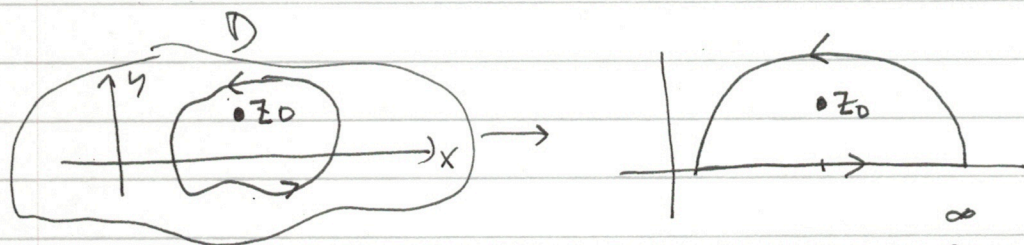


Relaciones de Cauchy - Kronig

Sea $f(z)$ analítica en D , con $\lim_{|z| \rightarrow \infty} |f(z)| = 0$

$$\text{Cauchy} \Rightarrow f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0} dz \quad (1)$$



~~$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0} dz$$~~

$$f(z_0) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{f(x)}{x - z_0} dx$$

$$z_0 \rightarrow x_0 \quad f(x_0) = \frac{1}{i\pi} \int_{-\infty}^{\infty} \frac{f(x)}{x - x_0} dx \quad (2)$$

$$f(x_0) = u(x_0) + i v(x_0) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{v(x)}{x - x_0} dx - \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{u(x)}{x - x_0} dx$$

$$\Rightarrow u(x_0) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{v(x)}{x - x_0} dx \quad (3)$$

$$v(x_0) = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{u(x)}{x - x_0} dx \quad (4)$$

cuando $f(-x) = f^*(x)$ [caso de $n(\omega) = 1$]

$$\Rightarrow \begin{cases} u(x_0) = \frac{2}{\pi} \int_0^{\infty} \frac{x v(x)}{x^2 - x_0^2} dx \\ v(x_0) = -\frac{2}{\pi} \int_0^{\infty} \frac{x_0 u(x)}{x^2 - x_0^2} dx \end{cases} \quad (5)$$

Kramers-Kronig



Como particular, $f(\omega) = \epsilon(\omega) - \epsilon_0 = \epsilon'(\omega) - \epsilon_0 - i\epsilon''(\omega)$

$$\Rightarrow \epsilon'(\omega) - \epsilon_0 = \frac{2}{\pi} P \int_0^{\infty} \frac{\epsilon''(\omega') \omega'}{\omega'^2 - \omega^2} d\omega'$$

$$\epsilon''(\omega) = \frac{2\omega}{\pi} P \int_0^{\infty} \frac{(\epsilon'(\omega') - \epsilon_0)}{\omega'^2 - \omega^2} d\omega'$$

Dispersion y
Absorcion estan
íntimamente
relacionadas.

$$D(t) = \int_{-\infty}^{\infty} \epsilon(t-t') E(t') dt' = \int_{-\infty}^{\infty} \epsilon(t') E(t-t') dt'$$

$$\Rightarrow \boxed{D(\omega) = \epsilon(\omega) E(\omega)}$$

y como $\epsilon(\omega) \xrightarrow{\omega \rightarrow \infty} \epsilon_0 \Rightarrow$ aplicar Cauchy a $\epsilon(\omega) - \epsilon_0$

$$\lim_{|z| \rightarrow \infty} (\epsilon(z) - \epsilon_0) = 0 \quad \checkmark$$

$\omega > \omega_p \rightarrow$ prop. de ondes

$\omega < \omega_p \rightarrow n$ imaginario $\rightarrow$ décaissement exponentiel

Relations de Kramers-Kronig (ver spectra)

Exemple: $\gamma_j \approx 0$

$$\Rightarrow n^2 = 1 + \frac{Ne^2}{\epsilon_0 m} \sum_j \frac{f_j}{\omega_j^2 - \omega^2}$$

$$\Rightarrow \underbrace{\epsilon(\omega) - \epsilon_0}_{\epsilon'(\omega) - \epsilon_0} = \frac{Ne^2}{m} \sum_j \frac{f_j}{\omega_j^2 - \omega^2}$$

re-ecrit comme, $\epsilon'(\omega) - \epsilon_0 = \frac{Ne^2}{m} \mathcal{P} \int_0^\infty \sum_j \frac{f_j \delta(\omega' - \omega_j)}{\omega'^2 - \omega^2} d\omega'$

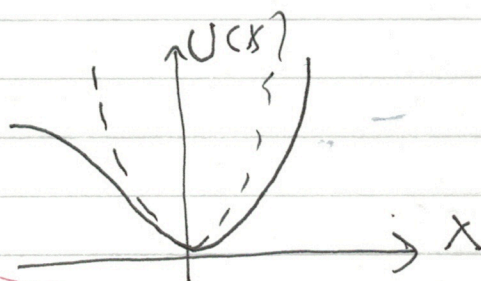
ce qui implique, $\epsilon''(\omega) = \frac{\pi Ne^2}{2\omega m} \sum_j f_j \delta(\omega - \omega_j)$.

