Electron-Phonon calculations with ABINIT
The role of the Fermi Surface

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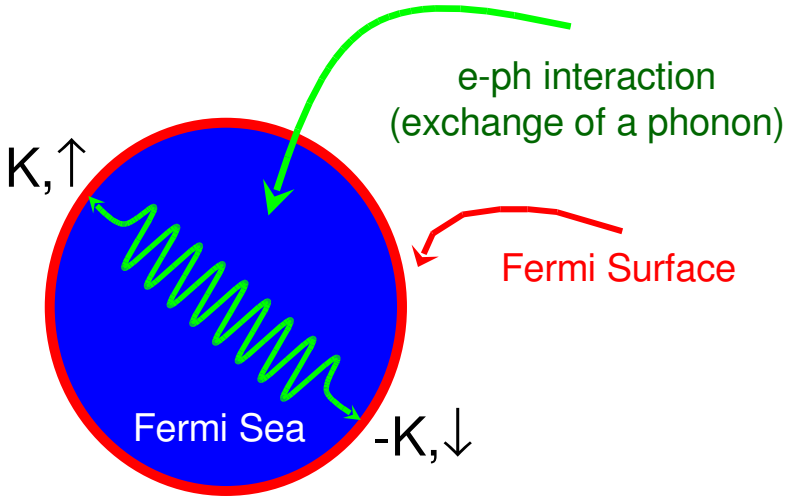
Outline

- Superconductivity from First Principles
  1. Conventional superconductivity
  2. e-ph calculations with Abinit
- The Role of the Fermi Surface
  1. Fermi surfaces and nesting functions
  2. An application in electron-doped graphite
- Future Developments

Main Idea

Superconductivity results from a phonon mediated attraction between electrons



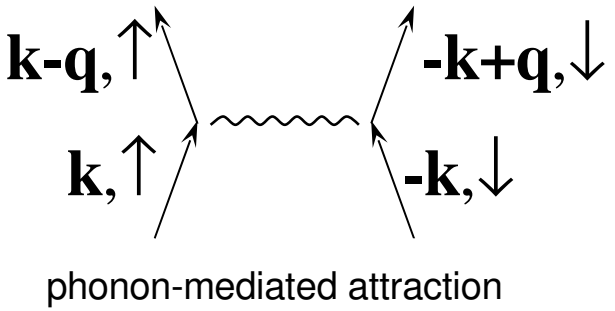
In brief:

1) Below the critical temperature T_c the normal metallic state is unstable

2) For $T < T_c$ electrons are paired together to create a boson-like state (*Cooper pair)*

