Kramer-Kronig analysis

Step-by-step guide

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Starting point:

- Single scattering distribution of bulk excitations in terms of dielectric function:

$$S(E) = \frac{N_{ZLP}t}{\pi a_0 m_0 v^2} \mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right] \ln\left[1 + \left(\frac{\beta}{\theta_E}\right)^2\right]$$

\cite{Egerton_book}

- Kramer-Kronig relations:

$$\mathrm{Re}\left[\frac{1}{\varepsilon(E)}\right] = 1 - \frac{2}{\pi}\mathcal{P}\int_0^\infty \mathrm{Im}\left[\frac{-1}{\varepsilon(E')}\right]\frac{E'dE'}{E'^2 - E^2}.$$

\cite{dapor2017}

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Extracting Im[-1/ε]

$$S(E) = \frac{N_{ZLP}t}{\pi a_0 m_0 v^2} \mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right] \ln\left[1+\left(\frac{\beta}{\theta_E}\right)^2\right]$$

$$\mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right] = \frac{\pi a_0 m_0 v^2}{N_{ZLP}t} \frac{S(E)}{\ln\left[1+\left(\frac{\beta}{\theta_E}\right)^2\right]}.$$

?

KNOWN

Finding K

$$\frac{N_{ZLP}t}{\pi a_0 m_0 v^2} \equiv K,$$

- Take E = 0 in

$$\mathrm{Re}\left[\frac{1}{\varepsilon(E)}\right] = 1 - \frac{2}{\pi}\mathcal{P}\int_0^\infty \mathrm{Im}\left[\frac{-1}{\varepsilon\left(E'\right)}\right]\frac{E'dE'}{E'^2 - E^2}.$$

- Gives

$$1 - \mathrm{Re}\left[\frac{1}{\varepsilon(0)}\right] = \frac{2}{\pi}\int_0^\infty \mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right]\frac{dE}{E}.$$

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Finding $\frac{N_{ZLP}t}{\pi a_0 m_0 v^2} \equiv K, \qquad 1 - \mathrm{Re}\left[\frac{1}{\varepsilon(0)}\right] = \frac{2}{\pi}\int_0^\infty \mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right]\frac{dE}{E}.$

- Dividing by E and integrating both sides of

$$\mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right] = \frac{\pi a_0 m_0 v^2}{N_{ZLP}t}\frac{S(E)}{\ln\left[1+\left(\frac{\beta}{\theta_E}\right)^2\right]}.$$

- Gives

$$\int_0^\infty \mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right]\frac{dE}{E} = \frac{\pi a_0 m_0 v^2}{N_{ZLP}t}\int_0^\infty \frac{S(E)}{\ln\left[1+\left(\frac{\beta}{\theta_E}\right)^2\right]}\frac{dE}{E}$$

Finding K

- Combining

$$\int_0^\infty \mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right]\frac{dE}{E} = \frac{\pi a_0 m_0 v^2}{N_{ZLP} t}\int_0^\infty \frac{S(E)}{\ln\left[1+\left(\frac{\beta}{\theta_E}\right)^2\right]}\frac{dE}{E} \quad \& \quad 1 - \mathrm{Re}\left[\frac{1}{\varepsilon(0)}\right] = \frac{2}{\pi}\int_0^\infty \mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right]\frac{dE}{E}.$$

- Gives

KNOWN

$$\frac{\int_0^\infty \frac{S(E)}{\ln\left[1+\left(\frac{\beta}{\theta_E}\right)^2\right]}\frac{dE}{E}}{\frac{\pi}{2}\left(1 - \mathrm{Re}\left[\frac{1}{\varepsilon(0)}\right]\right)} = \frac{N_{ZLP} t}{\pi a_0 m_0 v^2} \equiv K,$$

ALSO KNOWN for many materials

Can extract Im[-1/ε]!

$$\mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right] = \frac{\pi a_0 m_0 v^2}{N_{ZLP}\, t}\,\frac{S(E)}{\ln\left[1+\left(\frac{\beta}{\theta_E}\right)^2\right]}.$$

FOUND!

