woptic: optical conductivity and adaptive k-integration

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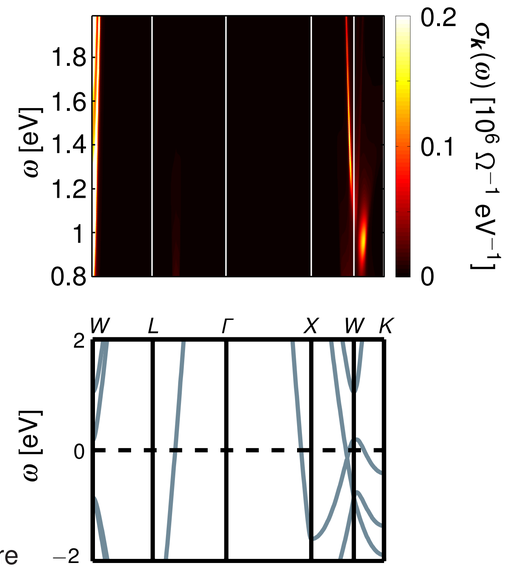
Brioullin-zone integration

- application of Bloch theorem
- indispensable for numerical study of periodic solids
- traditionally, uniform sampling
- in some cases, small k-space regions contribute disproportionately, e.g.:
  - transport
  - low-energy spectral properties
  - here: *optical conductivity* σ

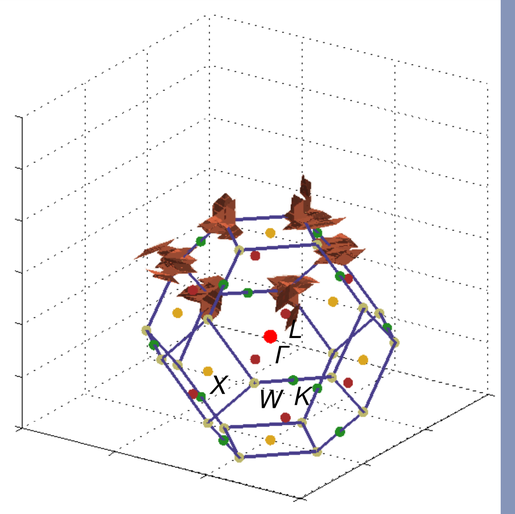
⇝ adaptive k-mesh refinement



fcc-Al: k-resolved contributions to σ, and bandstructure

Adaptive tetrahedral k-mesh

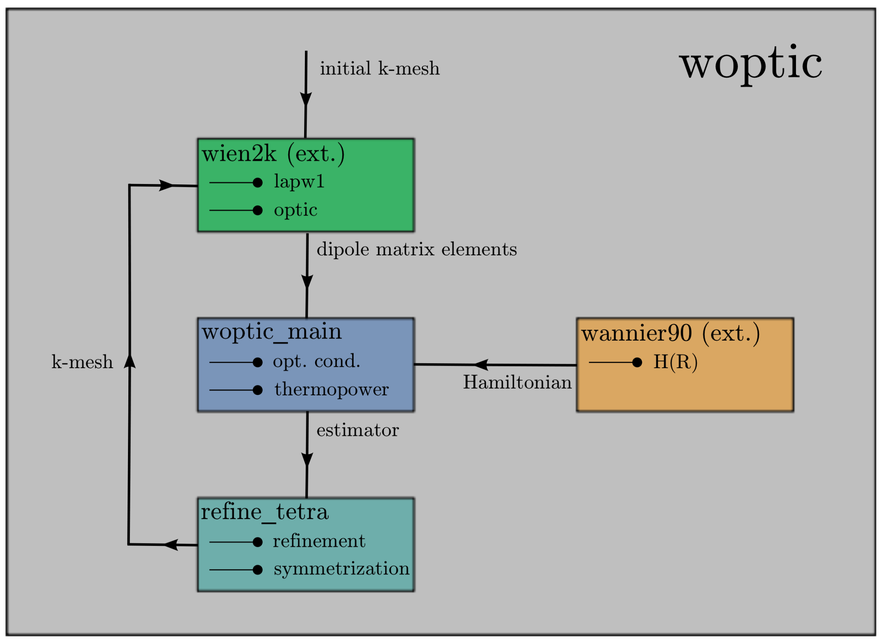
- k-space is divided into tetrahedra, which are successively selectively refined
- in 3d, refinement is not unique, sub-tetrahedra are not congruent
- Kuhn triangulation: 2 classes of tetrahedra



adaptive k-mesh for fcc-Al after six refinements

woptic: optical conductivity of interacting electrons

- part of Wien2Wannier package
- works with Wien2k, Wannier90, and any self-energy
- two main parts:
  - woptic_main computes σ
  - refine_tetra manages k-mesh
- Vertex corrections are neglected (in DMFT, they vanish)



