

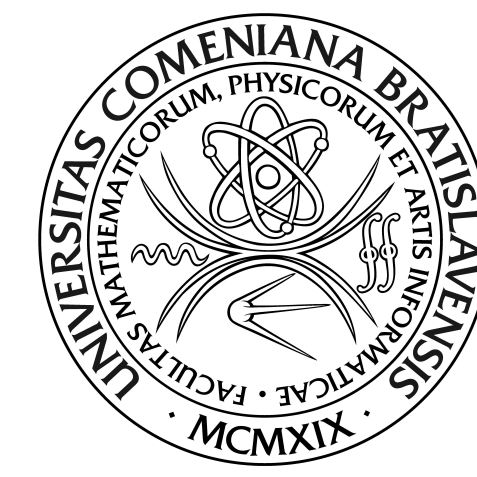
Extrapolation of complex optical conductivity of metals

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Introduction & Abstract

Recent measurements show that it is possible to observe quantum corrections to optical conductivity up to UV region. Although this anti-Drude behavior, increase of conductivity with frequency, should disappear at electron collision frequency, such transition has never been observed or described theoretically. It is well known that extrapolation of complex conductivity obtained from spectroscopic ellipsometry is ill-posed. A solution of this analytic continuation problem is not unique for experimental data with finite accuracy. However, we show that assuming physically appropriate properties of searched function $\sigma(\omega)$ (symmetry, smoothness, given number of maxima and asymptotic solution for low and high frequencies) one can significantly restrict the set of solutions. We present a simple numerical method using radial basis function approximation and a simulated annealing optimisation method which reasonably extrapolates optical conductivity from visible frequency range down to far infrared and up to ultraviolet region. We have obtained good agreement with the real part of optical conductivity obtained from transmission measurements in a wide frequency range.

Numerical Method

- $\sigma'_{data}(\omega) + i\sigma''_{data}(\omega)$ is measured complex conductivity for discrete values $\omega_j \in [\omega_{min}, \omega_{max}]$
- Define new variable $x \equiv \ln \hbar\omega/\pi kT$ and $y \equiv \sigma'(\omega)$ (Ref. [2]) and set of points (x_i, y_i) where

$$x_i = 0, 1, 2, \dots, \underbrace{8, 8.1, 8.2, \dots, 9.9, 10}_{\ln(\hbar\omega_j/kT)}, 11, 12, \dots, n \quad (1)$$

and y_i are fitting parameters to be optimized.

- Smooth function $y = f(x)$ is constructed as a cubic spline using RBF method for boundary conditions fixed to known dc-conductivity $(1, \sigma'_{dc})$ and $(n, 0)$
- Calculate real and imaginary part of complex conductivity $\sigma'_{\{y_i\}}(\omega) = f(x(\omega))$, $\sigma''_{\{y_i\}}(\omega) = \mathcal{H}[\sigma'_{\{y_i\}}(\omega)]$
- Simulated annealing - with respect to values y_i find local minimum of functional

$$\mathcal{F}[\sigma'_{\{y_i\}}(\omega)] = \sum_{\omega_j} (\sigma''_{data}(\omega_j) - \sigma''_{\{y_i\}}(\omega_j))^2 + (\sigma'_{data}(\omega_j) - \sigma'_{\{y_i\}}(\omega_j))^2, \quad (2)$$

- Accept only curves with precision better than precision of RBF spline.
- Many accepted curves do not satisfy requirement that conductivity of disordered conductors should change slowly on scale much less than Γ , see Ref. [1].
- Average curve of the accepted curves $\bar{\sigma}'(\omega) \equiv \sigma'_{\{y_i\}}(\omega)$ satisfies such requirement.
- The final extrapolated curve is found by minimizing

$$\tilde{\mathcal{F}}[\sigma'_{\{y_i\}}(\omega)] = \mathcal{F}[\sigma'_{\{y_i\}}(\omega)] + \lambda \int_{\omega_0}^{\omega_n} \left(\frac{d^2\sigma'(\omega)}{d\omega^2} - \frac{d^2\bar{\sigma}'(\omega)}{d\omega^2} \right)^2 d\omega, \quad (3)$$

