

16 Introduction to Superconducting Density Functional Theory

Antonio Sanna

Max-Planck Institut für Mikrostrukturphysik

Weinberg 2, 06120 Halle, Germany

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1 Introduction

Density functional theories (DFTs) have proved to be a very convenient approach to deal with the many body problem in condensed matter. The original formulation of Hohenberg, Kohn, and Sham [1, 2] as well as several of its extensions [3–7] are now largely applied to study realistic systems and predict their properties with great success.

Density functional theories are all based on a Hohenberg-Kohn type of theorem that proves the existence of a one-to-one mapping between a set of chosen densities and the relative external potentials, implying that it is possible to achieve exact predictions of any observable without having to deal with anything more complex than the density itself.

All the complexity of the many body problem is transferred to the construction of a (universal) functional of the density. A DFT framework is practically useless until a good approximation for the universal functional is available. Clearly the process of functional construction is far from being straightforward. Also, for those used to diagrammatic methods, where approximations are usually expressed in terms of including/excluding some specific process, DFT functionals are sometimes rather obscure. Rarely one can deduce their domain of validity a priori from pure theoretical considerations.

On the other hand the advantage of DFTs is that, once a valid approximation for the functional is constructed, this functional is usually a simple object that can be easily evaluated implemented and applied. DFT algorithms are quite simple, incredibly fast, and very little is required by the user who can focus, instead, on the analysis of results.

Superconducting density functional theory (SCDFT) is an extension of DFT to account for the very peculiar symmetry breaking that occurs in a superconductor [8, 9]. Proposed in 1988 [10] by Oliveira Gross and Kohn it was later revisited [11, 12] to include the multi-component DFT of Kreibich and Gross [13], adding in this way the effect of nuclear motion.

In this lecture it is assumed that the reader has already a basic knowledge of superconductivity and the fundamentals of Green functions and field theory. There are excellent introductions to superconductivity, like DeGennes [9] who discusses in great details BCS theory and the physics of superconducting materials, while the book of Fetter and Walecka [14] is a great reference for the many body formalism.

For what concerns the superconducting state and the topic of this lecture the main references that have been used are the book of Vonsovsky, Izyumov, and Kurmaev [15] and for the SCDFT theory the original research papers [10–12] as well as the PhD theses of Kurth [16], Lueders [17], and Marques [18].

2 Derivation of SCDFT

2.1 Hamiltonian

The starting point of SCDFT is the non relativistic Hamiltonian for interacting electrons *and* nuclei.

$$H = H_e + H_{en} + H_n + H_{ext}, \quad (1)$$

where e stands for electrons, n for nuclei and ext for external fields.

$$H_e = \sum_{\sigma} \int d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}) \left[-\frac{1}{2} \nabla^2 - \mu \right] \psi_{\sigma}(\mathbf{r}) + \frac{1}{2} \sum_{\sigma\sigma'} \int d\mathbf{r} d\mathbf{r}' \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma'}^{\dagger}(\mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} \psi_{\sigma'}(\mathbf{r}') \psi_{\sigma}(\mathbf{r}) \quad (2)$$

where ψ are the electronic field operators, μ the chemical potential, and $d\mathbf{r}$ is an abbreviation for the 3D volume differential.

Nuclei need to be considered explicitly (not just as source of an external potential like in conventional DFT [1]) because in most known superconductors the ionic dynamics provides an essential part of the superconducting coupling

$$H_n = - \int d\mathbf{R} \Phi^{\dagger}(\mathbf{R}) \frac{\nabla^2}{2M} \Phi(\mathbf{R}) + \frac{1}{2} \int d\mathbf{R} d\mathbf{R}' \Phi^{\dagger}(\mathbf{R}) \Phi^{\dagger}(\mathbf{R}') \frac{Z}{|\mathbf{R} - \mathbf{R}'|} \Phi(\mathbf{R}') \Phi(\mathbf{R}) \quad (3)$$

$$H_{en} = -\frac{1}{2} \sum_{\sigma} \int d\mathbf{R} d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}) \Phi^{\dagger}(\mathbf{R}) \frac{Z}{|\mathbf{R} - \mathbf{r}|} \Phi(\mathbf{R}) \psi_{\sigma}(\mathbf{r}) \quad (4)$$

where Φ are ionic field operators, M the mass, and Z the atomic number (assuming a single atom type to keep it simple).

The Hamiltonian still includes an external field that is necessary to break the *phase* symmetry and allow for a superconducting condensation [9]. In fact the normal state is a stationary point, and unless a continuous symmetry is broken in some way any perturbative approach based on this Hamiltonian will not lead to a superconducting state in perfect analogy with the theory of magnetism. From the knowledge of BCS [8, 19] and Eliashberg theory [15, 19, 20] it is expected that the most convenient way to introduce a symmetry breaking term that leads to superconductivity is to couple the system to an external superconductor¹ that can tunnel Cooper pairs in and out

$$H_{\Delta_{ext}} = \int d\mathbf{r} d\mathbf{r}' \Delta_{ext}^*(\mathbf{r}, \mathbf{r}') \psi_{\uparrow}(\mathbf{r}) \psi_{\downarrow}(\mathbf{r}') + h.c. \quad (5)$$

This form of the symmetry breaking field has the great advantage of being extremely simple (involving only two field operators) and will prove also to be theoretically quite convenient. At the same time it has the disadvantage of introducing in the original Hamiltonian a Cooper pair source and sink such that the particle number is not fixed anymore.

In addition to the symmetry breaking external field in Eq. (5) one should also add an external field coupling to the electronic density

$$H_{v_{ext}} = \int d\mathbf{r} v_{ext}(\mathbf{r}) \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}) \quad (6)$$

¹The symmetry breaking will be assumed of singlet type throughout this lecture.

and an external field that couples to the nuclei

$$H_{W_{ext}} = \int W_{ext}(\{\mathbf{R}_i\}) \prod_j d\mathbf{R}_j \Phi^\dagger(\mathbf{R}_j) \Phi(\mathbf{R}_j). \quad (7)$$

Unlike the electronic external potential, the ionic one couples all nuclei with each other (as it depends on the *set* of positions $\{\mathbf{R}_i\}$). This, not obvious, choice is made in order to be able, eventually, to construct a non interacting system of ions that actually behave like phonons under an external potential.

2.2 Hohenberg Kohn theorem

The SCDFT was introduced by Oliveira, Gross, and Kohn [10] as a generalization of finite temperature DFT to include the extra density (χ – called anomalous or superconducting) that couples with the proximity field Δ_{ext} . In its modern form [11, 12] SCDFT is based on the three densities

$$\rho(\mathbf{r}) = \text{Tr} \left[\varrho_0 \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}) \right] \quad (8)$$

$$\chi(\mathbf{r}, \mathbf{r}') = \text{Tr} [\varrho_0 \psi_{\uparrow}(\mathbf{r}) \psi_{\downarrow}(\mathbf{r}')] \quad (9)$$

$$\Gamma(\{\mathbf{R}_i\}) = \text{Tr} \left[\varrho_0 \prod_j \Phi^{\dagger}(\mathbf{R}_j) \Phi(\mathbf{R}_j) \right] \quad (10)$$

where ϱ_0 is the grand canonical density matrix (not to be confused with the electron density $\rho(\mathbf{r})$)

$$\varrho_0 = \frac{e^{-\beta(H-\mu N)}}{\text{Tr} [e^{\beta(H-\mu N)}]}, \quad (11)$$

N being the particle number operator.

SCDFT is based on a generalized Hohenberg-Kohn theorem at finite temperature, that states

1. There is a one-to-one mapping between the set of densities $\rho(\mathbf{r})$, $\chi(\mathbf{r}, \mathbf{r}')$, and $\Gamma(\{\mathbf{R}_i\})$ onto the set of external potentials $v_{ext}(\mathbf{r})$, $\Delta_{ext}(\mathbf{r}, \mathbf{r}')$, and $W_{ext}(\{\mathbf{R}_i\})$
2. There is a variational principle so that it exists a functional Ω that

$$\begin{aligned} \Omega[\rho_0, \chi_0, \Gamma_0] &= \Omega_0 \\ \Omega[\rho, \chi, \Gamma] &> \Omega_0 \quad \text{for} \quad \rho, \chi, \Gamma \neq \rho_0, \chi_0, \Gamma_0 \end{aligned} \quad (12)$$

where ρ_0, χ_0 , and Γ_0 are the ground state densities and Ω_0 the grand canonical potential.

The proof is a generalization of the finite temperature DFT proof of Mermin [7]. It is still worth to sketch it here. One defines the grand canonical functional as

$$\Omega[\varrho] = \text{Tr} \left[\varrho \left(H - \mu N + \frac{1}{\beta} \ln \varrho \right) \right] \quad (13)$$

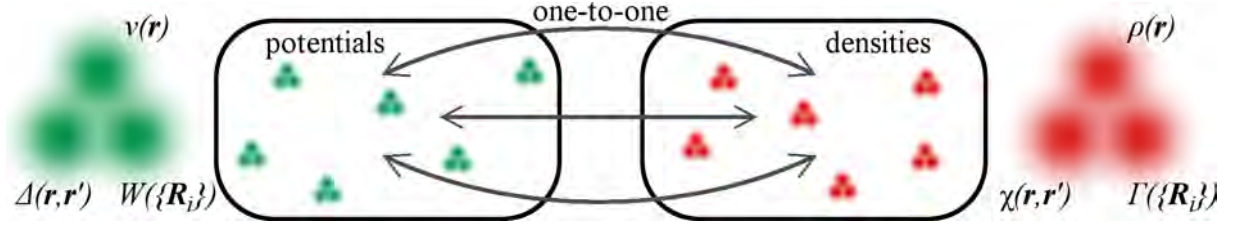


Fig. 1: Correspondence between potentials (v, Δ, W) and densities (ρ, χ, Γ) in SCDF.

where ϱ are density matrices. If ϱ is the grand canonical density matrix ($\varrho \rightarrow \varrho_0$) then $\Omega[\varrho_0]$ is in fact the grand canonical potential of the system $-\frac{1}{\beta} \ln \left\{ \text{Tr} \left[e^{-\beta(H-\mu N)} \right] \right\} \equiv \Omega_0$. From this, it is straightforward to prove that, independently of the specific form of H , $\Omega[\varrho_0] < \Omega[\varrho]$ for any $\varrho \neq \varrho_0$ (refer to appendix A in Ref. [7]).

