A numerical extrapolation method for complex conductivity of disordered metals.

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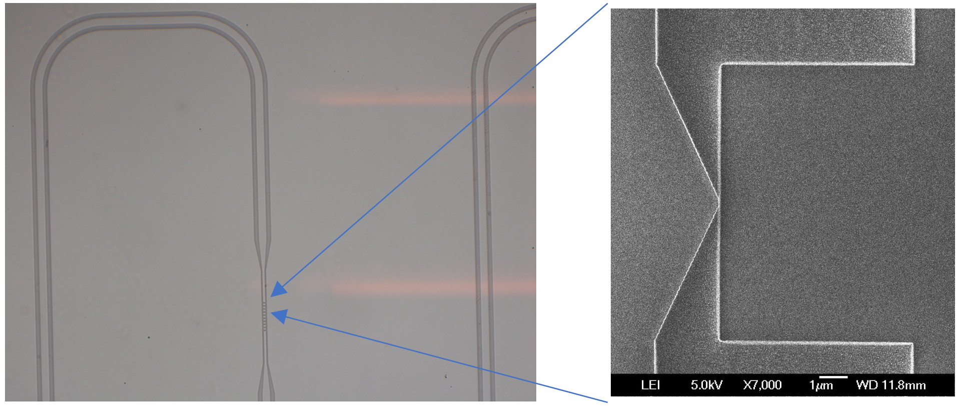
Strongly disordered metals

- MoC : Quantum correction to optical conductivity up to optical frequencies [1]
- NbN : Superconducting devices, e.g.:
  - photon detectors
  - parametric amplifiers



$$L(I) = L_k(1 + I^2/I_0^2);$$

$$L_k \sim \frac{\hbar R_n}{k_B T_c}$$

[1] Neilinger, P. et al, Phys. Rev. B. **100,** 241106, 2019.

Complex conductivity

$$\vec{j}(t) = \int_0^\infty d\tau \sigma(\tau) \vec{E}(\vec{r}, t-\tau)$$

$$\vec{j} = \sigma(\omega)\vec{E}(\omega) \qquad \sigma(\omega) = \int_0^\infty dt e^{i\omega t}\sigma(t)$$

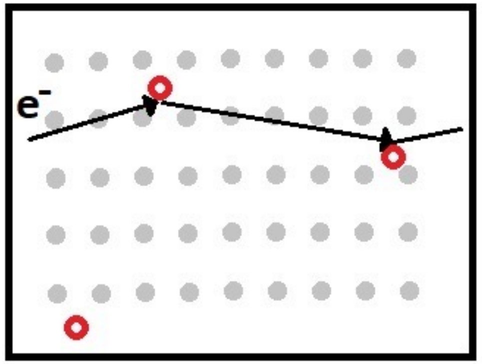
Causality ⇒ $\sigma(\omega)$ analytic in upper half-plane ... Kramers-Kronig relations

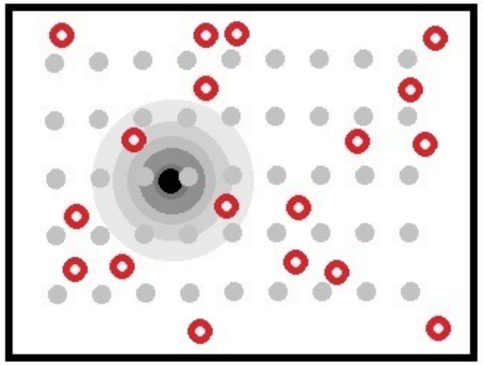
$$\sigma(\omega) = \sigma'(\omega) + i\sigma''(\omega)$$

$$\sigma'(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\sigma''(\omega')}{\omega' - \omega} d\omega' \qquad \sigma''(\omega) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\sigma'(\omega')}{\omega' - \omega} d\omega'$$