Numerical Simulation

- The procedure was tested on data (circles in Fig. 1) created from simple theoretical model of optical conductivity (dashed lines)
- We used simulated annealing with multiple melting of system to find an ensemble of accepted curves (few of them showed as grey lines)

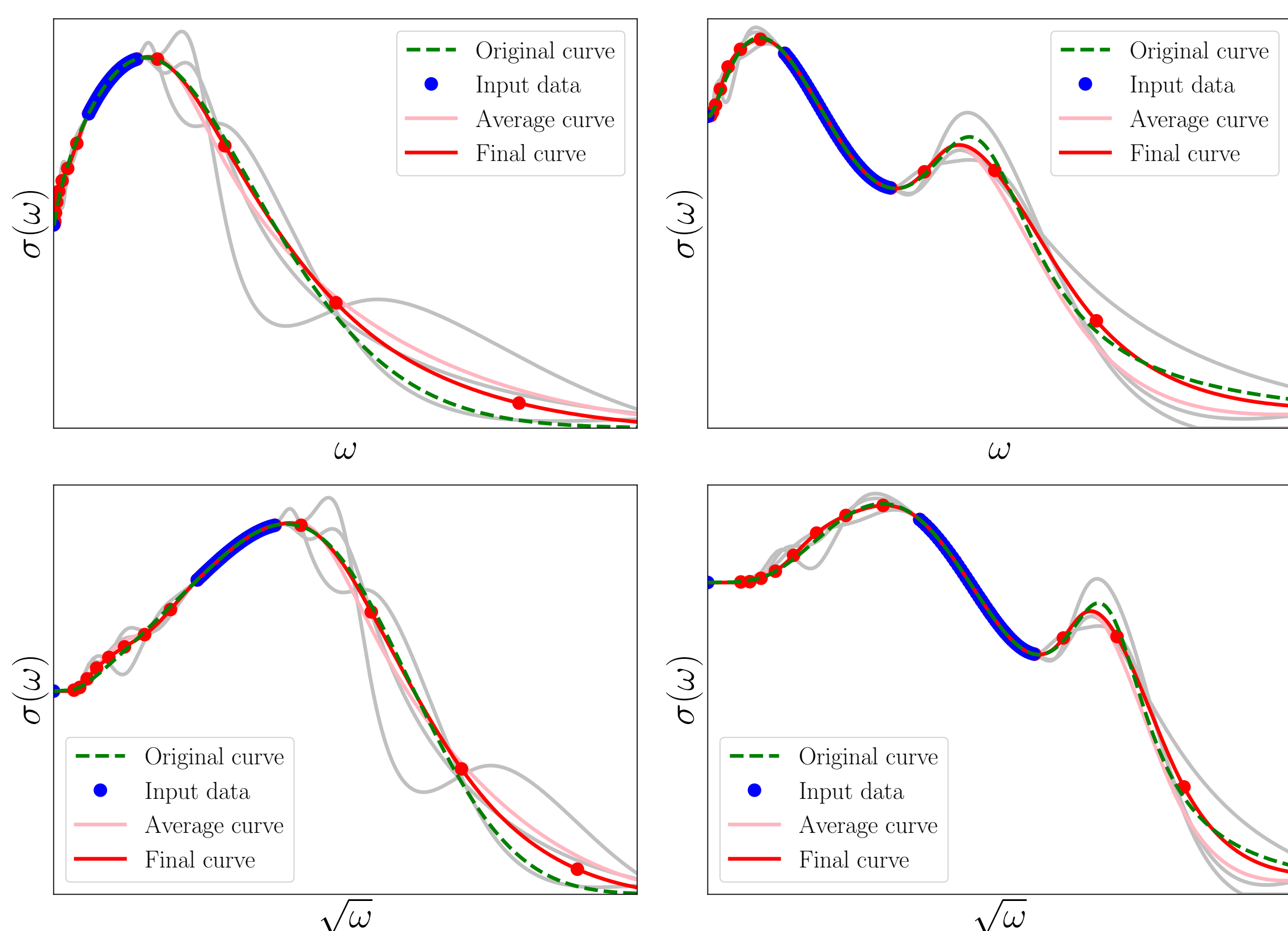


Figure 1: Left: simple Drude model of optical conductivity with square-root quantum corrections (MoC) Right: optical conductivity as a sum of two lorentzians with square-root quantum corrections (NbN)

