THE UNIVERSITY of York
DEPARTMENT OF PHYSICS

The electron-phonon interaction in ABINIT

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Why care about el-phon?

- Phonons are the main scattering mechanism for T > 0
- Thermal properties
- Resistance
- Molecular conduction
- Superconductivity

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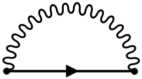
Outline

Migdal

- Use the Migdal approximation: 
- Separate the explicit coupling term (Frölich type Hamiltonian)

$$\hat{H} = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{e-ph}$$

$$\hat{H}_{e-ph} = \sum_{kq} \langle k+q \mid \nabla_\alpha V \mid k \rangle u_{q\alpha} c^\dagger_{k+q} c_k$$

$$\nabla V = \epsilon^{-1} \nabla V_0 \qquad \vec{u}_q = \sum_i \sqrt{\frac{\hbar}{2NM\omega_{qi}}} \vec{\epsilon}_{qi} (a_{qi} + a^\dagger_{qi})$$

Eliashberg

- The self-energy for the phonons is in the LR screening
- The self-energy *for the electrons*

$$\Sigma_{ep} = T \int_{FS} \int_{\Omega} \frac{\alpha^2 F(k, k', \Omega)}{N(0)} \left(\frac{2\Omega}{\omega^2 + \Omega^2}\right) G$$

- Eliashberg function (weighted DOS)

$$\alpha^2 F(k, k', \Omega) = N(0) \sum_j \left| g^j_{k,k'} \right|^2 \delta(\omega_{q,j} - \Omega)$$

$$g^j_{k,k'} = \frac{1}{\sqrt{2M\omega_{q,j}}} \vec{\epsilon}_{q,j} \cdot \langle k \mid \nabla V \mid k' \rangle$$

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EP quantities

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$$\lambda(k, k', \omega) = \int_0^\infty d\Omega \frac{2\Omega}{\omega^2 + \Omega^2} \alpha^2 F(k, k', \Omega)$$

- EP linewidth for the phonons (from Fermi GR)

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Superconductivity

- McMillan equation is popular

$$T_c = \frac{\omega_{log}}{1.2} \exp\left(\frac{-1.04(1+\lambda)}{\lambda - \mu^{\star}(1+0.62\lambda)}\right)$$

- where

$$\omega_{log} = \exp\left(\frac{2}{\lambda}\int_0^{\infty} d\Omega \alpha^2 F(\Omega) \frac{ln(\Omega)}{\Omega}\right)$$

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- telphon_2 merge the DDB files (mrgddb)
- telphon_3 merge the GKK files (mrggkk)
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- Read in the matrix elements for bare perturbations
- Calculate $g^{j}_{k,k'}$, eventually average over FS (smearing or tetrahedron)
- Complete irred $\vec{q}$
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- On dense grid calculate $\alpha^2 F(\Omega)$
- Calculate moments of $\alpha^2 F(\Omega)$
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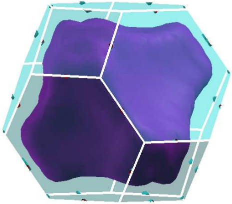
- FS output
- Nesting factor
- Interpolation checks
- $\longrightarrow$ see next talk, with examples!



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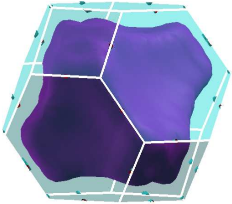

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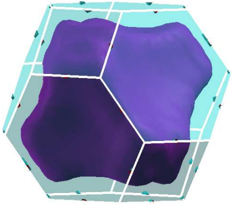

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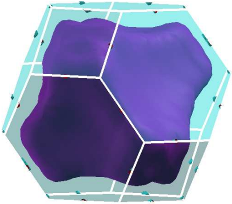

Higher moments of a2F

- Standard λ is special casea (n=0) of

$$\lambda < \omega^n >= 2 \int_0^\infty d\Omega[\alpha^2 F(\Omega)]\Omega^n \qquad (1)$$

