Optical Properties with Wien2k

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Menu

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    - Calculating ε: Random-Phase Approximation
2. Practical Calculations
    - `optic`: Momentum Matrix Elements
    - `joint`: Imaginary Part of Dielectric Tensor
    - `kram`: Derived Quantities
3. Examples

Ambrosch-Draxl and Sofo, Comp. Phys. Commun. 175, 1 (2006)

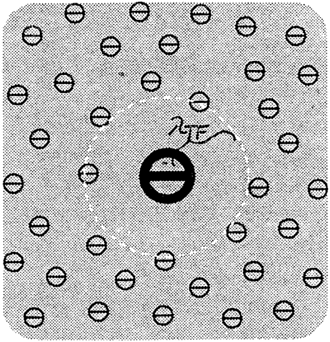
Appetizer

$$\mathrm{Im}\,\varepsilon_{ij}(\omega) \Rightarrow \left\{ \begin{array}{ll}
\text{optical conductivity} & \mathrm{Re}\,\sigma_{ij} = \dfrac{\omega}{4\pi}\,\mathrm{Im}\,\varepsilon_{ij} \\[2ex]
\text{refractive index} & n_{ii} = \sqrt{(|\varepsilon_{ii}| + \mathrm{Re}\,\varepsilon_{ii})/2} \\[2ex]
\text{extinction coefficient} & k_{ii} = \sqrt{(|\varepsilon_{ii}| - \mathrm{Re}\,\varepsilon_{ii})/2} \\[2ex]
\text{absorption coefficient} & \alpha_{ii} = 2\omega k/c \\[2ex]
\text{energy loss function} & L_{ij} = -\,\mathrm{Im}(\varepsilon^{-1})_{ij} \\[2ex]
\text{reflectivity} & R_{ii} = \dfrac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \\[2ex]
\text{sum rules} & N_{\mathrm{eff}} = \displaystyle\int_0^{\omega} \mathrm{d}\omega'\ \mathrm{Im}\,\varepsilon(\omega')
\end{array} \right.$$

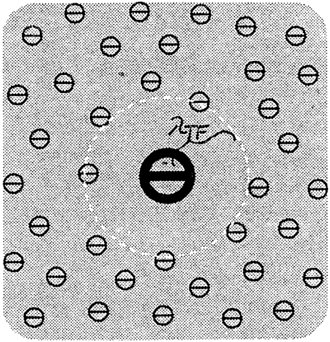
Screening

Consider a test charge Q in a solid:

$$V(\boldsymbol{r}-\boldsymbol{r}') = \frac{-Q}{|\boldsymbol{r}-\boldsymbol{r}'|} \longleftrightarrow V(\boldsymbol{q}) = -\frac{4\pi Q}{\boldsymbol{q}^2}$$



Screening



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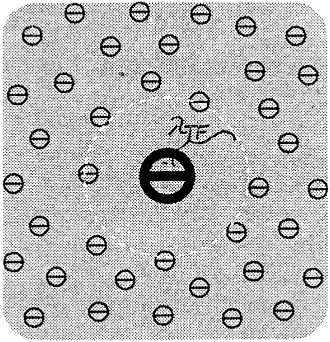
e^- will move to screen the charge
$\rightsquigarrow$ effective potential W;
dielectric function "$V = \varepsilon W$"

Screening



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e^- will move to screen the charge
⇝ effective potential W;
dielectric function "$V = \varepsilon W$"

Simplest model: Thomas-Fermi

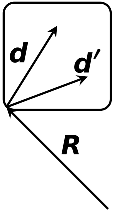
$$W(\boldsymbol{r}) = \frac{e^{-\boldsymbol{k}_{TF}\boldsymbol{r}}}{\boldsymbol{r}} \longleftrightarrow W(\boldsymbol{q}) = \frac{4\pi}{\boldsymbol{k}_{TF}{}^2 + \boldsymbol{q}^2}$$

$$\boldsymbol{k}_{TF}^2 = 4\pi\mathcal{N}(E_F)$$

Ansatz for W

$$W \sim \int \mathrm{d}\boldsymbol{r}' \mathrm{d}t \, \varepsilon^{-1}(\boldsymbol{r}'; t) \, V(\boldsymbol{r} - \boldsymbol{r}'; t - t')$$