3) Only electrons close to the Fermi Surface (FS) can pair

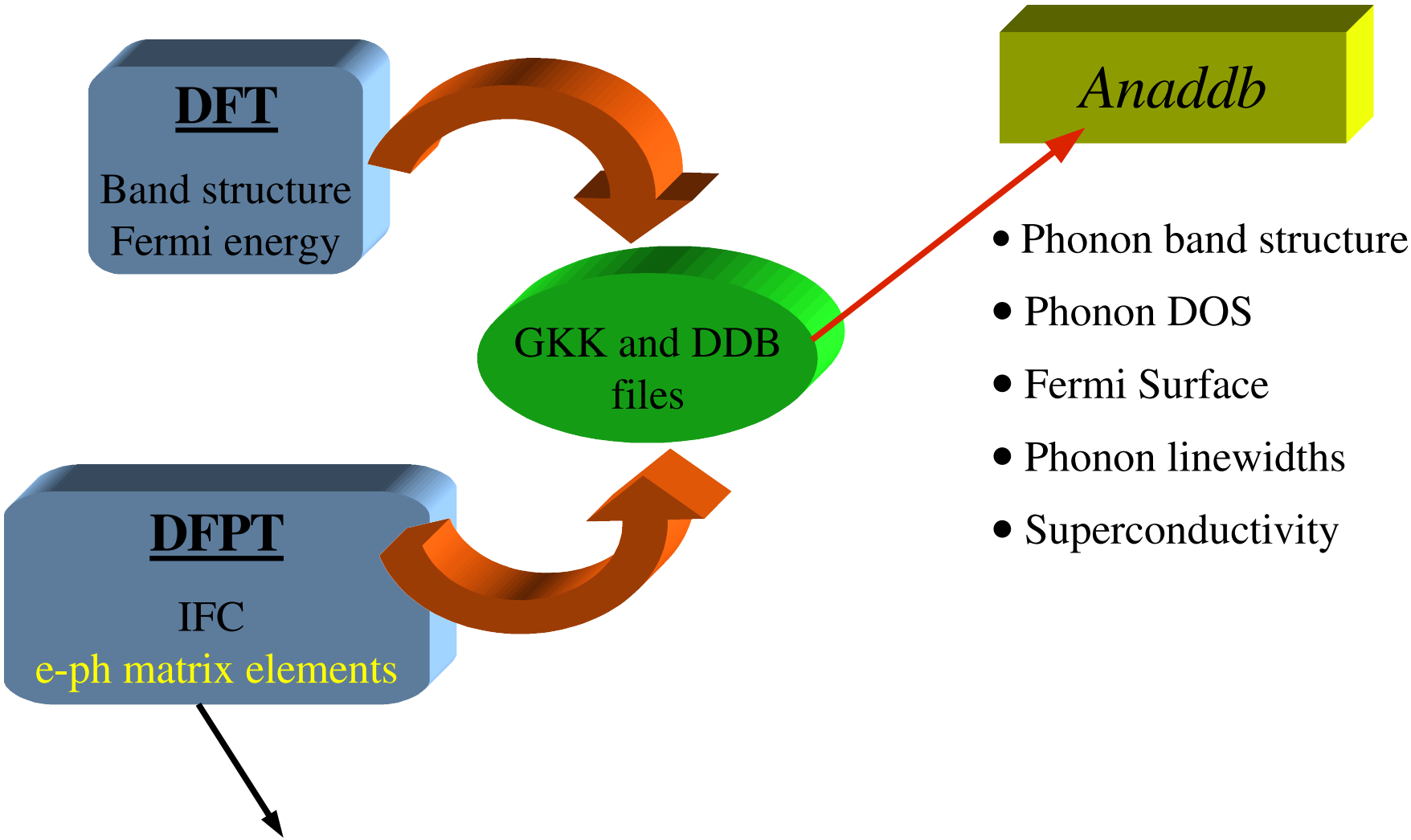
4) A pair does not lose energy by interacting with the lattice



phonon-mediated attraction

What do we need to study superconductivity from *first principles*?

The Code



$$M^{\nu}_{m\mathbf{k}+\mathbf{q},n\mathbf{k}} = \langle \Psi_{m\mathbf{k}+\mathbf{q}} | \delta V^{\nu\mathbf{q}}_{eff}(\mathbf{r}) | \Psi_{n\mathbf{k}} \rangle$$

All the **3*natom** perturbations must be calculated!

E-ph Formalism

From the e-ph matrix elements we can calculate:

1) Eliashberg function $\alpha^2F(\omega)$

$$\alpha^2F(\Omega) \propto \sum_{mn\mathbf{k}} \sum_{\nu\mathbf{q}} \frac{\left|M^{\nu}_{m\mathbf{k}+\mathbf{q},n\mathbf{k}}\right|^2}{\omega_{\mathbf{q}\nu}} \delta(\Omega - \omega_{\mathbf{q}\nu})\, \delta(\epsilon_{n\mathbf{k}})\, \delta(\epsilon_{m\mathbf{k}+\mathbf{q}})$$

2) Coupling costant λ

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

3) McMillan expression for T_c

$$T_c = \frac{\omega_{\log}}{1.20} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^{\star}(1+0.62\lambda)}\right]$$

Free Parameter

where:

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

Anaddb Output File

```
Q point =    5.000000E-01    5.000000E-01    5.000000E-01

Mode number    Frequency (Ha)  Linewidth (Ha)  Lambda(q,n)
       1       -1.129601E-03    2.264127E-06    6.001508E-02
       2       -1.129575E-03    2.264127E-06    6.001790E-02
       3        1.231081E-03    6.118777E-06    1.365531E-01

Superconductivity : isotropic evaluation of parameters from
electron-phonon coupling.

 isotropic lambda =     4.703691E+00

 omegalog     =     1.762804E-04 (Ha)     5.566487E+01 (Kelvin)
 input mustar =     1.360000E-01
 MacMillan Tc =     3.543208E-05 (Ha)     1.118855E+01 (Kelvin)
```

