# #10 Kramers-Kronigove relacije

## I Analitička svojstva odzivnih funkcija
## II Primjena Kramers-Kronigovih relacija

predavanja 20**

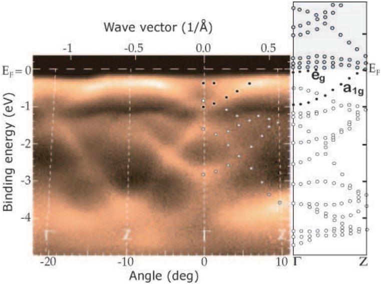
# Motivacija I i II

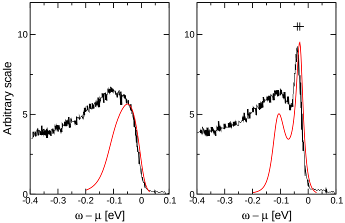
*što je zajedničko odzivnim funkcijama u elektrodinamici kontinuuma i raznim vlastitim energijama u mikroskopskoj fizici čvrstog stanja?*

- ARPES (kutno razlučiva fotoemisija elektrona; $\hbar\omega = 22$ eV)

$$(-)\mathcal{G}_2(\mathbf{p},\omega) = \frac{(-)\Sigma_2(\mathbf{p},\omega)}{\left[\omega - \varepsilon(\mathbf{p}) - \Sigma_1(\mathbf{p},\omega)\right]^2 + \left[\Sigma_2(\mathbf{p},\omega)\right]^2}$$

- fitanje eksperimentalnih rezultata - suglasno s K-K relacijama



# Analitička svojstva odzivnih funkcija

- analitička svojstva odzivnih funkcija u FČS

  *(i)* $\alpha(z)$ je analitička funkcija za $\mathrm{Im}\, z \geq 0$
  *(ii)* $\alpha(z)/z$ opada brže od $|z|^{-1}$ za $|z| \to \infty$
  *(iii)* $\alpha_1(z) = \alpha_1(-z)$ i $\alpha_2(z) = -\alpha_2(-z)$

- niskofrekventni dio u dielektričnoj susceptibilnosti

$$4\pi\chi(\omega) \approx \frac{-\Omega_{pl}^2}{\omega(\omega + i\Gamma_1)} + \frac{-\omega_p^2}{\omega^2 + i\gamma\omega - \omega_{\mathrm{TO}}^2} + \dots$$

- doprinos optičkih fonona? $(\surd)$

$$4\pi\chi^f(z) = -\omega_p^2/[z^2 + i\gamma z - \omega_{\mathrm{TO}}^2]$$

- doprinos vodljivih elektrona? $(\times)$

$$4\pi\chi^{el}(z) = -\Omega_{pl}^2/[z(z + i\Gamma_1)]$$

# Nelokalnost u vremenu

*izotropni homogeni sustavi s lokalnom vezom u* $\mathbf{x}$

- susceptibilnost $[\chi_{\alpha\beta}(\mathbf{x}, t; \mathbf{x}', t') \approx \delta_{\alpha,\beta}\delta(\mathbf{x} - \mathbf{x}')\chi(\mathbf{x}, t - t')]$

$$\mathbf{P}(\mathbf{x}, t) = \int_{-\infty}^{\infty} \mathrm{d}\tau\, \chi(\mathbf{x}, \tau)\mathbf{E}(\mathbf{x}, t - \tau)$$

- dielektrični pomak $[\chi(\mathbf{x}, \tau) \approx \chi(\tau);\ \chi(\mathbf{k}, \tau) = (-1/k^2)\tilde{\chi}(\mathbf{k}, \tau)]$

$$\mathbf{D}(\mathbf{x}, t) = \mathbf{E}(\mathbf{x}, t) + 4\pi \int_{-\infty}^{\infty} \mathrm{d}\tau\, \chi(\mathbf{x}, \tau)\mathbf{E}(\mathbf{x}, t - \tau)$$