Ansatz for *W*



$$\boldsymbol{r} = \boldsymbol{R} + \boldsymbol{d}$$

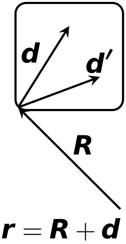
$$W \sim \int \mathrm{d}\boldsymbol{r}'\mathrm{d}t\,\varepsilon^{-1}(\boldsymbol{r}';t)\,V(\boldsymbol{r}-\boldsymbol{r}';t-t')$$

Bare $V(\boldsymbol{r},\boldsymbol{r}';t,t') = V(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t')$ is translation invariant and instantaneous

Response depends on position in unit cell, is retarded

$$\varepsilon^{-1}{}_{\tilde{\boldsymbol{R}}}(\boldsymbol{d}_1,\boldsymbol{d}_2;t)$$

Ansatz for W



$$W \sim \int \mathrm{d}\boldsymbol{r}' \mathrm{d}t \, \varepsilon^{-1}(\boldsymbol{r}'; t) \, V(\boldsymbol{r} - \boldsymbol{r}'; t - t')$$

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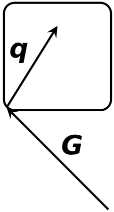
Response depends on position in unit cell, is retarded

$$\rightsquigarrow \; W_{\boldsymbol{R}}(\boldsymbol{d}, \boldsymbol{d}'; t) = \sum_{\tilde{\boldsymbol{R}}} \int \mathrm{d}\boldsymbol{d}_1 \mathrm{d}\boldsymbol{d}_2 \; \varepsilon^{-1}{}_{\tilde{\boldsymbol{R}}}(\boldsymbol{d}_1, \boldsymbol{d}_2; t)$$

$$\cdot \, V(\boldsymbol{R} + \boldsymbol{d} - \boldsymbol{d}' - [\boldsymbol{d}_1 - \boldsymbol{d}_2 - \tilde{\boldsymbol{R}}])$$

The Dielectric Function



$$\boldsymbol{k} = \boldsymbol{G} + \boldsymbol{q}$$

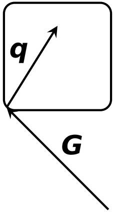
$$W_G(\boldsymbol{q},\omega) = \sum_{\boldsymbol{G}'} {\varepsilon^{-1}}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q},\omega)\; V_{\boldsymbol{G}'}(\boldsymbol{q},\omega)$$

light is long-wavelength:

$$W_G(\boldsymbol{q},\omega) \approx {\varepsilon^{-1}}_{\boldsymbol{G}\boldsymbol{0}}(\boldsymbol{q},\omega)\; V_{\boldsymbol{0}}(\boldsymbol{q},\omega)$$

$$\boldsymbol{G}' = \boldsymbol{0},\; \boldsymbol{q} \to \boldsymbol{0}$$

The Dielectric Function



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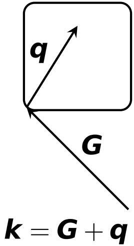
$$W_G(\boldsymbol{q},\omega) \approx \varepsilon^{-1}{}_{\boldsymbol{G}\boldsymbol{0}}(\boldsymbol{q},\omega)\ V_{\boldsymbol{0}}(\boldsymbol{q},\omega)$$

“macroscopic” ε (u.c. average):

$$W(\boldsymbol{q},\omega) = \varepsilon^{-1}{}_{\boldsymbol{0}\boldsymbol{0}}(\boldsymbol{q},\omega)\ V_{\boldsymbol{0}}(\boldsymbol{q},\omega)$$

$$\varepsilon_{\mathrm{M}}(\boldsymbol{q},\omega) = \frac{1}{\varepsilon^{-1}{}_{\boldsymbol{0}\boldsymbol{0}}(\boldsymbol{q},\omega)}$$

