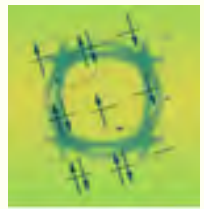
Introduction to SuperConducting DFT

Antonio Sanna

Max Planck Institute of Microstructure Physics

Halle (Germany)



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goals, Hamiltonian and order parameter

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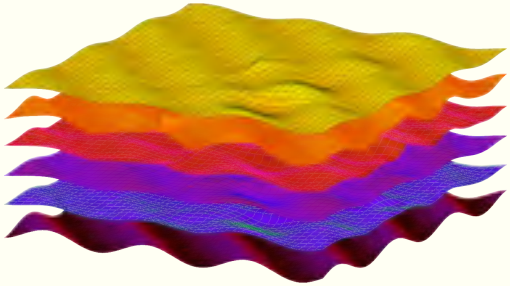
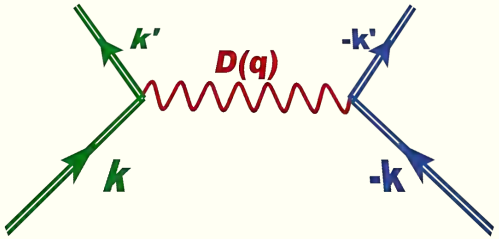
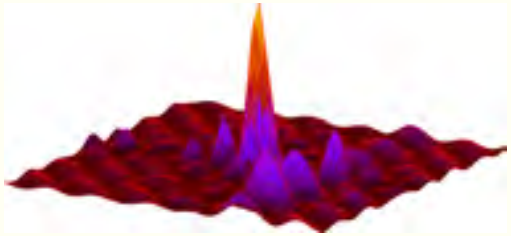
Theories of Superconductivity



$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4, ...)$



$\bar{G}(\mathbf{r}_1, \mathbf{r}_2, \omega)$

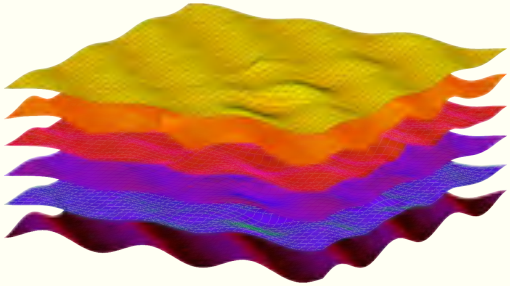


$\rho(\mathbf{r}_1)$, $\chi(\mathbf{r}_1, \mathbf{r}_2)$

MODELS (BCS)

- Analytic or numerically trivial
- Full solution of the model: you get the wavefunction
- (relatively) Easy to get a physical understanding
- Oversimplification of reality
- No quantitative predictions are possible

Theories of Superconductivity



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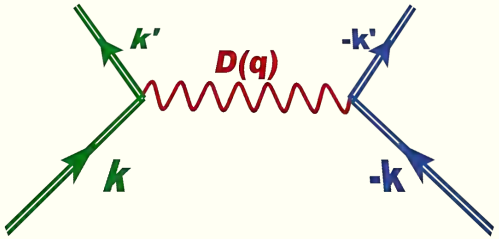

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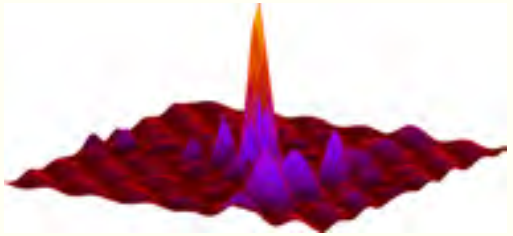
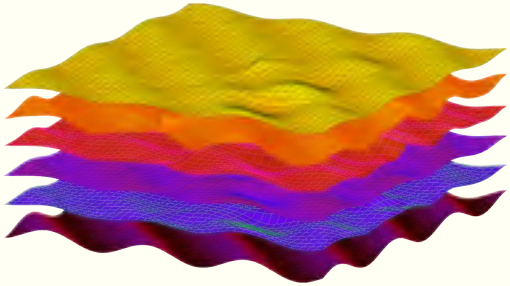


$\rho(\mathbf{r}_1)$, $\chi(\mathbf{r}_1, \mathbf{r}_2)$

Green's Function Methods (Eliashberg)

- Computationally intensive
- Physical interpretation neither too easy nor too difficult
- Powerful and arbitrarily accurate (if you can afford it)
- (if you are good) You get whatever your favorite experimentalist can measure

Theories of Superconductivity



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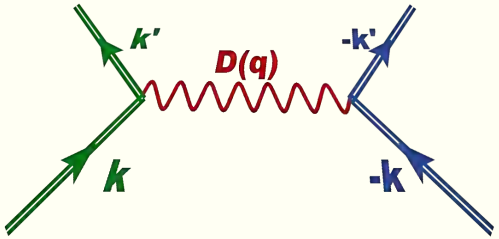

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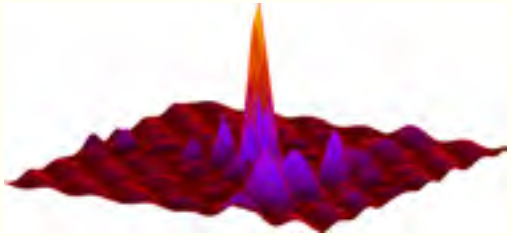


$\rho(\mathbf{r}_1)$, $\chi(\mathbf{r}_1, \mathbf{r}_2)$

(SC) DFT

- Computationally cheap
- You need functionals; functional are hard to derive
- Physical interpretation not straightforward
- Powerful and (as) accurate (as your functionals)

Hamiltonian (Sec 2.1)

$$
\begin{aligned}
H &= H_e + H_{en} + H_n + H_{ext} \\
H_e &= \sum_\sigma \int d\boldsymbol{r} \psi_\sigma^\dagger(\boldsymbol{r}) \left[-\frac{1}{2}\nabla^2 - \mu \right] \psi_\sigma(\boldsymbol{r}) \\
&+ \frac{1}{2} \sum_{\sigma\sigma'} \int d\boldsymbol{r} d\boldsymbol{r}' \psi_\sigma^\dagger(\boldsymbol{r}) \psi_{\sigma'}^\dagger(\boldsymbol{r}') \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|} \psi_{\sigma'}(\boldsymbol{r}') \psi_\sigma(\boldsymbol{r}) \\
H_n &= -\int d\boldsymbol{R} \Phi^\dagger(\boldsymbol{R}) \frac{\nabla^2}{2M} \Phi(\boldsymbol{R}) \\
&+ \frac{1}{2} \int d\boldsymbol{R} d\boldsymbol{R}' \Phi^\dagger(\boldsymbol{R}) \Phi^\dagger(\boldsymbol{R}') \frac{Z^2}{|\boldsymbol{R} - \boldsymbol{R}'|} \Phi(\boldsymbol{R}') \Phi(\boldsymbol{R}) \\
H_{en} &= -\sum_\sigma \int d\boldsymbol{R} d\boldsymbol{r} \psi_\sigma^\dagger(\boldsymbol{r}) \Phi^\dagger(\boldsymbol{R}) \frac{Z}{|\boldsymbol{R} - \boldsymbol{r}|} \Phi(\boldsymbol{R}) \psi_\sigma(\boldsymbol{r}) \\
H_{\Delta_{ext}} &= \int d\boldsymbol{r} d\boldsymbol{r}' \Delta_{ext}^*(\boldsymbol{r}, \boldsymbol{r}') \psi_\uparrow(\boldsymbol{r}) \psi_\downarrow(\boldsymbol{r}') + h.c.
\end{aligned}
$$