The Role of the Fermi Surface

The shape of the FS affects $\alpha^2F(\omega)$ through the double delta:

$$\alpha^2F(\Omega) \propto \sum_{mn\mathbf{k}} \sum_{\nu\mathbf{q}} \frac{|M^{\nu}_{m\mathbf{k}+\mathbf{q},n\mathbf{k}}|^2}{\omega_{\mathbf{q}\nu}} \delta(\Omega - \omega_{\mathbf{q}\nu})\, \delta(\epsilon_{n\mathbf{k}})\, \delta(\epsilon_{m\mathbf{k}+\mathbf{q}})$$

Interband and intraband nesting

$$\chi_{nm}(\mathbf{q}) = \sum_{\mathbf{k}} \delta(\epsilon_{n\mathbf{k}})\, \delta(\epsilon_{m\mathbf{k}+\mathbf{q}})$$

Related input variables:

to plot the Fermi Surface: `prtfsurf`

to calculate and interpolate the nesting: `prtnest`

Fermi Surfaces with ABINIT

- Simple as using `prtfsurf=1` in a SCF or NSCF calculation
- Output in the XcrysDen file format, but others are possible
- Not only bands at ε_F
- FS deformation due to a *frozen phonon*

Abinit intput file

```
prtfsurf 1

kptopt   1

kptrlatt 30  0  0
          0 30  0
          0  0 30
....
....
```

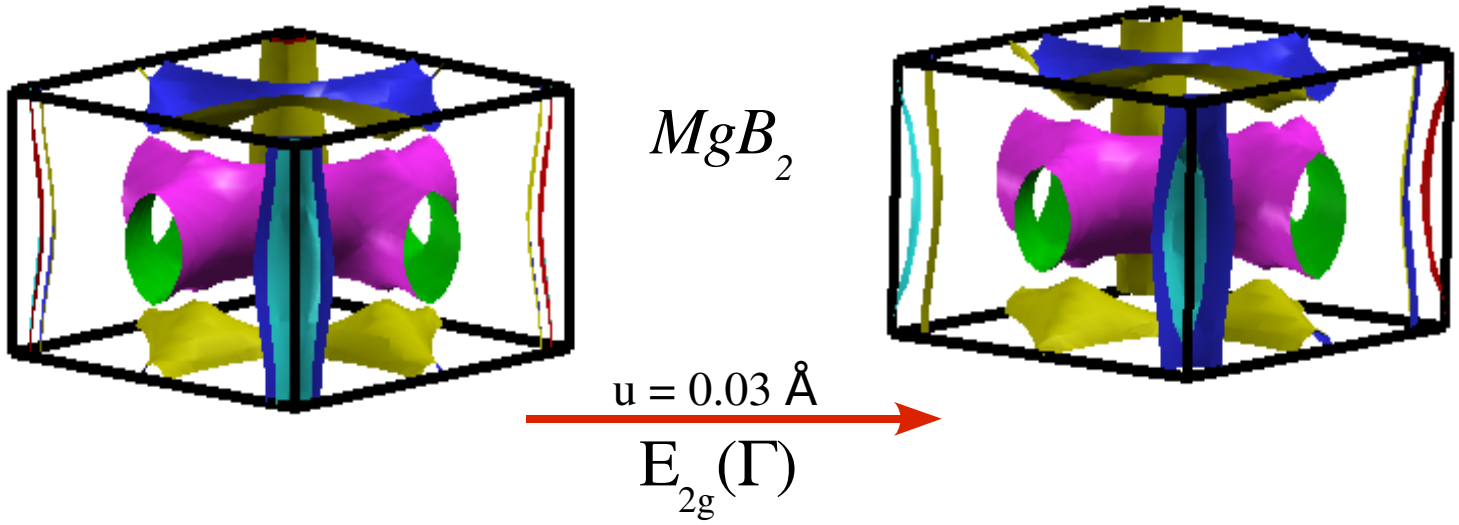
Dense k-grids are a must but only the k-points in the IBZ are needed

Limitations:

