Impurities in inhomogeneous superconductors from Density Functional Theory (DFT)

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Introduction

- The juKKR code [1] is a DFT-based calculation method using Green's functions through the Korringa-Kohn-Rostoker (KKR) method
- The KKR method shows interesting features, such as :
  - single site and multiple scattering problem separation
  - dealing with reduced symmetry system / impurities
- To perform calculations that include superconductivity behaviours, the juKKR code is being extended with the Bogoliubov-de Gennes (BdG) formalism [2]

At the moment, the BdG formalism has been successfully implemented for homogeneous superconductor calculations [3].
Work in progress : Implementing the BdG formalism for inhomogeneous superconductors. This will allow to investigate behaviours of exotic materials, such as Majorana qubits or Yu-Shiba-Rusinov chains.

The KKR method

- In the KKR method, we define the Green's function as the resolvent of the Hamiltonian, which can be formulated as [4] :

Structure constants

$$\mathcal{G}(\boldsymbol{r}+\boldsymbol{R}^n, \boldsymbol{r}'+\boldsymbol{R}^{n'}; E) = \underbrace{\delta_{nn'}\sqrt{E}\sum_{L} H_L^n(\boldsymbol{r}_>; E) R_L^n(\boldsymbol{r}_<; E)}_{\text{single site}} + \underbrace{\sum_{LL'} R_L^n(\boldsymbol{r}; E) G_{LL'}^{nn'}(E) R_{L'}^{n'}(\boldsymbol{r}'; E)}_{\text{multiple scattering}}$$

- The electronic density is obtained from the imaginary part of the Green's function :

$$\rho(\boldsymbol{r}) = -\frac{1}{\pi} Im \sum_{\sigma} \int_{-\infty}^{E_F} dE\, G^{\sigma,\sigma}(\boldsymbol{r}, \boldsymbol{r}; E)$$

Impurities within the KKR-Green function method

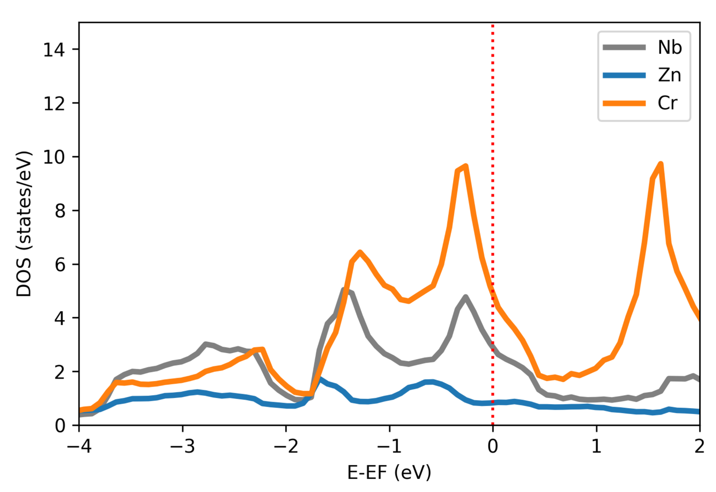
- The Green's function $\mathcal{G}$ of a perturbed system which Hamiltonian is $\mathcal{H} = \mathcal{H}_0 + \Delta\mathcal{V}$ can be obtained from the Green's function $\mathcal{G}_0$ of the unperturbed system through the Dyson equation [4] :

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \Delta\mathcal{V} \mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \mathcal{T} \mathcal{G}_0$$

- The problem of calculating the Green function of the perturbed system is then translated into finding the T-matrix of the system :

$$\mathcal{T}(E) = \Delta\mathcal{V}(1 + \mathcal{G}_0(\mathrm{E})\mathcal{T}(E))$$

Effect of impurities on the DOS of bcc Nb



This graph shows how the DOS of homogeneous bcc Nb (grey) is affected by a Zn/Cr impurity (blue/orange).

We can see that the population at the Fermi level (red dotted-line) can either significantly increase or decrease, depending on the impurity.

The Bogoliubov de Gennes Method

- Superconductivity can be described using the Bogoliubov-de Gennes (BdG) equations. These can be formulated in the effective single particle picture of density functional theory [2]:

$$H_{\mathrm{BdG}} = \begin{pmatrix} -\nabla^2 - E_{\mathrm{F}} + V^{\mathrm{eff}}(\vec{x}) & \Delta^{\mathrm{eff}}(\vec{x}) \\ \Delta^{\mathrm{eff}\,*}(\vec{x}) & \nabla^2 + E_{\mathrm{F}} - V^{\mathrm{eff}\,*}(\vec{x}) \end{pmatrix}$$

$$\Psi_n(\vec{x}) = \begin{pmatrix} u_n(\vec{x}) \\ v_n(\vec{x}) \end{pmatrix} \begin{matrix} \text{electron like} \\ \text{hole like} \end{matrix}$$