SC order parameter

One can define a superconducting density or order parameter as:

$$\chi(r, r') := \left\langle GS \left| \hat{\psi}_\uparrow(r)\hat{\psi}_\downarrow(r') \right| GS \right\rangle$$

we can test it on the BCS wavefunction:

$$|GS\rangle \to |BCS\rangle = \prod_k \left(u_k + v_k a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} \right) |0\rangle$$

and after a good half of an hour of commutators

$$\begin{aligned}
\chi(r, r') &:= \left\langle BCS \left| \hat{\psi}_\uparrow(r)\hat{\psi}_\downarrow(r') \right| BCS \right\rangle \\
&= -\sum_k \phi_{k\uparrow}(r)\phi_{-k\downarrow}(r') \left[\left(|u_k|^2 + |v_k|^2 \right) u_k^* v_k \right] \\
&= -\sum_k \phi_{k\uparrow}(r)\phi_{-k\downarrow}(r') \frac{\Delta_k}{2E_k}
\end{aligned}$$

OGK/HK Theorem (Sec 2.2)

Oliveira-Gross-Kohn theorem $\equiv$ Hohenberg-Kohn theorem for SCDFT

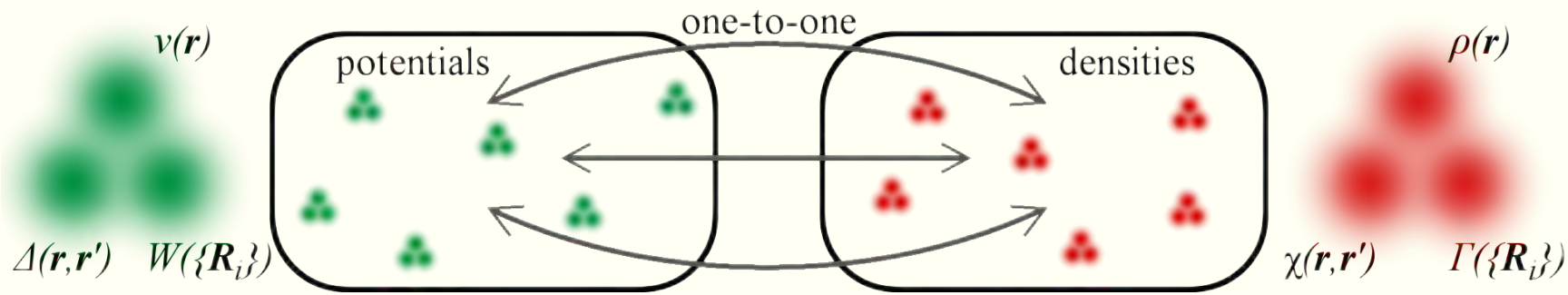
Modern SCDFT is based on the three densities:

$$\begin{aligned}
\rho(\boldsymbol{r}) &= \mathrm{Tr}\left[\varrho_0 \sum_\sigma \psi_\sigma^\dagger(\boldsymbol{r})\,\psi_\sigma(\boldsymbol{r})\right] \\
\chi(\boldsymbol{r},\boldsymbol{r}') &= \mathrm{Tr}\left[\varrho_0\,\psi_\uparrow(\boldsymbol{r})\,\psi_\downarrow(\boldsymbol{r}')\right] \\
\Gamma(\{\boldsymbol{R}_i\}) &= \mathrm{Tr}\left[\varrho_0 \prod_j \Phi^\dagger(\boldsymbol{R}_j)\,\Phi(\boldsymbol{R}_j)\right]
\end{aligned}$$

at finite temperature.
ϱ_0 is the grand canonical density matrix:

$$\varrho_0 = \frac{e^{-\beta(H-\mu N)}}{\mathrm{Tr}\left[e^{\beta(H-\mu N)}\right]},$$

OGK/HK Theorem (Sec 2.2)

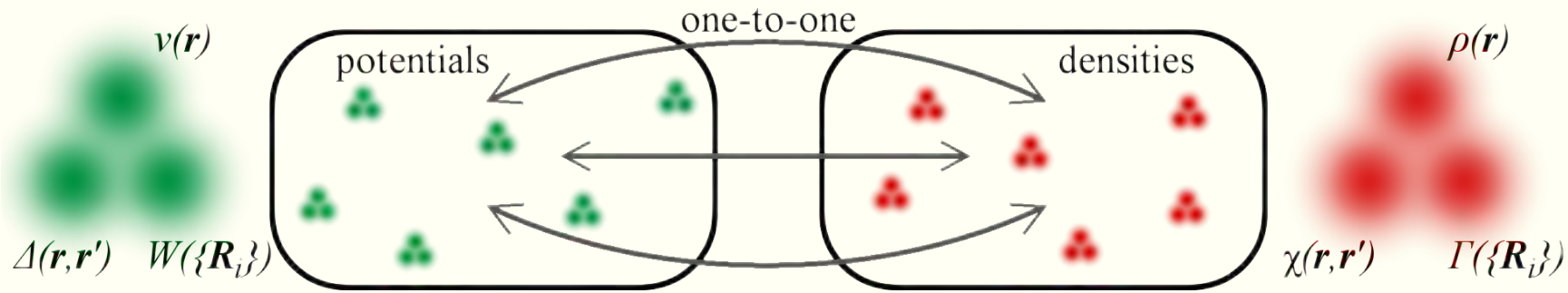


1. There is a one-to-one mapping between the set of densities $\rho(\boldsymbol{r})$, $\chi(\boldsymbol{r},\boldsymbol{r}')$, $\Gamma(\{\boldsymbol{R}_i\})$ onto the set f external potentials $v_{ext}(\boldsymbol{r})$, $\Delta_{ext}(\boldsymbol{r},\boldsymbol{r}')$, $W_{ext}(\{\boldsymbol{R}_i\})$
2.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

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

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

OGK/HK Theorem (Sec 2.2)



$\Omega[\rho, \chi, \Gamma]$ can be written as:

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

where $F[\rho, \chi, \Gamma]$ is a universal (material independent) functional.