A second step is to prove by *reductio ad absurdum* that one set of densities can minimize two different sets of external potentials. So let us assume that both $v_{ext}, \Delta_{ext}, W_{ext}$ and $v'_{ext}, \Delta'_{ext}, W'_{ext}$ lead to the same densities ρ, χ, Γ . Clearly H and H' the two Hamiltonians corresponding to the two sets of external potentials are different² as are the corresponding density matrices ϱ and ϱ' . By using the minimum principle one can write the following set of relations

$$\begin{aligned} \Omega' &\equiv \text{Tr} \left\{ \varrho'_0 \left[H' - \mu N \frac{1}{\beta} \ln(\varrho'_0) \right] \right\} < \text{Tr} \left\{ \varrho_0 \left[H' - \mu N \frac{1}{\beta} \ln(\varrho_0) \right] \right\} \\ &= \Omega + \text{Tr} \left\{ \varrho_0 \left[(H_{v'_{ext}} - H_{v_{ext}}) + (H_{\Gamma'_{ext}} - H_{\Gamma_{ext}}) + (H_{\Delta'_{ext}} - H_{\Delta_{ext}}) \right] \right\} \end{aligned} \quad (14)$$

where the last equation uses the assumption that the two systems have the same densities. The argument can be repeated starting from Ω , i.e., swapping primed and un-primed quantities, leading to another inequality

$$\Omega < \Omega' + \text{Tr} \left\{ \varrho'_0 \left[(H_{v_{ext}} - H_{v'_{ext}}) + (H_{\Gamma_{ext}} - H_{\Gamma'_{ext}}) + (H_{\Delta_{ext}} - H_{\Delta'_{ext}}) \right] \right\}. \quad (15)$$

Summing Eq. (14) and (15) and inconsistency emerges

$$\Omega' + \Omega < \Omega + \Omega'. \quad (16)$$

This implies that the assumption was absurd and two different sets of potentials can not lead to the same set of densities. Establishing the one-to-one mapping between densities and potentials is the first part of the Hohenberg-Kohn theorem for SCDF.

To prove the second part one has to notice that, since all observables are obviously functionals of the external potentials, they are also functionals of the densities (due to the one-to-one relation). Since this includes the thermodynamic potential Ω , one can rewrite the minimum principle proved above in terms of the densities (instead of using the density matrix) that is the second and last point of the Hohenberg-Kohn theorem for SCDF.

²This is because the external potentials couple differently with the field operators. With this in mind one can easily extend the theorem to add extra densities and potentials [21, 22].

The fact that all observables are functional of the densities and that H is the sum of internal interactions (Eq. (1)) and couplings with external fields (Eqs. (5), (6), and (7)) allows to write $\Omega[\rho, \chi, \Gamma]$ as

$$\begin{aligned} \Omega[\rho, \chi, \Gamma] = & F[\rho, \chi, \Gamma] + \int d\mathbf{r} v_{ext}(\mathbf{r}) \rho(\mathbf{r}) \\ & + \int \Gamma(\{\mathbf{R}_i\}) W_{ext}(\{\mathbf{R}_i\}) \prod_j d\mathbf{R}_j + \int d\mathbf{r} d\mathbf{r}' \Delta_{ext}^*(\mathbf{r}, \mathbf{r}') \chi(\mathbf{r}, \mathbf{r}') + c.c. \end{aligned} \quad (17)$$

which defines the universal functional $F[\rho, \chi, \Gamma]$. This functional is called universal because, not depending on the external potentials, it is system independent and uniquely fixed by the choice of the Hamiltonian and the chosen set of densities. Still, one retains an explicit dependence on the external potentials, because this coupling is necessary to bind the minimization to a specific physical problem.

2.3 The Kohn-Sham system

As for conventional DFT, in order to move from an exact one-to-one mapping derived in the previous section to a useful computational framework one needs to introduce the Kohn-Sham system [2], a non-interacting system with external potentials such that it is minimized by the same densities as the physical (interacting) one.

The thermodynamic potential of this support system is defined as

$$\begin{aligned} \Omega_s[\rho, \chi, \Gamma] = & T_{s,e}[\rho, \chi, \Gamma] + T_{s,n}[\rho, \chi, \Gamma] - \frac{1}{\beta} S[\rho, \chi, \Gamma] + \int d\mathbf{r} v_s(\mathbf{r}) \rho(\mathbf{r}) \\ & + \int \Gamma(\{\mathbf{R}_i\}) W_s(\{\mathbf{R}_i\}) \prod_j d\mathbf{R}_j + \int d\mathbf{r} d\mathbf{r}' \Delta_s^*(\mathbf{r}, \mathbf{r}') \chi(\mathbf{r}, \mathbf{r}') + c.c. \end{aligned} \quad (18)$$

where T are kinetic energy functionals and S is the entropy functional; the Kohn-Sham “external” potentials must be chosen as

$$\begin{aligned} v_s(\mathbf{r}) &= v_{ext}(\mathbf{r}) + v_H(\mathbf{r}) + v_{xc}(\mathbf{r}) \\ \Delta_s(\mathbf{r}, \mathbf{r}') &= \Delta_{ext}(\mathbf{r}, \mathbf{r}') + \Delta_{xc}(\mathbf{r}, \mathbf{r}') \\ W_s(\{\mathbf{R}_i\}) &= W_{ext}(\{\mathbf{R}_i\}) + W_H(\{\mathbf{R}_i\}) + W_{xc}(\{\mathbf{R}_i\}) \end{aligned} \quad (19)$$

where the subscript H stands for Hartree terms³ and xc are the exchange-correlation potentials defined as

$$\begin{aligned} v_{xc}[\rho, \chi, \Gamma] &= \frac{\delta F_{xc}[\rho, \chi, \Gamma]}{\delta \rho} \\ \Delta_{xc}[\rho, \chi, \Gamma] &= \frac{\delta F_{xc}[\rho, \chi, \Gamma]}{\delta \chi} \\ W_{xc}[\rho, \chi, \Gamma] &= \frac{\delta F_{xc}[\rho, \chi, \Gamma]}{\delta \Gamma} \end{aligned} \quad (20)$$

³An Hartree contribution to Δ_s is not included because such a term does not exist in perturbation theory [15,19].

where

$$F_{xc}[\rho, \chi, \Gamma] = F[\rho, \chi, \Gamma] - T_{s,n}[\rho, \chi, \Gamma] - T_{s,n}[\rho, \chi, \Gamma] + \frac{1}{\beta} S[\rho, \chi, \Gamma]. \quad (21)$$

With these definitions, it is easy to see by functional differentiation of Eq. (18) and (17) that they are minimized by the same densities.

Having defined the Kohn-Sham potentials one can now write the Kohn-Sham equations for SCDF. The ionic equation has the familiar form

$$\left[\sum_j \frac{\nabla_j^2}{2M_j} + W_s(\{\mathbf{R}_i\}) \right] \Phi_n(\{\mathbf{R}_i\}) = \mathcal{E}_n \Phi_n(\{\mathbf{R}_i\}), \quad (22)$$

where M_j is the mass of the atom with label j , \mathcal{E}_n the eigenvalues and Φ_n the ionic eigenstates. The electronic equations are obtained from the electronic Hamiltonian

$$H_s = \sum_{\sigma} \int d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}) \left[\frac{-\nabla^2}{2} + v_s(\mathbf{r}) - \mu \right] \psi_{\sigma}(\mathbf{r}) + \int d\mathbf{r} d\mathbf{r}' [\Delta_s^*(\mathbf{r}, \mathbf{r}') \psi_{\uparrow}(\mathbf{r}) \psi_{\downarrow}(\mathbf{r}') + h.c.]. \quad (23)$$

This Hamiltonian is non diagonal in the field operators because of the coupling induced by the anomalous potential Δ_s^* . It is diagonalized by a Bogoliubov-Valatin transformation [9]

$$\psi_{\sigma}(\mathbf{r}) = \sum_i \left[u_i(\mathbf{r}) \gamma_{i\sigma} - \text{sgn}(\sigma) v_i(\mathbf{r}) \gamma_{i\sigma}^{\dagger} \right] \quad (24)$$

leading to the diagonalization conditions

$$\left[-\frac{\nabla^2}{2} + v_s(\mathbf{r}) - \mu \right] u_i(\mathbf{r}) + \int \Delta_s(\mathbf{r}, \mathbf{r}') v_i(\mathbf{r}') d\mathbf{r}' = E_i u_i(\mathbf{r}) \quad (25)$$

$$-\left[-\frac{\nabla^2}{2} + v_s(\mathbf{r}) - \mu \right] v_i(\mathbf{r}) + \int \Delta_s^*(\mathbf{r}, \mathbf{r}') u_i(\mathbf{r}') d\mathbf{r}' = E_i v_i(\mathbf{r}) \quad (26)$$

that are the electronic Kohn-Sham equation for SCDF. Their mathematical form is well known in superconductivity literature as the Bogoliubov-deGennes (BdG) equations [9] mostly used, within the BCS model, to describe superconducting structures in real space. In SCDF these equations become exact for the calculation of the total energy and the densities

$$\rho(\mathbf{r}) = 2 \sum_i \left[|u_i(\mathbf{r})|^2 f(E_i) + |v_i(\mathbf{r})|^2 f(-E_i) \right] \quad (27)$$

$$\chi(\mathbf{r}, \mathbf{r}') = \sum_i \left[u_i(\mathbf{r}) v_i^*(\mathbf{r}') f(-E_i) - v_i^*(\mathbf{r}) u_i(\mathbf{r}') f(E_i) \right]. \quad (28)$$

In absence of superconductivity both χ and Δ are zero and Eq. (25) becomes the conventional Kohn-Sham equation of DFT⁴

$$\left[-\frac{\nabla^2}{2} + v_s(\mathbf{r}) - \mu \right] \varphi_{nk}(\mathbf{r}) = \xi_{nk} \varphi_{nk}(\mathbf{r}), \quad (29)$$

In the same limit Eq. (26) would be a DFT Kohn-Sham like equation with inverted eigenvalues, that can be seen as an equation for holes instead of electrons. The non-particle-conserving type of superconducting coupling, as a matter of fact, connects these two equations.

⁴Actually slightly more general because it would still include the full effect of temperature and ionic motion since it is still coupled with Eq. (22) via the potentials in (19) and (20).

