10. OP and OPc

OP—Optical Properties—computes Optical Properties from KK-determined reflectance and phase. 33 different functions may be calculated. The program can also subtract a model dielectric function from the data.

OPc is the console version.

Switches: `/h`, `/q`, and

`/V`*nnn*	—unit cell Volume is *nnn*
`/Wp`*nnn*	—Plasma frequency is *nnn*
`/W`*nnn*, *mmm*	—calculate between frequencies *nnn* and *mmm*
`/W`*mmm*	—calculate from 0.0 to maximum frequency *mmm*
`/ALL or /all`	—do ALL functions (33 files created)
`/P<file>`	—Partial dielectric function, $\epsilon - \epsilon_{DL}$

The unit cell volume is needed for sum rules. The plasma frequency is used for self-energy and effective mass. Max frequency (`/Wm`*nnn*) can be used to limit file size.

The switch for "Partial dielectric function" subtracts a Drude-Lorentz model from $<\epsilon(\omega)>$ before calculation of the optical function. It either uses parameters in a `*.PRM` file produced by DLFIT or asks the user for these parameters.

Response function switches:

`/S1 or /S`	—σ_1	`/S2`	—σ_2
`/E1 or /E`	—ϵ_1	`/E2`	—ϵ_2
`/N`	—refractive index, n	`/K`	—extinction coefficient, κ
`/A`	—Absorption coefficient, α		
`/R`	—Reflectance, $\mathscr{R}$	`/RPH`	—$\mathscr{R}$ is in file from KK
`/L`	—Loss function, $-\operatorname{Im} 1/\epsilon$		
`/M`	—effective Mass, m^*/m		
`/T`	—$1/\tau(\omega)$		
`/I`	—−Imag(self-energy), $-\Sigma_2$	`/RE`	—REal(self-energy), Σ_1
`/SU`	—SUm rule on $\sigma_1(\omega)$, N_{eff}	`/SL`	—Sum r. Loss function
`/Wps`	—superfluid plasma frequency, ω_{ps}		
`/LL`	—London Length, λ_L		
`/SK`	—SKin depth, δ		
`/F`	—Free carrier: ϵ_1 vs $1/\omega^2$		
`/D`	—Drude model: $1/\sigma_1$ vs ω^2		

Examples:

`OP F1A006 /S1`

Calculate conductivity (σ_1) from file `F1A006.RPH`

`OP F1A006 -sum -v162.1 -q`

Calculate Sum rule from file `F1A006.RPH`; output in `F1A006.SUM`. Unit cell volume = 162.1 Å^3. Be quick.

OP uses as input an `RPH` file, containing in 3 colums the frequency (cm^{-1}), the power reflectance $\mathscr{R}$, and the phase shift on reflection ϕ. This file is produced either by KK or, for simulated data, by DLCalc.

The complex (amplitude) reflectivity is $\sqrt{\mathscr{R}}e^{i\phi}$. The complex refractive index is calculated from the reflectivity:

$$N = \frac{1+\sqrt{\mathscr{R}}e^{i\phi}}{1-\sqrt{\mathscr{R}}e^{i\phi}}.$$

and the complex dielectric function is

$$\epsilon = \epsilon_1 + i\epsilon_2 = N^2.$$

Here are the functions that OP calculates. The frequencies are in wavenumbers (cm^{-1}), with $\omega[\,\mathrm{cm}^{-1}] = f[\mathrm{Hz}]/c = \omega[\mathrm{rad/s}]/2\pi c$. The computed results are in SI, mostly.

Some of the functions depend on $\Delta\epsilon$. If there is a single low energy band, with all the high frequency behavior lumped into ϵ_∞ then

$$\Delta\epsilon = \epsilon - \epsilon_\infty.$$

More generally, one may want to subtract off the contributions of phonons, interband transitons, etc. In this case, $\Delta\epsilon$ is the Partial dielectric function, $\epsilon - \epsilon_{DL}$ that you invoke with /P<file>.

