5. KK

KK—Kramers-Kronig transform—performs a Kramers-Kronig transform for (single-bounce) reflectance $\mathscr{R}$ *and* (slab) transmittance $\mathscr{T}$ data. KK uses graphics window to show you some of the intermediate steps.

You will need to specify the extrapolations to be used outside the data. In 2012 these were changed significantly.

At high frequencies, you must use a `<compound name>.XRO` file. These are generated by the xro program described on page 32. Examples would be `Ag.xro` or `YBa2Cu3O6.93.xro`. The xro files extend from 80,660 cm^{-1} (10 eV) to 241,980,000 cm^{-1} (30,000 eV). Above this range, the data are extrapolated as $\mathscr{R} \sim \omega^{-4}$ as appropriate for completely free electrons.

Unless your data extend to 80,600 cm^{-1} or so (unlikely if you do not have vacuum ultraviolet instrumentation) there will be a gap. Optical data typically stop between 20,000 and 40,000 cm^{-1}, or 2.5 and 5 eV. There are 4 methods of bridging the gap between your measured data and the `.xro` data:

1. A power law in $1/\omega$: $\mathscr{R} = A + B/\omega + C/\omega^2 + D/\omega^3 + \ldots$ (Say `L#` at the prompt.)
2. A power law in ω: $\mathscr{R} = A + B\omega + C\omega^2 + D\omega^3 + \ldots$ (Say `W#` at the prompt.)
3. A cubic spline can also be used. (Not recommended, but sometimes it works.)
4. No bridge. This is equivalent to a straight line connection.

For the two power laws you are shown a plot of $\mathscr{R}$ in the bridge region, and asked to select the points used in the fit. You also specify the order (the highest power of ω used in the fit).* The order is 3 in the above equations. The earlier extrapolation (in KKold) used $1/\omega^D$ with D in the range 0 to 4. Thus the power law in $1/\omega$ is probably the best choice. The default is to use $1/\omega$.

Sometimes the x-ray (xro) calculation produces a rather high reflectance in the 80,000–300,000 cm-1 region. The reflectance is "high" if it is well above the measured data in the visible/uv. The bridge will have a positive slope, and can contribute to a negative $\sigma_1(\omega)$ in the KK results. To work around this, use the `/W` or `/G` option. Before asking about the fit over the bridge region, KK will then show the high-frequency end of the data and the low end of the x-ray-extension reflectance. You will be asked to click twice to select the new start and end of the gap. Generally you will (1) click just right of the first data point (keeping all the data†) and (2) in the xro data where it has fallen below the measured data. This click pushes the start of the x-ray extension to higher energies and uses a power law over the wider gap.

In verbose mode (`\v`), KK will ask if you want to widen the gap. Verbose mode also asks if you want to keep (include) the low- and high-frequency extrapolated data (reflectance and phase). These options are also available with `/KL` and `/KH` switches. If you do keep the extrapolations in the output file, be sure to remove the extrapolation data before making plots for publication!

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* If the order is too large, the fitting routine produces a singular matrix. In this case, KK reduces the order by 1 and tries again. You are limited to order ≤ 9.

† You may of course click somewhere inside your data if you want to trim what seem like unreliable uv data.

There are several low frequency extrapolations possible, controlled by a parameter `COND`. For KK of $\mathscr{R}$, one has:

>0	⇒	`COND` is the known DC conductivity, in $\Omega^{-1}\text{cm}^{-1}$	
=0 or i	⇒	Reflectance is assumed constant to DC	
-1 or m	⇒	Metallic conductivity assumed:	$\mathscr{R} = 1 - A\omega^{1/2}$
-2 or t	⇒	Two-fluid model:	$\mathscr{R} = 1 - A\omega^{2}$
-3 or l	⇒	Marginal Fermi Liquid:	$\mathscr{R} = 1 - A\omega^{1}$
-4 or s	⇒	Superconducting:	$\mathscr{R} = 1 - A\omega^{4}$
-5 or f	⇒	Use a parameter file. (You will be asked for the name of the `*.PAR` file.)	

