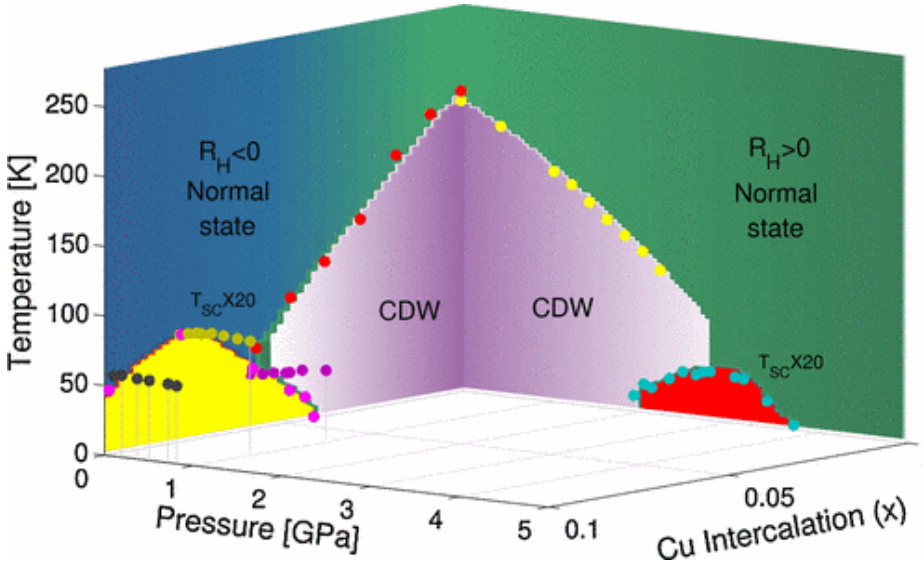
Advanced SIESTA Workshop 2025

Lindhard response function

Bogdan Guster

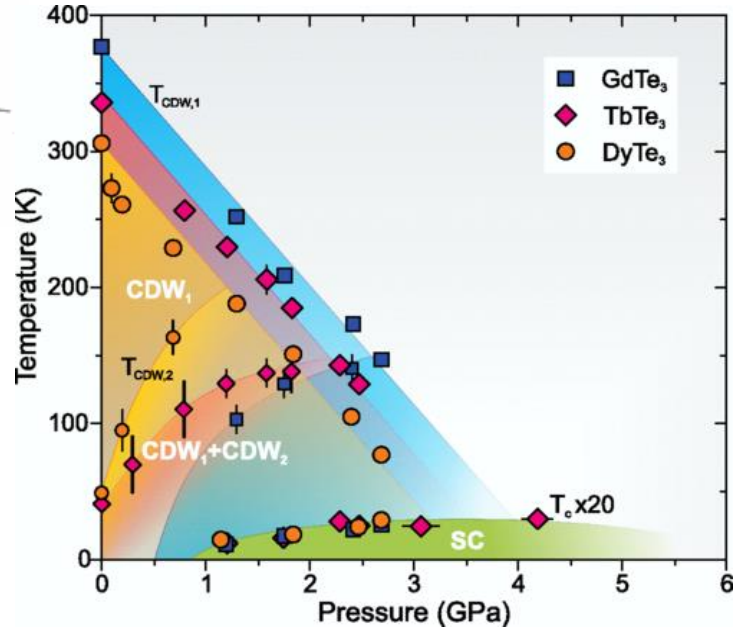
Broad survey over popular metals phase diagrams