Kohn-Sham System (Sec 2.3)

We introduce a **non interacting** system:

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

constructed to have the same density of the interacting one:

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

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

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constructed to have the same density of the interacting one:

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

Kohn-Sham Equations (Sec 2.3)

Ionic equation:

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

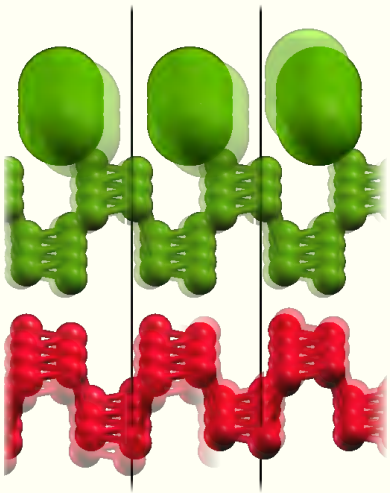
Electronic equations:

$$\begin{aligned}
\left[-\frac{\nabla^2}{2} + v_s(\boldsymbol{r}) - \mu\right] u_i(\boldsymbol{r}) + \int \Delta_s(\boldsymbol{r}, \boldsymbol{r}')\, v_i(\boldsymbol{r}')\, d\boldsymbol{r}' &= E_i u_i(\boldsymbol{r}) \\
-\left[-\frac{\nabla^2}{2} + v_s(\boldsymbol{r}) - \mu\right] v_i(\boldsymbol{r}) + \int \Delta_s^*(\boldsymbol{r}, \boldsymbol{r}')\, u_i(\boldsymbol{r}')\, d\boldsymbol{r}' &= E_i v_i(\boldsymbol{r})
\end{aligned}$$

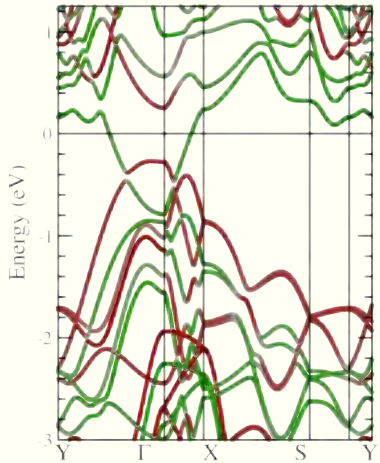
Decoupling Approximation (Sec 2.4)

I Decouple electrons from ions separating static and dynamic part of the interaction, including the latter in a perturbative fashion.

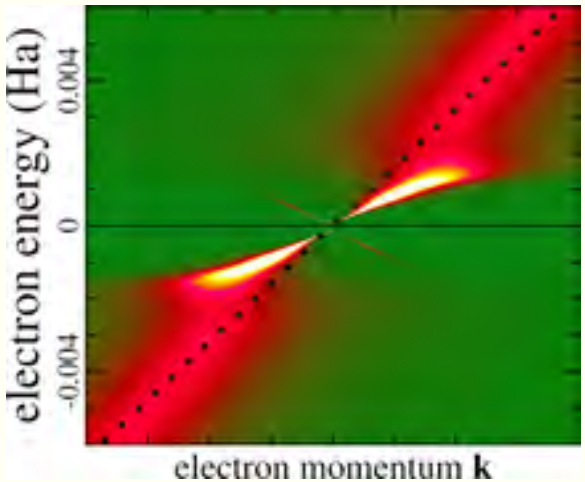
II Decouple the high energy chemical scale (responsible for bonding) from low energy pairing interactions (responsible for superconductivity).



phonons



chemistry



superconductivity

Phonons and el-ph (Sec 2.4.1)

The electron-lattice interaction in H is simplified to:

$$\begin{aligned}\tilde{H}_{e-ph} &= \sum_{mn\sigma}\sum_{\nu \boldsymbol{k}\boldsymbol{q}} g^{\nu}_{m\boldsymbol{k}+\boldsymbol{q},n\boldsymbol{k}} \sum_{\sigma} \psi^{\dagger}_{\sigma m\boldsymbol{k}+\boldsymbol{q}} \psi_{\sigma n\boldsymbol{k}} b_{\nu\boldsymbol{q}} \\ &= \sum_{\nu\boldsymbol{q}} \sqrt{\frac{\hbar}{2\omega_{\boldsymbol{q}\nu}}} \int d\boldsymbol{r} \Delta V^{\boldsymbol{q}\nu}_{scf}(\boldsymbol{r}) \psi^{\dagger}_{\sigma}(\boldsymbol{r}) \psi_{\sigma}(\boldsymbol{r}) b_{\nu\boldsymbol{q}}\end{aligned}$$

the coupling comes **from the Kohn Sham system of conventional DFT**:

$$g^{\nu}_{m\boldsymbol{k}+\boldsymbol{q},n\boldsymbol{k}} = \sqrt{\frac{\hbar}{2\omega_{\boldsymbol{q}\nu}}} \left\langle \varphi_{m\boldsymbol{k}+\boldsymbol{q}} \left| \Delta V^{\boldsymbol{q}\nu}_{scf} \right| \varphi_{n\boldsymbol{k}} \right\rangle$$

Electronic decoupling (Sec 2.4.2)

Back to the electronic equations

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

they can be written in a basis set of normal state Kohn Sham orbitals:

$$u_i(\boldsymbol{r})=\sum_{n\boldsymbol{k}}u_{i,n\boldsymbol{k}}\,\varphi_{n\boldsymbol{k}}(\boldsymbol{r}) \qquad v_i(\boldsymbol{r})=\sum_{n\boldsymbol{k}}v_{i,n\boldsymbol{k}}\,\varphi_{n\boldsymbol{k}}(\boldsymbol{r})$$
$$\Delta_s(\boldsymbol{r},\boldsymbol{r}')=\sum_{nn'\boldsymbol{k}\boldsymbol{k}'}\Delta_{s,nn'\boldsymbol{k}\boldsymbol{k}'}\,\varphi_{n\boldsymbol{k}}(\boldsymbol{r})\,\varphi_{n'\boldsymbol{k}'}(\boldsymbol{r}')$$

leading to:

$$\xi_{n\boldsymbol{k}}\,u_{i,n\boldsymbol{k}}+\sum_{n'\boldsymbol{k}'}\Delta_{s,nn'\boldsymbol{k}\boldsymbol{k}'}\,v_{i,n'\boldsymbol{k}'} = E_i\,u_{i,n\boldsymbol{k}}$$
$$-\xi_{n\boldsymbol{k}}\,v_{i,n\boldsymbol{k}}+\sum_{n'\boldsymbol{k}'}\Delta^*_{s,nn'\boldsymbol{k}\boldsymbol{k}'}\,u_{i,n'\boldsymbol{k}'} = E_i\,v_{i,n\boldsymbol{k}}$$

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

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Electronic decoupling (Sec 2.4.2)

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Electronic decoupling approximation:

$$\begin{aligned} u_i(\boldsymbol{r}) \equiv u_{n\boldsymbol{k}}(\boldsymbol{r}) &= u_{n\boldsymbol{k}}\varphi_{n\boldsymbol{k}}(\boldsymbol{r}) \\ u_i(\boldsymbol{r}) \equiv v_{n\boldsymbol{k}}(\boldsymbol{r}) &= v_{n\boldsymbol{k}}\varphi_{n\boldsymbol{k}}(\boldsymbol{r}), \end{aligned}$$

that implies $\Delta_{s,nn'\boldsymbol{k}\boldsymbol{k}'} \to \delta_{n\boldsymbol{k},n'\boldsymbol{k}'}\Delta_{s,n\boldsymbol{k}}$
Meaning: Superconductivity doesn't induce either structural phase transitions nor inter-band hybridizations