- realnost dielektričnog pomaka

$$\mathbf{D}(\mathbf{x}, t) = \int (\mathrm{d}\omega/2\pi)\, \mathrm{e}^{-i\omega t}\, \mathbf{D}(\mathbf{x}, \omega) \rightarrow \mathbf{D}^*(\mathbf{x}, \omega) = \mathbf{D}(\mathbf{x}, -\omega)$$

# Nelokalnost u vremenu

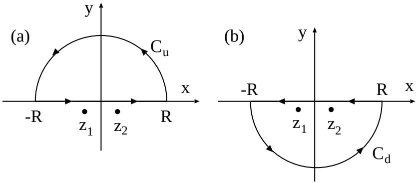
*primjer: ionski izolatori*

- dielektrična susceptibilnost $[\nu_0^2 = \omega_{\mathrm{TO}}^2 - (\gamma/2)^2]$

$$\chi(\tau) = \int (\mathrm{d}\omega/2\pi)\, \mathrm{e}^{-i\omega\tau}\, \chi(\omega), \qquad 4\pi\chi(\omega) = \frac{\omega_p^2}{\omega_{\mathrm{TO}}^2 - \omega^2 - i\gamma\omega}$$

- integracija za $\tau < 0$ daje 0; nultočke su: $z_{1,2} = \mp\nu_0 - i\gamma/2$
- za $\tau > 0$

$$4\pi\chi(\tau) = \frac{1}{2\pi}\oint_{C_d} \mathrm{d}z\, \frac{\omega_p^2}{(z-z_1)(z-z_2)} \mathrm{e}^{-iz\tau} = \omega_p^2\, \mathrm{e}^{-\gamma\tau/2}\, \frac{\sin\nu_0\tau}{\nu_0}\theta(\tau)$$



# Nelokalnost u vremenu

*primjer: ionski izolatori → rješenje*

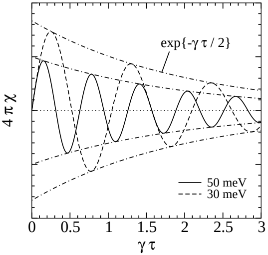
- inducirana polarizacija

$$\mathbf{P}(\mathbf{x}, t) = \int \mathrm{d}\tau\, \chi(\tau) \mathbf{E}(\mathbf{x}, t - \tau)$$

- kauzalnost: posljedica $[\mathbf{P}(\mathbf{x}, t)]$ slijedi uzrok $[\mathbf{E}(\mathbf{x}, t - \tau)] \Rightarrow \theta(\tau)$

$$4\pi\chi(\tau) = \omega_p^2\, \mathrm{e}^{-\gamma\tau/2}\, (\sin \nu_0 \tau / \nu_0) \theta(\tau)$$

- nelokalnost u vremenu: $\Rightarrow \exp\{-\gamma\tau/2\}$ $[\hbar\nu_0 = 50,\ 30\ \mathrm{meV},$ $\hbar\gamma = 5\ \mathrm{meV}]$



# Struktura dielektričnog pomaka

*na koji se način realnost polja $\mathbf{E}(\mathbf{x}, t)$ i $\mathbf{D}(\mathbf{x}, t)$ te analitička svojstva funkcije $4\pi\chi(\tau)$ odražavaju na strukturu polja $\mathbf{D}(\mathbf{x}, t)$?*

- električno polje

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{E}_0(\mathbf{x}) \cos \omega t \equiv \mathbf{E}(\mathbf{x}, \omega)\mathrm{e}^{-i\omega t} + \mathbf{E}(\mathbf{x}, -\omega)\mathrm{e}^{i\omega t}$$

- dielektrična funkcija $[\varepsilon(\omega) = 1 + 4\pi\chi(\omega)]$

$$\varepsilon_1(\omega) = \varepsilon_1(-\omega), \quad \varepsilon_2(\omega) = -\varepsilon_2(-\omega)$$