Transition Metal Dichalcogenides

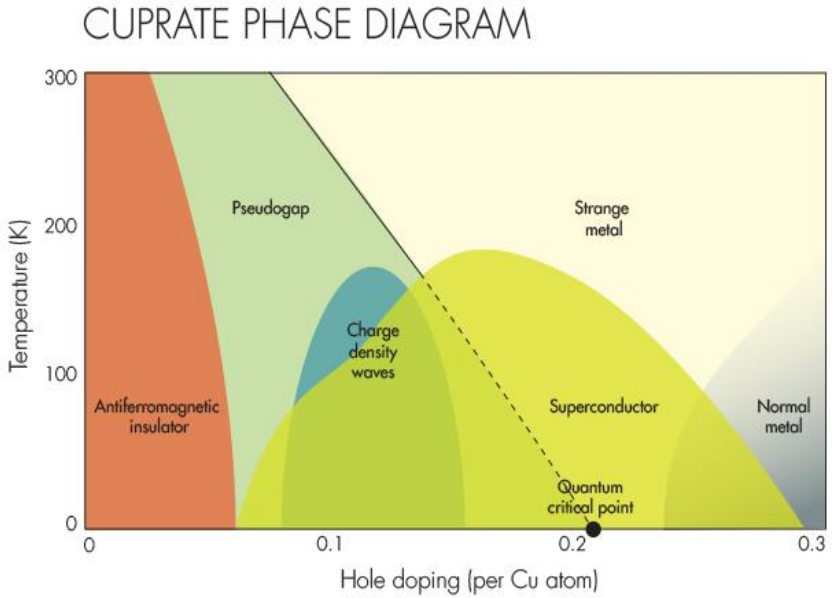


Phys. Rev. Lett. 103, 236401

Tellurides

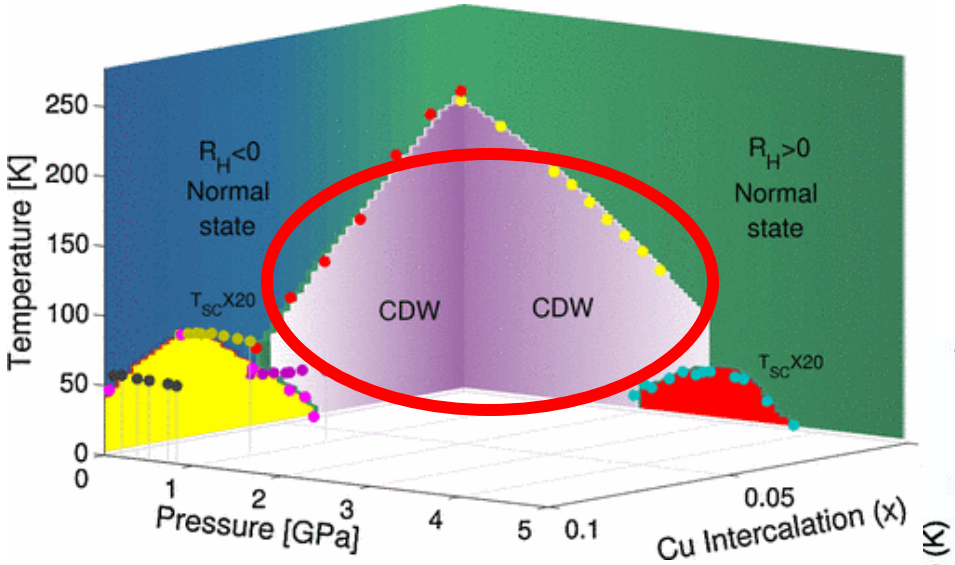


Phys. Rev. B 91, 205114



Where about Lindhard function is useful?

Transition Metal Dichalcogenides



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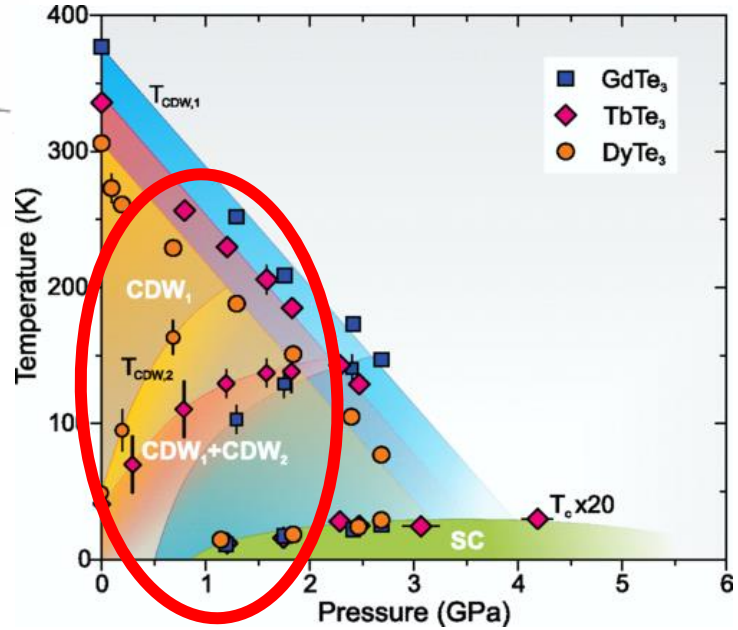