- Added calculation of $\lambda < \omega^n >$ for n=2,3,4,5
- Used to estimate the temperature relaxation rate of hot electrons

$$\gamma_T = \frac{3\hbar\lambda < \omega^2 >}{\pi k_B T_e}\left(1 - \frac{\hbar^2 \lambda < \omega^4 >}{12\lambda < \omega^2 > k_B^2 T_e T_L} + \ldots\right) \qquad (2)$$

from Allen PRL **59** 1460 (1987)

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- Interpolating phonons and elphon matrices separately
- Basis at random qpoint could be different
- Standard diagonalization routines give monotonically increasing order for ω and γ_{qj}

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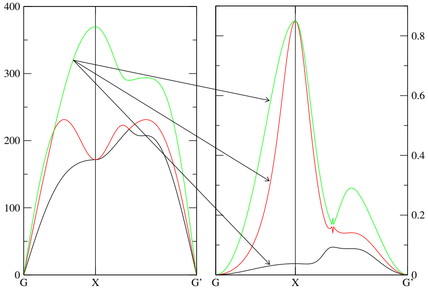
Mode separation II

Straight diag of dynamical matrix and γ matrix



Mode separation III

- Which linewidth belongs to which phonon mode?
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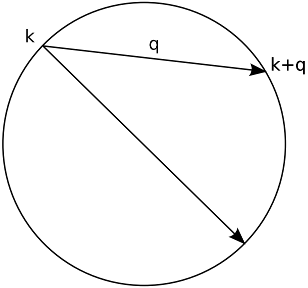
- J.-P. Crocombette implemented the calculation of the phonon contribution to the resistivity
- Momentum relaxation due to scattering off phonons



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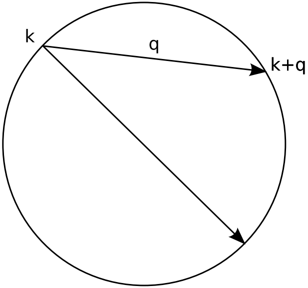

Phonon resistivity contribution II

- Transport spectral function $\alpha_{tr}F = \alpha^2_{out}F - \alpha^2_{in}F$

$$\alpha^2_{out}F(\omega) = \frac{1}{N(0)\langle v_x^2 \rangle} \sum_{\nu} \sum_{kjk'j'} | g_{q\nu}^{kjk'j'} |^2 v_x(k) v_x(k) \delta(\epsilon_{kj}) \delta(\epsilon_{k'j'}) \delta(\omega - \omega_{q\nu})$$

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- T dependent resistance and thermal conductivity (isotropic)

$$\rho(T) = \frac{\pi \Omega_{cell} k_B T}{N(0)\langle v_x^2 \rangle} \int_0^\infty \frac{d\omega}{\omega} \frac{x^2}{sinh^2(x)} \alpha_{tr}F(\omega) \quad x = \frac{\omega}{k_B T}$$

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Limitations/problems

- No anisotropy (yet)
- Memory use (can page to disk, but still)
- Symmetrization: still need all 3*N_{atom} perturbations
  - Phase difference between kpoints and perturbations
  - Adding matrices from different kpoints → gauge dependency

$$g_{k,k'}^{q_3} = g_{S_1k,S_1k'}^{q_1} + g_{S_2k,S_2k'}^{q_2}$$

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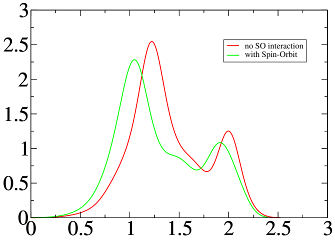
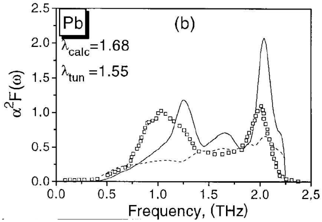
FCC lead

- Compare Eliashberg function with litterature
- Spin-orbit coupling is essential





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2. Potential for many extensions: superconductivity, (anisotropic) transport
3. Input for Raman spectra? Higher order or resonant Raman
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