3.1.3) Analiticidade

Vamos estudar a susceptibilidade generalizada χ_{ij}.

$$\overline{\delta A_i(t)} = \sum_j \int_{-\infty}^{t} dt' \, \chi_{ij}(t-t') \, f_j(t')$$

$$\Rightarrow \overline{\delta A_i(\omega)} = \sum_j \chi_{ij}(\omega) \, f_j(\omega)$$

Em geral a resposta $x(t)$ é tal que

$$x(t) = \int \chi(t,t') \, f(t') \, dt'$$

i) Resposta é linear com o termo forçante (resposta linear)

ii) Invariância por translação da origem dos tempos

$$\Rightarrow \chi(t,t') = \chi(t-t')$$

iii) Causalidade $\chi(t) = 0$ se $t<0$

$$\Rightarrow \chi(\omega) = \int_{-\infty}^{\infty} \chi(t) \, e^{i\omega t} dt = \int_{0}^{\infty} \chi(t) \, e^{i\omega t} dt$$

possui prolongamento analítico para $\omega = z$ tal que $\mathrm{Im}\, z > 0$ pois $z = \omega + i v$ $\quad izt = i\omega t - vt$ se $t>0 \Rightarrow$ convergência para $v>0$.

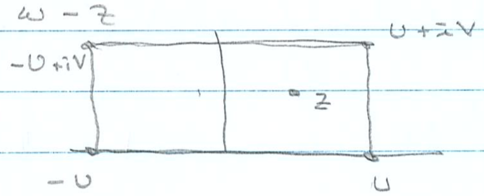
$$\Rightarrow \chi(z) = \int_{0}^{\infty} \chi(t) \, e^{izt} dt = \int_{0}^{\infty} dt \, e^{izt} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \chi(\omega)$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\chi(\omega)}{\omega - z} \, d\omega$$

que é a fórmula de Cauchy

$$\chi(z) = \frac{1}{2\pi i} \oint \frac{\chi(\omega)\, d\omega}{\omega - z}$$

integrada em



onde $\mathrm{Im}\, z > 0$

e $\int |\chi(\omega)|^2 d\omega < \infty$.

Se $z = \omega + i\epsilon$ $(\epsilon \downarrow 0)$ Temos:

$$\chi(\omega) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\chi(\omega')\, d\omega'}{\omega' - \omega - i\epsilon} =$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega'\, \chi(\omega') \left\{ P\left(\frac{1}{\omega' - \omega}\right) + i\pi\delta(\omega' - \omega) \right\}$$

$$\Rightarrow \chi(\omega) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega' \frac{\chi(\omega')}{\omega' - \omega} + \frac{\chi(\omega)}{2}$$

$$\Rightarrow \chi(\omega) = \frac{1}{\pi i} \int_{-\infty}^{\infty} d\omega' \frac{\chi(\omega')}{\omega' - \omega}$$

Seja $\chi(\omega) = \chi'(\omega) + i\chi''(\omega)$

$$\Rightarrow \chi'(\omega) + i\chi''(\omega) = \frac{1}{\pi i} \int_{-\infty}^{\infty} d\omega' \frac{\chi'(\omega') + i\chi''(\omega')}{\omega' - \omega}$$

$$\Rightarrow \chi'(\omega) = \frac{1}{\pi} \int \frac{\chi''(\omega')}{\omega' - \omega} d\omega' \quad \text{e}$$

$$\chi''(\omega) = -\frac{1}{\pi} \int \frac{\chi'(\omega')}{\omega' - \omega} d\omega'$$

Relações de dispersão
Fórmulas de Plemelj ou Kramers-Kronig

"Transformadas de Hilbert"

voltemos à $X(\omega) = \int_0^\infty x(t)\, e^{i\omega t} dt \qquad \omega \in \mathbb{R}$.

$$\Rightarrow X'(\omega) = \frac{X(\omega) + X^*(\omega)}{2} = \frac{1}{2}\int_0^\infty x(t)\, e^{i\omega t} dt +$$

$$+ \frac{1}{2}\int_0^\infty x^*(t)\, e^{-i\omega t} dt \qquad (t \to -t \text{ na } 2^{a} \text{ integral})$$

$$X'(\omega) = \frac{1}{2}\int_0^\infty x(t)\, e^{i\omega t} dt + \frac{1}{2}\int_{-\infty}^0 x^*(-t)\, e^{i\omega t} dt$$

$$= \frac{1}{2}\int_{-\infty}^\infty \tilde{x}(t)\, e^{i\omega t} dt \qquad \text{onde } \tilde{x}(t) = \begin{cases} x(t) & \text{se } t > 0 \\ x^*(-t) & \text{se } t < 0 \end{cases}$$