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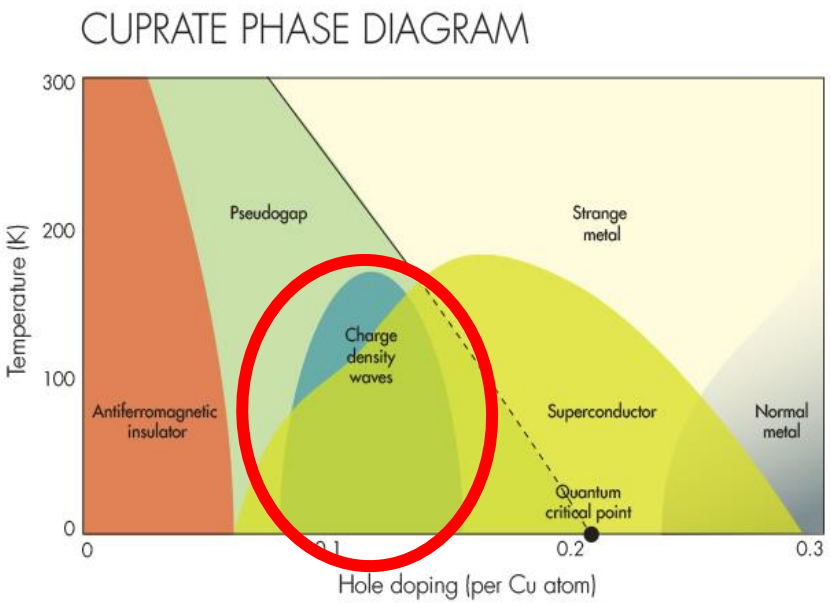

Where about Lindhard function is useful?

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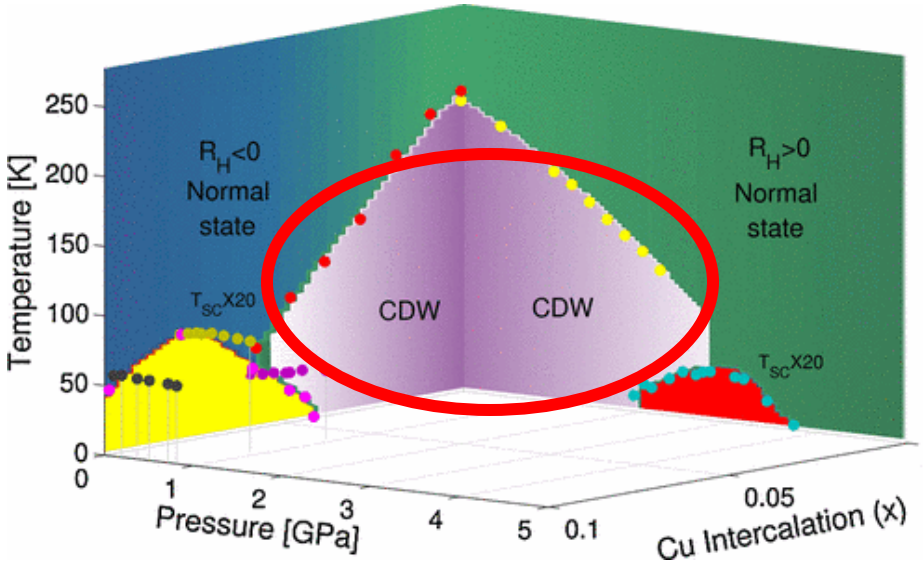