And: $E_{n\boldsymbol{k}} = \pm\sqrt{\xi^2_{n\boldsymbol{k}} + |\Delta_s(n\boldsymbol{k})|^2}$,

$$\rho(\boldsymbol{r}) = \sum_{n\boldsymbol{k}} \left[1 - \frac{\xi^2_{n\boldsymbol{k}}}{|E_{n\boldsymbol{k}}|}\tanh\left(\frac{\beta|E_{n\boldsymbol{k}}|}{2}\right)\right]|\varphi_{n\boldsymbol{k}}(\boldsymbol{r})|^2$$

$$\chi(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{2}\sum_{n\boldsymbol{k}} \frac{\Delta_s(n\boldsymbol{k})}{|E_{n\boldsymbol{k}}|}\tanh\left(\frac{\beta|E_{n\boldsymbol{k}}|}{2}\right)\varphi_{n\boldsymbol{k}}(\boldsymbol{r})\,\varphi^*_{n\boldsymbol{k}}(\boldsymbol{r}')$$

Electronic decoupling (Sec 2.4.2)

$$\begin{aligned} \xi_{n\boldsymbol{k}}\, u_{i,n\boldsymbol{k}} + \sum_{n'\boldsymbol{k}'} \Delta_{s,nn'\boldsymbol{k}\boldsymbol{k}'}\, v_{i,n'\boldsymbol{k}'} &= E_i\, u_{i,n\boldsymbol{k}} \\ -\xi_{n\boldsymbol{k}}\, v_{i,n\boldsymbol{k}} + \sum_{n'\boldsymbol{k}'} \Delta^*_{s,nn'\boldsymbol{k}\boldsymbol{k}'}\, u_{i,n'\boldsymbol{k}'} &= E_i\, v_{i,n\boldsymbol{k}} \end{aligned}$$

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And: $E_{n\boldsymbol{k}} = \pm\sqrt{\xi^2_{n\boldsymbol{k}} + |\Delta_s(n\boldsymbol{k})|^2}$,

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First Summary

I Hamiltonian for electrons and nuclei

II The nuclear part is simplified with a Born Oppenheimer approximation and the electron phonon taken from the Kohn Sham system.

III Add a symmetry breaking term to induce superconductivity

IV Set up a finite temperature formalism

V Prove the OGK theorem and set up the Kohn Sham system

VI Introduce some *basic* approximations

A theoretical framework is now set. Now we need functionals

Éliashberg Theory (Sec 3.1)

To construct a functional we set up a perturbative approach:
Our Hmiltonian:

$$H \to H_e + H_{ee} + \tilde{H}_{en} + H_{ext}$$

si split into:

$$\begin{aligned} H_0 &= H_s + H_{ext} \\ H_I &= H_{ee} + \tilde{H}_{en} - H_{DC} \end{aligned}$$

where:

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

Differing from a *GW* (like) set-up for:

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

Éliashberg Theory (Sec 3.1)

Conventional diagrammatic can be restored by introducing:

$$\bar{\psi}(\boldsymbol{r}) = \begin{pmatrix} \psi_{\uparrow}(\boldsymbol{r}) \\ \psi^{\dagger}_{\downarrow}(\boldsymbol{r}) \end{pmatrix} \qquad \bar{\psi}^{\dagger}(\boldsymbol{r}) = \begin{pmatrix} \psi^{\dagger}_{\uparrow}(\boldsymbol{r}) & \psi_{\downarrow}(\boldsymbol{r}) \end{pmatrix}.$$

and *rewriting* H_0 and H_I as:

$$\begin{aligned} H_0 &= \int d\boldsymbol{r} \bar{\psi}^{\dagger}(\boldsymbol{r}) \bar{H}_0(\boldsymbol{r}, \boldsymbol{r}') \bar{\psi}(\boldsymbol{r}') \\ H_I &= \int d\boldsymbol{r} \bar{\psi}^{\dagger}(\boldsymbol{r}) \left[\sum_{\nu \boldsymbol{q}} \sqrt{\frac{\hbar}{2\omega_{\boldsymbol{q}\nu}}} \int d\boldsymbol{r} \Delta V^{\boldsymbol{q}\nu}_{scf}(\boldsymbol{r}) \bar{\sigma}_3 b_{\nu\boldsymbol{q}} - v_s(\boldsymbol{r}) \right] \bar{\psi}(\boldsymbol{r}) \\ &+ \frac{1}{2} \int d\boldsymbol{r} d\boldsymbol{r}' \left[\bar{\psi}^{\dagger}(\boldsymbol{r}) \bar{\sigma}_3 \bar{\psi}(\boldsymbol{r}) \right] \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|} \left[\bar{\psi}^{\dagger}(\boldsymbol{r}') \bar{\sigma}_3 \bar{\psi}(\boldsymbol{r}') \right]. \end{aligned}$$

formally we are back to *GW* but in terms of 2×2 matrices:

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

Éliashberg Theory (Sec 3.1)

Dyson equation:

$$\bar{G}\left(\boldsymbol{r}, \boldsymbol{r}', \omega_i\right) = \bar{G}_0\left(\boldsymbol{r}, \boldsymbol{r}', \omega_i\right) + \bar{G}_0\left(\boldsymbol{r}, \boldsymbol{r}', \omega_i\right) \bar{\Sigma}\left(\boldsymbol{r}, \boldsymbol{r}', \omega_i\right) \bar{G}\left(\boldsymbol{r}, \boldsymbol{r}', \omega_i\right)$$

Approximation: A *GW* self energy:

$$\bar{\Sigma} = \underbrace{\quad + \quad}_{\bar{\Sigma}_{xc}} - \bar{\Sigma}_{DC}$$

Sham Schlüter connection (Sec 3.2)

between SCDFT and Éliashberg

Eliashberg theory is the DFT-based Dyson equation:

$$\bar{G}\left(n\boldsymbol{k},\omega_i\right) = \bar{G}_0\left(n\boldsymbol{k},\omega_i\right) + \bar{G}_0\left(n\boldsymbol{k},\omega_i\right)\bar{\Sigma}\left(n\boldsymbol{k},\omega_i\right)\bar{G}\left(n\boldsymbol{k},\omega_i\right),$$

Now we consider an alternative, SCDFT-based, Dyson equation:

$$\bar{G}\left(n\boldsymbol{k},\omega_i\right) = \bar{G}_s\left(n\boldsymbol{k},\omega_i\right) + \bar{G}_s\left(n\boldsymbol{k},\omega_i\right)\bar{\Sigma}_s\left(n\boldsymbol{k},\omega_i\right)\bar{G}\left(n\boldsymbol{k},\omega_i\right),$$

$$\bar{\Sigma}_s = \bar{\Sigma}_{xc} - \begin{pmatrix} v_{xc}\left(n\boldsymbol{k}\right) & \Delta_{xc}\left(n\boldsymbol{k}\right) \\ \Delta_{xc}^*\left(n\boldsymbol{k}\right) & -v_{xc}\left(n\boldsymbol{k}\right) \end{pmatrix}.$$

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Sham Schlüter connection (Sec 3.2)