$$\sigma'(\omega) = H[\sigma''(\omega')]$$

Quantum corrections to conductivity



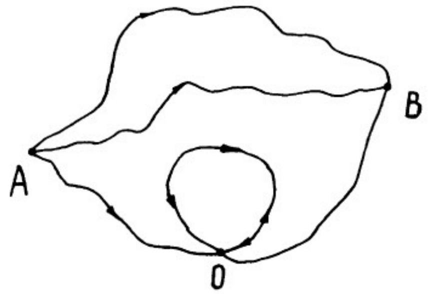


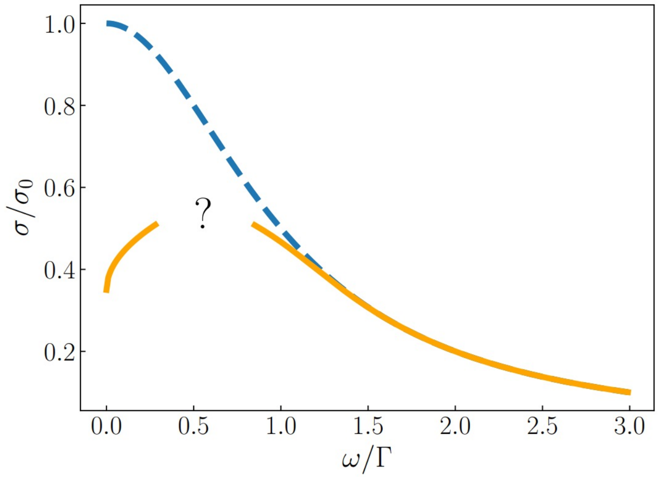
$$\Gamma = 1/\tau$$

Localized state

Metal-insulator transistion

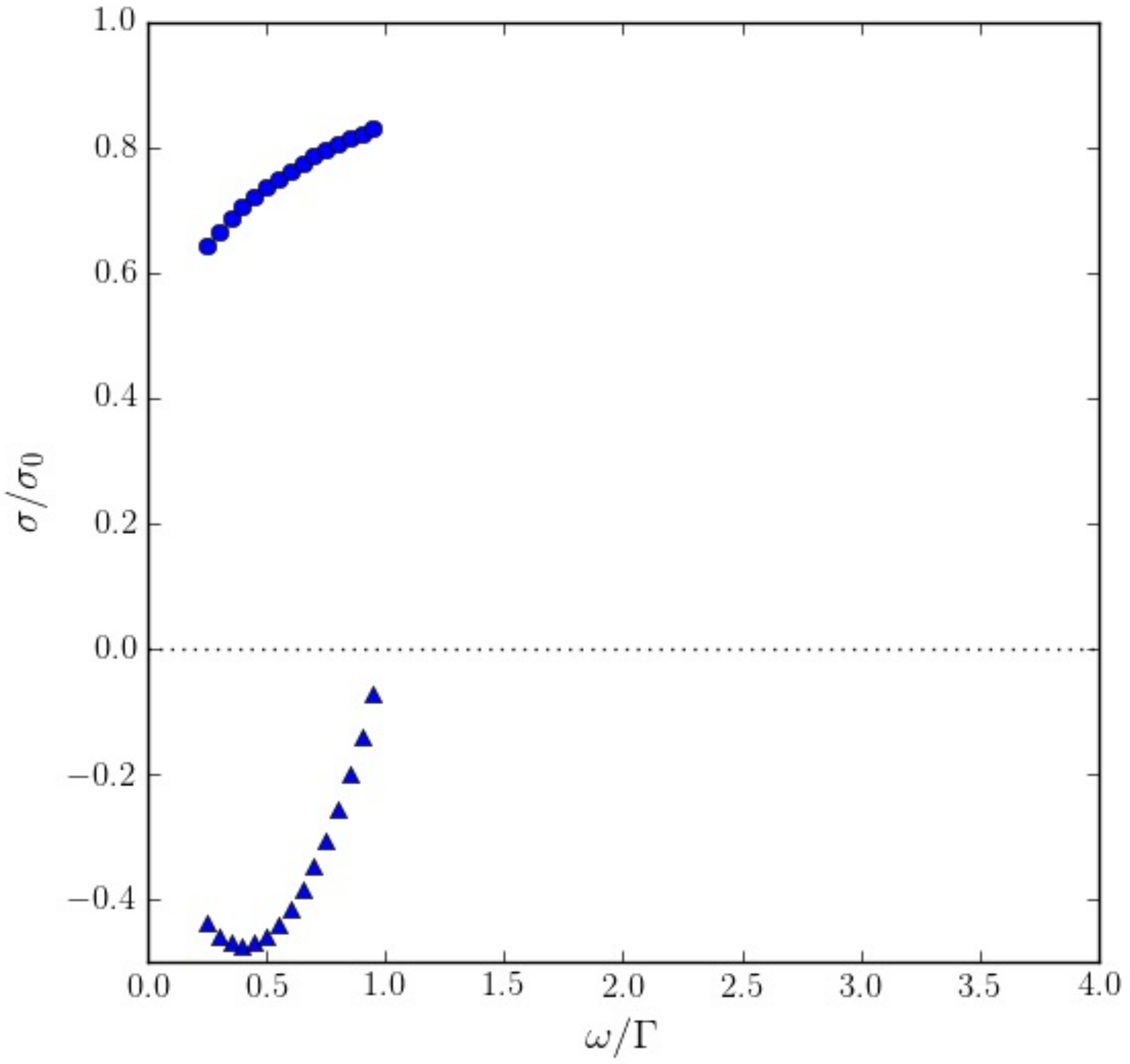
$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega/\Gamma}$$





[2] P. W. Anderson, Phys. Rev. **109**, 1492 (1958) .