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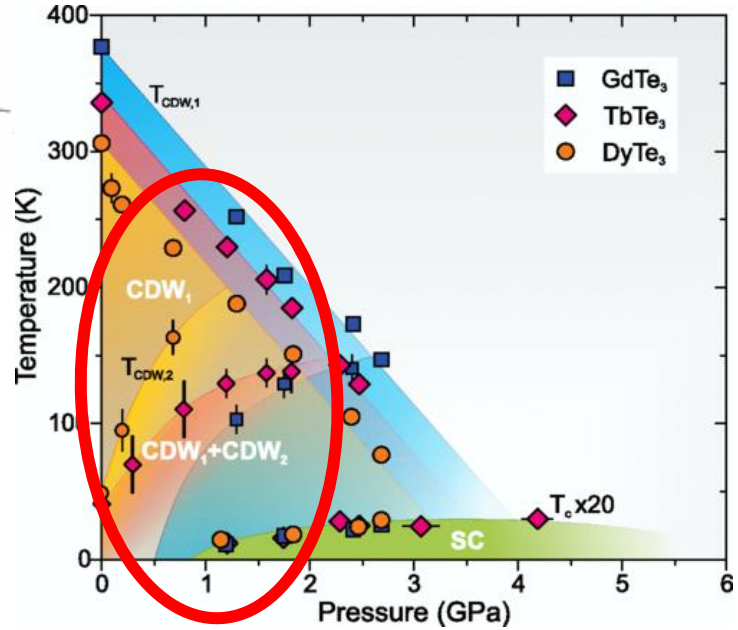

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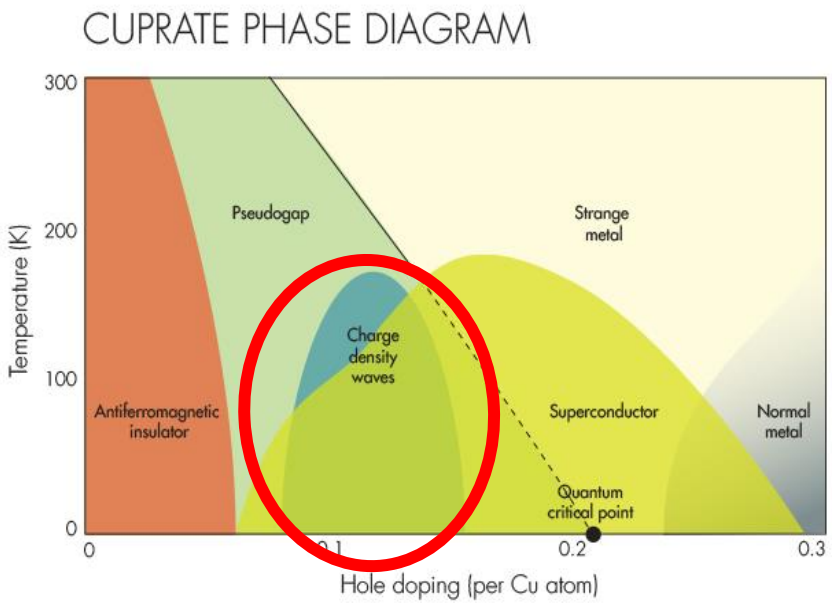


Lindhard function can provide insight into the behaviour of Charge Density Waves

General aspects of Lindhard response function

$$\chi_0(\mathbf{q},\omega) = \frac{1}{V}\sum_{n,n'}\sum_{\mathbf{k}} \frac{f(\varepsilon_{n\mathbf{k}}) - f(\varepsilon_{n'\mathbf{k}+\mathbf{q}})}{\hbar\omega + \varepsilon_{n\mathbf{k}} - \varepsilon_{n'\mathbf{k}+\mathbf{q}} + i\eta} \left|\langle n\mathbf{k}|e^{i\mathbf{q}\cdot\mathbf{r}}|n'\mathbf{k}+\mathbf{q}\rangle\right|^2$$

$$f(\varepsilon_{n\mathbf{k}}) = \frac{1}{e^{(\varepsilon_{n\mathbf{k}}-\varepsilon_F)/k_BT}+1}$$