De $\sum_j f_j = Z$, $\Rightarrow \int_0^\infty \omega \epsilon''(\omega) d\omega = \frac{\pi Ne^2 Z}{2m}$ Règle de somme.

Susceptibilidad No lineal de un oscilador anarmónico clásico (Modelo de Lorentz)

(i) Medio No-centrosimétrico

$$U \approx \frac{1}{2} m \omega_0^2 x^2 + \frac{1}{3} m \alpha x^3 \quad (1)$$



$$F_{rest} = -m \omega_0^2 x - m \alpha x^2 \quad (2)$$

→ notar que $U(-x) \neq U(x)$

$$\Rightarrow \ddot{x} + 2\gamma \dot{x} + \omega_0^2 x + \alpha x^2 = -e E(t)/m \quad (3)$$

Tomamos $E(t) = E_1 e^{-i\omega_1 t} + E_2 e^{-i\omega_2 t} + c.c.$ (4)

"buena" elección para mostrar la fenomenología de ~~los~~ los medios cuasiestáticos.

usar Teo. de perturbaciones. [x es pequeño]

$$E(t) \rightarrow \lambda E(t), \quad \lambda \in [0, 1]$$

$$\ddot{x} + 2\gamma \dot{x} + \omega_0^2 x + \alpha x^2 = -\lambda e E/m \quad (4')$$

$$x = \lambda x^{(1)} + \lambda^2 x^{(2)} + \lambda^3 x^{(3)} + \dots \quad (5)$$

Reempl. en (4') e igualar potencias de λ .

$$(6) \left\{ \begin{aligned} \Rightarrow \ddot{X}^{(1)} + 2\gamma \dot{X}^{(1)} + \omega_0^2 X^{(1)} &= -eE^{(1)}/m & (\text{orden } \lambda) \\ \ddot{X}^{(2)} + 2\gamma \dot{X}^{(2)} + \omega_0^2 X^{(2)} + a[X^{(1)}]^2 &= 0 & (\text{orden } \lambda^2) \\ \ddot{X}^{(3)} + 2\gamma \dot{X}^{(3)} + \omega_0^2 X^{(3)} + 2aX^{(1)}X^{(2)} &= 0 & (\text{orden } \lambda^3) \end{aligned} \right.$$

Como $E(t) = E_1(t) + E_2(t)$, tomamos $X^{(1)}(t) = X_1^{(1)}(t) + X_2^{(1)}(t)$

$$X^{(1)}(t) = X^{(1)}(\omega_1)e^{-i\omega_1 t} + X^{(1)}(\omega_2)e^{-i\omega_2 t} + c.c. \quad (7)$$

se obtiene: $X^{(1)}(\omega_j) = -\frac{e}{m} \frac{E_j}{D(\omega_j)}$ (8)

donde $D(\omega_j) \equiv \omega_0^2 - \omega^2 - 2i\gamma\omega$ (9)

se toma ahora $[X^{(1)}(t)]^2$ y se reemplaza en la ec. para $X^{(2)}$:

$$\ddot{X}^{(2)} + 2\gamma \dot{X}^{(2)} + \omega_0^2 X^{(2)} = -a[X^{(1)}]^2 \quad \leftarrow \text{F efectiva} \quad (10)$$

contiene frecuencias $\pm 2\omega_1, \pm 2\omega_2, \pm(\omega_1 + \omega_2), \pm(\omega_1 - \omega_2), \phi$.

por lo tanto,

$$X^{(2)}(t) = X^{(2)}(2\omega_1)e^{-i2\omega_1 t} + X^{(2)}(2\omega_2)e^{-i2\omega_2 t} + X^{(2)}(\omega_1 + \omega_2)e^{-i(\omega_1 + \omega_2)t} + X^{(2)}(\omega_1 - \omega_2)e^{-i(\omega_1 - \omega_2)t} + X^{(2)}(0) + c.c. \quad (11)$$

se obtiene:

$$X^{(2)}(2\omega_1) = \frac{-e(e/m)^2 E_1^2}{D(2\omega_1) D^2(\omega_1)} ; \quad X^{(2)}(2\omega_2) = \frac{-e(e/m)^2 E_2^2}{D(2\omega_2) D^2(\omega_2)}$$

$$X^{(2)}(\omega_1 + \omega_2) = \frac{-2e(e/m)^2 E_1 E_2}{D(\omega_1 + \omega_2) D(\omega_1) D(\omega_2)}$$

$$X^{(2)}(\omega_1 - \omega_2) = \frac{-2e(e/m)^2 E_1 E_2^*}{D(\omega_1 - \omega_2) D(\omega_1) D(-\omega_2)}$$

$$X^{(2)}(\phi) = \frac{-2e(e/m)^2 E_1 E_1^*}{D(\phi) D(\omega_1) D(-\omega_1)} + \frac{-2e(e/m)^2 E_2 E_2^*}{D(\phi) D(\omega_2) D(-\omega_2)}$$