2.3.1 Transformation to momentum space

Eq. (29) can be solved in the superconducting state (i.e., keeping the non-zero χ in the functional $v_s[\rho, \chi, F]$), introducing the corresponding eigenfunctions $\varphi_{nk}(\mathbf{r})$. These would be different from the conventional KS orbitals, but can be used as a basis set to express the BdG equations in \mathbf{k} space. Introducing the expansion

$$u_i(\mathbf{r}) = \sum_{nk} u_{i,nk} \varphi_{nk}(\mathbf{r}) \quad (30)$$

$$v_i(\mathbf{r}) = \sum_{nk} v_{i,nk} \varphi_{nk}(\mathbf{r}) \quad (31)$$

$$\Delta_s(\mathbf{r}, \mathbf{r}') = \sum_{nn'kk'} \Delta_{s,nn'kk'} \varphi_{nk}(\mathbf{r}) \varphi_{n'k'}(\mathbf{r}') \quad (32)$$

inserting into Eqs. (25), (26) and using the orthogonality of the basis set gives

$$\begin{aligned} \xi_{nk} u_{i,nk} + \sum_{n'k'} \Delta_{s,nn'kk'} v_{i,n'k'} &= E_i u_{i,nk} \\ -\xi_{nk} v_{i,nk} + \sum_{n'k'} \Delta_{s,nn'kk'}^* u_{i,n'k'} &= E_i v_{i,nk} \end{aligned} \quad (33)$$

a form of the BdG equations particularly useful for introducing approximations.

2.4 Decoupling approximations

The SCDF formalism developed so far is exact but useless unless one is able to derive a valid approximation for the exchange correlation functional F_{xc} entering Eq. (20). However the problem introduced in Sec. 2.1 is a very complicated one and cannot be tackled without introducing key approximations to strip it to the bone. The goal of an ab-initio approach is to introduce controlled (or at least controllable) approximations. Luckily in the problem of interacting electrons and nuclei there is a lot of experience and many established approximations that can be introduced give results of broad validity.

The most important approximations, that will be discussed in this section, are meant to decouple as much as possible the many degrees of freedom (and densities) of the problem

1. Decouple electrons from ions separating the static and dynamic parts of the interaction, including the latter in a perturbative fashion.
2. Decouple the high energy chemical scale (responsible for bonding) from low energy pairing interactions (responsible for superconductivity).

2.4.1 Phonons and electron-phonon interaction

The formalism so far describes a set of interacting electrons and ions. This correlated electron-nuclear dynamics is enormously complex and far from being satisfactorily solved. However,

if one considers only systems close to their equilibrium it is reasonable to assume that atoms are locked to a lattice position and only small oscillations can occur. The assumption allows to treat ionic oscillations as a perturbation on a static field, greatly simplifying the problem. There is some excellent literature (like [23–25]) discussing these issue in great detail. Here the focus will be on the main approximations that are presently used in implementations of SCDFT.

A key approximation is to ignore the effect of superconductivity on the lattice dynamics and on the electron-phonon interaction. This, as the superconducting transition is usually of second order, is exact close to the critical temperature, where the superconducting density becomes infinitesimally small. This allows to study the lattice dynamics in the normal state.

To compute phonons and the electron-phonon interaction one usually relies on conventional Kohn-Sham density functional theory and the electron-phonon scattering matrix elements are defined as

$$g_{m\mathbf{k}+\mathbf{q},n\mathbf{k}}^{\nu} = \sqrt{\frac{\hbar}{2\omega_{q\nu}}} \left\langle \varphi_{m\mathbf{k}+\mathbf{q}} \left| \Delta V_{scf}^{q\nu} \right| \varphi_{n\mathbf{k}} \right\rangle \quad (34)$$

where \mathbf{k} and \mathbf{q} are the electron and phonon momenta, m and n Kohn-Sham band indices, $\varphi_{n\mathbf{k}}$ the Kohn-Sham states, ν is the phonon branch, $\omega_{q\nu}$ the phonon frequency and $\Delta V_{scf}^{q\nu}$ the variation in the Kohn-Sham potential due to the ionic displacement corresponding to the phonon mode. By means of density functional perturbation theory [25] these matrix elements can be computed accurately and at a reasonable computational cost for any bulk superconductor. The electron-phonon interaction of the Kohn-Sham system reads

$$\tilde{H}_{e-ph} = \sum_{mn\sigma} \sum_{\nu\mathbf{k}\mathbf{q}} g_{m\mathbf{k}+\mathbf{q},n\mathbf{k}}^{\nu} \sum_{\sigma} \psi_{\sigma m\mathbf{k}+\mathbf{q}}^{\dagger} \psi_{\sigma n\mathbf{k}} b_{\nu\mathbf{q}} = \sum_{\nu\mathbf{q}} \sqrt{\frac{\hbar}{2\omega_{q\nu}}} \int d\mathbf{r} \Delta V_{scf}^{q\nu}(\mathbf{r}) \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}) b_{\nu\mathbf{q}}, \quad (35)$$

where $\psi_{\sigma n\mathbf{k}}^{\dagger}$ and $\psi_{\sigma n\mathbf{k}}$ are creation and destruction operators for Kohn-Sham states and $b_{\nu\mathbf{q}}$ is a phonon operator.

The step of approximating the dynamic part of H_{en} with \tilde{H}_{en} can certainly be justified empirically by its success in applications [26, 25] but is theoretically not very rigorous. The main supporting argument is essentially that if the Kohn-Sham band structure is close to the interacting one so will likely be their response to a lattice motion. Clearly if Kohn-Sham bands are far off from the interacting ones (like in strongly correlated systems) the Kohn-Sham electron-phonon coupling is also expected to be a poor approximation to the real one.

2.4.2 Band decoupling approximation

The electronic BdG Kohn-Sham equations (33) can be enormously simplified by assuming that the superconducting condensation will be a small perturbation to the non-superconducting system. As already pointed out in the previous section, since the superconducting transition is usually of second order the assumption becomes exact close to T_C so that it will not affect the estimation of T_C itself.

This assumption, first of all, implies that the superconducting transition will not induce a structural one, therefore $\Delta_s(\mathbf{r}, \mathbf{r})$ should maintain the original lattice periodicity and the \mathbf{k} quantum

number in Eq. (29) must be conserved [16, 17]. In other words the summations in equation Eqs. (30) and (31) should only run over the band index n and not over \mathbf{k} .

The summation over n means that the superconducting transition can still induce an *hybridization* between different bands corresponding to the same \mathbf{k} -point. However, unless bands are degenerate (or close to degeneracy with respect to the energy scale set by Δ_s that is of the order 10 meV) this hybridization must be extremely small. Therefore, apart for anomalous cases, one can introduce a second and stronger approximation by ignoring this superconductivity induced band hybridization effect. Then Eqs. (30) and (31) reduce to

$$u_i(\mathbf{r}) \equiv u_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}\varphi_{n\mathbf{k}}(\mathbf{r}) \quad (36)$$

$$u_i(\mathbf{r}) \equiv v_{n\mathbf{k}}(\mathbf{r}) = v_{n\mathbf{k}}\varphi_{n\mathbf{k}}(\mathbf{r}),$$

which implies $\Delta_{s,mn'\mathbf{k}\mathbf{k}'} \rightarrow \delta_{n\mathbf{k},n'\mathbf{k}'}\Delta_{s,n\mathbf{k}}$.

Inserting Eq. (36) into (33) one can formally solve these equations obtaining

$$u_{n\mathbf{k}} = \frac{1}{\sqrt{2}} \operatorname{sgn}(E_{n\mathbf{k}}) e^{\phi_{n\mathbf{k}}} \sqrt{1 + \frac{\xi_{n\mathbf{k}}}{|E_{n\mathbf{k}}|}} \quad (37)$$

$$v_{n\mathbf{k}} = \frac{1}{\sqrt{2}} \sqrt{1 - \frac{\xi_{n\mathbf{k}}}{|E_{n\mathbf{k}}|}} \quad (38)$$

with $e^{\phi_{n\mathbf{k}}} = \Delta_s(n\mathbf{k}) / |\Delta_s(n\mathbf{k})|$ and $E_{n\mathbf{k}} = \pm \sqrt{\xi_{n\mathbf{k}}^2 + |\Delta_s(n\mathbf{k})|^2}$. While the densities in Eq. (27) and (28) take on the simple form

$$\rho(\mathbf{r}) = \sum_{n\mathbf{k}} \left[1 - \frac{\xi_{n\mathbf{k}}^2}{|E_{n\mathbf{k}}|} \tanh\left(\frac{\beta|E_{n\mathbf{k}}|}{2}\right) \right] |\varphi_{n\mathbf{k}}(\mathbf{r})|^2 \quad (39)$$

$$\chi(\mathbf{r}, \mathbf{r}') = \frac{1}{2} \sum_{n\mathbf{k}} \frac{\Delta_s(n\mathbf{k})}{|E_{n\mathbf{k}}|} \tanh\left(\frac{\beta|E_{n\mathbf{k}}|}{2}\right) \varphi_{n\mathbf{k}}(\mathbf{r}) \varphi_{n\mathbf{k}}^*(\mathbf{r}'). \quad (40)$$

The whole superconducting problem is now reduced to the construction of the matrix elements of the Kohn-Sham potential $\Delta_s(n\mathbf{k})$ that are defined by the solution of Eq. (20). The explicit dependence on χ in that equation can be substituted with a dependence on Δ_s (using Eq. (40))

$$\Delta_{xc} = \frac{\delta F_{xc}[\rho, \chi[\Delta_s, \rho, \Gamma], \Gamma]}{\delta \chi} \quad (41)$$

The above equation is a closed (self-consistent) equation for the Kohn-Sham potential and is usually called the SCDFT gap equation.

At this stage one needs some approximation for the $F_{xc}[\rho, \chi, \Gamma]$ functional. A simple functional will be derived in the following sections by first creating a link between SCDFT and many body perturbation theory.

3 Connection between SCDFE and Eliashberg theory

A DFT exchange-correlation functional contains information on the interacting behavior of the many body system. This type of information can be extracted from different approaches like models, solvable exact limits of the theory, empirical data, perturbative methods and more. Perturbation methods have the advantage of allowing for a systematic improvement, it is formally possible to reach arbitrary high accuracy, although in reality one is usually strongly limited by computational costs and convergence issues.

Nevertheless it is nice to construct an exchange correlation functional starting from many body perturbation theory and to keep exact control on what type of physics the functional will describe and what would be its limits.

It will be shown in Sec. 3.2 how to set up a link between many body perturbation theory and SCDFE. The focus will be on a specific many body approximation for superconductivity that goes under the name of Eliashberg theory and will be briefly reviewed in Sec. 3.1. Eventually, in Sec. 3.3, the exact link will be studied for a model superconductor.

3.1 A survey on Eliashberg theory of superconductivity

This section gives a formal introduction to Eliashberg theory of superconductivity that is the most popular theory used for superconductivity predictions, especially in the simplified form of the McMillan equation [27].