[3] B. L. Altshuler and A. G. Aronov. edited by Pollak, M. and Efros, A. L., North-Holland, Amsterdam, 1985.



Measurement of optical conductivity

- Spectroscopic ellipsometry
- Limited experimental window
- Kramers-Kronig analysis
- Highly disordered metals → Quantum corrections to optical conductivity

Ill-posed problems

- Not unique solution / the procedure of obtaining solution is unstable
  - Inverse problems
  - Cauchy problem for Laplace equation
  - Integral equations
  - Analytic continuation

$$\boldsymbol{A}q = f$$

$$\boldsymbol{A}(q + \delta q) = f + \delta f$$

$$\delta q = \boldsymbol{A}^{-1}\delta f$$

$$\frac{\|\delta q\|}{\|q\|} \le \|\boldsymbol{A}\|\|\boldsymbol{A}^{-1}\|\frac{\|\delta f\|}{\|f\|}$$

Analytic continuation:

Def:

$f(x)$ analytic in $U \subset V \subset \mathbb{C}$

$F(z)$ analytic in V, such that $\forall z \in U: F(z) = f(z)$

Can be turn to integral equation problem:

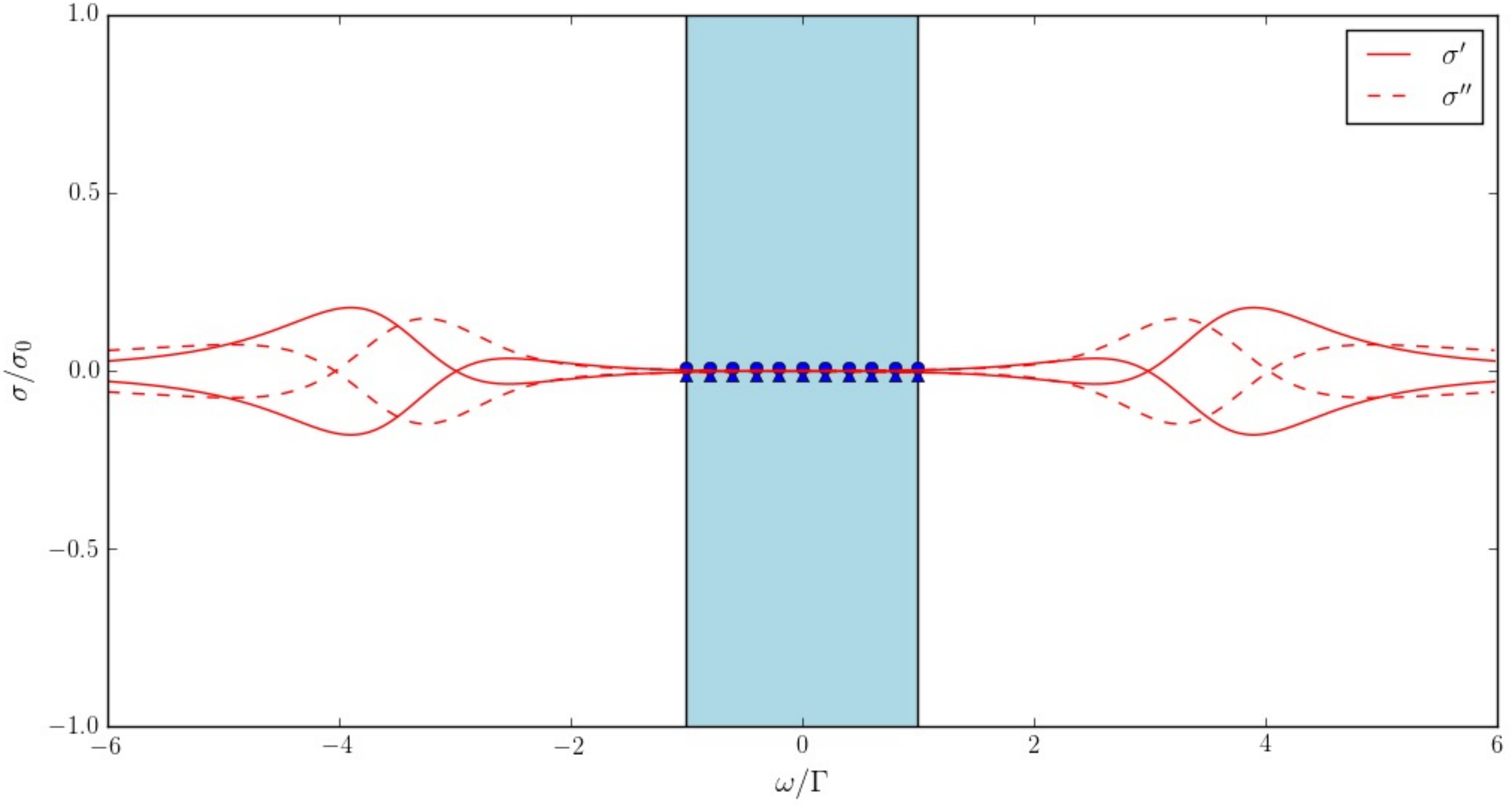
$$\Delta_i(\omega) = \frac{2}{\pi} \int_1^\infty \frac{\Delta_r(s)}{\omega - s} ds$$