The Dielectric Function



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“macroscopic” ε (u.c. average):

$$W(\boldsymbol{q},\omega) = \varepsilon^{-1}{}_{\boldsymbol{00}}(\boldsymbol{q},\omega)\ V_{\boldsymbol{0}}(\boldsymbol{q},\omega)$$

$$\varepsilon_{\mathrm{M}}(\boldsymbol{q},\omega) = \frac{1}{\varepsilon^{-1}{}_{\boldsymbol{00}}(\boldsymbol{q},\omega)}$$

neglect local-field effects:

$$\varepsilon_{\mathrm{M}}(\boldsymbol{q},\omega) \approx \varepsilon_{\boldsymbol{00}}(\boldsymbol{q},\omega)$$

Calculating ε: The RPA

$$V(\boldsymbol{q}) = \varepsilon(\boldsymbol{q},\omega)\, W(\boldsymbol{q},\omega)$$

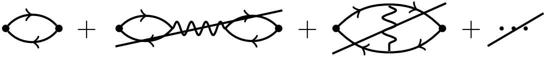
- Poisson: $\boldsymbol{q}^2 W = 4\pi\,(-Q + \delta n) \quad \longleftrightarrow \quad W = V + \frac{4\pi}{\boldsymbol{q}^2}\delta n$
- linear response: $\delta n = \ \chi V$

Calculating ε: The RPA

$$\boxed{V(\boldsymbol{q}) = \varepsilon(\boldsymbol{q},\omega)\,W(\boldsymbol{q},\omega)}$$

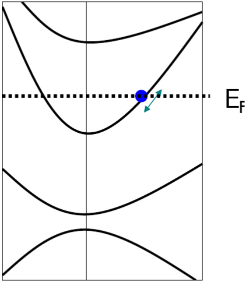
- Poisson: $\boldsymbol{q}^2 W = 4\pi\,(-Q + \delta n) \quad \longleftrightarrow \quad W = V + \frac{4\pi}{\boldsymbol{q}^2}\delta n$
- linear response: $\delta n = \cancel{\chi V}\; P\,W \quad \longrightarrow \quad V = (1 - \frac{4\pi}{\boldsymbol{q}^2}P)\,W$
- “random-phase” approximation: P to lowest order

$P =$

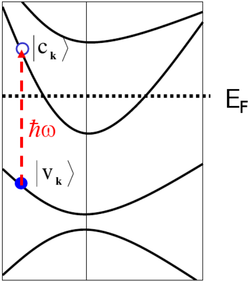


$\sim G^0(1,2)\,G^0(2,1)$

Intra- and Interband transitions



intraband



interband

free e$^-$: Lindhard formula

$$P = \frac{4\pi}{\boldsymbol{q}^2\Omega}\sum_{\boldsymbol{k}} \frac{f(\epsilon_{\boldsymbol{k}+\boldsymbol{q}}) - f(\epsilon_{\boldsymbol{k}})}{\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}} - \omega}$$

Bloch e$^-$:

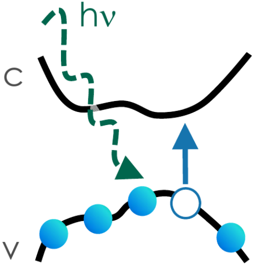
$$P = \frac{4\pi}{\boldsymbol{q}^2\Omega}\sum_{\boldsymbol{k}nn'} A^{nn'}_{\boldsymbol{kq}} \frac{f(\epsilon_{\boldsymbol{k}+\boldsymbol{q}}) - f(\epsilon_{\boldsymbol{k}})}{\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}} - \omega}$$

Intra- and Interband transitions

intraband: Drude model,
(ω_p: plasma frequency)

$$\mathrm{Im}\,\varepsilon^{\mathrm{intra}} = \frac{\Gamma {\omega_\mathrm{p}}^2}{\omega\left(\omega^2 + \Gamma^2\right)}$$

interband:



joint density of states:

$$\rho(\omega) = \sum_{c,v} \int \mathrm{d}\boldsymbol{k}\; \delta\Big(\epsilon_c(\boldsymbol{k}) - \epsilon_v(\boldsymbol{k}) - \omega\Big)$$