KNOWN

Finding Re[1/ε]

- Use:

$$\mathrm{Re}\left[\frac{1}{\varepsilon(E)}\right] = 1 - \frac{2}{\pi}\mathcal{P}\int_0^\infty \mathrm{Im}\left[\frac{-1}{\varepsilon\left(E'\right)}\right]\frac{E' dE'}{E'^2 - E^2}.$$

- But: for discrete spectrum: singularity at *E* = *E'*

  → use causality dielectric function

Finding Re[1/ε]

- Using:

$$\mathrm{Re}\left[\frac{1}{\varepsilon(E)}\right] = \mathcal{C}\left\{\frac{1}{\varepsilon(t)} - \delta(t)\right\} = \mathcal{F}\{p(t)\}, \qquad \mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right] = \mathcal{S}\left\{\frac{1}{\varepsilon(t)} - \delta(t)\right\} = i\mathcal{F}\{q(t)\},$$

- And, due to causality:

$$p(t) = \mathrm{sgn}[q(t)]$$

- Resulting in:

$$\mathrm{Re}\left[\frac{1}{\varepsilon(E)}\right] = \mathcal{C}\left\{\mathrm{sgn}\left[\mathcal{S}^{-1}\left\{\mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right]\right\}\right]\right\}$$

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Finding dielectric function

- Yippy!!

$$\varepsilon(E) = \varepsilon_1(E) + i\varepsilon_2(E) = \frac{\mathrm{Re}[1/\varepsilon(E)] + i\,\mathrm{Im}[-1/\varepsilon(E)]}{\{\mathrm{Re}[1/\varepsilon(E)]\}^2 + \{\mathrm{Im}[-1/\varepsilon(E)]\}^2}.$$

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Cool cool cool, BUT

- Assumed single scattering $S(E)$ distribution of bulk excitations to be know…

- In reality the recorded spectrum consists of bulk excitations, surface excitations and relativistic losses.

Obtaining $S_b(E)$

- $S_b(E)$ obtainable from bulk excitations through Fourier log deconvolution method
- → need to obtain bulk excitations from total spectrum

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Obtaining $S_b(E)$

- Assume no relativistic losses:

$$\begin{aligned} S_{tot}(E) &= S_b(E) + S_s(E) \\ &= C_b(E)\,\mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right] + C_s(E)\left(\mathrm{Im}\left[\frac{-4}{1+\varepsilon(E)}\right] - \mathrm{Im}\left[\frac{-1}{\varepsilon(E)}\right]\right) \end{aligned}$$

- Difficult to extract ε from this function

\cite{thesis_ascunce}

Plan of attack

- Assume:

$$S_{tot}(E) = S_b^{'}(E)$$

- Calculate ε' with KK-analysis
- Calculate

$$S_s^{'}(E) = C_s(E)\left(\mathrm{Im}\left[\frac{-4}{1+\varepsilon^{'}(E)}\right] - \mathrm{Im}\left[\frac{-1}{\varepsilon^{'}(E)}\right]\right)$$

- Better approximation:

$$S_b^{''}(E) = S_{tot}(E) - S_s^{'}(E)$$

  - Calculate ε'' with KK-analysis
  - Calculate S_s''
  - Approximate S_b'''
    - Calculate ε''' with KK-analysis
    - Calculate S_s'''
    - Approximate S_b''''

Repeat until convergence

Including relativistic losses

- Kröger function:

$$\frac{d^2P_s}{d\Omega\ dE} = \frac{1}{\pi^2 a_0 k_0 T} \frac{\theta}{(\theta^2+\theta_E^2)^2} \mathrm{Im}\left[\frac{(\varepsilon_a-\varepsilon_b)^2}{\varepsilon_a^2\varepsilon_b} R_c\right]$$

- Similar approach probably

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What is the dielectric function?

- Description of reaction of the entire solid to the passing electron:
  - Real part: permittivity, polarizability
  - Imaginary part: energy dissipation

Interpretations of the dielectric function

- Real part:
  - Crosses zero: transitions in the system (plasmons, interband, …)
  - Number of crosses: character of material (metallic, semi-conductor, …)
- Imaginary part:
  - Damping on transitions

High energy range

- $\varepsilon_1 \rightarrow 1$, ε_2 small

$$\varepsilon(\omega) = \varepsilon_1 + i\varepsilon_2 = 1 + \chi = 1 - \frac{\omega_p^2}{\omega^2 + \Gamma^2} + \frac{i\,\Gamma\omega_p^2}{\omega\left(\omega^2 + \Gamma^2\right)}$$

