omega'-\omega} \\ \chi''(\omega) &= -\mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi'(\omega')}{\omega'-\omega} \end{aligned}}$$

Kramers-Kronig relations

- By knowing either χ' or χ'', we can find the other component and the entire χ

$$\chi(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''(\omega')}{\omega'-\omega-i\varepsilon}$$

This is a consequence of causality!

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3) Power dissipated in the system due to external fields

$$P = \frac{d}{dt} \langle \psi(t) | H | \psi(t) \rangle \underset{\uparrow}{=} - \sum_i \langle O_i(t) \rangle \dot{A}_i(t)$$

Feynmann-Heller thm.

• Total energy dissipated:

$$W = \int_{-\infty}^{\infty} dt\, P = -\int_{-\infty}^{\infty} dt\, dt'\, \chi_{ij}(t-t')\, \dot{A}_i(t)\, A_j(t')$$

implicit sum over i,j

$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (-i\omega)\, A_i^*(\omega)\, \chi_{ij}(\omega)\, A_j(\omega)$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{4\pi} (-i\omega)\, A_i(-\omega) [\chi_{ij}(\omega) - \chi_{ji}(-\omega)]\, A_j(\omega)$$

where we used that $A_i(t)$ - real $\Rightarrow A_i^*(\omega) = A_i(-\omega)$

• If A_i and A_j transform the same way under time-reversal

$$\chi_{ji}(\omega) = \chi_{ij}^*(-\omega) = \chi_{ij}(\omega)$$

Onsager relation

$$\Rightarrow W = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \omega\, A_i(-\omega)\, \chi''_{ij}(\omega)\, A_j(\omega)$$

As stated above, $\chi''_{ij}(\omega)$ is related to dissipation!

• More generally, define correlation function $S_{ij}(t)$

$$S_{ij}(t) = \langle O_i(t)\, O_j(0) \rangle$$

and spectral function / density $\rho_{ij}(\omega)$

$$2\pi\hbar\, \rho_{ij}(\omega) = S_{ij}(\omega) = \frac{1}{Z} \sum_{m,n} e^{-\beta\hbar\omega_m} \langle m | O_i | n \rangle \langle n | O_j | m \rangle \cdot 2\pi\delta(\omega - \omega_n + \omega_m)$$

• Interchanging m and n yields a "detailed balance" relation

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$$S_{ij}(-\omega) = e^{-\beta\hbar\omega} S^{*}_{ij}(\omega) = e^{-\beta\hbar\omega} S_{ji}(\omega)$$

- Using the spectral decomposition, one can check that

$$2i\chi''_{ij}(\omega) = \chi_{ij}(\omega) - \chi_{ji}(-\omega) = -\frac{i}{\hbar}(1-e^{-\beta\hbar\omega}) S_{ij}(\omega)$$

$$\boxed{\begin{aligned} &\chi''_{ij}(\omega) = -\frac{1}{2\hbar}(1-e^{-\beta\hbar\omega}) S_{ij}(\omega) = -\pi(1-e^{-\beta\hbar\omega})\rho_{ij}(\omega) \\ \Longleftrightarrow\quad &\chi''_{ij}(\omega) = -\frac{1}{2\hbar}\left(S_{ij}(\omega) - S_{ji}(-\omega)\right) \end{aligned}}$$

Fluctuation–Dissipation theorem

- In the limit $T \to \infty$, we recover the classical result

$$\chi''_{ij}(\omega) = -\frac{\omega}{2k_BT} S_{ij}(\omega)$$

4) Sum rules are identities that follow from the symmetries of the response functions.

- First consider a single electron system

$$H = \frac{p^2}{2m} + V(x)$$

$$\left.\begin{aligned} &[x,p] = i\hbar \\ &[p^2,x] = -2i\hbar p \\ &[H,x] = -\frac{i\hbar p}{m} \end{aligned}\right\} \Rightarrow \langle n|p|0\rangle = \langle n|\frac{i}{\hbar}m[H,x]|0\rangle = im(\omega_n-\omega_0)\langle n|x|0\rangle$$

$$-\hbar = i\langle 0|[x,p]|0\rangle = i\sum_n\left[\langle 0|x|n\rangle\langle n|p|0\rangle - \langle 0|p|n\rangle\langle n|x|0\rangle\right]$$

$$= -2m\sum_n(\omega_n-\omega_0)|\langle n|x|0\rangle|^2$$

$$= -2m \sum_n (\omega_n - \omega_0) |\langle n|x|0\rangle|$$

$$\Rightarrow \quad \sum_n (E_n - E_0) |\langle n|x|0\rangle|^2 = \frac{\hbar^2}{2m}$$

- This generalizes to a system of N electrons as

$$\sum_n (E_n - E_0) |\langle n|\rho_q^\dagger|0\rangle|^2 = N \frac{\hbar^2 q^2}{2m}$$

where ρ_q is the momentum-space particle density

- At $T \to 0$ we have for a single $O = \rho_q^\dagger$

$$S(q,\omega) = 2\pi \sum_n |\langle n|\rho_q^\dagger|0\rangle|^2 \delta(\omega - \omega_n + \omega_0)$$

$$\boxed{\int_0^\infty \frac{d\omega}{2\pi} \omega S(q,\omega) = \sum_n (\omega_n - \omega_0) |\langle n|\rho_q^\dagger|0\rangle|^2 = N \frac{\hbar q^2}{2m}}$$

f-sum rule

- Recall the dielectric response function

$$\varepsilon(q,\omega) = 1 - \frac{4\pi e^2}{q^2} \chi(q,\omega)$$

$$\mathrm{Im}(\varepsilon(q,\omega)) = -\frac{4\pi e^2}{q^2} \chi''(q,\omega) = \frac{2\pi e^2}{\hbar q^2} S(q,\omega)$$

$$\Rightarrow \int_0^\infty d\omega \cdot \omega \, \mathrm{Im}(\varepsilon(q,\omega)) = N \cdot \frac{2\pi^2 e^2}{m} = \frac{\pi}{2} \omega_p^2$$

plasma frequency

• Similarly, the conductivity is given by

$$\varepsilon(q,\omega) = \frac{4\pi i}{\omega}\sigma(q,\omega)$$

$$\operatorname{Im}(\varepsilon(q,\omega)) = \frac{4\pi}{\omega}\operatorname{Re}(\sigma(q,\omega))$$

$$\Rightarrow \boxed{\int_0^\infty d\omega \cdot \operatorname{Re}(\sigma(q,\omega)) = \frac{\omega_p^2}{8}}$$

Conductivity sum rule

Does this hold in a superconductor?