Extrapolation of real data

- Procedure was applied to data measured on disordered conductors MoC and NbN by spectroscopic ellipsometry with different dc-conductivity measured by van der Pauw method.
- Finite temperature is included by transformation

$$\omega \mapsto \Omega = \sqrt{\omega^2 + (\pi k_B T / \hbar)^2} \quad (4)$$

- Back-transformation allows to compare extrapolation with temperature dependent transport measurements (light blue on fig.2).

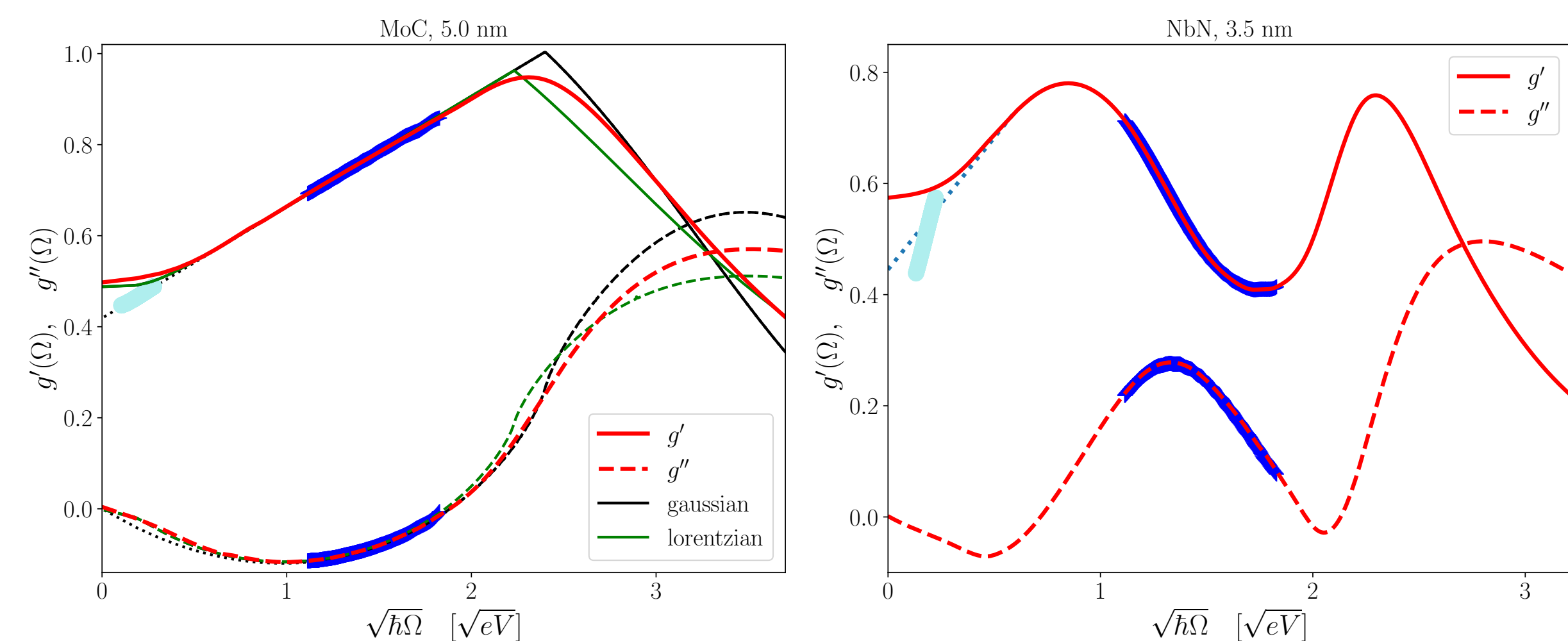


Figure 2: Extrapolation of normalized sheet conductance (orange line) obtained from spectroscopic ellipsometry for MoC and NbN thin films compared with theoretical curves (grey lines) proposed in Ref. [1]