Da mesma forma:

$$X''(\omega) = \frac{X(\omega) - X^*(\omega)}{2i} = \frac{1}{2i}\int_0^\infty x(t)\, e^{i\omega t} dt \, -$$

$$- \frac{1}{2i}\int_0^\infty x^*(t)\, e^{-i\omega t} dt \qquad (t \to -t \text{ na } 2^{a} \text{ integral})$$

$$X''(\omega) = \frac{1}{2i}\int_0^\infty x(t) e^{i\omega t} dt - \frac{1}{2i}\int_{-\infty}^0 x^*(-t)\, e^{i\omega t}$$

$$= -\frac{i}{2}\int_{-\infty}^\infty \varepsilon(t)\, \tilde{x}(t)\, e^{i\omega t} dt \qquad \text{onde } \varepsilon(t) = \begin{cases} 1 & \text{se } t > 0 \\ -1 & \text{se } t < 0 \end{cases}$$

$$\left.\begin{aligned} \Rightarrow \mathcal{F}^{-1}[X'(\omega)] &= \frac{\tilde{x}(t)}{2} \\ \mathcal{F}^{-1}[X''(\omega)] &= -\frac{i}{2}\,\varepsilon(t)\,\tilde{x}(t) \end{aligned}\right\} \Rightarrow \mathcal{F}^{-1}[X''(\omega)] = -i\,\varepsilon(t)\, \mathcal{F}^{-1}[X'(\omega)]$$

Vamos definir $p(t) = \mathcal{F}^{-1}[\chi''(\omega)] = \frac{1}{2\pi}\int_{-\infty}^{\infty} \chi''(\omega) e^{-i\omega t} d\omega$

e $q(t) = i\,\varepsilon(t)\,p(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} Q(\omega) e^{-i\omega t} d\omega$.

$\Rightarrow Q(\omega) = \int_{-\infty}^{\infty} i\,\varepsilon(t)\,p(t)\, e^{i\omega t} dt$.

mas, usando que $\varepsilon(t) e^{i\omega t} = \frac{1}{\pi i} \fint \frac{e^{i\omega' t}}{\omega' - \omega} d\omega'$

Temos $Q(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty} dt\, p(t) \int_{-\infty}^{\infty} \frac{d\omega'}{\omega' - \omega} e^{i\omega' t}$

$\Rightarrow Q(\omega) = \frac{1}{\pi} \fint_{-\infty}^{\infty} d\omega' \frac{\chi''(\omega')}{\omega' - \omega} = \chi'(\omega)$ (pela 1ª Transf. de Hilbert)

$\Rightarrow \chi(\omega) = \chi'(\omega) + i\chi''(\omega)$

$= \int_{-\infty}^{\infty} i\,\varepsilon(t)\,p(t)\, e^{i\omega t} dt + i\int_{-\infty}^{\infty} p(t)\, e^{i\omega t} dt$

$= \int_{-\infty}^{\infty} i \underbrace{[\varepsilon(t) + 1]}_{\begin{cases} 0 & \text{se } t<0 \\ 2 & \text{se } t>0 \end{cases}} p(t)\, e^{i\omega t} = 2i\int_{0}^{\infty} p(t)\, e^{i\omega t} dt$

$\Rightarrow \chi(\omega) = \int_{-\infty}^{\infty} \chi(t)\, e^{i\omega t} dt = \int_{0}^{\infty} \chi(t)\, e^{i\omega t} dt$

$= \int_{0}^{\infty} 2i\, p(t)\, e^{i\omega t} dt \Rightarrow \chi(t) = 2i\,p(t) \quad t>0$

$\Rightarrow \chi(t) = 2i\chi''(t)$ se $t>0$, onde $p(t) = \chi''(t) = \mathcal{F}^{-1}[\chi''(\omega)]$

Vamos usar este resultado na fórmula de Kubo

$$\chi(t) = -\beta\Theta(t)\dot{C}(t) \Rightarrow 2i\chi''(t) = -\beta\Theta(t)\dot{C}(t)$$

ou $\chi''(t) = \frac{i}{2}\beta\dot{C}(t)$

$\Rightarrow \chi''(t)$ é uma função ímpar de t porque $C(t)$ é uma função par de t.
$\chi''(t)$ é imaginária pura $\Rightarrow$

$$\chi(t) = 2i\chi''(t) = 2i\int \frac{d\omega}{2\pi} e^{-i\omega t}\chi''(\omega)$$

$\chi''(\omega) = -\chi''(-\omega)$ e $\chi''(\omega) \in \mathbb{R}$.