Ahora usando $P^{(1)}(\omega) = \chi^{(1)}(\omega) E(\omega)$

y como $P^{(1)}(\omega) = -N e x^{(1)}(\omega) \Rightarrow \boxed{\chi^{(1)}(\omega_j) = \frac{N(e^2/m)}{D(\omega_j)}} \quad (12)$

Suscept. No-lineal:

$$P^{(2)}(2\omega) = \chi^{(2)}(2\omega, \omega, \omega) E^2(\omega)$$

donde, $P^{(2)}(2\omega) = -N e x^{(2)}(2\omega)$

$$\Rightarrow \chi^{(2)}(2\omega_1, \omega_1, \omega_1) = \frac{N(e^3/m^2)e}{D(2\omega_1) D^2(\omega_1)} \quad (13)$$

que puede re-esccribirse como:

$$\chi^{(2)}(2\omega_1, \omega_1, \omega_1) = \frac{me}{N^2 e^3} \chi^{(1)}(2\omega_1) [\chi^{(1)}(\omega_1)]^2 \quad (14)$$

De manera similar, se obtiene:

$$\chi^{(2)}(\omega_1 + \omega_2, \omega_1, \omega_2) = \frac{N(e^3/m^2)a}{D(\omega_1 + \omega_2)D(\omega_1)D(\omega_2)} \quad (15)$$

$$\circ \quad \chi^{(2)}(\omega_1 + \omega_2, \omega_1, \omega_2) = \frac{ma}{N^2 e^3} \chi^{(1)}(\omega_1 + \omega_2) \chi^{(1)}(\omega_1) \chi^{(1)}(\omega_2) \quad (15')$$

$$\chi^{(2)}(\omega_1 - \omega_2, \omega_1, \omega_2) = \frac{N(e^3/m^2)a}{D(\omega_1 - \omega_2)D(\omega_1)D(\omega_2)} \quad (16)$$

$$= \frac{ma}{N^2 e^3} \chi^{(1)}(\omega_1 - \omega_2) \chi^{(1)}(\omega_1) \chi^{(1)}(-\omega_2) \quad (16')$$

$$\chi^{(2)}(0, \omega_1, \omega_1) = \frac{N(e^3/m^2)a}{D(0)D(\omega_1)D(-\omega_1)} = \frac{ma}{N^2 e^3} \chi^{(1)}(0) \chi^{(1)}(\omega_1) \chi^{(1)}(-\omega_1) \quad (17)$$

Regla de Miller: $\frac{\chi^{(2)}(\omega_1 + \omega_2, \omega_1, \omega_2)}{\chi^{(1)}(\omega_1 + \omega_2) \chi^{(1)}(\omega_1) \chi^{(1)}(\omega_2)} = \frac{ma}{N^2 e^3}$

$\approx \text{cte. (obs. experimental!)} \quad \text{!}$

$$\Rightarrow \frac{ma}{N^2 e^3} \approx \text{cte.}$$

$$m\omega_0^2 d \approx ma d^2 \Rightarrow \boxed{\alpha = \omega_0^2 / d}$$

$$N \approx 1/d^3$$

Estimación de $\chi^{(2)}$

$$\chi^{(2)}(\omega_1 + \omega_2, \omega_1, \omega_2) = \frac{N(e^3/m^2)e}{D(\omega_1 + \omega_2)D(\omega_1)D(\omega_2)}$$

$\chi^{(2)}(\omega_1 + \omega_2)$
 $\chi^{(1)}(\omega_1)\chi^{(1)}(\omega_2)$

Miller: $\frac{ma}{N^2 e^3} = \text{cte.}$

N es muy o menos cte ($\approx 10^{22}$ /cc)
 $m \checkmark$ $e \checkmark$ a no se conoce

Asumir: contrib. lineal y cuadrática son del mismo Orden

$\Rightarrow m\omega_0^2 d = m e d^2$, donde $d \sim$ tamaño atómico

$\Rightarrow \boxed{a = \omega_0^2 / d}$

Aprox. $D(\omega) \approx \omega_0^2$, $N \approx 1/d^3$, $e = \omega_0^2 / d$

$\Rightarrow \chi^{(2)} \approx \frac{e^3}{m^2 \omega_0^4 d^4}$

$\omega_0 = 10^{16}$ rad/sec.

$d \approx 3 \text{ \AA}$

$e = 4.8 \times 10^{-10}$ esu

$m = 9.1 \times 10^{-28}$ gr.

$\Rightarrow \chi^{(2)} \approx 1.7 \times 10^{-8}$ (esu)

↓
en acuerdo con valores experimentales