$$\Delta_i(\omega_m) = \frac{2}{\pi} \sum_{n=0}^{N} \frac{1}{\omega_m - s_n} \Delta_r(\omega_n) \Delta s$$

The precision decreases with distance from known interval as [3]:

$$\alpha(x) = \frac{4}{\pi} e^{-x\pi/2}$$

[3]: L. N. Trefethen, BIT. Num Math. pp. 1-15 (2020)



1.0
0.5
0.0
−0.5
−1.0
−6
−4
−2
0
2
4
6
ω/Γ
σ/σ_0
σ'
σ''

Regularization

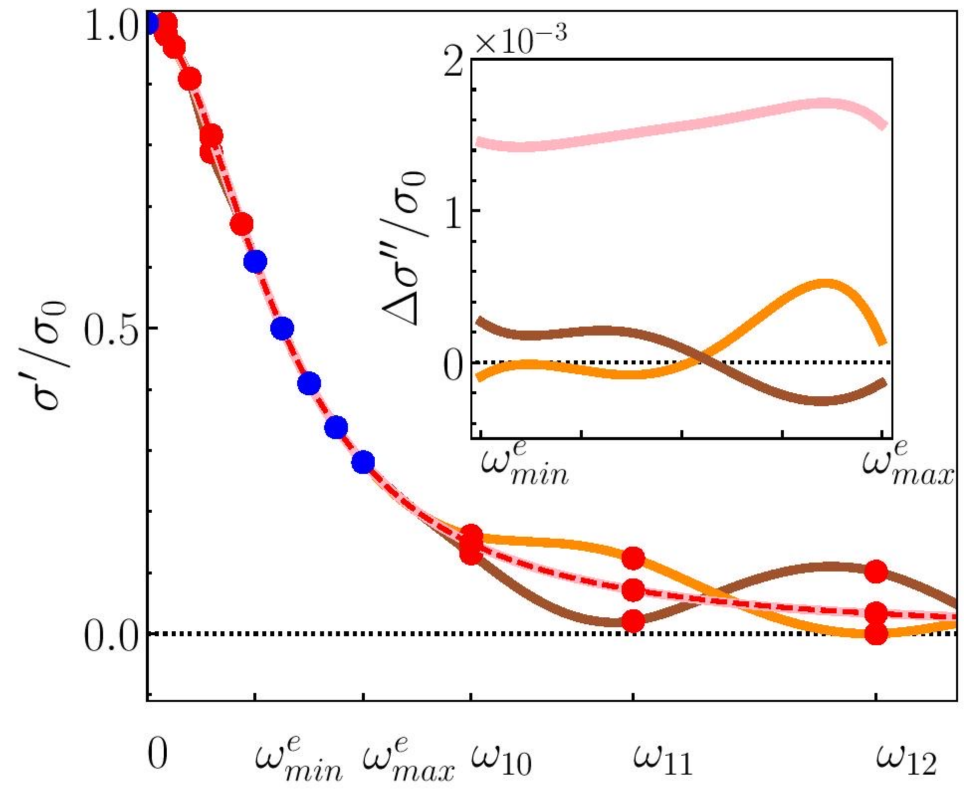
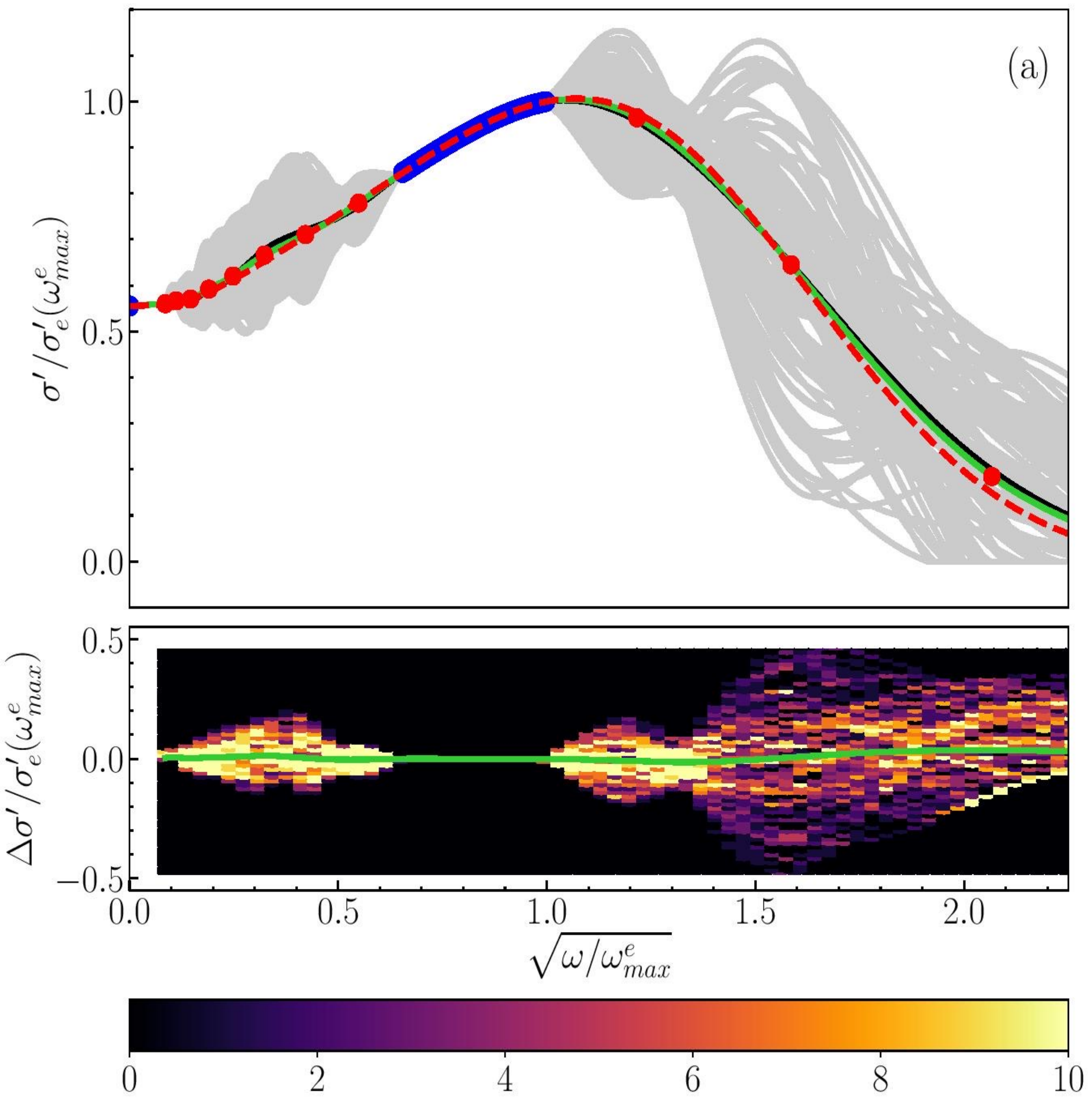


Fig.5: Principle of finding of feasible curves

- Disordered metals has large ralaxation rate Γ
- Searched function is smooth and changes on large scales
- Averaging in an ensamble of solutions fitting the data