- f – Fermi-Dirac (FD) distribution
- $\varepsilon_{n\mathbf{k}}$ – electronic energy eigenvalue of band n with wavevector $\mathbf{k}$
- $\varepsilon_{n\mathbf{k+q}}$ – electronic energy eigenvalue of band n with wavevector $\mathbf{k}$ after scattering by $\mathbf{q}$
- ω – phonon energy (or more generally frequency of perturbation)

but, in the case of Fermi surface nesting, static limit will suffice ($\omega \to 0$)

$$\chi_0(\mathbf{q}) = \frac{1}{V}\sum_{n,n'}\sum_{\mathbf{k}} \frac{f(\varepsilon_{n\mathbf{k}}) - f(\varepsilon_{n'\mathbf{k}+\mathbf{q}})}{\varepsilon_{n\mathbf{k}} - \varepsilon_{n'\mathbf{k}+\mathbf{q}} + i\eta} \left|\langle n\mathbf{k}|e^{i\mathbf{q}\cdot\mathbf{r}}|n'\mathbf{k}+\mathbf{q}\rangle\right|^2$$

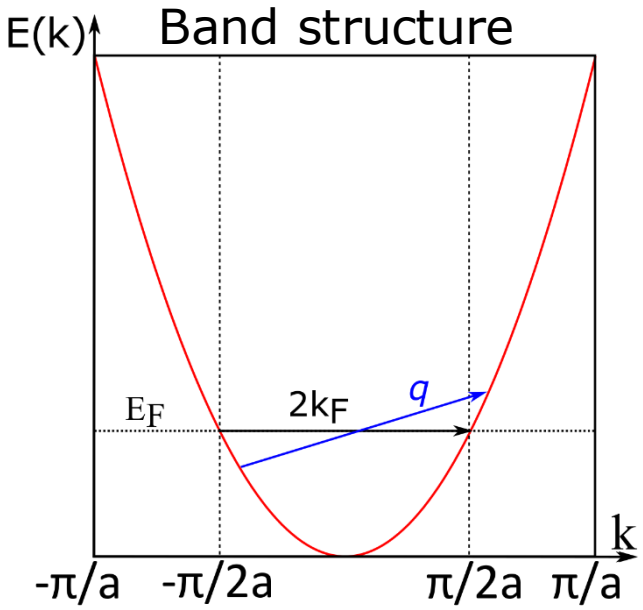
General aspects of Lindhard response function

$$\chi_0(\mathbf{q}) = \frac{1}{V} \sum_{n,n'} \sum_{\mathbf{k}} \frac{f(\varepsilon_{n\mathbf{k}}) - f(\varepsilon_{n'\mathbf{k}+\mathbf{q}})}{\varepsilon_{n\mathbf{k}} - \varepsilon_{n'\mathbf{k}+\mathbf{q}} + i\eta} |\langle n\mathbf{k}|e^{i\mathbf{q}\cdot\mathbf{r}}|n'\mathbf{k}+\mathbf{q}\rangle|^2$$

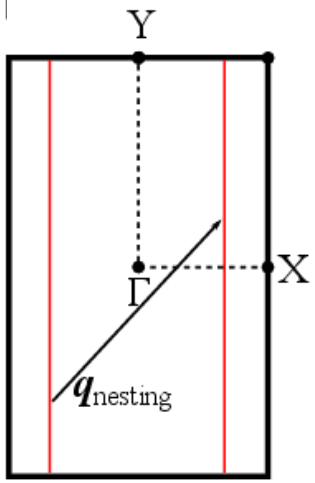
assuming matrix elements have maximum overlap this simplifies to:

$$\chi_0(\mathbf{q}) = \frac{2}{V} \sum_{\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k}}) - f(\varepsilon_{\mathbf{k}+\mathbf{q}})}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}}$$