Voltando a $\chi(z)$ tem-se

$$\chi(z) = \int_0^\infty \chi(t) e^{izt}\,dt = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi}\frac{\chi''(\omega')}{\omega'-z}.$$

onde assume-se convergência em $\omega' = \infty$. Senão,

$$\chi(z) \to \chi(z) - \chi(0) = \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi''(\omega')}{\omega'-z} - \int\frac{d\omega'}{\pi}\frac{\chi''(\omega')}{\omega'}$$

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

$\chi(0)$ é um valor não conhecido!

Fazendo $z = \omega + i\epsilon$

$$\chi(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\chi''(\omega')}{\omega'-\omega}\, d\omega' + i\chi''(\omega)$$

$$\Rightarrow \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\chi''(\omega')}{\omega'-\omega}\, d\omega' = \chi'(\omega)$$ como já se esperava.

Susceptibilidade estática: $\chi = \lim_{\omega \to 0} \chi(\omega + i\eta)$

$$\chi(z) = -\beta\int_0^{\infty} dt\, e^{izt}\, \dot{C}(t) = -\beta e^{izt} C(t)\Big|_0^{\infty} +$$

$$+ \beta\int_0^{\infty} iz\, e^{izt} C(t)\, dt = \beta\left[C(0) - C(\infty)\right] +$$

$$+ iz\beta\int_0^{\infty} dt\, e^{izt}\left(C(t) - C(\infty)\right)$$; se $z \to 0$ e a integral converge $\boxed{\chi(0) = \beta C(t=0)}$

Susceptibilidade isotérmica: $\chi_T = \beta C(t=0) = \chi(0)$. Então, quando $C(\infty) \to 0$ e a integral converge

$$\chi(z) = \beta C(0) + iz\beta\int_0^{\infty} dt\, e^{izt} C(t) = \chi + iz\beta C(z)$$

$$(\chi(z) - \chi)\frac{1}{iz\beta} = C(z) \Rightarrow \boxed{\frac{1}{iz\beta}\left(\chi(z)\chi^{-1} - 1\right)\chi = C(z)}$$

Mas já vimos que

$$\frac{d}{dt}\overline{\delta A_i}(t) = \beta\,\Theta(t)\sum_j \dot{C}_{ij}(t) f_j \Rightarrow \int_0^{\infty} \frac{d}{dt}\overline{\delta A}(t)\, e^{izt}\, dt = \beta\int_0^{\infty} \dot{C}(t)\, e^{izt}\, dt$$

$$e^{izt}\,\overline{\delta A}(t)\Big|_0^\infty - iz\int_0^\infty \overline{\delta A}(t)\, e^{izt}\, dt = \beta\, C(t) f\Big|_0^\infty - iz\beta\int_0^\infty e^{izt}\, C(t) f\, dt$$

$$\Rightarrow -\overline{\delta A}(t=0) - iz\,\overline{\delta A}(z) = -\beta\, C(t=0) f - iz\beta\, C(z) f.$$

como $\overline{\delta A}(t=0) = \chi f$ e $\beta C(t=0) = \chi$ Temos

$$-iz\,\overline{\delta A}(z) = -iz\beta\, C(z) f \;\Rightarrow\; \overline{\delta A}(z) = \beta\, C(z) f$$

ou ainda $\overline{\delta A}(z) = \dfrac{1}{iz}\left(\chi(z)\chi^{-1} - 1\right)\underbrace{\chi f}_{\overline{\delta A}(t=0)}$

$$\Rightarrow \boxed{\overline{\delta A}(z) = \frac{1}{iz}\left(\chi(z)\chi^{-1} - 1\right)\overline{\delta A}(t=0)}$$

Novamente, como $C(z) = \dfrac{1}{iz\beta}\left(\chi(z) - \chi\right)$

podemos escrever:

$$C(z) = \frac{1}{iz\beta}\left[\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\chi''(\omega')\, d\omega'}{\omega' - z} - \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\chi''(\omega')\, d\omega'}{\omega'}\right]$$

$$\boxed{C(z) = -\frac{i}{\beta}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\,\frac{\chi''(\omega')}{\omega'(\omega' - z)}}$$

Como $\chi''(t) = \dfrac{i}{2}\beta\,\dot{C}(t)$ e $\chi''(t) = \dfrac{1}{2\pi}\displaystyle\int_{-\infty}^{\infty} d\omega\, \chi''(\omega)\, e^{-i\omega t}$

$$C(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} C(\omega)\, e^{-i\omega t}\, d\omega \;\Rightarrow\; \dot{C}(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} -i\omega\, C(\omega)\, e^{-i\omega t}\, d\omega$$

$$\boxed{\chi''(\omega) = \frac{\beta\omega}{2}\, C(\omega)}$$ Teo. de flutuação e dissipação (clássico.