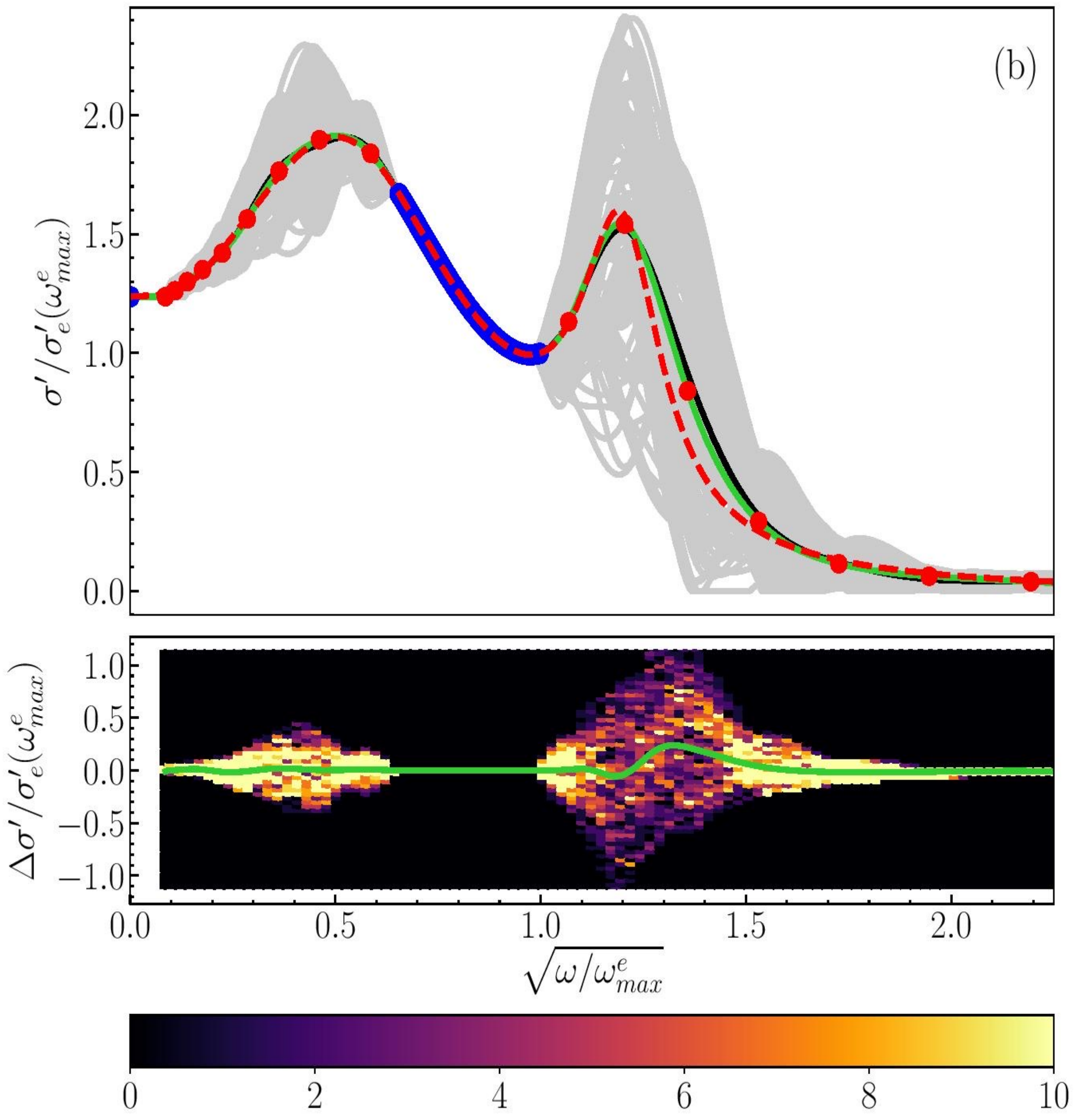
Numerical results

- Minimized functional:

$$\mathcal{F}[\sigma'_{\{y_i\}}(\omega)] = \sum_{\omega^e_j}\left(\sigma''_e(\omega^e_j) - \sigma''_{\{y_i\}}(\omega^e_j)]\right)^2 + \sum_{\omega^e_j}\left(\sigma'_e(\omega^e_j) - \sigma'_{\{y_i\}}(\omega^e_j)\right)^2$$

- Input data (blue points) generated by restriction of domain of model function:

$$g_1(\omega, T) = e^{-\Omega^2/\Gamma_1^2} + Q(\sqrt{\Omega/\Gamma_1} - 1)e^{-4\Omega^2/\Gamma_1^2}$$