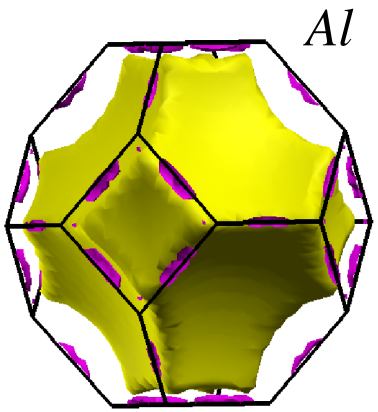
(1) Only Gamma centered k-meshes

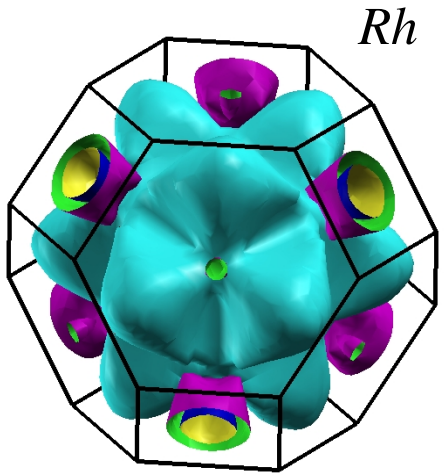
(2) Avoid non zero off diagonal terms if `kptrlatt` is used

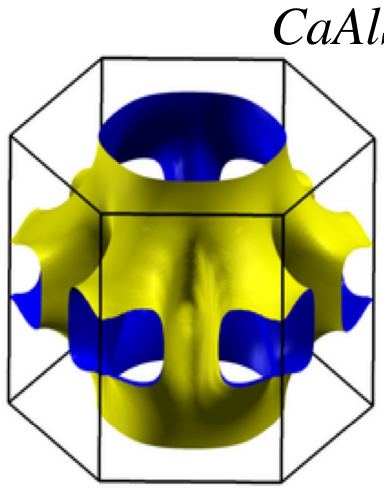
- FS + *frozen phonon* displacements...



- and *ab initio* nice pictures!







Nesting Functions

- Useful to analize the FS geometry and identify important scattering processes
- Smearing and tetrahedron method
- Total nesting, intraband and interband contributions
- Evaluated on the coarse q-grid used for phonons
- Linear interpolation along an arbitrary q-path or on a 3D mesh

anaddb input file

```
prtnest 1          #print the nesting

kptrlatt 4 0 0
         0 4 0
         0 0 4 #needed

elphsmear 0.01 #not used if tetra

nqpath 7           #q-path for the
                   #interpolation
qpath
 0.0 0.0 0.0
 ... ... ...
 1/2 3/4 1/4
```

$$\chi_{nm}(\mathbf{q}) = \sum_{\mathbf{k}} \delta(\epsilon_{n\mathbf{k}})\, \delta(\epsilon_{m\mathbf{k}+\mathbf{q}})$$

Intraband and interband

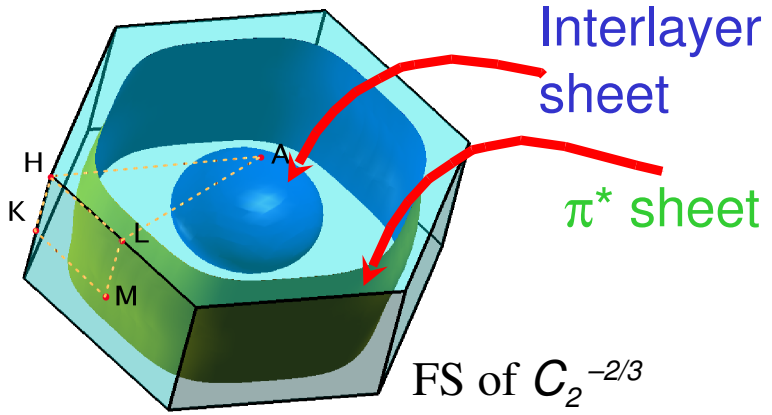
$$\chi(\mathbf{q}) = \sum_{nm} \sum_{\mathbf{k}} \delta(\epsilon_{n\mathbf{k}})\, \delta(\epsilon_{m\mathbf{k}+\mathbf{q}})$$

Total nesting

Example: e-ph in Doped Graphite

FS with 2 sheets $\Rightarrow$ 3 scattering processes:

1. π^*- π^* intraband scattering (green)
2. interlayer-interlayer (blue)
3. π^*- interlayer (red)