- dielektrični pomak $[\varepsilon(-\omega) = \varepsilon^*(\omega)]$

$$\begin{aligned} \mathbf{D}(\mathbf{x}, t) &= (1/2)\mathbf{E}_0(\mathbf{x})\left[\varepsilon(\omega)\mathrm{e}^{-i\omega t} + \varepsilon^*(\omega)\mathrm{e}^{i\omega t}\right] \\ &= \frac{1}{2}\mathbf{E}_0(\mathbf{x})\left\{\frac{1}{2}\left[\varepsilon + \varepsilon^*\right]\left(\mathrm{e}^{-i\omega t} + \mathrm{e}^{i\omega t}\right) + \frac{1}{2}\left[\varepsilon - \varepsilon^*\right]\left(\mathrm{e}^{-i\omega t} - \mathrm{e}^{i\omega t}\right)\right\} \\ &= \mathbf{E}_0(\mathbf{x})\left[\varepsilon_1(\omega) \cos \omega t + \varepsilon_2(\omega) \sin \omega t\right] \end{aligned}$$

- doprinos u fazi uz $\varepsilon_1(\omega)$
- pomak u fazi za $\pi/2$ uz $\varepsilon_2(\omega)$ (apsorpcije energije u mediju)

# Kramers-Kronigove relacije

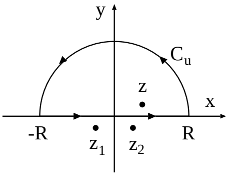
*promatramo odzivnu funkciju* $\alpha(z)$

- Cauchyjev teorem

$$\alpha(z) \;=\; \frac{1}{2\pi i}\oint_{C_u} \mathrm{d}z' \,\frac{\alpha(z')}{z'-z}$$

- za $z \rightarrow \omega + i\eta$ daje

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



# Kramers-Kronigove relacije

*standardne transformacije*

- koristimo identitet
$$1/[\omega' - \omega - i\eta] = \mathcal{P}\big(1/[\omega' - \omega]\big) + \pi i \delta(\omega' - \omega)$$
- rezultat $[\alpha_1(\omega) = \alpha_1(-\omega)$ i $\alpha_2(\omega) = -\alpha_2(-\omega)]$

$$\alpha_1(\omega) + i\alpha_2(\omega) = \frac{1}{\pi i}\mathcal{P}\int_{-\infty}^{\infty} \mathrm{d}\omega' \, \frac{[\alpha_1(\omega') + i\alpha_2(\omega')]}{\omega' - \omega}$$

- standardna simetrizirana forma

$$\alpha_1(\omega) = \frac{2}{\pi}\mathcal{P}\int_0^{\infty} \mathrm{d}\omega' \, \frac{\omega'\alpha_2(\omega')}{\omega'^2 - \omega^2}$$
$$\alpha_2(\omega) = -\frac{2}{\pi}\mathcal{P}\int_0^{\infty} \mathrm{d}\omega' \, \frac{\omega\alpha_1(\omega')}{\omega'^2 - \omega^2}$$

# Kramers-Kronigove relacije u vodičima

*na koji način možemo prilagoditi Drudeovu susceptibilnost?*

- analitička forma ukupne susceptibilnosti u vodičima

$$\alpha(z) = 4\pi\chi(z) - \frac{4\pi i\sigma^{\mathrm{dc}}}{z} \rightarrow \alpha^{el}(z) = \frac{-i\Omega_{pl}^2}{\Gamma_1(z + i\Gamma_1)}$$

- Kramers-Kronigove relacije

$$\begin{aligned}\chi_1(\omega) &= \frac{2}{\pi}\mathcal{P}\int_0^\infty \mathrm{d}\omega' \, \frac{\omega'\chi_2(\omega')}{\omega'^2 - \omega^2} \\ \chi_2(\omega) &= \frac{\sigma^{\mathrm{dc}}}{\omega} - \frac{2}{\pi}\mathcal{P}\int_0^\infty \mathrm{d}\omega' \, \frac{\omega\chi_1(\omega')}{\omega'^2 - \omega^2}\end{aligned}$$