1. `Sigma_1`

   The real part of the optical conducivity (in $\Omega^{-1}\mathrm{cm}^{-1}$) is

$$\sigma_1 = \frac{\omega\epsilon_2}{60}.$$

This can be compared to the expression in cgs:

$$\sigma_1 = \frac{\omega\epsilon_2}{4\pi},$$

with ω in sec^{-1} and σ_1 also in sec^{-1}.

2. `Sigma_2`

   The imaginary part of the optical conducivity (in $\Omega^{-1}\mathrm{cm}^{-1}$) is

$$\sigma_2 = -\frac{\omega(\epsilon_1 - 1)}{60}.$$

3. `Epsilon_1`

$$\epsilon_1 = \mathrm{Re}(\epsilon)$$

4. `Epsilon_2`

$$\epsilon_2 = \mathrm{Im}(\epsilon)$$

5. `Reflectance`

The power reflectance is

$$\mathscr{R} = \left|\frac{N-1}{N+1}\right|^2.$$

OP actually computes this rather than just reading the values from the `.RPH` file.

6. `Refr Index`

$$n = \mathrm{Re}(N)$$

7. `Ext Coeff.`

$$\kappa = \mathrm{Im}(N)$$

8. `Alpha`

The absorption coefficient (in cm^{-1}) is

$$\alpha = 4\pi\omega\kappa,$$

correct for ω in cm^{-1}. In cgs, this is

$$\alpha = 2\omega\kappa/c.$$

9. `Loss Fnctn`

The energy loss function is

$$L = \frac{\epsilon_2}{(\epsilon_1^2 + \epsilon_2^2)} = -\,\mathrm{Im}\,\frac{1}{\epsilon}.$$

10. `Surface Loss Fnctn`

The "surface" energy loss function is

$$L_s = \frac{\epsilon_2}{((\epsilon_1 - 1)^2 + \epsilon_2^2)} = -\,\mathrm{Im}\,\frac{1}{\epsilon - 1}.$$

11. `-Imag self-energy`

In some theories, the imaginary part of the self energy Σ plays the role of a scattering rate, with the dielectric function written as

$$\epsilon(\omega) = \epsilon_\infty - \frac{\omega_p^2}{\omega[\omega - 2\Sigma(\omega/2)]}.$$

with ω_p the plasma frequency and ϵ_∞ the limiting high frequency value. The factors of 2 occur because the excitations are created in pairs (electron-hole pairs or quasiparticle pairs). (These factors do not appear in all theoretical treatments.) The imaginary part of Σ is related to the quasiparticle lifetime through $1/\tau^*(\omega) = -2\,\mathrm{Im}\,\Sigma(\omega/2)(m_b/m^*(\omega))$ with m^* the effective mass and m_b the band mass.

OP computes $-\operatorname{Im}\Sigma$ via

$$-\operatorname{Im}\Sigma = \frac{\omega_p^2}{2\omega\Delta\epsilon} + \omega/2.$$

with $\Delta\epsilon = \epsilon - \epsilon_\infty$. You must enter the plasma frequency and ϵ_∞.

After computing the right had side of the above equation,OP divides the frequencies by 2, so that the dielectric function value at 400 cm^{-1} (for example) generates the $-\operatorname{Im}\Sigma$ value at 200 cm^{-1}.

Note that optical phonons and interband transitions may occur and these can be included in the ϵ_∞ function. OP allows you to subtract these from the data through its `/P<file>` capability.

`12. Real self-energy`

The real part of Σ is related to the effective mass m^* of the interacting carriers by

$$m^*(\omega)/m_b = 1 - 2\operatorname{Re}\Sigma(\omega/2)/\omega.$$

Hence, OP computes

$$\operatorname{Re}\Sigma(\omega/2) = \frac{\omega_p^2}{(2\omega\Delta\epsilon)} + \omega/2.$$

After computing the right had side of the above equation, OP divides the frequencies by 2, so that the dielectric function value at 400 cm^{-1} (for example) generates the $\operatorname{Re}\Sigma$ value at 200 cm^{-1}.