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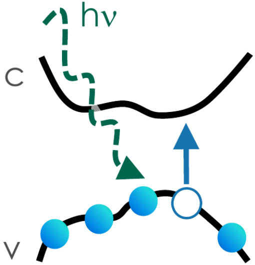

joint density of states:

$$\rho(\omega) = \sum_{c,v} \int \mathrm{d}\boldsymbol{k}\ \delta\Big(\epsilon_c(\boldsymbol{k}) - \epsilon_v(\boldsymbol{k}) - \omega\Big)$$

v-*c* transition probability
("selection rules") given by
momentum matrix elements

$$\mathrm{Im}\,\varepsilon_{ij}(\omega, \mathbf{0}) \propto \frac{1}{\omega^2} \sum_{c,v} \int \mathrm{d}\boldsymbol{k}\ \delta\Big(\epsilon_c(\boldsymbol{k}) - \epsilon_v(\boldsymbol{k}) - \omega\Big)\ \langle c\boldsymbol{k}|\widehat{p}_i|v\boldsymbol{k}\rangle \langle v\boldsymbol{k}|\widehat{p}_j|c\boldsymbol{k}\rangle$$

Symmetry Constraints

$\varepsilon_{ij} = \varepsilon_{ji}$ is always symmetric.

Additional constraints from crystal symmetry:

$$\varepsilon = U^{-1}\,\varepsilon\,U$$

cubic $\begin{pmatrix} 1 & 0 & 0 \\ & 1 & 0 \\ & & 1 \end{pmatrix}$

tetragonal,
trigonal,
hexagonal $\begin{pmatrix} 1 & 0 & 0 \\ & 1 & 0 \\ & & 3 \end{pmatrix}$

orthorhombic $\begin{pmatrix} 1 & 0 & 0 \\ & 2 & 0 \\ & & 3 \end{pmatrix}$

monoclinic $\begin{pmatrix} 1 & 4 & 0 \\ & 2 & 0 \\ & & 3 \end{pmatrix}$

triclinic $\begin{pmatrix} 1 & 4 & 5 \\ & 2 & 6 \\ & & 3 \end{pmatrix}$

Program Flow

`lapw1` Kohn-Sham eigenstates

`optic` momentum matrix elements (*case*`.symmat`)

`joint` imaginary part of dielectric tensor (`case.joint`)

`kram` derived quantities

- Kramers-Kronig

$$\mathrm{Re}\,\varepsilon_{ij} = \delta_{ij} + \tfrac{2}{\pi}\,\mathcal{P}\int_0^\infty \mathrm{d}\Omega\;\frac{\Omega}{\Omega^2-\omega^2}\;\mathrm{Im}\,\varepsilon_{ij}$$

⇝ all optical constants

`optic`: Momentum Matrix Elements

⓪ normal SCF run ⟶ converged density

① `x kgen` ⟶ dense k-mesh (check convergence!)

② `x lapw1` *-options* ⟶ eigenvectors on dense mesh

③ `x lapw2 -fermi` *-options* ⟶ *case*`.weight`

- metals: “`TETRA 101.0`” in *case*`.in2`

④ `x optic` *-options* ⟶ momentum matrix elements

case`.symmat:` $\langle c\boldsymbol{k}|\widehat{p}_i|v\boldsymbol{k}\rangle\,\langle v\boldsymbol{k}|\widehat{p}_j|c\boldsymbol{k}\rangle$

core-level spectra: Kevin Jorissen’s lecture tomorrow 10:30

`optic`: Input and Output

case.inop

```
99999 1            #k-points,  1st k-point
-5.0 3.0 9999      Emin Emax [Ry],  NBvalMAX
2                  #indep. elements (symmetry/SOC)
1                  Re xx
3                  Re zz
OFF 3              write mommat2?, #spheres
1 2 3              spheres to sum over
```