One can start from the Hamiltonian, Eq. (1). After decoupling the lattice dynamics as discussed in Sec. 2.4.1 only the electronic part and the electron-phonon interaction part \tilde{H}_{en} introduced in Sec. 2.4.1 are retained

$$H \rightarrow H_e + H_{ee} + \tilde{H}_{en} + H_{ext} \quad (42)$$

where now H_{ext} contains the anomalous coupling in Eq. (5) as well as the static electron-ion coupling (as in normal DFT).⁵

H is then split in a zero-approximation H_0 plus an interaction part H_I . A convenient choice for the zero approximation is H_{ext} plus the Kohn-Sham Hamiltonian entering in Eq. (29)

$$H_s = \sum_{\sigma} \int d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}) \left[-\frac{\nabla^2}{2} + v_s(\mathbf{r}) - \mu \right] \psi_{\sigma}(\mathbf{r}), \quad (43)$$

while everything else goes into H_I . So

$$H_0 = H_s + H_{ext} \quad (44)$$

$$H_I = H_{ee} + \tilde{H}_{en} - H_{DC} \quad (45)$$

where the last term removes extra xc effects already included in H_s , therefore avoiding any *double counting*

$$H_{DC} = \sum_{\sigma} \int d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}) v_s(\mathbf{r}) \psi_{\sigma}(\mathbf{r}). \quad (46)$$

⁵Often in the literature on Eliashberg theory the external potential $\Delta_{ext}(\mathbf{r}, \mathbf{r}')$ is taken to be local ($\Delta_{ext}(\mathbf{r})$) here is introduced as non-local to be consistent with the SCDFE formalism.

The reference Kohn-Sham system to which we refer here is that of normal DFT and not of SCDFD (alternatively one could consider v_s as the SCDFD limit for $\chi = 0$, i.e., formally retaining the effects of the multi-component formalism and its dependence on Γ).

Unfortunately conventional many body perturbation theory [14] can not be directly applied to $H_0 + H_I$ because the particle source in Eq. (5) introduces new processes forbidden in a particle conserving theory.

There is a trick that allows to transform H back into a standard form: the Nambu-Gor'kov formalism. One defines two new electronic field operators

$$\bar{\psi}(\mathbf{r}) = \begin{pmatrix} \psi_{\uparrow}(\mathbf{r}) \\ \psi_{\downarrow}(\mathbf{r}) \end{pmatrix} \quad (47)$$

$$\bar{\psi}^{\dagger}(\mathbf{r}) = \left(\psi_{\uparrow}^{\dagger}(\mathbf{r}) \quad \psi_{\downarrow}(\mathbf{r}) \right). \quad (48)$$

that still obey Fermionic commutation rules. With these two-component fields $\bar{\psi}$ one can rewrite H_0 and H_I as

$$H_0 = \int d\mathbf{r} \bar{\psi}^{\dagger}(\mathbf{r}) \bar{H}_0(\mathbf{r}, \mathbf{r}') \bar{\psi}(\mathbf{r}') \quad (49)$$

$$H_I = \int d\mathbf{r} \bar{\psi}^{\dagger}(\mathbf{r}) \left[\sum_{vq} \sqrt{\frac{\hbar}{2\omega_{qv}}} \int d\mathbf{r}' \Delta V_{scf}^{qv}(\mathbf{r}) \bar{\sigma}_3 b_{vq} - v_s(\mathbf{r}) \right] \bar{\psi}(\mathbf{r}) \\ + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \left[\bar{\psi}^{\dagger}(\mathbf{r}) \bar{\sigma}_3 \bar{\psi}(\mathbf{r}') \right] \frac{1}{|\mathbf{r} - \mathbf{r}'|} \left[\bar{\psi}^{\dagger}(\mathbf{r}') \bar{\sigma}_3 \bar{\psi}(\mathbf{r}') \right]. \quad (50)$$

where $\bar{\sigma}_3$ is the Pauli matrix $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and \bar{H}_0 is defined as

$$\bar{H}_0(\mathbf{r}, \mathbf{r}') = \begin{pmatrix} \left[-\frac{\nabla^2}{2} + v_s(\mathbf{r}) - \mu \right] \delta(\mathbf{r} - \mathbf{r}') & \Delta_{ext}(\mathbf{r}, \mathbf{r}') \\ \Delta_{ext}^*(\mathbf{r}, \mathbf{r}') & - \left[-\frac{\nabla^2}{2} + v_s(\mathbf{r}) - \mu \right] \delta(\mathbf{r} - \mathbf{r}') \end{pmatrix}. \quad (51)$$

The Hamiltonian in this new form does not feature anymore source terms for the new field $\bar{\psi}$, therefore the perturbative expansion for H_I will have exactly the same contributions (diagrams) as in conventional perturbation theory. The difference is that Green functions and self energy will have a 2×2 matrix structure and vertices will carry the extra $\bar{\sigma}_3$ terms. The Green function is defined as

$$\bar{G}(\tau\mathbf{r}, \tau'\mathbf{r}') := - \begin{pmatrix} \left\langle T \psi_{H,\uparrow}(\tau\mathbf{r}) \psi_{H,\uparrow}^{\dagger}(\tau'\mathbf{r}') \right\rangle & \left\langle T \psi_{H,\uparrow}(\tau\mathbf{r}) \psi_{H,\downarrow}(\tau'\mathbf{r}') \right\rangle \\ \left\langle T \psi_{H,\downarrow}^{\dagger}(\tau\mathbf{r}) \psi_{H,\uparrow}^{\dagger}(\tau'\mathbf{r}') \right\rangle & \left\langle T \psi_{H,\downarrow}^{\dagger}(\tau\mathbf{r}) \psi_{H,\downarrow}(\tau'\mathbf{r}') \right\rangle \end{pmatrix}, \quad (52)$$

where the H subscript refers to the Heisenberg picture, T is the time ordering operator for the imaginary time coordinate τ and the $\langle \dots \rangle$ is used as short notation for the thermodynamic average as in Eq. (8). Comparing with Eq. (8) one can show that normal and anomalous densities can be easily extracted from \bar{G}

$$\rho(\mathbf{r}) = \lim_{\tau' \rightarrow \tau^+} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} \bar{G}^{(11)}(\tau\mathbf{r}, \tau'\mathbf{r}') = \lim_{\mathbf{r}' \rightarrow \mathbf{r}} \frac{1}{\beta} \sum_i \bar{G}^{(11)}(\mathbf{r}, \tau'\mathbf{r}', \omega_i) \quad (53)$$

$$\chi(\mathbf{r}, \mathbf{r}') = \lim_{\tau' \rightarrow \tau^+} \bar{G}^{(12)}(\tau\mathbf{r}, \tau'\mathbf{r}') = \frac{1}{\beta} \sum_i \bar{G}^{(12)}(\mathbf{r}, \tau'\mathbf{r}', \omega_i) \quad (54)$$

where the (ij) superscript indicates the matrix component of \bar{G} , and the second equality comes from the transform from imaginary time to Matsubara frequencies (ω_i) according to the standard relation⁶ $\bar{G}(\mathbf{r}, \mathbf{r}', \omega_i) = \int d\tau e^{i\omega_i\tau} \bar{G}(0, \mathbf{r}, \tau \mathbf{r}')$.

\bar{G} is obtained by solving the Dyson equation

$$\bar{G}(\mathbf{r}, \mathbf{r}', \omega_i) = \bar{G}_0(\mathbf{r}, \mathbf{r}', \omega_i) + \bar{G}_0(\mathbf{r}, \mathbf{r}', \omega_i) \bar{\Sigma}(\mathbf{r}, \mathbf{r}', \omega_i) \bar{G}(\mathbf{r}, \mathbf{r}', \omega_i), \quad (55)$$

where $\bar{G}_0(\mathbf{r}, \mathbf{r}', \omega_i)$ is the Green function corresponding to the non interacting Hamiltonian H_0 . What is now left is to introduce an approximation for the self energy $\bar{\Sigma}$. Leaving aside (for the moment) contributions stemming from the double counting term H_{DC} , the first order contribution is

$$\bar{\Sigma}^{(1)} = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \text{[diagram 4]}, \quad (56)$$

where wavy lines are phonon propagators, dashed lines the (bare) Coulomb interaction and arrowed lines are the Green functions. The first term is an Hartree-like phonon driven electron-electron interaction. A careful analysis of this diagram shows that its contribution is rather small, essentially introducing a shift (of the order of the phononic energy scale) on the eigenvalues of H_0 . Conventionally this contribution is not included in Eliashberg theory because it is irrelevant in comparison to the intrinsic error one commits computing the eigenvalues of H_0 .⁷ The second term is the conventional Hartree diagram. It is exactly cancelled by a corresponding term in v_s since one assumes that the Kohn-Sham Hamiltonian leads to the same density of the interacting system.

The third and fourth terms are exchange-like diagrams that contain those electron-electron scattering processes that are essential to superconductivity.

Quite clearly the first order set of diagrams in $\bar{\Sigma}^{(1)}$ would not be sufficient to obtain any reasonable result. Consider that electrons are now interacting only with the bare Coulomb interaction while in real materials (especially in metals) the electronic interaction is very effectively screened. Like in GW theory [28, 29] it is possible to boost the order of the approximation by dressing propagators and Green functions (the phonon propagator is already dressed as it is computed externally). Therefore defining the following approximation

$$\bar{\Sigma} = \underbrace{\text{[diagram 3]} + \text{[diagram 4]}}_{\bar{\Sigma}_{xc}} - \bar{\Sigma}_{DC} \quad (57)$$

where $\bar{\Sigma}_{DC}$ is simply $\bar{\tau}_3 v_{xc}$.

⁶To keep the formalism as simple as possible convergence factors $e^{i\omega_i\eta}$ will be omitted [14].

⁷In the multi-component formalism discussed in Sec. 2.3 this term would be already included in v_s (since in Eq. (20) there is a functional dependence on the ionic density). However, Eliashberg theory usually starts from the conventional Kohn-Sham Hamiltonian where v_s is only a functional of the electronic density and ions only appear as a static external potential.

The computational cost to apply the approximation above would still be too expensive. Just looking at the Coulomb diagram essentially corresponds to a self consistent GW approach in the 2×2 Nambu-Gor'kov space! One should instead rely on the same approximations discussed in Sec. 2.4.2, assuming that the electronic states are already well described by the Kohn-Sham Hamiltonian and neglect inter-band hybridization. Essentially the self energy still is that of Eq. (57) but the diagonal part of the second diagram is removed together with $\bar{\Sigma}_{DC}$ (that was inserted in the first place to avoid the double counting of xc terms).