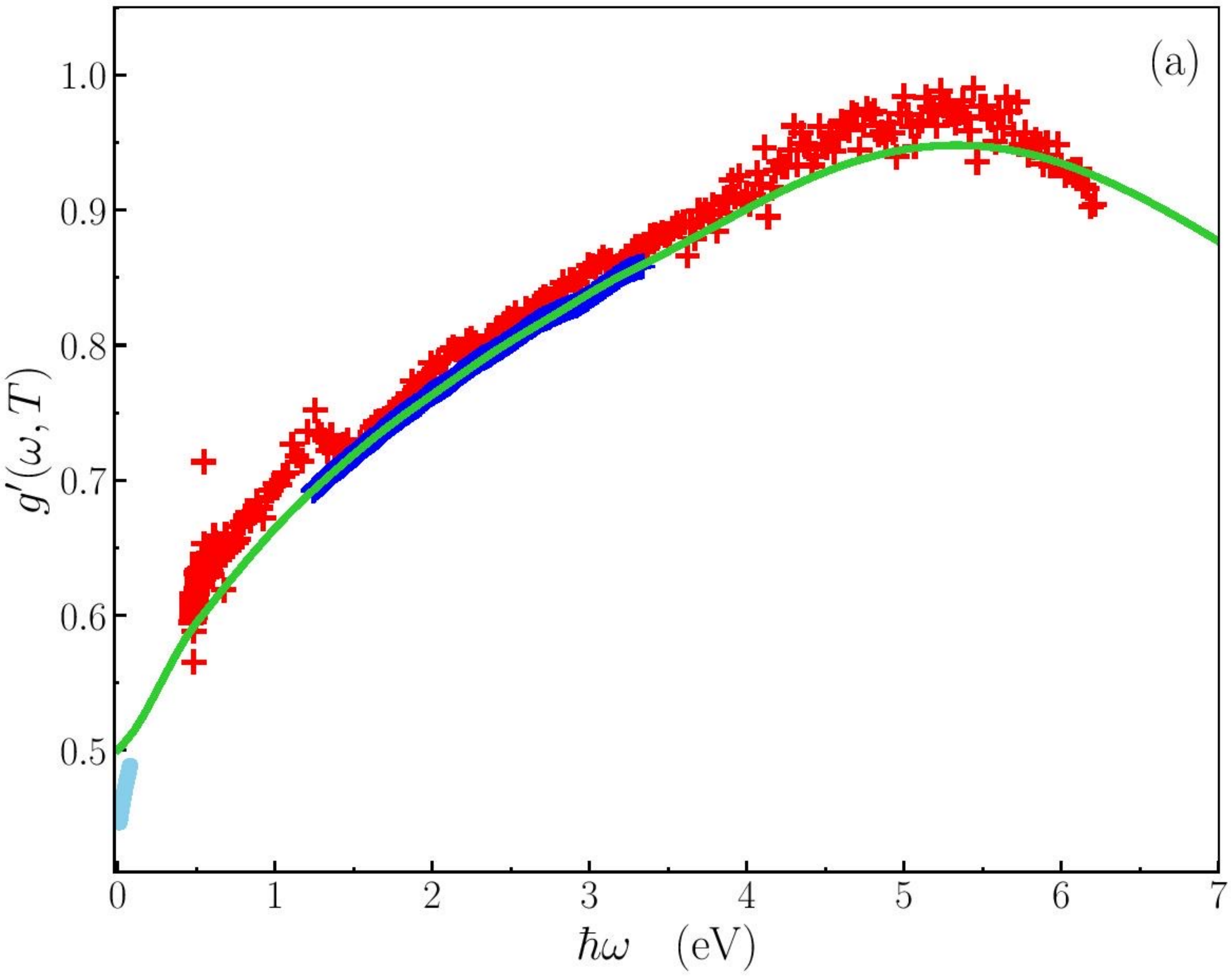
Numerical results

- Model function:

$$g_2(\omega, T) = \frac{1}{1+(\Omega/\Gamma_{2,1})^2} + Q(\sqrt{\Omega/\Gamma_{2,1}} - 1)e^{-4\Omega^2/\Gamma_{2,1}^2} + \frac{r_2}{1+((\Omega-\Omega_2)/\Gamma_{2,2})^2}$$