symmetry

1: $\mathrm{Re}\langle xx\rangle$
2: $\mathrm{Re}\langle yy\rangle$
3: $\mathrm{Re}\langle zz\rangle$
4: $\mathrm{Re}\langle xy\rangle$
5: $\mathrm{Re}\langle xz\rangle$
6: $\mathrm{Re}\langle yz\rangle$

spin-orbit

7: $\mathrm{Im}\langle xy\rangle$
8: $\mathrm{Im}\langle xz\rangle$
9: $\mathrm{Im}\langle yz\rangle$

case.symmat

$\langle v\mathbf{k}|\widehat{p}_i|c\mathbf{k}\rangle\,\langle c\mathbf{k}|\widehat{p}_j|v\mathbf{k}\rangle$

case.mommat2 (if ON)

$\langle v\mathbf{k}|\widehat{p}_i|c\mathbf{k}\rangle$

joint: Im(ε), (Joint) Density of States

case.injoint

```
1 9999 9999     lower, upper, upper-val bandindex
0.0 .001 1.0    Emin (≥ 0), dE, Emax [Ry]
eV              units [eV / ryd  / cm-1]
4               mode
2               #indep. elements
0.1 0.1         broadenings Γ for Drude (mode=6,7)
```

case.joint

$$\left.\begin{array}{c} \mathrm{Im}\,\varepsilon_{ij} \\ \rho \end{array}\right\} \sim \sum_{c,v} \int \mathrm{d}\boldsymbol{k}\, \delta\Big(\epsilon_c(\boldsymbol{k}) - \epsilon_v(\boldsymbol{k}) - \omega\Big) \left\{\begin{array}{c} \langle c\boldsymbol{k}|\widehat{p}_i|v\boldsymbol{k}\rangle \, \langle v\boldsymbol{k}|\widehat{p}_j|c\boldsymbol{k}\rangle \\ 1 \end{array}\right.$$

`joint`: Modes of Operation

“physical” (all bands)

1 joint DOS

3 regular DOS

4 $\operatorname{Im}\varepsilon$ interband

6 $\operatorname{Im}\varepsilon$ intraband (Drude)

$$\operatorname{Im}\varepsilon_{ij} \sim \sum_{c,v,\boldsymbol{k}} \delta\Big(\epsilon_c(\boldsymbol{k}) - \epsilon_v(\boldsymbol{k}) - \omega\Big)\ \langle c\boldsymbol{k}|\widehat{p}_i|v\boldsymbol{k}\rangle\,\langle v\boldsymbol{k}|\widehat{p}_j|c\boldsymbol{k}\rangle$$

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1 joint DOS
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band analysis

0 joint DOS
2 DOS
5 interband
7 intraband

$$\operatorname{Im}\varepsilon_{ij} \sim \sum_{c,v,\boldsymbol{k}} \delta\Big(\epsilon_c(\boldsymbol{k}) - \epsilon_v(\boldsymbol{k}) - \omega\Big)\ \langle c\boldsymbol{k}|\widehat{p}_i|v\boldsymbol{k}\rangle\,\langle v\boldsymbol{k}|\widehat{p}_j|c\boldsymbol{k}\rangle$$

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- 1 joint DOS
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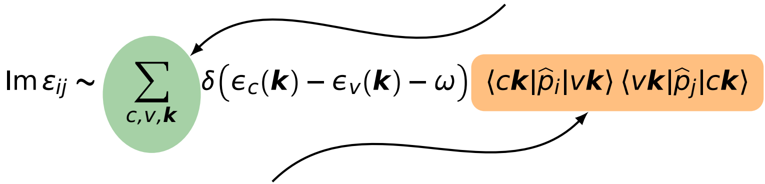
band analysis

- 0 joint DOS
- 2 DOS
- 5 interband
- 7 intraband



$$\mathrm{Im}\,\varepsilon_{ij} \sim \sum_{c,v,\boldsymbol{k}} \delta\Big(\epsilon_c(\boldsymbol{k}) - \epsilon_v(\boldsymbol{k}) - \omega\Big) \langle c\boldsymbol{k}|\widehat{p}_i|v\boldsymbol{k}\rangle \langle v\boldsymbol{k}|\widehat{p}_j|c\boldsymbol{k}\rangle$$