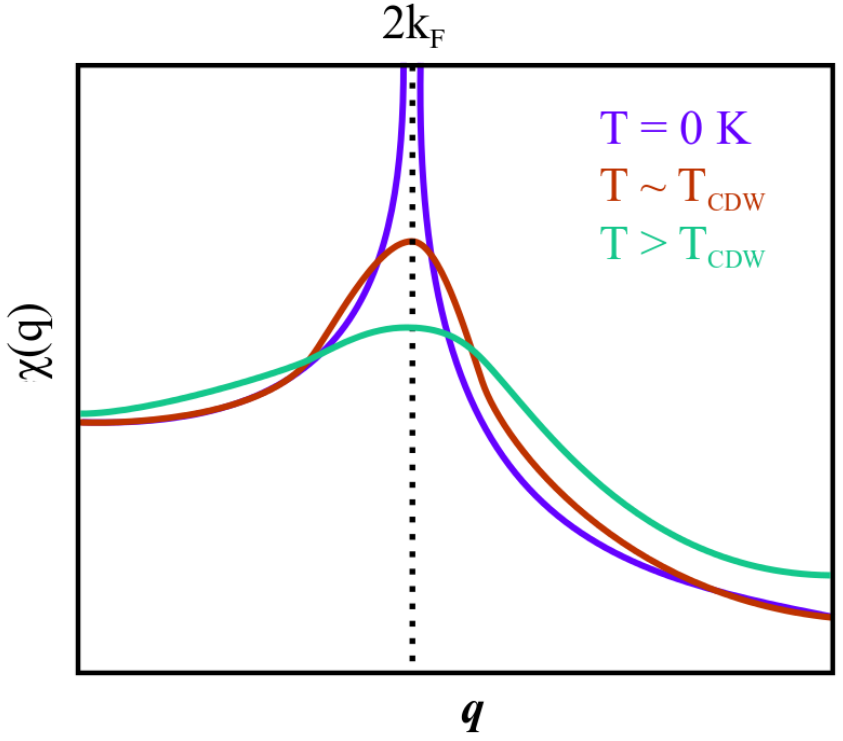
General aspects of Fermi Surface Nesting

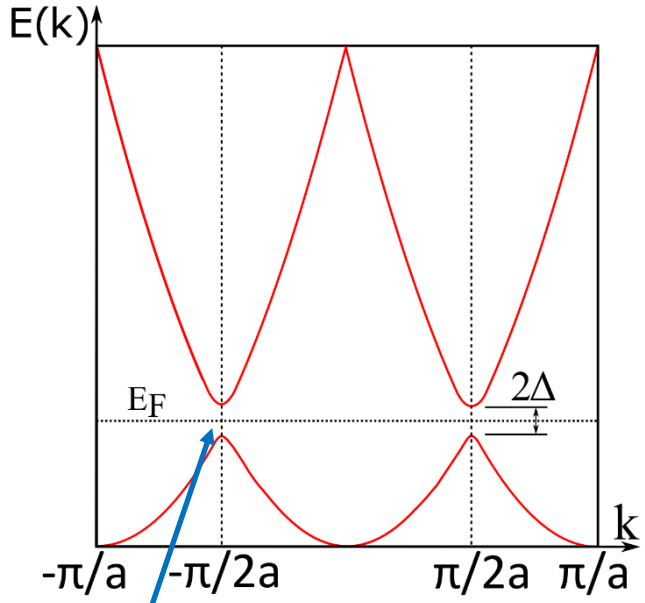


Fermi surface



$$\chi_0(\mathbf{q}) = \frac{2}{V}\sum_{\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k}}) - f(\varepsilon_{\mathbf{k}+\mathbf{q}})}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}}$$