- Transmission and complex refractive index calculated from extrapolated conductivities are compared with measurement (Fig.3 and 4).

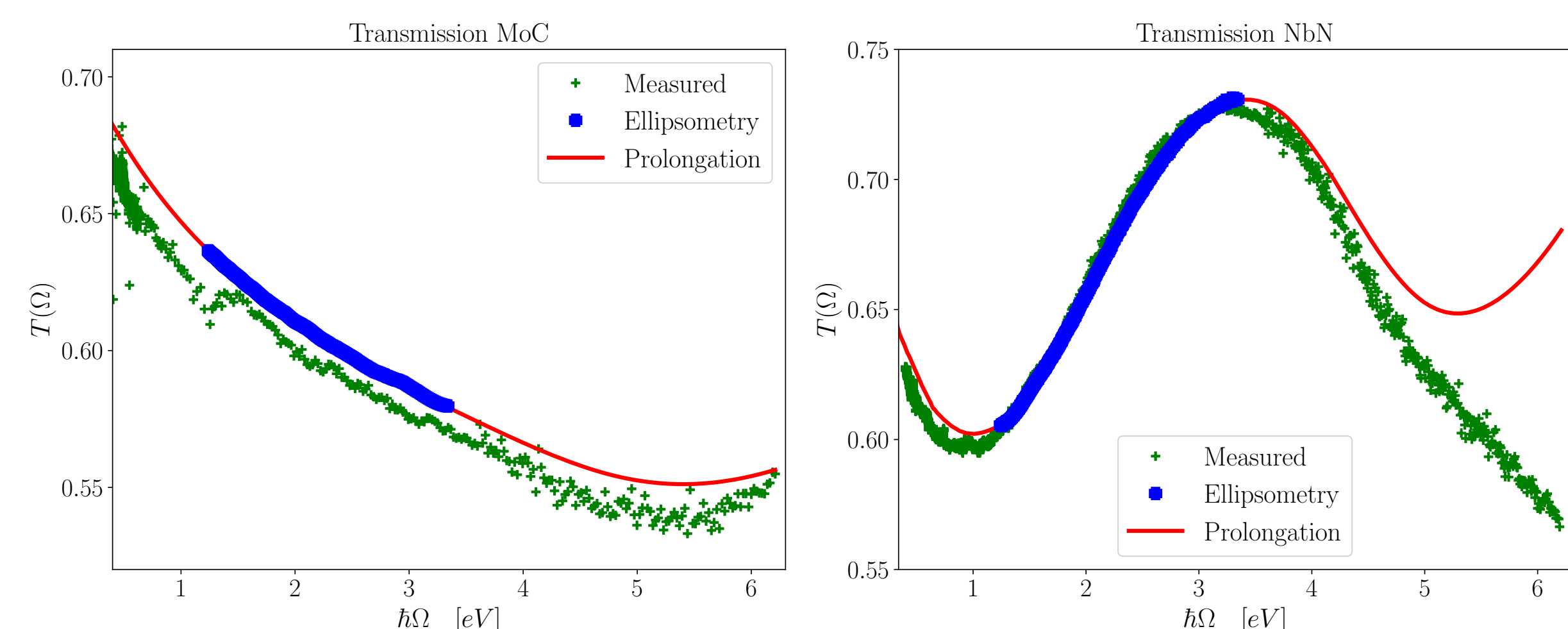


Figure 3: Transmission of MoC and NbN sample on sapphire substrate normalized to transmission of substrate (green "+"), transmission obtained from extrapolated conductivity (red line)