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Crossings with +slope ε_1

- Well defined collective response (i.e. peak/transition?)
  - Condittion for plasma resonance

$$E(\varepsilon_1 = 0) = [E_p^2 - (\Delta E_p)^2]^{1/2}$$

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Cherenkov radiation

- When: $\varepsilon_1(E) > c^2/v^2$

Damping

- Stopping power:

$$\frac{dE}{dz} = \frac{2\hbar^2}{\pi a_0 m_0 v^2} \int\int \frac{q_y \omega \,\mathrm{Im}[-1/\varepsilon(q,\omega)]}{q_y^2 + (\omega/v)^2} \, dq_y \, d\omega$$

Low loss electron energy spectrum

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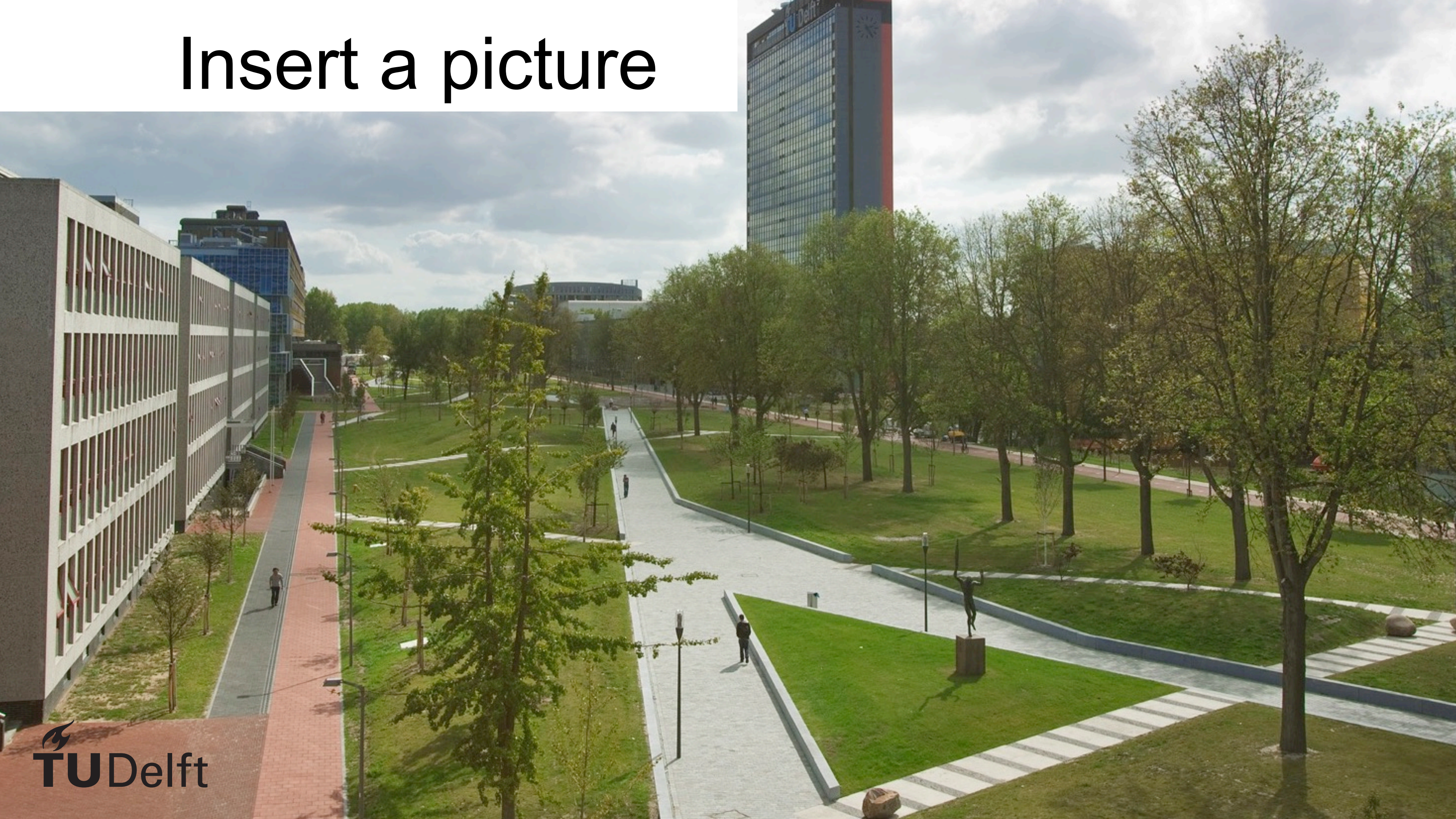

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