In the basis of Kohn-Sham states this self energy then takes the form

$$\bar{\Sigma}(\mathbf{n}\mathbf{k}, \omega_i) = -\frac{1}{\beta} \sum_j \sum_{mq'} \bar{\sigma}_3 \bar{G}(\mathbf{n}\mathbf{k}, \omega_i) \bar{\sigma}_3 \left[\sum_v g_{m\mathbf{k}+\mathbf{q}, \mathbf{n}\mathbf{k}}^v D_v(\mathbf{q}, \omega_i - \omega_j) + \bar{\sigma}_1 W(\mathbf{n}\mathbf{k}, m\mathbf{k} + \mathbf{q}) \right], \quad (58)$$

where ω_i are the Matsubara frequencies, $\bar{\sigma}_1$ is the Pauli matrix $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $D_v(\mathbf{q}, \omega_i - \omega_j) = -2\omega_{vq} / \left[(\omega_i - \omega_j)^2 + \omega_{vq}^2 \right]$ is the phonon propagator and W the screened Coulomb interaction. $\bar{G}(\mathbf{n}\mathbf{k}, \omega_i)$ is the Nambu-Gor'kov Green function that in momentum space is

$$\bar{G}(\mathbf{n}\mathbf{k}, \omega_i) = \int_0^\beta d\tau e^{-i\omega_i(\tau-\tau')} \int d\mathbf{r}\mathbf{r}' \varphi_{\mathbf{n}\mathbf{k}}^*(\mathbf{r}) \bar{G}(\tau\mathbf{r}, \tau'\mathbf{r}') \varphi_{\mathbf{n}\mathbf{k}}(\mathbf{r}') \quad (59)$$

and is the solution of the Dyson equation

$$\bar{G}(\mathbf{n}\mathbf{k}, \omega_i) = \bar{G}_0(\mathbf{n}\mathbf{k}, \omega_i) + \bar{G}_0(\mathbf{n}\mathbf{k}, \omega_i) \bar{\Sigma}(\mathbf{n}\mathbf{k}, \omega_i) \bar{G}(\mathbf{n}\mathbf{k}, \omega_i), \quad (60)$$

where $\bar{G}_0(\mathbf{n}\mathbf{k}, \omega_i)$ is the Green function corresponding to the non interacting Hamiltonian H_0 . The above equation is Eliashberg theory of superconductivity. Its solution is usually achieved by first expanding this matrix equation into Pauli matrices and separating it into components. The decomposition has the advantage to lead to a more explicit form of \bar{G} and help the physical interpretation. \bar{G} is expressed as

$$\bar{G}(\mathbf{n}\mathbf{k}, \omega_i) = \frac{\begin{pmatrix} i\omega_i Z(\mathbf{n}\mathbf{k}, \omega_i) + [\xi_{\mathbf{n}\mathbf{k}} + \mathcal{X}(\mathbf{n}\mathbf{k}, \omega_i)] & \phi(\mathbf{n}\mathbf{k}, \omega_i) \\ \phi(\mathbf{n}\mathbf{k}, \omega_i) & i\omega_i Z(\mathbf{n}\mathbf{k}, \omega_i) - [\xi_{\mathbf{n}\mathbf{k}} + \mathcal{X}(\mathbf{n}\mathbf{k}, \omega_i)] \end{pmatrix}}{[i\omega_i Z(\mathbf{n}\mathbf{k}, \omega_i)]^2 - [\xi_{\mathbf{n}\mathbf{k}} + \mathcal{X}(\mathbf{n}\mathbf{k}, \omega_i)]^2 - \phi^2(\mathbf{n}\mathbf{k}, \omega_i)}, \quad (61)$$

where \mathcal{X} (not to be confused with the superconducting order parameter) shifts the non interacting energies, Z behaves as a mass term, and ϕ/Z is the function giving the superconducting gap (this interpretation is evident by analytically continuing \bar{G} to the real frequency axis $i\omega_i \rightarrow \omega$). These are now scalar functions and here they are assumed to be real valued.⁸

The interested reader can refer to more specialized literature with extra focus on application and numerical implementation, like the classic Review of Carbotte [31] or the excellent review of Ummarino in this same lecture series [32].

⁸One can show that for the Hamiltonian (1) the ϕ , Z and \mathcal{X} functions satisfy a set of equations with real coefficients. In spite of this the solution could still be non trivially complex, as in the famous three crystal experiment [30], but this unusual situation will be neglected.

3.2 The Sham Schlüter connection

In Sec. 2 the SCDFD framework was derived and a set of quite general approximations was introduced in order to decouple the superconducting and the normal state problem. In the previous section the Eliashberg theory of superconductivity was reviewed and derived in the same approximations assumed for SCDFD.

Following the work of Marques [18], this section is devoted to set up a formal connection between the two theories, by extending the Sham Schlüter connection to SCDFD.

The connection is based on a Dyson equation similar to Eq. (60), however instead of using the normal state Kohn-Sham Hamiltonian H_0 (Eq. (49)) as reference Hamiltonian for the perturbation expansion, one should use the SCDFD Kohn-Sham system

$$\bar{H}_s(\mathbf{r}, \mathbf{r}') = \begin{pmatrix} \left[-\frac{\nabla^2}{2} + v_s(\mathbf{r}) - \mu \right] \delta(\mathbf{r} - \mathbf{r}') & \Delta_s(\mathbf{r}, \mathbf{r}') \\ \Delta_s^*(\mathbf{r}, \mathbf{r}') & -\left[-\frac{\nabla^2}{2} + v_s(\mathbf{r}) - \mu \right] \delta(\mathbf{r} - \mathbf{r}') \end{pmatrix} \quad (62)$$

leading to the following form of the Dyson equation

$$\bar{G}(\mathbf{n}\mathbf{k}, \omega_i) = \bar{G}_s(\mathbf{n}\mathbf{k}, \omega_i) + \bar{G}_s(\mathbf{n}\mathbf{k}, \omega_i) \bar{\Sigma}_s(\mathbf{n}\mathbf{k}, \omega_i) \bar{G}(\mathbf{n}\mathbf{k}, \omega_i), \quad (63)$$

that differs from Eq. (60) as \bar{G}_s is the Green function of the SCDFD Kohn-Sham system and $\bar{\Sigma}_s(\mathbf{n}\mathbf{k}, \omega_i)$ is the self energy in which the double counting correction refers to SCDFD (not to DFT as in Eq. (57))

$$\bar{\Sigma}_s = \bar{\Sigma}_{xc} - \bar{\Sigma}_{DC}^{SC}, \quad (64)$$

where $\bar{\Sigma}_{DC}^{SC}$ reads

$$\bar{\Sigma}_{DC}^{SC}(\mathbf{n}\mathbf{k}) = \begin{pmatrix} v_{xc}(\mathbf{n}\mathbf{k}) & \Delta_{xc}(\mathbf{n}\mathbf{k}) \\ \Delta_{xc}^*(\mathbf{n}\mathbf{k}) & -v_{xc}(\mathbf{n}\mathbf{k}) \end{pmatrix}. \quad (65)$$

Then one uses the fact that *both* \bar{G} and \bar{G}_s when inserted into Eq. (53) provide the exact density of the system. It is easy to see that in the Kohn-Sham basis this implies

$$\sum_i \sum_{\mathbf{n}\mathbf{k}} \bar{G}^{(11)}(\mathbf{n}\mathbf{k}, \omega_i) = \sum_i \sum_{\mathbf{n}\mathbf{k}} \bar{G}_s^{(11)}(\mathbf{n}\mathbf{k}, \omega_i) \equiv \sum_i \sum_{\mathbf{n}\mathbf{k}} \frac{-(i\omega_i + \xi_{\mathbf{n}\mathbf{k}})}{\omega_i^2 + \xi_{\mathbf{n}\mathbf{k}}^2 + \Delta_s^2(\mathbf{n}\mathbf{k})} \quad (66)$$

$$\sum_i \bar{G}^{(12)}(\mathbf{n}\mathbf{k}, \omega_i) = \sum_i \bar{G}_s^{(12)}(\mathbf{n}\mathbf{k}, \omega_i) \equiv \sum_i \frac{-\Delta_s(\mathbf{n}\mathbf{k})}{\omega_i^2 + \xi_{\mathbf{n}\mathbf{k}}^2 + \Delta_s^2(\mathbf{n}\mathbf{k})}, \quad (67)$$

where the second equality uses the explicit form of G_s that, belonging to a non interacting system, is simply $\frac{1}{i\omega_i \bar{I} - \bar{H}_s}$, with \bar{I} being the 2×2 identity matrix. These constraints used in Eq. (63) lead obviously to a set of conditions for v_{xc} and Δ_{xc} .

However, if Σ_{xc} is assumed in the Eliashberg approximation, the diagonal part of Eq. (65) should be dropped, as discussed in Sec. 3.1, and one single scalar condition is sufficient (all other matrix components would be redundant)

$$\begin{aligned} & \sum_i \left[\bar{\Sigma}_{xc}^{(11)}(\mathbf{n}\mathbf{k}, \omega_i) \bar{G}_s^{(11)}(\mathbf{n}\mathbf{k}, \omega_i) \bar{G}^{(12)}(\mathbf{n}\mathbf{k}, \omega_i) + \bar{\Sigma}_{xc}^{(11)}(\mathbf{n}\mathbf{k}, \omega_i) \bar{G}_s^{(12)}(\mathbf{n}\mathbf{k}, -\omega_i) \bar{G}^{(11)}(\mathbf{n}\mathbf{k}, \omega_i) \right. \\ & \quad \left. - \bar{\Sigma}_{xc}^{(21)}(\mathbf{n}\mathbf{k}, \omega_i) \bar{G}_s^{(12)}(\mathbf{n}\mathbf{k}, \omega_i) \bar{G}^{(12)}(\mathbf{n}\mathbf{k}, \omega_i) + \bar{\Sigma}_{xc}^{(21)}(\mathbf{n}\mathbf{k}, \omega_i) \bar{G}_s^{(11)}(\mathbf{n}\mathbf{k}, -\omega_i) \bar{G}^{(11)}(\mathbf{n}\mathbf{k}, \omega_i) \right] \\ & = \sum_i \left[\Delta_{xc}(\mathbf{n}\mathbf{k}) \bar{G}_s^{(11)}(\mathbf{n}\mathbf{k}, \omega_i) \bar{G}^{(11)}(\mathbf{n}\mathbf{k}, \omega_i) - \Delta_{xc}^*(\mathbf{n}\mathbf{k}) \bar{G}_s^{(12)}(\mathbf{n}\mathbf{k}, -\omega_i) \bar{G}^{(12)}(\mathbf{n}\mathbf{k}, \omega_i) \right]. \quad (68) \end{aligned}$$