- for non-interacting electrons (c: conduction, v: valence):

$$\sigma_{\alpha\beta}(\Omega) \sim \sum_{c,v,\boldsymbol{k}} \frac{\delta(\varepsilon_c(\boldsymbol{k})-\varepsilon_v(\boldsymbol{k})-\Omega)}{\Omega} \nabla^{\alpha}_{vc}(\boldsymbol{k}) \nabla^{\beta}_{cv}(\boldsymbol{k})$$

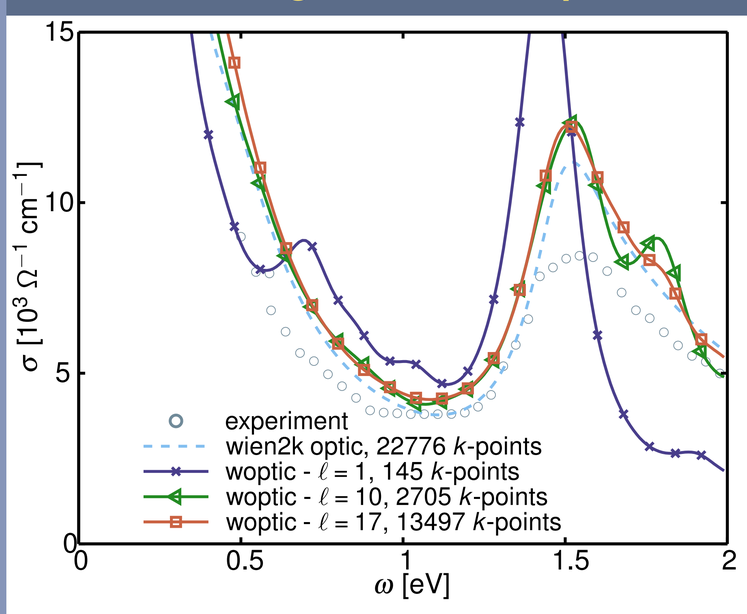
- for interacting electrons (⇝ spectral density $A_{nm}(\boldsymbol{k},\omega)$):

$$\sigma_{\alpha\beta}(\Omega) \sim \sum_{\boldsymbol{k},\omega} \frac{f(\omega)-f(\omega+\Omega)}{\Omega} \operatorname{tr}\left\{\nabla^{\alpha} A(\boldsymbol{k},\omega+\Omega) \nabla^{\beta} A(\boldsymbol{k},\omega)\right\}$$

f = Fermi function, $\qquad \nabla^{\alpha}_{nm} = \langle \psi_{n\boldsymbol{k}} | \partial_{\beta} | \psi_{m\boldsymbol{k}} \rangle$

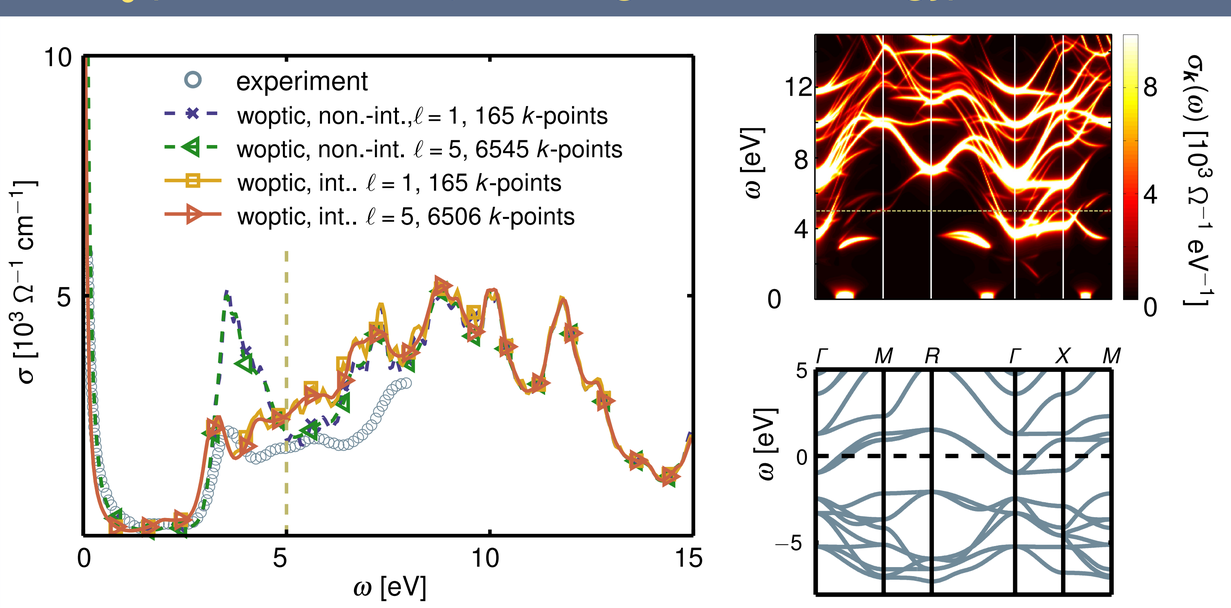
- The trace is expensive, adaptive integration worthwhile