“sphere analysis”

$$|c\boldsymbol{k}\rangle = \sum_{\alpha}^{\mathrm{MT,I}} |c\boldsymbol{k}\rangle_\alpha$$

NB: cross-terms are missed!

case.`inop`

```
OFF 3  mommat2?, #spheres
1 2 3  spheres to sum over
```

`kram`: Kramers-Kronig Analysis

case.inkram

```
0.1        interband broadening
0.0        energy shift (scissors operator)
1          add intraband contributions?  1/0
12.6 12.6  plasma frequencies  (joint, mode=6)
 0.1  0.1  broadenings Γ for Drude models
```

output

- *case*.epsilon
  $\mathrm{Re}\,\varepsilon, \mathrm{Im}\,\varepsilon$
- *case*.absorp
  $\mathrm{Re}\,\sigma, \alpha$
- *case*.reflectivity
  R
- *case*.sigmak
  $\mathrm{Re}\,\sigma, \mathrm{Im}\,\sigma$
- *case*.eloss
  loss function
- *case*.refraction
  n, k
- *case*.sumrules

More Stuff You May Need to Know

spin-polarized calculations

Kramers-Kronig is not additive.

1. `x joint -up && x joint -dn`
2. `addjoint-updn`
3. `x kram`

More Stuff You May Need to Know

spin-polarized calculations

1. `x joint -up && x joint -dn`
2. `addjoint-updn`
3. `x kram`

procedure for metals

1. `x joint (mode=6)` ⟶ plasma frequencies $\omega_{\mathrm{p}_{ij}}$
2. `x joint (mode=4)` ⟶ interband $\mathrm{Im}\,\varepsilon$
3. `x kram (intra=1,` insert ω_{p} `)`

$$\mathrm{Im}\,\varepsilon^{\mathrm{intra}} = \frac{\Gamma {\omega_{\mathrm{p}}}^2}{\omega\left(\omega^2+\Gamma^2\right)}, \qquad \mathrm{Re}\,\varepsilon^{\mathrm{intra}} = 1 - \frac{{\omega_{\mathrm{p}}}^2}{\omega^2+\Gamma^2}$$

More Stuff You May Need to Know

spin-polarized calculations

1. `x joint -up && x joint -dn`
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procedure for metals

1. `x joint (mode=6)` ⟶ plasma frequencies $\omega_{\mathrm{p}_{ij}}$
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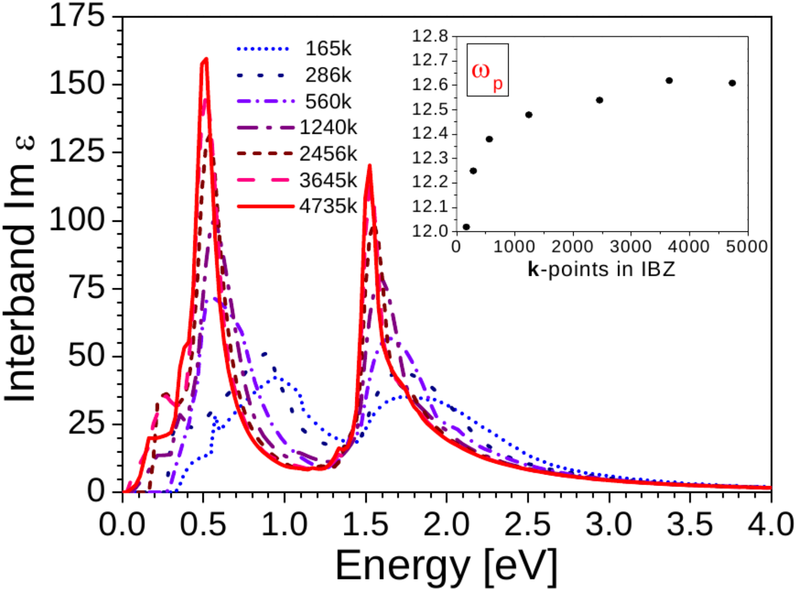
Kramers-Kronig needs $\mathrm{Im}\,\varepsilon$ in a large energy range