Both $\bar{G}$ and $\bar{G}_s$ provide the exact density of the system:

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

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

inserting this constrain in the (SCDFT)Dyson equation:

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

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\end{aligned}$$

Sham Schlüter connection (Sec 3.2)

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\begin{aligned}
\Delta^{*}_{xc}(n\boldsymbol{k}) = \frac{1}{\Xi(n\boldsymbol{k})}\Bigg[& \frac{1}{\beta}\sum_{i}\bar{\Sigma}^{(11)}_{xc}(n\boldsymbol{k},\omega_i)\,\bar{G}^{(11)}_{s}(n\boldsymbol{k},\omega_i)\,\bar{G}^{(12)}(n\boldsymbol{k},\omega_i) \\
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\end{aligned}
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$\Delta^{*}_{xc}(n\boldsymbol{k})$

Kohn Sham potential that leads to the interacting superconducting density

$\Sigma^{(IJ)}_{xc}(n\boldsymbol{k},\omega_i)$

diagrammatic irreducible self energy

$G^{(IJ)}_{s}(n\boldsymbol{k},\omega_i)$

SCDFT Kohn Sham Green's function (it depends on $\Delta^{*}_{xc}(n\boldsymbol{k})$)

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A simple model (Sec 3.3)

Pick up an Einstein phonon mode:

$$g^{\nu}_{m\boldsymbol{k}+\boldsymbol{q},n\boldsymbol{k}} = \sqrt{\frac{\lambda\omega_{ph}}{N_F}}$$

Fix a constant DOS:

$$N(\xi) = \sum_{n,\boldsymbol{k}} \delta(\xi - \xi_{n\boldsymbol{k}}) = N_F$$

... and *solve* the corresponding SCDFT Sham-Schlüter equation:

$$\Delta^{*}_{xc}(n\boldsymbol{k}) = \mathcal{S}\left[\Delta^{*}_{xc}, \bar{\Sigma}_{xc}\right]$$

A simple model (Sec 3.3)

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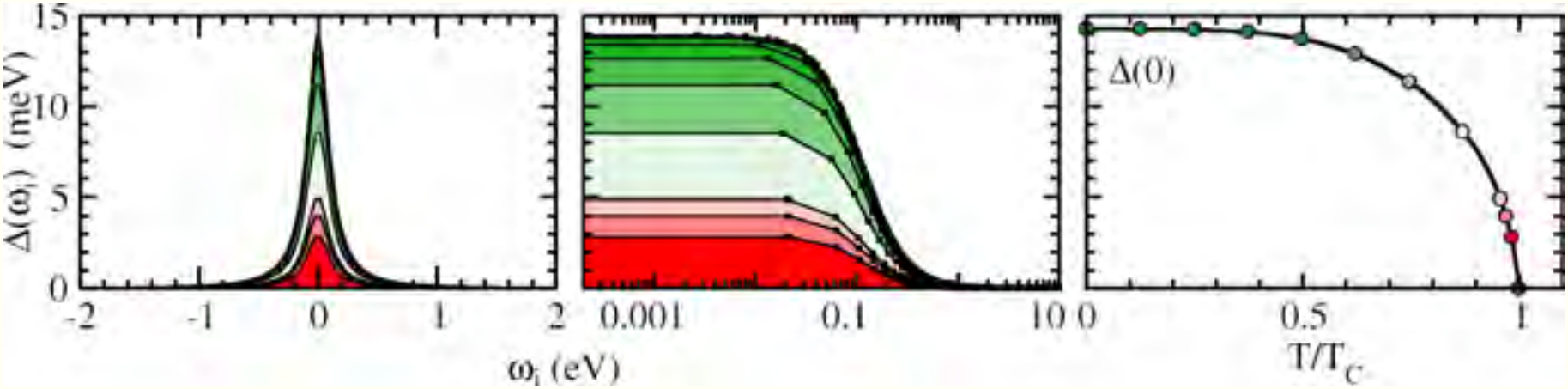
Éliashberg gap:



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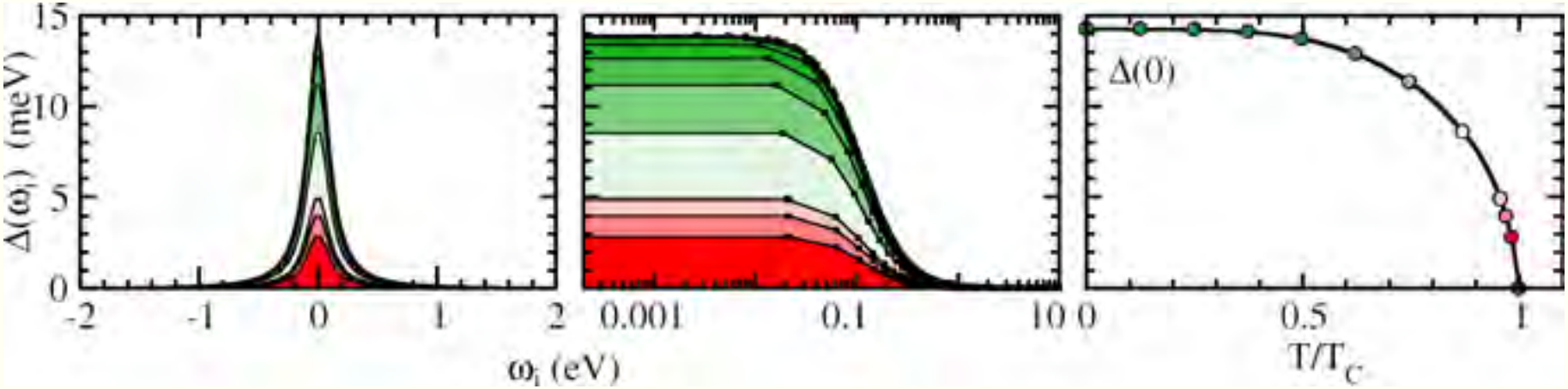
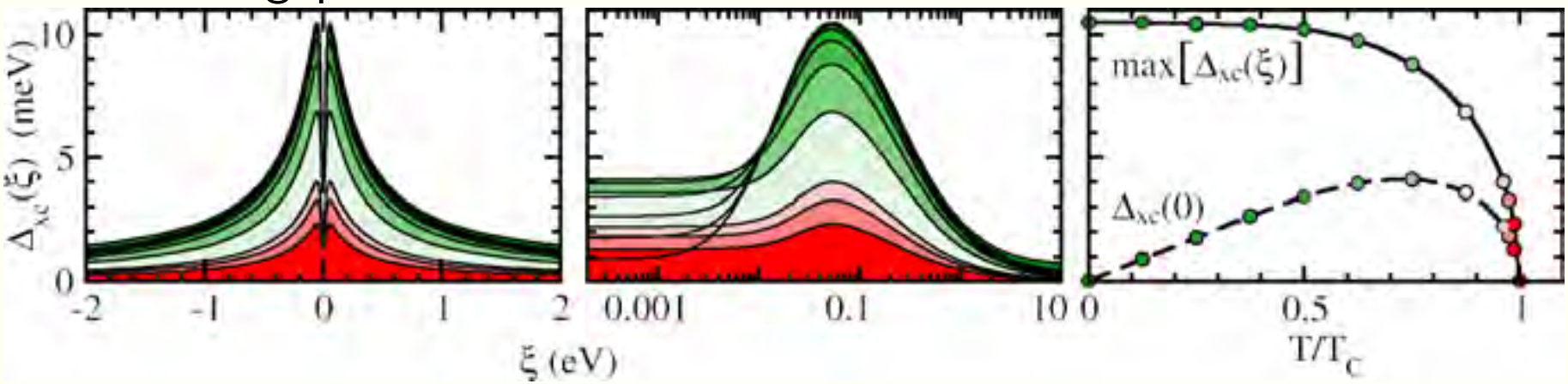