fcc-Al: convergence and comparison to Wien2k



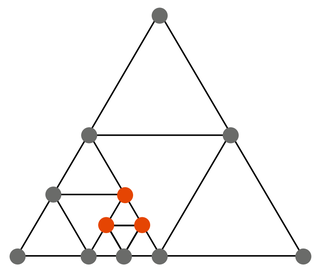
- contributions to σ strongly peaked in k
- match Wien2k results, but much cheaper
- precise shape depends on broadening scheme
  - Wien2k: Lorentzian (0.1 eV)
  - woptic: $\Sigma \leftarrow -\mathrm{i}\delta$
- ℓ: # refinement iterations

$SrVO_3$ (correlated metal, including DMFT self-energy)



Tetrahedral Hygiene

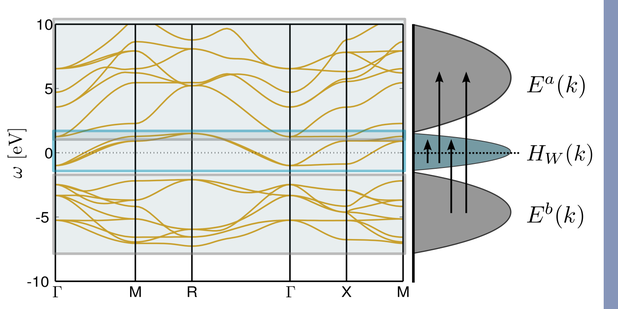
- enforce *regularity:* at most one "hanging node" per edge, to avoid unstable convergence
- and *shape stability:* no highly-distorted tetrahedra, to avoid large errors
- no k-point is wasted
  - k-points re-used in subsequent iterations, lapw1 and optic only called for new ones
  - take advantage of symmetries
- tetrahedron T selected for refinement if integration error estimate $\quad \varepsilon_T \geq \Theta \max_{T'} \varepsilon_{T'} \quad (\Theta = \text{"harshness"})$



hanging nodes (red) in 2d;
for regularity, refine center triangle

Practical considerations

- inputs:
  - momentum matrix elements $\nabla^{\alpha}_{nm}(\boldsymbol{k})$ (from Wien2k's optic)
  - Hamiltonian $H(\boldsymbol{k})$ (from Wannier90)
  - self-energy $\Sigma(\boldsymbol{k},\omega)$ (e.g. from DMFT)
- random-phase problem:
  - $\psi_{\boldsymbol{k}}$ has random phase in Wien2k (independent diagonalizations)
  - may affect σ in interacting case
  - to be fixed by interpolating $\nabla(\boldsymbol{k})$



modes of operation:

- full momentum-matrix $\nabla^{\alpha}_{nm}(\boldsymbol{k})$
- Peierls approximation: $\nabla \mapsto \frac{\partial H}{\partial \boldsymbol{k}}$
- 2 non-interacting modes

References

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Take-home messages

- woptic calculates the optical conductivity
  - from a many-body calculation
  - using an adaptive k-mesh
- the two are separated, refine_tetra could be used for other quantities
- distributed as part of Wien2Wannier:
  `http://www.wien2k.at/reg_user/unsupported/wien2wannier/`
- "random-phase problem" is being worked on