$$\mathrm{Re}\,\varepsilon_{ij} = \delta_{ij} + \frac{2}{\pi}\mathcal{P}\int_0^\infty \mathrm{d}\Omega\, \frac{\Omega}{\Omega^2 - \omega^2}\,\mathrm{Im}\,\varepsilon_{ij}$$

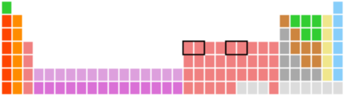
Some Limitations

- linear optical properties only
  - $W = \varepsilon^{-1(1)} V + \cancel{\varepsilon^{-1(2)} V^2} + \cdots$
- Kohn-Sham eigenstates interpreted as excited states
  ⇝ "scissors" operator: $\epsilon_c(\boldsymbol{k}) \rightarrow \epsilon_c^{\mathrm{LDA}}(\boldsymbol{k}) + \Delta$
- independent-particle approx. (no $\mathrm{e}^- – \mathrm{h}^+$ interaction)
  ⇝ Bethe-Salpeter (BSE) → Peter Blaha's lecture (13:00)
- LDA/GGA are not exact
  ⇝ hybrid DFT, effective potentials → Peter Blaha
  ⇝ DFT+U, LDA+DMFT → my lecture (tomorrow 9:00)

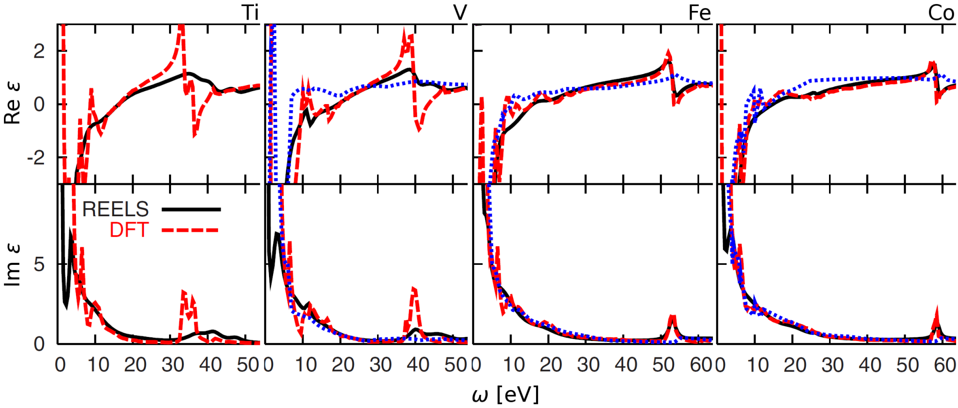
Example: Al, k-Mesh Convergence



Comparison to Experiment



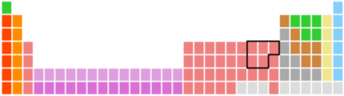
REELS = reflection electron energy loss spectroscopy



Optical Constants for 17 Elemental Metals

Werner *et al.*, Phys. Chem. Ref. Data 38, 1013 (2009)