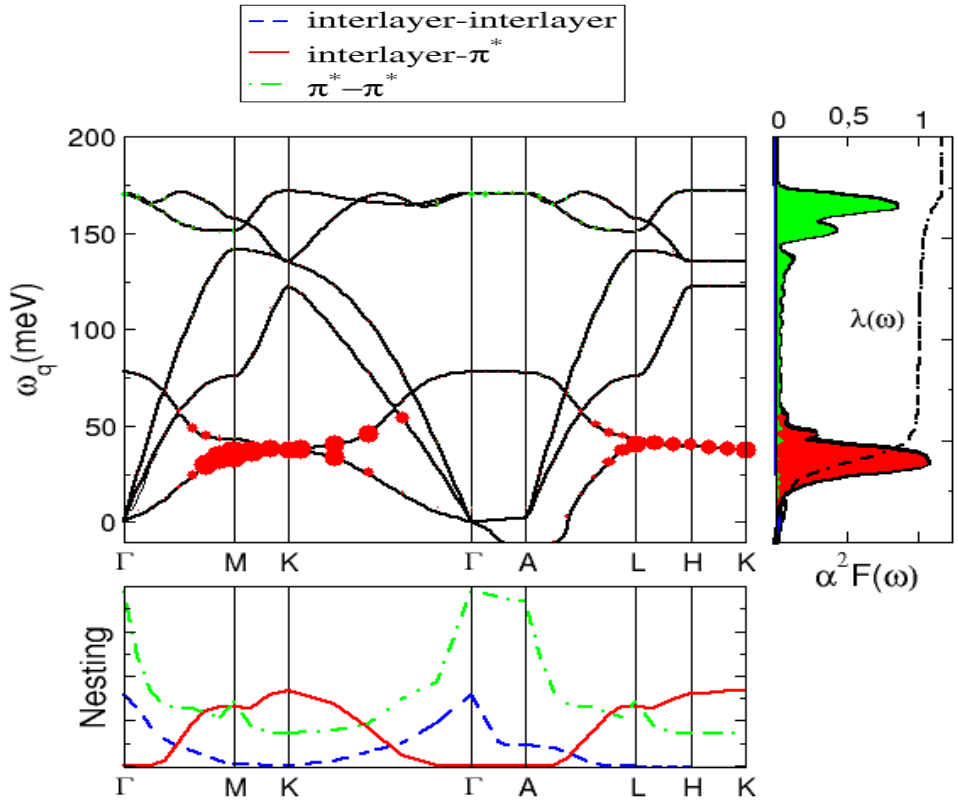
Three contributions to the total nesting:

$$\chi = \chi_{\pi^*-\pi^*} + \chi_{\pi^*-\text{in}} + \chi_{\text{in-in}}$$

Three contributions to the e-ph coupling:

$$\alpha^2 F = \alpha^2 F_{\pi^*-\pi^*} + \alpha^2 F_{\pi^*-\text{in}} + \alpha^2 F_{\text{in-in}}$$

$$\lambda = \lambda_{\pi^*-\pi^*} + \lambda_{\pi^*-\text{in}} + \lambda_{\text{in-in}}$$



Wish List

- Symmetrization of the e-ph elements wrt perturbations:
    1) reduce CPU time required by LR
    2) reduce memory required by anaddb
    3) reduce size of GKK files
- Interpolation of e-ph matrix elements on a denser k-grid
    1) improve the converge of the integrals over the FS
    2) linear or Fourier interpolation?
- Decrease the memory allocated
- Interface with other FS-viewer (not only XcrysDen)

THANK YOU FOR YOUR ATTENTION

E-ph matrix elements

$$M^{\nu}_{m\mathbf{k}+\mathbf{q},n\mathbf{k}} = \langle \Psi_{m\mathbf{k}+\mathbf{q}} | \delta V^{\nu\mathbf{q}}_{eff}(\mathbf{r}) | \Psi_{n\mathbf{k}} \rangle$$

→ Scattering of an electron due to a phonon ($\mathbf{q}$, ν)

RECIPE

- LR calculation for the elemental perturbations ($\mathbf{q}$, j, α)
  - atom
  - reduced direction
- Save matrix elements of $\delta V^{\mathbf{q},j,\alpha}$ in the GKK file (only for **k**'s and **q**'s in the irreducible wedge)
- Run anaddb to:

  a) build e-ph elements: ($\mathbf{q}$, j, α) ⇒ ($\mathbf{q}$, ν)

  b) reconstruct elements in the full BZ

LIMITATION

All the **3*natom** elemental perturbations must be calculated!