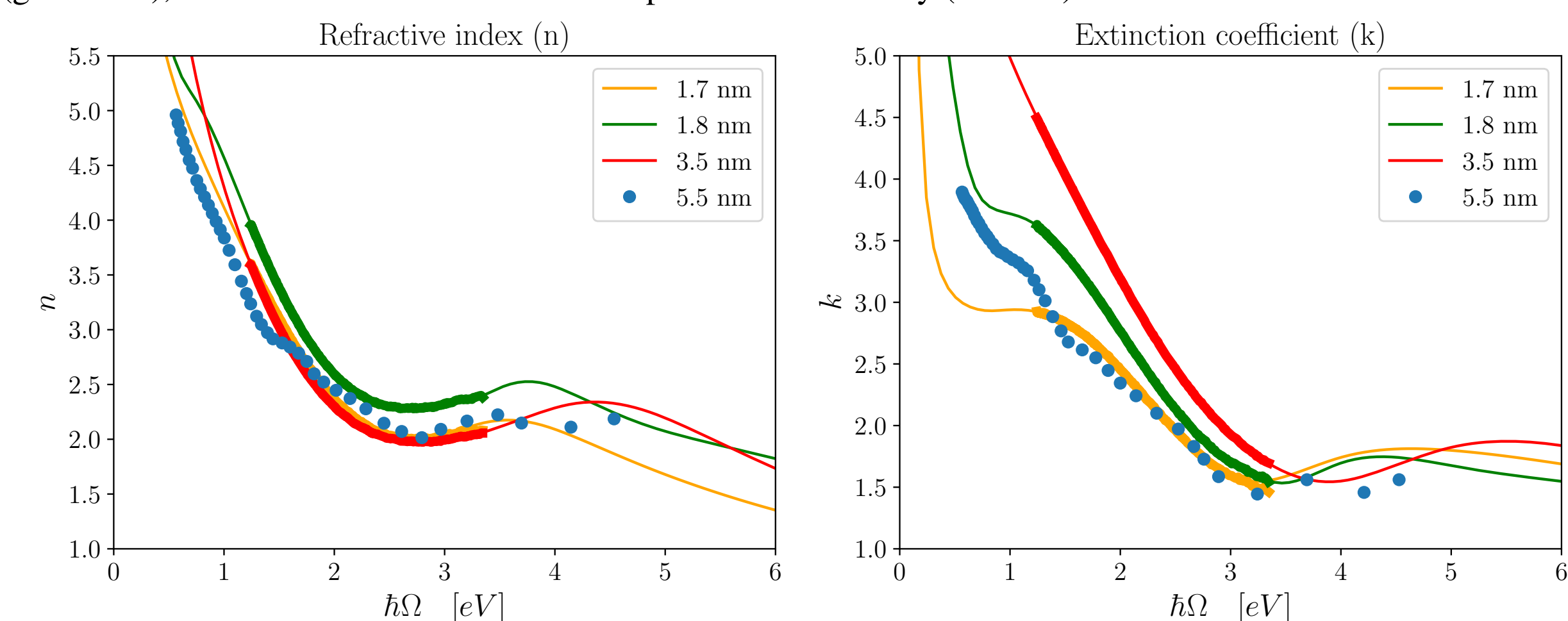


Figure 4: Real and imaginary part of refractive index of 5.5 nm thin NbN films measured in Ref. [3] compared with refractive index obtained from extrapolation for different thicknesses

Conclusions

Numerical procedure of extrapolation of complex conductivity of weakly disordered metals based on Kramers-Kronig analysis and general physical properties is presented. It is shown, that requirement of slow variation of conductivity on energy scales $\ll \Gamma$ is crucial and final extrapolated curve exhibit quantum correction visible from temperature dependence of dc-conductivity. Extrapolation of optical conductivity obtained from spectroscopic ellipsometry in visible range is in agreement with transmission measurement in infrared and ultraviolet range.

References

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Acknowledgements

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