The use of a parameter file (-5, f, or `/P<file>`) is strongly recommended. KK will use the parameters to calculate the low frequency reflectance or transmittance.*

You also need to specify the file names for input or output. The file order on command line is: Data, X-ray, Parameter, Output. KK will construct the output name from the data file name, with extension `.rph` or `.tph` if the name is not specified.

The data can be scaled or shifted and are clipped to 0.↔1. range.†

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

`/F<file>`	— Use `<file>` (`.XRO`) for high freq extrapolation
`/BL<number>`	— Bridge with $\mathscr{R} = A + B/\omega + C/\omega^2 + \ldots$ up to `<number>`
`/BW<number>`	— Bridge with $\mathscr{R} = A + B\omega + C\omega^2 + \ldots$ up to `<number>`
`/BS`	— Bridge with cubic spline (which sometimes does not work...)
`/BN`	— No bridge (equivalent to a straight line)
`/W or /G`	— Widen Gap using mouse to select highest data and lowest .xro points to keep
`/C`*nn*	— low frequency extrapolation using $\sigma_{dc} = nnn$
`/I or /C0`	— Reflectance is assumed constant to DC (default)
`/C or /C-1`	— Metallic conductivity assumed: $\mathscr{R} = 1 - A\omega^{1/2}$
`/L or /C-2`	— London (two-fluid) model: $\mathscr{R} = 1 - A\omega^{2}$
`/M or /C-3`	— Marginal-Fermi Liquid: $\mathscr{R} = 1 - A\omega^{1}$
`/S or /C-4`	— Superconducting: $\mathscr{R} = 1 - A\omega^{4}$
`/P<file>`	— Use `<file>` (.PAR or .PRM) for low frequency extrapolation (preferred)
`/KH`	— Keep high frequency extrapolation points
`/KL`	— Keep low frequency extrapolation points
`/T`	— transform of Transmittance
`/TPH`	— transform Transmittance and write *.TPH file
`/X`*nnn* `or /x`*nnn*	— film thickness (Angstroms) (for $\mathscr{T}$)
`/Y`*nnn*`,`*mmm*	— Scale data as $Y \leftarrow nnn * (Y - mmm)$
`/COLi,j`	— Data in Columns i, j.

* If the fit is not good at low frequencies, you may want to pick out the data up to say 500 cm^{-1} and optimize the parameters for a good low-frequency fit.

† The actual clipping algorithm allows the data to be 1.0 as long as it is 1.0 at all lower frequencies; otherwise 0.999999 is the largest value allowed.

Examples:

`KK F1A100.rnm  YBa2Cu3O6.93.xro /t /c-1 -q`

Transform `f1a100.rnm`, a transmittance file. Use built-in defaults, except extend low-frequency region as metal. Use `YBa2Cu3O6.93.xro` at high frequencies.

`KK F1A100.RAW  /FYBa2Cu3O6.93 /PYBa2Cu3O6.93.PAR /BL4 /KH`

`KK F1A100.RAW  YBa2Cu3O6.93 YBa2Cu3O6.93.PAR /BL4 /KH`

Transform `f1a100.raw`. The low frequencies are extrapolated using the parameters in `YBa2Cu3O6.93.PAR`. Use `YBa2Cu3O6.93.xro` in the x-ray region. Bridge with $\mathscr{R} = A + B/\omega + C/\omega^2 + D/\omega^3 + E/\omega^4$. Keep the high-frequency extrapolation data.* Note: the two command-line strings produce identical results.

KK produces an `RPH` file, where the three data columns are frequency, reflectance, and phase shift on reflectance; ω, $\mathscr{R}$, ϕ. From these, the complex refractive index is

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

The program OP can calculate a wide variety of optical constants from the `RPH` file. See pages 15–26 for the list and formulas.

* If you use `/KH` be sure to remove the extrapolation data before making plots for publication! Ditto for `/KL`.