# Transverzalno pravilo suma u izolatorima

*dielektrična funkcija u području* $\omega \gg \omega_{\mathrm{TO}}$

- aproksimativni izraz

$$\varepsilon_1(\omega) = 1 + 4\pi\chi_1(\omega) \approx 1 - \frac{\omega_p^2}{\omega^2}, \qquad \varepsilon_2(\omega) \approx 0$$

- Kramers-Kronigova relacija I

$$\varepsilon_1(\omega) = 1 + 4\pi\chi_1(\omega) = 1 - 8\int_0^\infty \mathrm{d}\omega' \, \frac{\omega'\chi_2(\omega')}{\omega^2} = 1 - \frac{\omega_p^2}{\omega^2}$$

- rezultat $[\chi_2(\omega) = \sigma_1(\omega)/\omega]$

$$8\int_0^\infty \mathrm{d}\omega \, \omega\chi_2^f(\omega) = 8\int_0^\infty \mathrm{d}\omega \, \sigma_1^f(\omega) = \omega_p^2$$

# Transverzalno pravilo suma u vodičima

- vodiči s dvije vrpce

$$\varepsilon(\omega) = 1 + (4\pi i/\omega)\sigma^{\rm intra}(\omega) + 4\pi\chi^{\rm inter}(\omega)$$

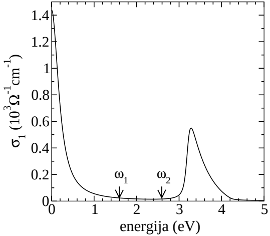
- unutarvrpčano pravilo suma

$$8\int_0^\infty {\rm d}\omega\, \sigma_1^{\rm intra}(\omega) = \Omega^2_{{\rm intra},\alpha} = \Omega^2_{pl}$$

- Kramers-Kronigova relacija I

$$\varepsilon_1(\omega) \approx 1 + \frac{2}{\pi}\int_{\omega_2}^\infty {\rm d}\omega'\, \frac{\varepsilon_2(\omega')}{\omega'} - \frac{2}{\pi\omega^2}\int_0^{\omega_1} {\rm d}\omega'\, \omega'\varepsilon_2(\omega')$$

$$\varepsilon_1(\omega) \approx \varepsilon_\infty - \frac{\Omega^2_{pl}}{\omega^2}$$



# Dielektrične konstante u izolatorima

*dielektrične konstante u Lyddane-Sachs-Tellerovoj relaciji*

- izolatori s međuvrpčanim pobuđenjima

$$\varepsilon(\omega) = 1 + 4\pi\chi^f(\omega) + 4\pi\chi^{\mathrm{inter}}(\omega)$$

- viskofrekventna dielektrična konstanta $[\omega_{\mathrm{TO}} \ll \omega \ll \omega_2]$

$$\varepsilon_\infty \approx 1 + 8\int_{\omega_2}^{\infty} \mathrm{d}\omega' \, \frac{\chi_2^{\mathrm{inter}}(\omega')}{\omega'}$$

- $\omega = 0$ dielektrična konstanta $[\omega \ll \omega_{\mathrm{TO}}]$

$$\varepsilon_0 = \varepsilon_1(0) \approx 1 + 8\int_0^{\infty} \mathrm{d}\omega' \, \frac{\chi_2(\omega')}{\omega'} = \varepsilon_\infty + \varepsilon_\infty \frac{\omega_{\mathrm{LO}}^2 - \omega_{\mathrm{TO}}^2}{\omega_{\mathrm{TO}}^2}$$

- Lyddane-Sachs-Tellerova relacija?

# Nultočke dielektrične funkcije

*kako su vezane nultočke od $\varepsilon(\omega)$ s frekvencijama $\Omega_i^2$ iz pravila suma?*

- primjer: $\omega_{pl} \approx \Omega_{pl}/\sqrt{\varepsilon_\infty}$
- na koji način utječu energije gušenja na oblik funkcije $\varepsilon(\omega)$?
- a na koji način broj nositelja naboja $n^*_{\alpha\alpha}$?