KS-SCDFT gap:



The KS spectrum is NOT a good approximation of the interacting one

A simple functional (Sec 3.3)

What if ... we take the Sham-Schlüter equation:

$$\Delta^*_{xc}(n\boldsymbol{k}) = \mathcal{S}\left[\Delta^*_{xc}, \bar{\Sigma}_{xc}\right]$$

and *arbitrarily* substitute $\bar{G} \to \bar{G}_s$...

Then

- We have no more dependence on the many body system
- $\mathcal{S}$ can be summed analytically
  (becoming an explicit function of Δ_s)

we get a GAP equation:

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

A simple functional (Sec 3.3)

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Note:

- The very first SCDFT functional was made like this
  with a few extra corrections
- Such a functional is **not too bad** and can be used for simulations
  although now there is better stuff
- The gap equation is essentially a modified BCS equation
  as simple as BCS but far better.

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Computational procedure :

- Compute the electronic structure (KS)
- Compute phonons and electron-phonon matrix elements
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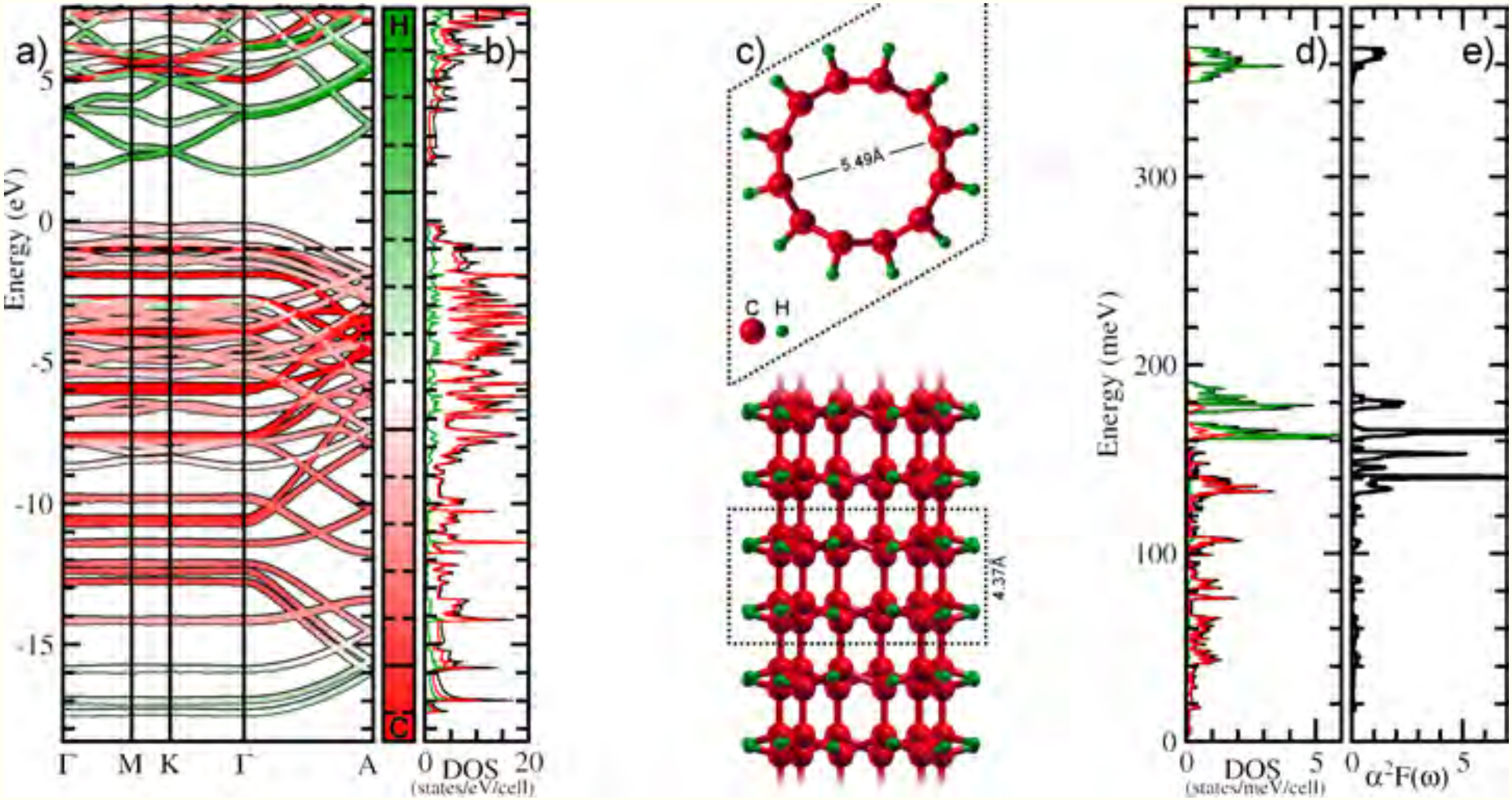
Example: a C-H tube (Sec 4)