This can be further simplified by the assumption that the order parameter and the gap functions are real, which is usually the case even for unconventional superconductors, leading to the following form of the connection

$$\begin{aligned} \Delta_{xc}^*(n\mathbf{k}) = \frac{1}{\Xi(n\mathbf{k})} \frac{1}{\beta} \left[\right. & \sum_i \bar{\Sigma}_{xc}^{(11)}(n\mathbf{k}, \omega_i) \bar{G}_s^{(11)}(n\mathbf{k}, +\omega_i) \bar{G}^{(12)}(n\mathbf{k}, \omega_i) \\ & + \sum_i \bar{\Sigma}_{xc}^{(11)}(n\mathbf{k}, \omega_i) \bar{G}_s^{(12)}(n\mathbf{k}, -\omega_i) \bar{G}^{(11)}(n\mathbf{k}, \omega_i) \\ & - \sum_i \bar{\Sigma}_{xc}^{(21)}(n\mathbf{k}, \omega_i) \bar{G}_s^{(12)}(n\mathbf{k}, +\omega_i) \bar{G}^{(12)}(n\mathbf{k}, \omega_i) \\ & \left. + \sum_i \bar{\Sigma}_{xc}^{(12)}(n\mathbf{k}, \omega_i) \bar{G}_s^{(11)}(n\mathbf{k}, -\omega_i) \bar{G}^{(11)}(n\mathbf{k}, \omega_i) \right], \end{aligned} \quad (69)$$

where

$$\Xi(n\mathbf{k}) = \frac{1}{\beta} \sum_i \left[\bar{G}_s^{(11)}(n\mathbf{k}, \omega_i) \bar{G}^{(11)}(n\mathbf{k}, \omega_i) - \bar{G}_s^{(12)}(n\mathbf{k}, -\omega_i) \bar{G}^{(12)}(n\mathbf{k}, \omega_i) \right]. \quad (70)$$

Equation (69) above is the Sham-Schlüter connection for SCDFT as derived by Marques [18]. For *any* given many body self energy it returns the anomalous Kohn-Sham potential of SCDFT (Δ_{xc}) that, by construction, leads to the same anomalous density of the interacting system described by that self energy (in this work always assumed in the Eliashberg approximation).

Note that the equation has to be seen as a self-consistent equation for Δ_{xc} because it also enters the right hand side in the definition of \bar{G}_s (see Eq. (66)–(67)), this equation is equivalent to Eq. (41), the gap equation of SCDFT, and its right hand side is therefore the functional derivative of F_{xc} with respect to the anomalous density. At the present stage it is not, however, an explicit function but expressed numerically in terms of Matsubara frequencies as it depends on $\bar{\Sigma}$ and is not useful for material studies. On the other hand it is a perfect tool to get more insights on the properties of the SCDFT Kohn-Sham system. This will be the topic of the next section where the Sham-Schlüter connection will be analyzed numerically for a model system.

3.3 Analysis of a model

In this section Eliashberg equations and Sham-Schlüter connection will be solved numerically for a simple system of electrons interacting only via an isotropic (momentum independent) electron-phonon coupling provided by a single Einstein phonon mode.

$$g_{m\mathbf{k}+\mathbf{q},n\mathbf{k}}^v = \sqrt{\frac{\lambda\omega_{ph}}{N_F}}, \quad (71)$$

where N_F is the density of states at the Fermi level, ω_{ph} is the energy of the Einstein mode and λ is the BCS-like electron-phonon coupling. For this example it will be assumed that $\lambda = 1$ and $\omega_{ph} = 60 \text{ meV}$. It is also assumed that the density of non-interacting states is constant

$$N(\xi) = \sum_{n,\mathbf{k}} \delta(\xi - \xi_{n\mathbf{k}}) = N_F. \quad (72)$$

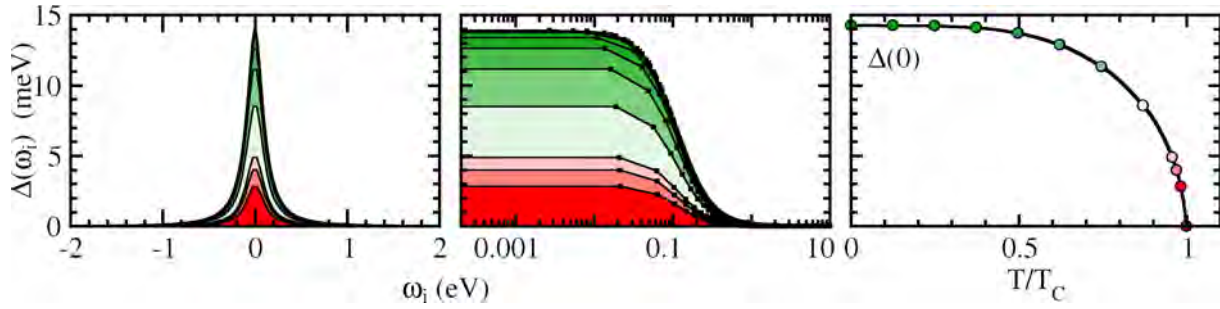


Fig. 2: Exact anomalous potential $\Delta(\xi)$ corresponding to the Eliashberg approximation to the self energy computed for a model pairing interaction. Colors encode the temperature as indicated in the right-most panel.

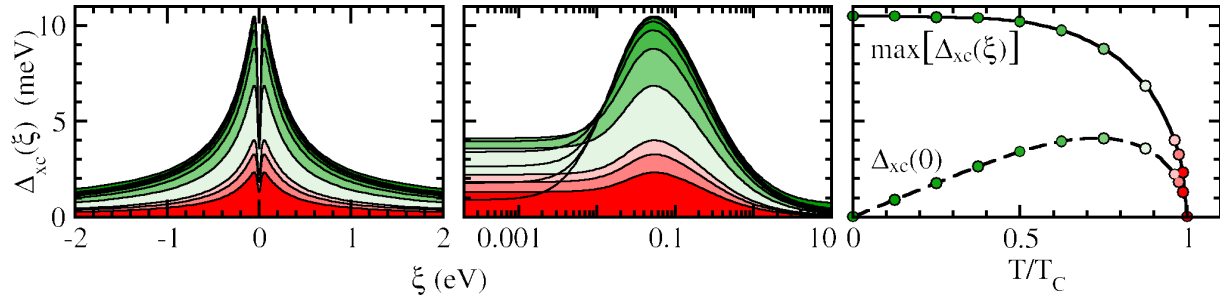


Fig. 3: Exact Kohn-Sham anomalous potential $\Delta_{xc}(\xi)$ corresponding to the Eliashberg approximation to the self energy computed for a model pairing interaction.

This model is completely isotropic meaning that Green functions and potentials will lose their dependence on $n\mathbf{k}$ and will only depend on $\xi_{n\mathbf{k}}$ the non interacting Kohn-Sham eigenenergy. Via Eq. (58) the coupling defined above enters the Sham-Schlüter connection (69) that can be solved numerically.⁹

The critical temperature T_C of the model is 80 K. The interacting Green function (see Eq. (61)) is uniquely defined by the two functions $\Delta(n\mathbf{k}, \omega_i)$ and $Z(n\mathbf{k}, \omega_i)$, while in this particle hole symmetric model χ is zero. Furthermore, since the pairing in Eq. (71) is just a constant, Z and Δ do not depend on $\xi_{n\mathbf{k}}$ either but only on ω_i .

The superconducting gap $\Delta(n\mathbf{k}, \omega_i)$ is plotted in Fig. 2 as a function of the Matsubara frequency ω_i and temperature. This function decreases monotonically with $|\omega_i|$ a fact that is directly linked with the experimental evidence that the superconducting gap has its maximum close to the Fermi level. Together with T_C the gap at the Fermi level ($\Delta(\xi = 0, \omega = 0)$) is the most important property of a superconductor because it is connected with the superconductor excitation spectrum and therefore with its unique response properties. The temperature dependence of Δ is shown in the right panel of Fig. 2 and has a standard BCS-like behavior.

In conventional DFT we are used to assume that the single particle spectrum of the Kohn-Sham system is quite similar to the interacting one and only in some pathological cases, like strongly correlated materials, the differences are really large. However, in SCDFT the properties of Δ_{xc}

⁹One can either proceed in two steps solving first the Dyson-Eliashberg equation (60) and then insert the resulting components of $\bar{\Sigma}$ and \bar{G} into Eq. (69) that is eventually solved for Δ_{xc} . Alternatively, one can also directly solve Eq. (69) self consistently until convergence is achieved both for $\bar{\Sigma}$, \bar{G} , and \bar{G}_s .

are quite different from those of Δ although formally Δ_{xc} also plays the role of a superconducting gap for the SCDFT Kohn-Sham system. Like Δ , Δ_{xc} shows a sharp feature at low energy. The width of this peak is broader but one should consider that the energy width on the imaginary axis is not quite the same as on the physical axis. Moreover, and this is the most important aspect, the Kohn-Sham gap has a dip close to the Fermi energy, showing a non-monotonic behavior in energy. The dip is lower at low temperature so that in the zero temperature limit the superconducting gap at the Fermi level is actually zero. A completely unphysical property. Not a conceptual problem as such, but just a reminder of the limitations of the Kohn-Sham system: the excitation spectrum of the superconducting Kohn-Sham system is not like that of the real interacting superconductor. The correct way to obtain the superconducting gap (or any other observable apart from density and total energy) in SCDFT is by constructing the functional of the densities for that observable. In this case the gap functional $\Delta[\rho, \chi, \Gamma]$. This was done for SCDFT [33, 34] but its construction would go beyond the goals of this lecture.

3.4 A simple SCDFT functional

As proved by Marques [18], the Sham-Schlüter connection can be used to derive a valid SCDFT functional (LM2005 [11, 12]). The main conceptual step is that G and G_s , while in general quite different, are connected by the sum rules (66) and (67) and it is likely not completely inaccurate to perform the substitution $G \rightarrow G_s$ into the Sham-Schlüter connection, both on explicit occurrences and on those coming from the G dependence of the self energy $\bar{\Sigma}_{xc}$ in Eq. (57). In this way the Sham-Schlüter connection becomes a closed equation in Δ_{xc} , i.e., an approximation for the SCDFT gap equation (41). In other word the substitution leads directly to an explicit expression for F_{xc} (or rather its functional derivative Δ_{xc}). The predictive power of such a simple functional was then improved by a set of procedures the details of which can be found in the original works [11, 12]. From a perturbative point of view this procedure is equivalent to choosing a many body self energy in first order (like in Eq. (56)) not in the non-interacting Green function \bar{G}_0 but in the SCDFT Kohn-Sham ones \bar{G}_s .