`13. Gamma_1`

$$\Gamma_1 = -\operatorname{Im}[\frac{\omega_p^2}{\omega\Delta\epsilon} - \omega]$$

`14. Gamma_2`

$$\Gamma_2 = \operatorname{Re}[\frac{\omega_p^2}{\omega\Delta\epsilon} - \omega]$$

`15. m*/m`

$$m*/m = -\frac{\omega_p^2}{\omega^2}\operatorname{Re}(\frac{1}{\Delta\epsilon})$$

`16. tau^-1*`

$$1/\tau = -\omega[\frac{\operatorname{Im}(\Delta\epsilon)}{\operatorname{Re}(\Delta\epsilon)}]$$

17. `Sumrule S_1`

This is the main sumrule function calculated by OP. The f-sum rule for solids can be written

$$\int_0^\infty \sigma_1(\omega')d\omega' = \frac{\omega_{p,tot}^2}{8},$$

where $\omega_{p,tot} = \sqrt{4\pi n_{tot} e^2/m}$ is the plasma frequency for all the electrons in the solid. We may write a partial sum rule (for the conduction band, say) as

$$\int_0^\omega \sigma_1(\omega')d\omega' = \frac{\pi n e^2}{2m^*},$$

where m^* is the average effective mass of the band. If the upper limit is above the free-carrier contribution and below the onset of the interband transitions, the right hand side becomes $\omega_p^2/8$ with ω_p the conduction band plasma frequency.

Next, write $n = N_{\mathit{eff}}/V_c$ and let m be the free electron mass. The density is in the number of effective electrons per unit cell volume (or formula volume). Then, OP calculates

$$N_{\mathit{eff}} \frac{m}{m*} = \frac{2mV_c}{\pi e^2} \int_0^\omega \sigma_1(\omega')d\omega'$$

with .

18. `Sumrule LossFn`

We may write a partial sum rule (for the conduction band, say) of the loss function as

$$\frac{1}{4\pi}\int_0^\omega \omega' L(\omega')d\omega' = \frac{\pi n e^2}{2m^*},$$

where m^* is the average effective mass of the band. If the upper limit is above the free-carrier contribution and below the onset of the interband transitions, the right hand side becomes $\omega_p^2/8$ with ω_p the conduction band plasma frequency. (The factor of $1/4\pi$ is the same as appears in $\omega\epsilon_2/4\pi = \sigma_1$.) Thus,

$$N_{\mathit{eff}} \frac{m}{m*} = \frac{mV_c}{2\pi^2 e^2} \int_0^\omega \omega' L(\omega')d\omega'$$

19. `Sumrule SurfaceLossFn`

Same as 18, but for L_s.

20. `Superfluid plasma freq`

A superfluid has a dielectric function that is

$$\epsilon = \epsilon_\infty - \frac{\omega_{ps}^2}{\omega^2}$$

with ω_{ps} the superfluid plasma frequency. OP calculates

$$\omega_{ps} = \sqrt{\omega^2 |\operatorname{Re}(\Delta\epsilon)|}$$

where the absolute value is used instead of a minus sign to avoid numerical problems. Be sure that ϵ is negative when you invoke this function!

If ω_{ps} is (nearly) constant in frequency, the behavior is that of a superfluid.

21. `London penetra. depth`

The dielectric function in 20 is that of a London superconductor, so one may also calculate λ_L as

$$\lambda_L = \frac{10^8}{2\pi\sqrt{\omega^2|\operatorname{Re}(\Delta\epsilon)|}}$$

The factor of 10^8 makes the units of $\lambda_L(\omega)$ in Å.