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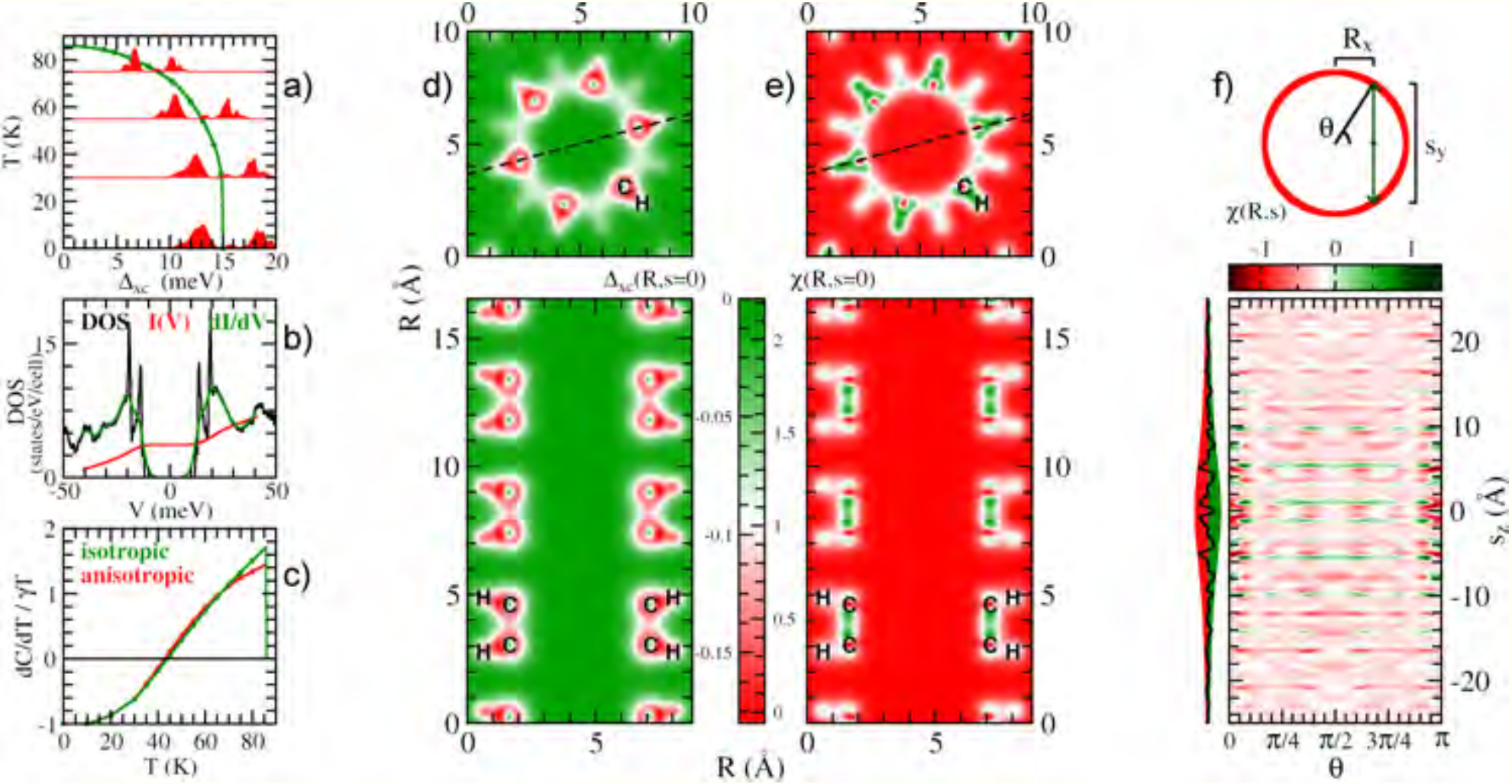

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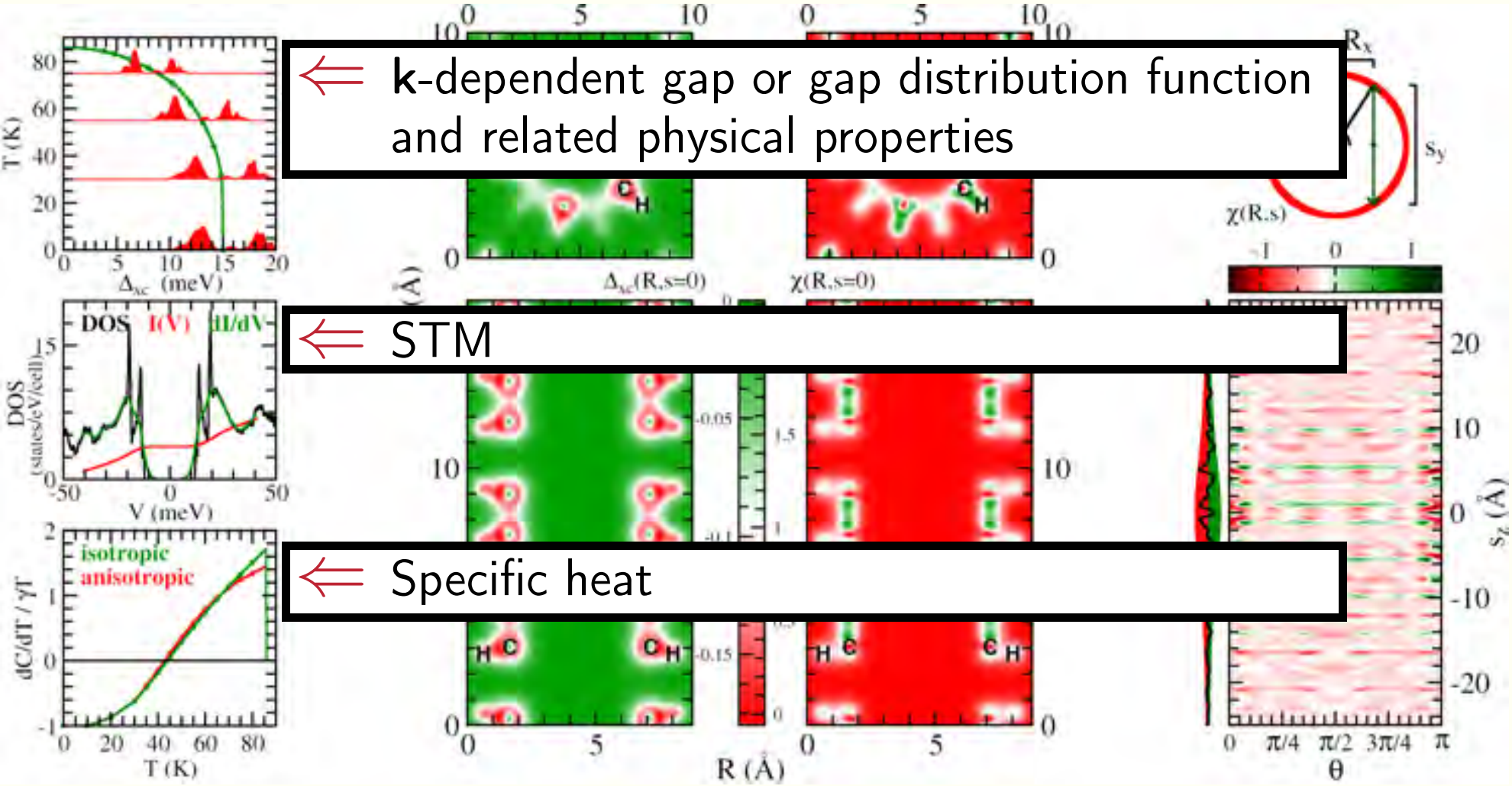