- Simulated annealing
- RBF spline

Extrapolation of experimental data



$g = g' + ig'' = \sigma \cdot Z_0 \cdot d$

$\Omega = \sqrt{\omega^2 + k_B T/\hbar}$

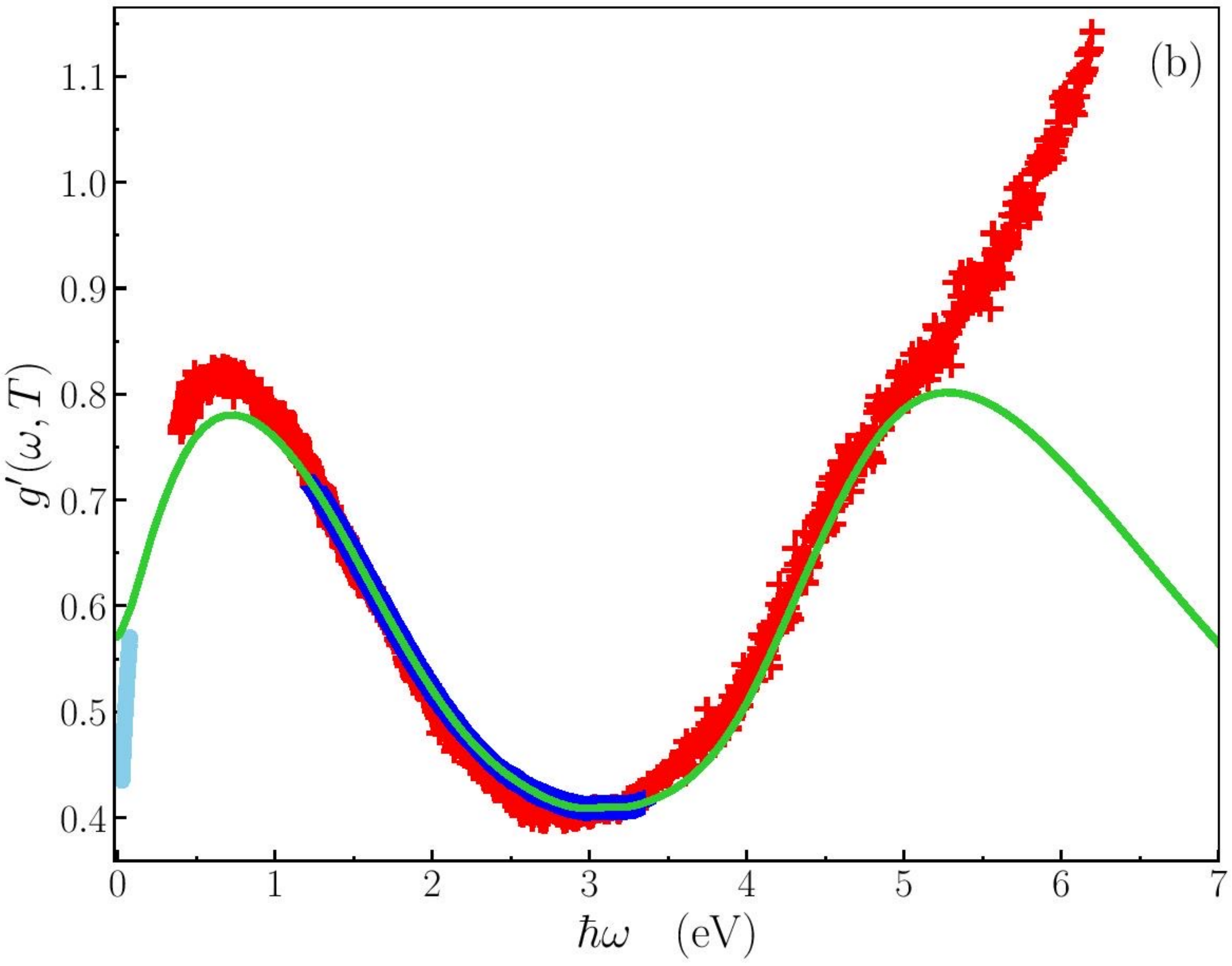
- **MoC**
  - $d = 5.0$ nm, $\epsilon_\infty = 1.4$
  - RT:

$$\omega \mapsto \Omega = \sqrt{\omega^2 + \gamma(T)^2}$$

$$\gamma(T) = \pi k_B T/\hbar$$

  - Transmission

Extrapolation of experimental data



$$g = g' + ig'' = \sigma \cdot Z_0 \cdot d$$

$$\Omega = \sqrt{\omega^2 + k_B T/\hbar}$$

- **NbN**
  - $d = 3{,}5$ nm, $\epsilon_\infty = 2.58$
  - RT, $\gamma(T) = \pi k_B T/\hbar$
  - Transmission