22. `Skin depth`

In the skin effect the electric field goes as $e^{-x/\delta}$ but of course the wave governed by a refractive indx N has a field which decays as $e^{-\kappa\omega x/c}$ (ω in rad/s) . Hence:

$$\delta = \frac{10^8}{2\pi\omega\kappa}.$$

The factor of 10^8 makes the units of $\delta(\omega)$ in Å.

23. `Epsilon_1 vs 1/w^2`

If

$$\epsilon = \epsilon_\infty - \frac{\omega_{ps}^2}{\omega^2}$$

then a plot of ϵ vs $1/\omega^2$ should be a straight line, with slope ω_{ps}^2. So this is equivalent to function 20.

24. `1/Sigma_1 vs w^2`

If the dielectric function is Drude like, then

$$\sigma_1 = \frac{\sigma_{dc}}{1+\omega^2\tau^2} = \frac{\omega_p^2/(4\pi\tau)}{\omega^2+1/\tau^2}$$

so a plot of $1/\sigma_1$ vs ω^2 should be a straight line with intercept $1/\tau$ and slope $4\pi\tau/\omega_p^2$.

25. `Abs(eps)`

$$|\epsilon| = \sqrt{\epsilon_1^2+\epsilon_2^2}$$

Not $\Delta\epsilon$!

26. `Abs(sigma)`

$$|\sigma| = \sqrt{\sigma_1^2+\sigma_2^2}$$

27. `Tan(delta)`

$$\tan\delta = \frac{\epsilon_2}{\epsilon_1}$$

28. `Abs(Tan(delta))`

$$\tan\delta_{abs} = |\frac{\epsilon_2}{\epsilon_1}|$$

29. `N_eff(free-el)`

Again, writing

$$\epsilon = \epsilon_\infty - \frac{\omega_{ps}^2}{\omega^2}$$

with ω_{ps} the superfluid plasma frequency. OP then writes $\omega_{ps}^2 = 4\pi n_s(\omega)e^2/m$ so that:

$$n_s(\omega) = \omega^2|\operatorname{Re}(\Delta\epsilon)|V_c C$$

30. `T slab (thick)`

Add intensities.

$$Damp = EXP(-Alpha * Thick)$$

$$\mathscr{T} == ((1. - \mathscr{R}_{sb}) * *2) * Damp/(1. - (\mathscr{R}_{sb} * *2) * (Damp * *2))$$

with $\mathscr{R}_{sb}$ the single bounce reflectance ($[(N-1)/(N+1]^2$.

31. `T slab (fringes)`

Add amplitude, getting the airy formula.

$$Delta = N * (2. * PI * \omega) * Thick$$

$$t1 = 2./(N + 1.)$$

$$t2 = 2. * N/(N + 1.)$$

$$rin = (N - 1.)/(N + 1.)$$

$$t = \frac{t1 * t2 * CEXP(i * Delta)}{(1. - rin * *2 * CEXP(2. * i * Delta))}$$

$$\mathscr{T} = tt*$$

32. `R slab (thick)`

Add intensities.

$$Damp = EXP(-2. * Alpha * Thick)$$

$$\mathscr{R} = \mathscr{R}_{sb} + \frac{\mathscr{R}_{sb} * ((1. - \mathscr{R}_{sb})^2) * Damp}{(1. - (\mathscr{R}_{sb}^2) * Damp)}$$

with $\mathscr{R}_{sb}$ the single bounce reflectance: $[\mathscr{R}_{sb} = (N-1)/(N+1)]^2$.

33. R slab (fringes)

$$Delta = N * (2\pi\omega) * Thick$$

! N(ω/c)d is the phase angle in the complex exponential.

$$t_1 = 2./(N + 1.)$$

$$t_2 = 2. * N/(N + 1.)$$

$$r_{in} = (N - 1.)/(N + 1.)$$

$$r_{fp} = (1. - N)/(1. + N) + \frac{t1 * rin * t2 * CEXP(2. * i * Delta)}{*(1. - rin * *2 * CEXP(2. * i * Delta))}$$

$$\mathscr{R} = r_{fp} rfp*$$

Add amplitude