It is extremely important to observe that upon this transformation of Eq. (69) all the Matsubara summations can be carried out analytically. From this comes one of the main computational advantages of the SCDFT scheme: it does not involve numerical Matsubara integrations. The explicit form of Δ_{xc} reads

$$\Delta_{xc}(nk) = \mathcal{Z}(nk)\Delta_{xc}(nk) + \frac{1}{2} \sum_{n'k'} \mathcal{K}(nk, n'k') \frac{\tanh\left(\frac{\beta}{2} E_{n'k'}\right)}{E_{n'k'}} \Delta_{xc}(n'k'), \quad (73)$$

where the two kernels \mathcal{K} and \mathcal{Z} are

$$\mathcal{Z}(nk) = \sum_{n'k'} \sum_{\nu} |g_{mk+q, nk}^{\nu}|^2 [I'(\xi_{nk}, \xi_{n'k'}, \omega_{q\nu}) + I'(\xi_{nk}, -\xi_{n'k'}, \omega_{q\nu})] \quad (74)$$

$$\mathcal{K}(nk, n'k') = W(nk, n'k') - \frac{\sum_{\nu} |g_{n'k+q, nk}^{\nu}|^2 [I(\xi_{nk}, \xi_{n'k'}, \omega) - I(\xi_{nk}, -\xi_{n'k'}, \omega)]}{\tanh\left(\frac{\beta}{2} \xi_{nk}\right) \tanh\left(\frac{\beta}{2} \xi_{n'k'}\right)}, \quad (75)$$

with $k' \equiv k + q$, and where

$$\begin{aligned}
 I'(\xi, \xi', \omega) &= \frac{d}{d\xi} I(\xi, \xi', \omega) \\
 I(\xi, \xi', \omega) &= J(\xi, \xi', \omega) - J(\xi, \xi', -\omega) \\
 J(\xi, \xi', \omega) &= [f_\beta(\xi) + b_\beta(\omega)] \frac{f_\beta(\xi') - f_\beta(\xi - \omega)}{\xi - \xi' - \omega}
 \end{aligned} \tag{76}$$

f_β and b_β being Fermi and Bose functions. In Eq. (75) the screened Coulomb interaction W is assumed to be static. More recent extensions to this functional have included dynamical effects as well [35]. Also this LM2005 functional is not particularly accurate in describing the effect of the electron-phonon coupling, overestimating it at strong coupling and underestimating it in the weak coupling limit, presently more accurate functionals exist [33]. However this functional has the advantage of providing a gap function that does not feature the dip at the Fermi level discussed in the previous section; instead Δ_{xc} at the Fermi level is by experience quite close to the physical superconducting gap.

It should be noted that Eq. (73) has the form of a BCS gap equation, however unlike the BCS equation that relies on a model, this equation is derived from first principles and the kernels are not adjustable parameters but functionals of the densities. This functional dependence is implicit via a dependence on the Kohn-Sham orbitals and their matrix elements.

4 Example: Superconductivity of a doped carbon-hydrogen nanotube

There is a relatively large literature presenting applications of SCDFT using different approximations and functionals. Ranging from the study of classic superconductors [12, 36], strongly anisotropic systems [37–40], at high pressure [41, 34, 42], or investigations of different pairing mechanisms [43, 44, 35, 45], to cite only a few.

As discussed in the first part of this lecture, an SCDFT investigation starts from the characterization of the normal state. The normal state information is then used to construct the exchange correlation potential, or rather the kernels of the SCDFT gap equations (73). From the solution of the gap equation it is then possible to extract a broad variety of observables and properties of the superconductor.

To briefly exemplify this procedure it will be applied here to a realistic system, a crystal of hole doped, hydrogenated, carbon nanotubes. The structure is shown in the center of Fig. 4. Similar to graphane [46], it will be shown that this system also has a strong electron-phonon coupling and that it features nicely inhomogeneous superconducting properties. The possibility of its experimental synthesis however are not discussed here as neither the thermodynamic stability nor the effect of zero point motion nor the physical doping mechanism will be addressed.

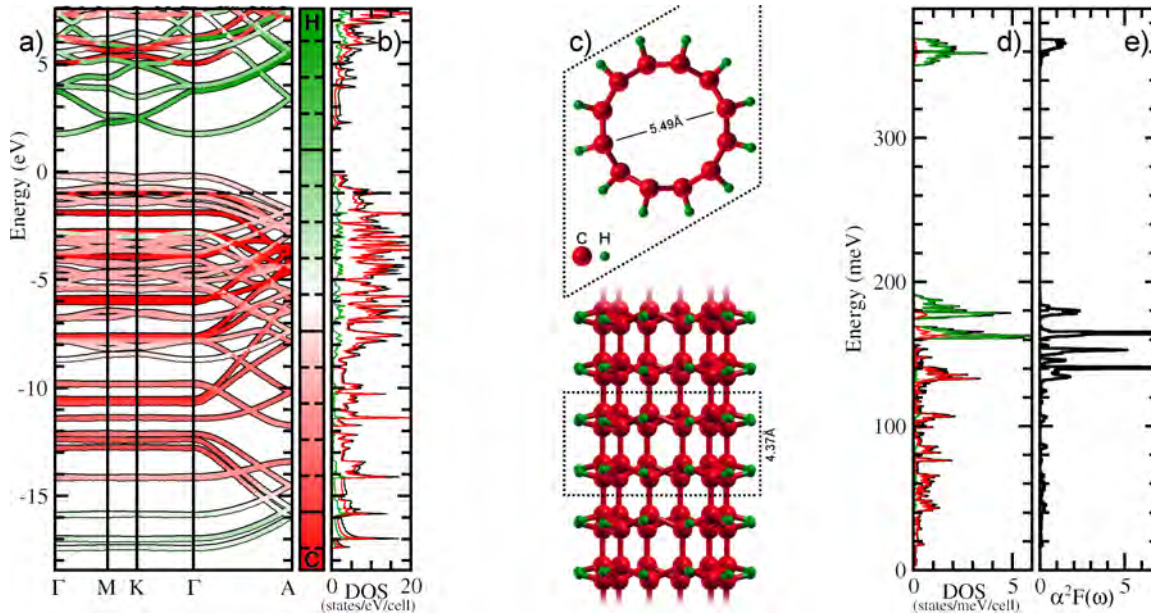


Fig. 4: Left: Electronic bands (a) and density states (DOS - b) of an hydrogenated carbon nanotube. The colorscale in the band plot gives the atomic projection of the Kohn-Sham states on atomic orbitals, from red (100% C) to green (65% H). The Fermi level of the undoped crystal is at zero. A dashed line shows the position of the Fermi level used for the simulation, corresponding to hole doping. Center (c): views of the nanotube structure, the dashed line indicates the periodic unit cell of the crystal. Right: phonon density of states (d - also decomposed in H and C components) and $\alpha^2F(\omega)$ function (e). The latter is an average of the electron-phonon matrix elements (34) on the Fermi surface of the system (Eq. (77)).

4.1 Normal state properties

The first step to apply SCDFT is to compute the normal state properties of the system: its Kohn-Sham eigenvalues and eigenstates, phonons, electron-phonon, and electron-electron coupling. From the band structure plot in Fig. 4 one can see that the undoped system is an insulator. A metallic state, a necessary precondition to superconductivity, could be realized, for example, by introducing boron substitutional impurities at the carbon sites, however here the doping will be simply induced by a rigid shift of the Fermi level (see Fig. 4a). While this over-simplified approach will neglect important effects as Kohn anomalies [47], it is still expected to provide a reasonable estimate of the superconducting coupling [46].

The phononic density of states is characterized by an high energy peak (350 meV) due to C-H bond stretching modes, a mid-energy region of hydrogen rocking modes, and a low energy part (below 150 meV) of C modes. The high-end of these carbon modes (C-C bond stretching) is the most relevant for the electron-phonon coupling, as shown by the $\alpha^2F(\omega)$ function

$$\alpha^2F(\omega) = \frac{1}{N_F} \sum_{nkn'k'} \sum_{\nu} |g_{nk,n'k'}^{\nu}|^2 \delta(\xi_{nk}) \delta(\xi_{n'k'}) \delta(\omega - \omega_{q\nu}) \quad (77)$$

with $k' \equiv k + q$.

Electronic states and phonon matrix elements are computed on a regular grid in momentum space, the size of which is set by convergence criteria and limited by the computational cost.

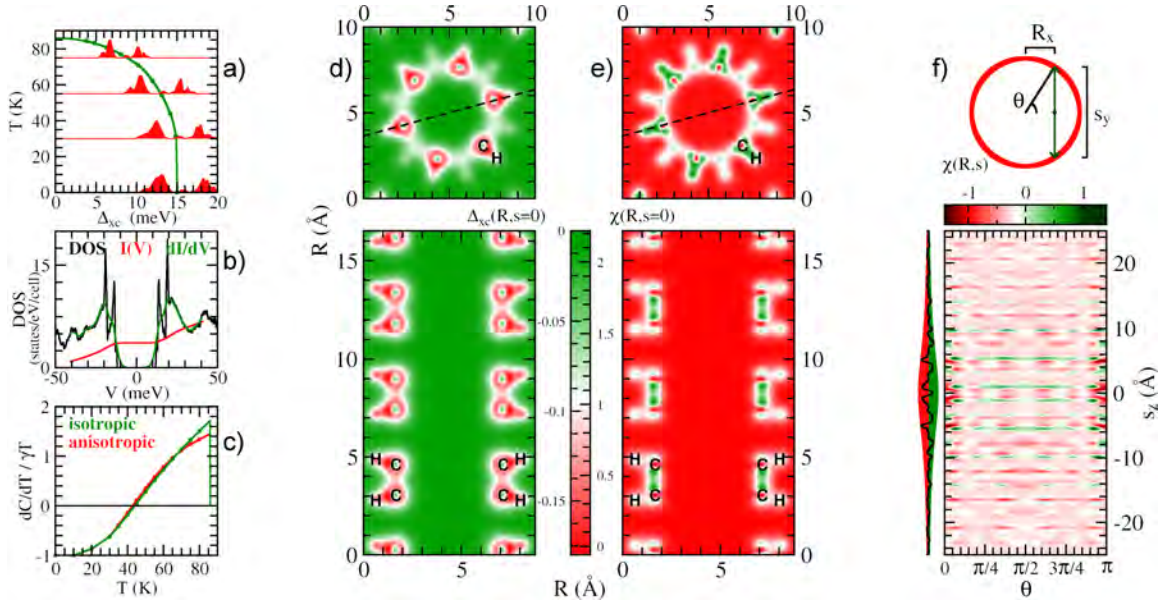


Fig. 5: *Left a):* Temperature dependence of the average Kohn-Sham superconducting gap (green line) and its distribution function $P(\Delta)$ (red - arbitrary vertical scale). *b)* Density of states (black), tunneling current (red - shifted upward, arbitrary units) and differential conductance (green) as computed from Eq. (79). *c)* Difference of specific heat in the normal and superconducting state as a function of temperature in isotropic and anisotropic approximation. *Center:* real space anomalous potential $\Delta(\mathbf{R}, s)$ and order parameter $\chi(\mathbf{R}, s)$ as a function of the Cooper pair center of mass \mathbf{R} . *Top:* xy cut of the tube, *bottom:* vertical cut of the tube. *Right f):* the order parameter as a function of the electronic distance across the tube surface (on the C layer). s_z refers to the vertical distance on the tube and θ gives the position of the two electrons on the xy plane as shown by the cartoon above the plot. The curve at the left of this plot is the $(\mathbf{R} = 0, s_z)$ cut highlighting the oscillatory behavior and its envelope function.