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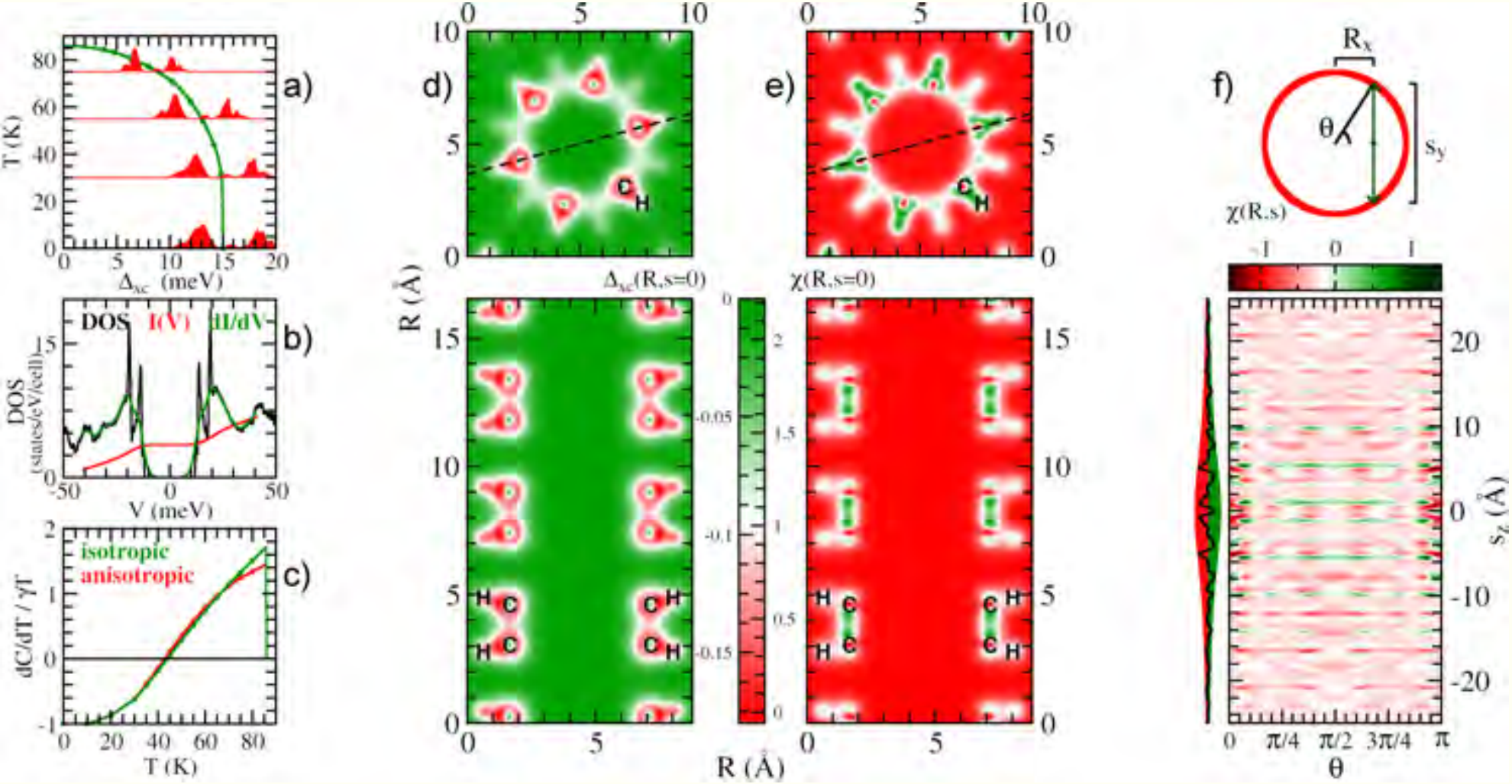

KS - SCDFT potential ⇑

⇑ SC order parameter $\chi(\boldsymbol{r}', \boldsymbol{r}')$ ⇑

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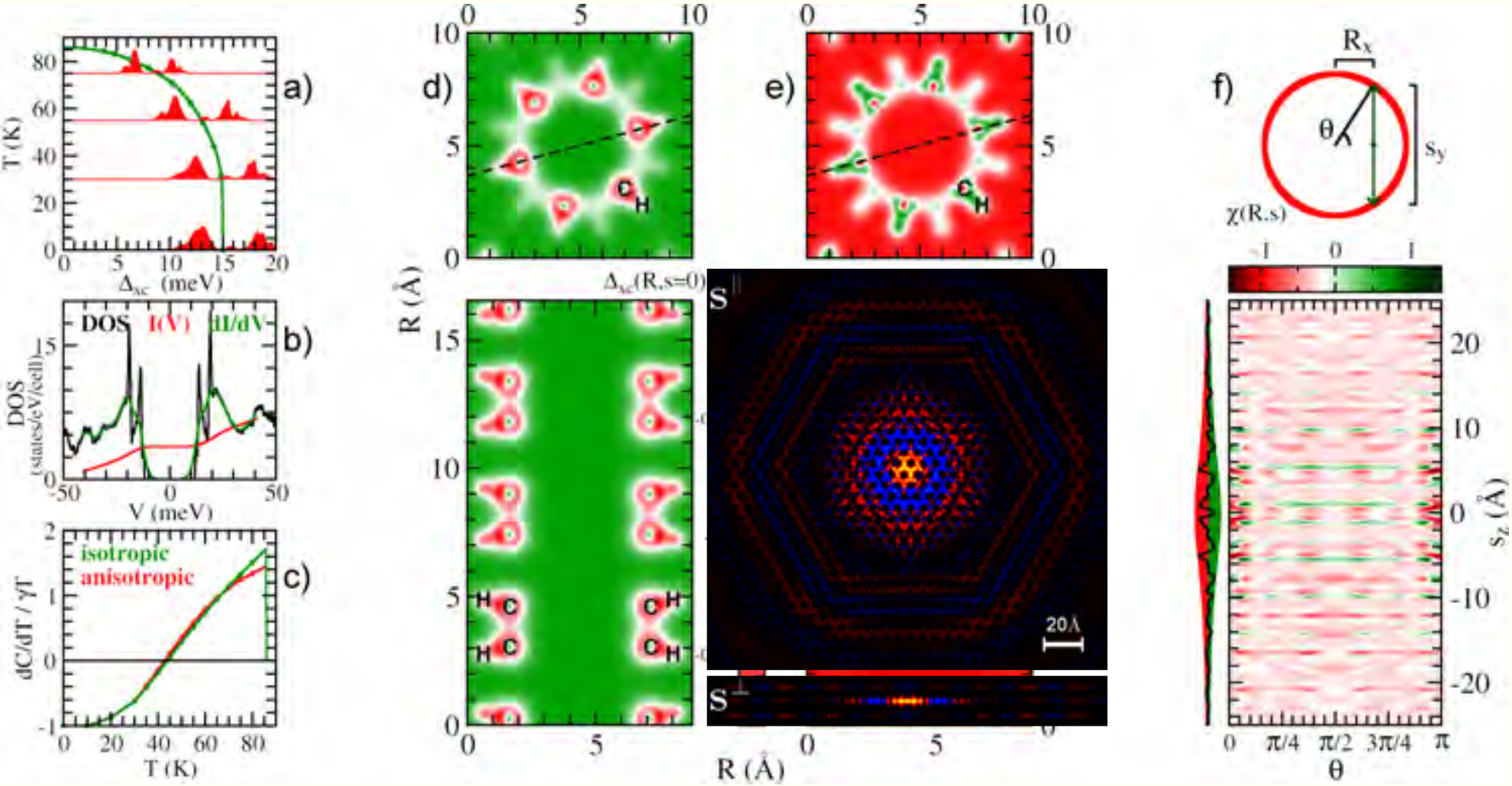

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Final Summary

I Hamiltonian for electrons and nuclei

II Density Functional-ization

III Use Many body theory to build a functional make approximations whenever you can.

IV Use the functional for production

IV Ask questions