Comparison to Experiment



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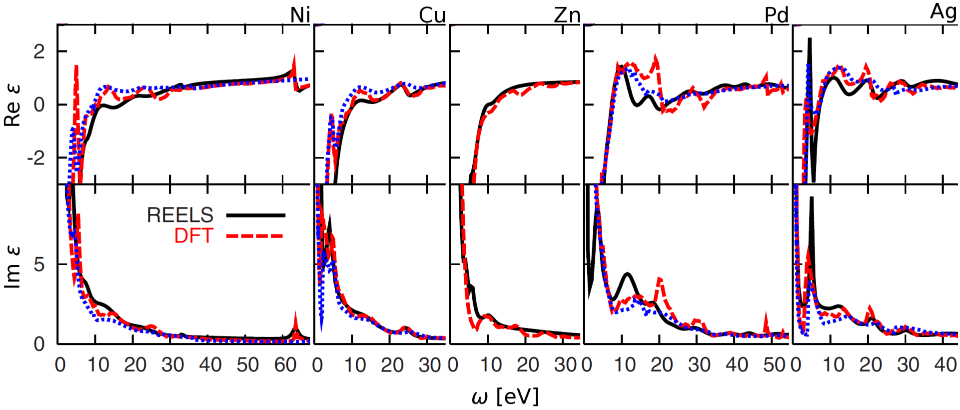
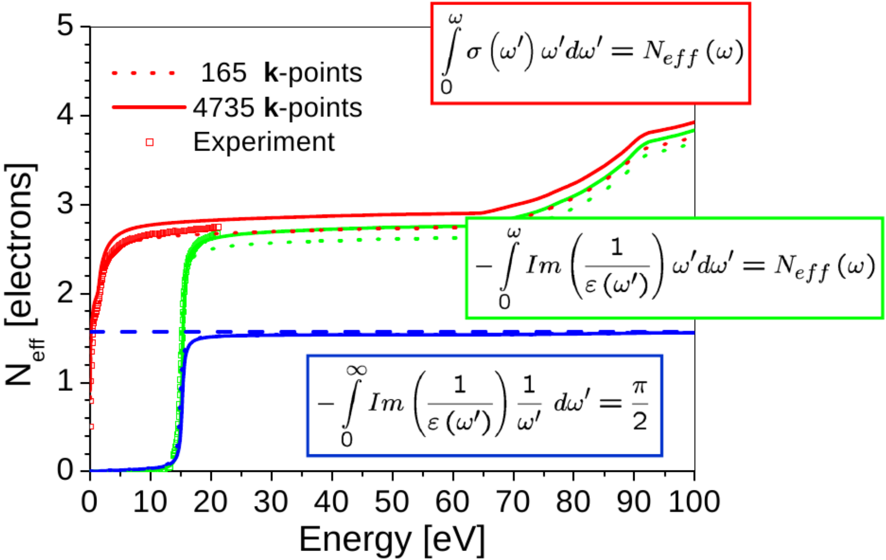


Optical Constants for 17 Elemental Metals

Werner *et al.*, Phys. Chem. Ref. Data 38, 1013 (2009)

Example: Al, Sum Rules

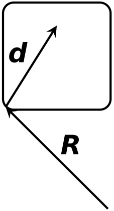


$$\int_0^{\omega} \sigma\left(\omega'\right)\omega' d\omega' = N_{eff}(\omega)$$

$$-\int_0^{\omega} Im\left(\frac{1}{\varepsilon(\omega')}\right)\omega' d\omega' = N_{eff}(\omega)$$

$$-\int_0^{\infty} Im\left(\frac{1}{\varepsilon(\omega')}\right)\frac{1}{\omega'}\, d\omega' = \frac{\pi}{2}$$

Reminder: Lattice Fourier Transform



$$\boldsymbol{r} = \boldsymbol{R} + \boldsymbol{d}$$
$$\boldsymbol{k} = \boldsymbol{G} + \boldsymbol{q}$$

A function defined on the unit cell becomes a discrete function on the reciprocal lattice:

$$f(\boldsymbol{d}) = f(\boldsymbol{d} + \boldsymbol{R}) \xleftrightarrow{\mathcal{F}} f_{\boldsymbol{G}} = \sum_{\boldsymbol{G}} \delta(\boldsymbol{k} - \boldsymbol{G}) f_{\boldsymbol{G}}$$

A discrete function on the direct lattice becomes a function defined in the first BZ:

$$f_{\boldsymbol{R}} = \sum_{\boldsymbol{R}} \delta(\boldsymbol{r} - \boldsymbol{R}) f_{\boldsymbol{R}} \xleftrightarrow{\mathcal{F}} f(\boldsymbol{q}) = f(\boldsymbol{q} + \boldsymbol{G})$$

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