However Eq. (73) requires a very accurate sampling especially of the states close to the Fermi level, because the kernels (74) are sharply peaked around $\xi = 0$. Therefore, an accurate interpolation scheme is necessary. As described in Ref [12] a convenient approach is to use a large set of random \mathbf{k} -points accumulated around the Fermi level and appropriately weighted. The properties of the corresponding states are then obtained by interpolation from calculations on regular grids: here a $10 \times 10 \times 20$ grid is used for the electronic states, a $2 \times 2 \times 10$ for the convergence of the potential- and \mathbf{k} -grids and a $1 \times 1 \times 2$ for the \mathbf{q} grid. Calculations were done within the norm-conserving pseudopotential approximation [48, 25]. Coulomb matrix elements were computed with the Sham-Kohn approach [49], as described in Ref. [12].

4.2 Solution of the gap equation and superconducting properties

Solving the SCDFT gap equation (73) using the LM2005 functional gives a critical temperature of 86 K. Fig. 5a) gives the temperature dependence of the average gap on the Fermi surface (average of $\Delta_{xc}(\xi = 0)$) as well as its distribution function

$$P(\Delta) = \frac{1}{N_F} \sum_{nk} \delta(\Delta - \Delta_{xc}(nk)) \delta(\xi_{nk}) \quad (78)$$

showing that the Kohn-Sham gap is distributed on two peaks that at $T = 0$ are centered at about 12.8 and 18.5 meV. The larger gap corresponding to one band with higher C projection (easily recognizable in Fig. 4) as a consequence of the fact that C modes have a stronger coupling than H modes. This predicted multigap behavior is usually observable experimentally in different ways [39, 50]. Tunneling spectroscopy, for example, probes rather directly the excitation spectrum: a tunneling current can be modeled as the convolution of the DOS of the superconductor with that of the tip. In the simplest approximation [51]

$$I(V) \sim \sum_{nk} \left[f_{\beta}(\xi_{nk}) - f_{\beta}(\xi_{nk} + V) \right] N_s(\xi_{nk} + V) \quad (79)$$

where N_s is the DOS in the superconducting state. It shown in Fig. 5b), where the current is computed for $T=10$ K.

Although indirectly, thermodynamic measurements also give information about the gap distribution function. This can be observed in the temperature dependence of the entropy or, more conveniently, of the difference in specific heat

$$\Delta C = C - C_N = \frac{1}{T} \frac{d}{dT} (S - S_N), \quad (80)$$

where the electronic entropy is

$$S = -2k_B \sum_{nk} \left\{ \left[1 - f_{\beta}(E_{nk}) \right] \ln \left(1 - f_{\beta}(E_{nk}) \right) + f_{\beta}(E_{nk}) \ln \left(f_{\beta}(E_{nk}) \right) \right\} \quad (81)$$

k_B being the Boltzmann constant. S_N is the corresponding quantity for the normal state ($\Delta_{xc} = 0$). ΔC is shown in Fig. 5c), both for a completely anisotropic calculation and for an isotropic one. In the anisotropic case ΔC tends to saturate towards T_C .

A more fundamental property that can be extracted from the solution of Eq. (73) is the Kohn-Sham potential Δ_{xc} and especially χ , the superconducting order parameter (40), that is the central object of theoretical superconductivity. These functions are discussed extensively in Ref. [38] and are the most rigorous representation of the concept of a Cooper pair. Instead of the $(\mathbf{r}, \mathbf{r}')$ dependence they are best plotted as a function of $\mathbf{R} = \frac{\mathbf{r} + \mathbf{r}'}{2}$ and relative distance $\mathbf{s} = \mathbf{r} - \mathbf{r}'$ as these can be interpreted as center of mass coordinate and electron-electron distance of the pair. The behavior of these functions is shown in the right side of Fig. 5. As discussed in Ref. [38] the \mathbf{R} dependence of Δ_{xc} tends to highlight those regions in space most involved in the Coulomb renormalization, in this case clearly the C–H bonding region. On the other hand χ is larger where the phonon coupling is stronger, in the present case mainly involving the covalent C–C bond of the tube surface.

As a function of \mathbf{s} these function show a typical oscillatory behavior. The envelope of the function has a maximum at $\mathbf{s} = 0$ and slowly decreases on the scale of the superconductor's coherence length. Fig. 5f) shows χ for two electrons located on the surface of the carbon tube, the oscillatory behavior is clearly visible as a function of \mathbf{s}_z , for vertical separation between the two electrons.

5 Summary and conclusion

Superconducting Density Functional Theory was reviewed to focus on its relation to conventional Eliashberg many body theory. Starting from the formal construction of the two theoretical frameworks, a connection was set-up using the Sham-Schlüter method. This connection is used to extract information on exact features of the Kohn-Sham system that reproduces the superconducting density in the Eliashberg approximation and to develop a simple functional for SCDFT. The methodology was then applied to the study of a realistic system: a hole doped hydrogenated carbon nanotube, that proves to be a strong superconductor with a critical temperature above 80 K. While this is the single most important number that characterizes the superconductivity, there are many other properties that can be extracted from SCDFT at an affordable computational cost. In fact the theory gives access to a rich variety of observables as momentum and position dependent properties like the gap distribution function or the local order parameter.

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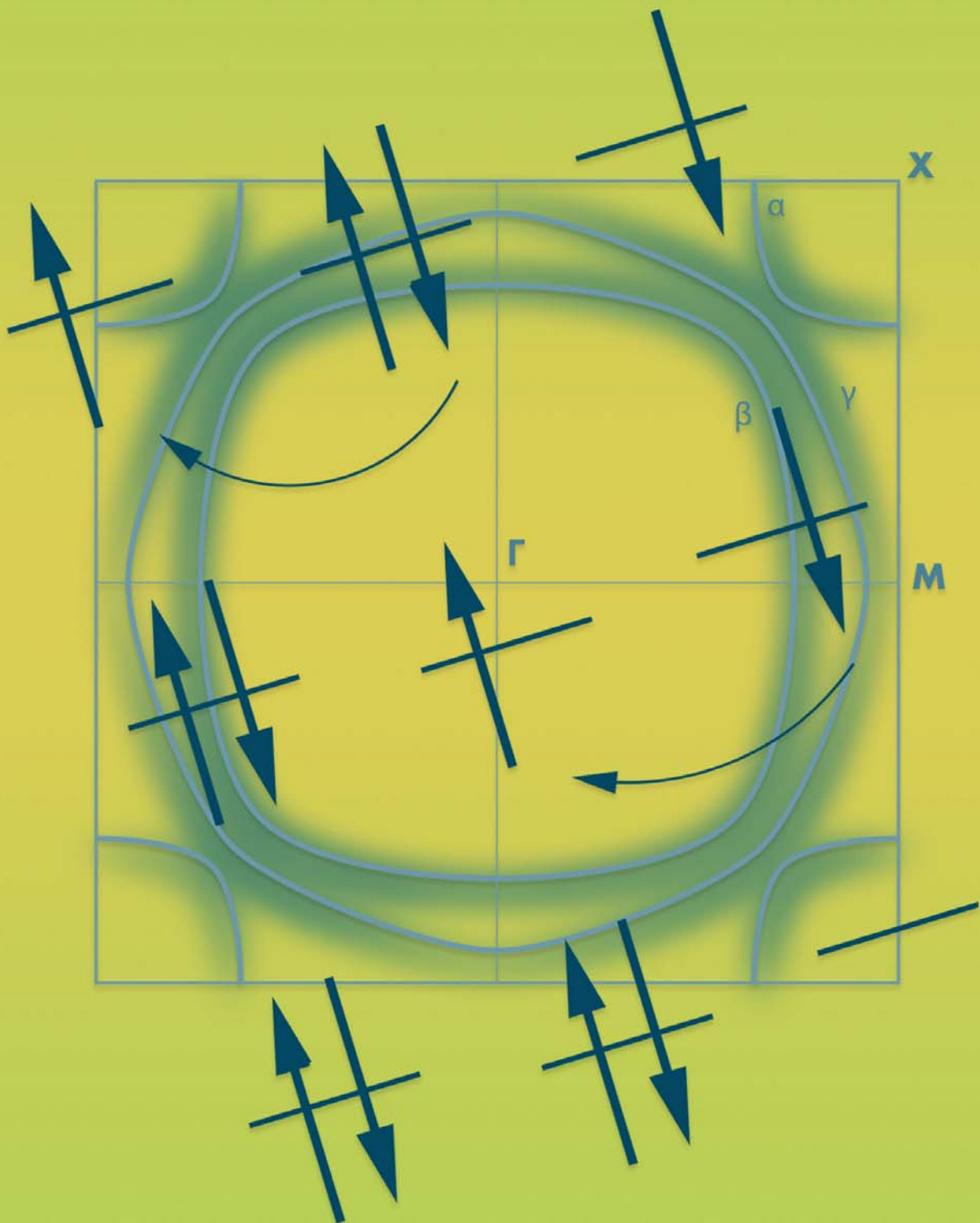
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