- Diagonalizing the BdG Hamiltonian gives the *normal* and *anomalous* densities:

$$\rho(\vec{x}) = \sum_n |u_n|^2(\vec{x}) f(\varepsilon_n) + |v_n|^2(\vec{x})[1 - f(\varepsilon_n)]$$

$$\chi(\vec{x}) = \sum_n u_n(\vec{x}) v_n^*(\vec{x})[1 - 2f(\varepsilon_n)]$$

- This determine the effective single particle potentials

$$V^{\mathrm{eff}}(\vec{x}) = V^{\mathrm{ext}}(\vec{x}) + \int \frac{\rho(\vec{x}')}{|\vec{x} - \vec{x}'|} \mathrm{d}^3x' + \underbrace{\frac{\delta E^0_{\mathrm{xc}}[\rho]}{\delta\rho(\vec{x})}}_{\text{LDA, GGA, ...}}$$

$$\Delta^{\mathrm{eff}}(\vec{x}) = \lambda \cdot \chi(\vec{x})$$

self-consistency

The coupling matrix determines the form of the pairing symmetry (e.g. s-wave) and assumes local pairing

The Coupling constant λ

In order to make accurate BdG calculations, experimental data is needed to determine the value of the coupling constant λ. This can be achieved in two ways :

1) By measuring the superconducting gap size

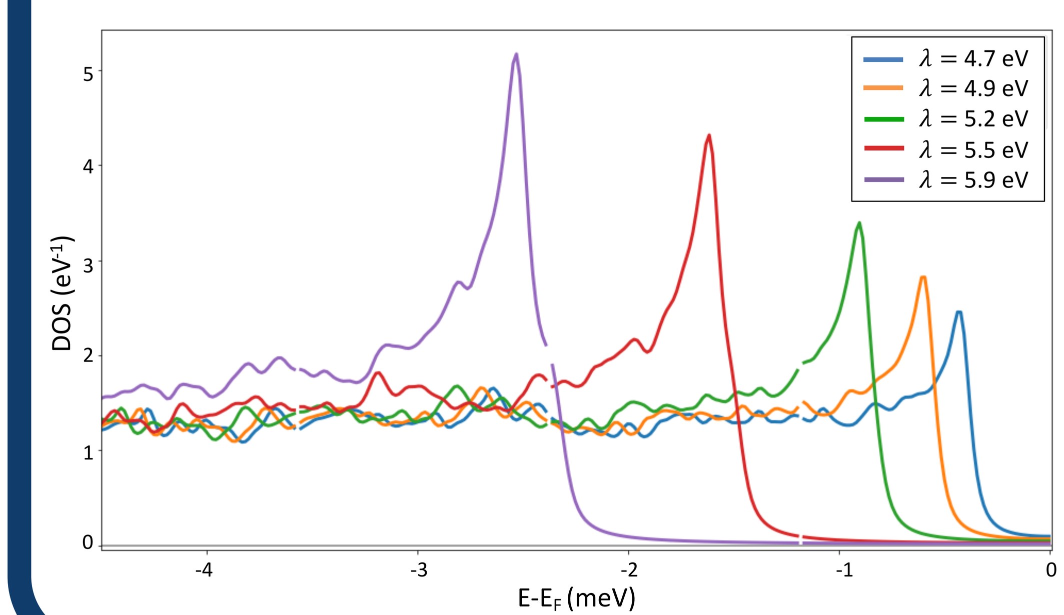
Variations of the coupling constant λ affect the size of the superconducting gap (cf. graphs). If the gap size is experimentally known, the value of λ is chosen such as the calculated superconducting gap size matches the measured one.

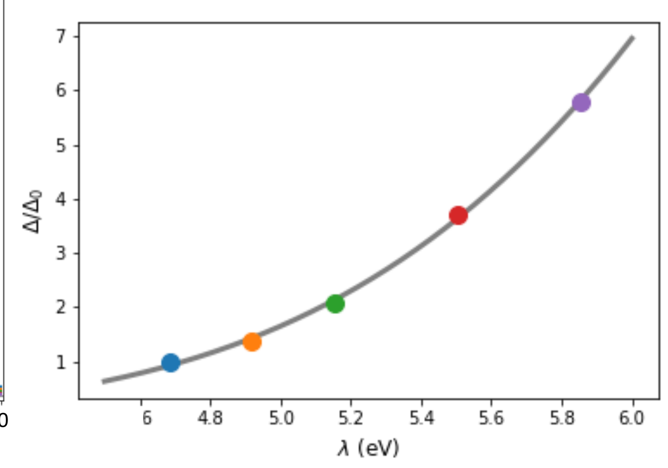
2) By measuring the critical temperature

The critical temperature T_c is linked to the coupling constant through [5] :

$$k_B T_C = 1.14\omega_D e^{-1/N_F\lambda}$$

ω_D = Debye frequency of phonons
N_F = DOS at Fermi level





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