Fermi surface nesting leads to a metal-insulator phase transition

Lindhard vs Bethe-Saltpeter

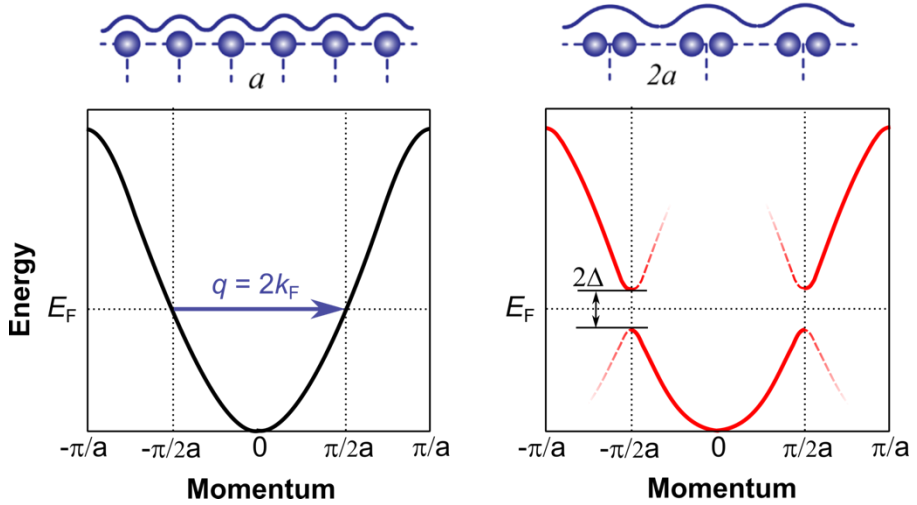
- Suitable for studying metals

Pros:

- Simple to implement
- Relatively easy to understand
- Computationally cheap

Cons (depending on what you do):

- Non-interacting electron-hole particle
- No Coulomb kernel
- No exciton binding
- Unsuitable in describing strong e-h interaction



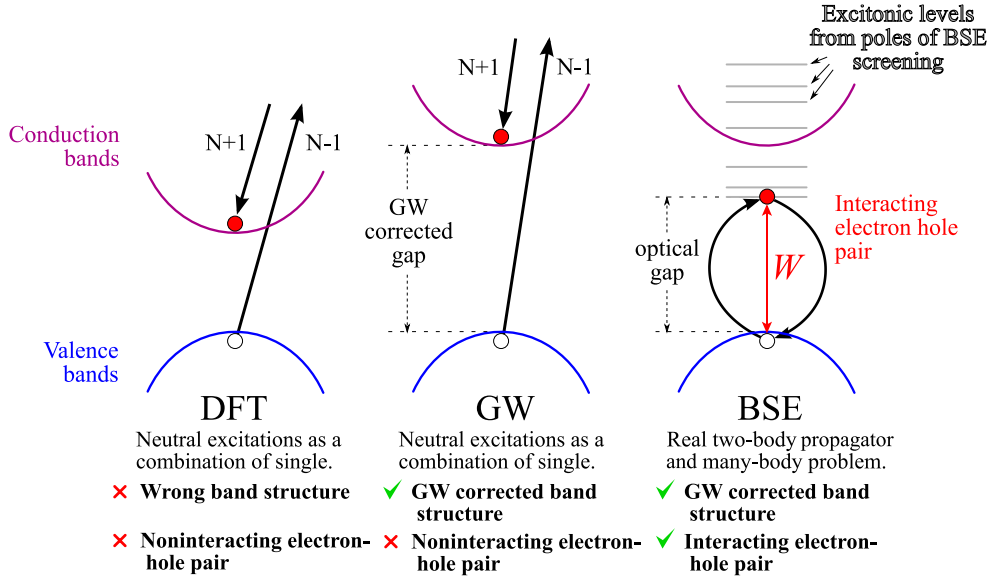
- Suitable for studying semiconductors

Pros:

- Includes the Coulomb kernel
- Useful in studying excitons
- Useful in providing absorption spectra

Cons (depending on what you do):

- Technically demanding to implement
- Computationally costly
- Requires quasiparticles energies (e.g. G0W0)



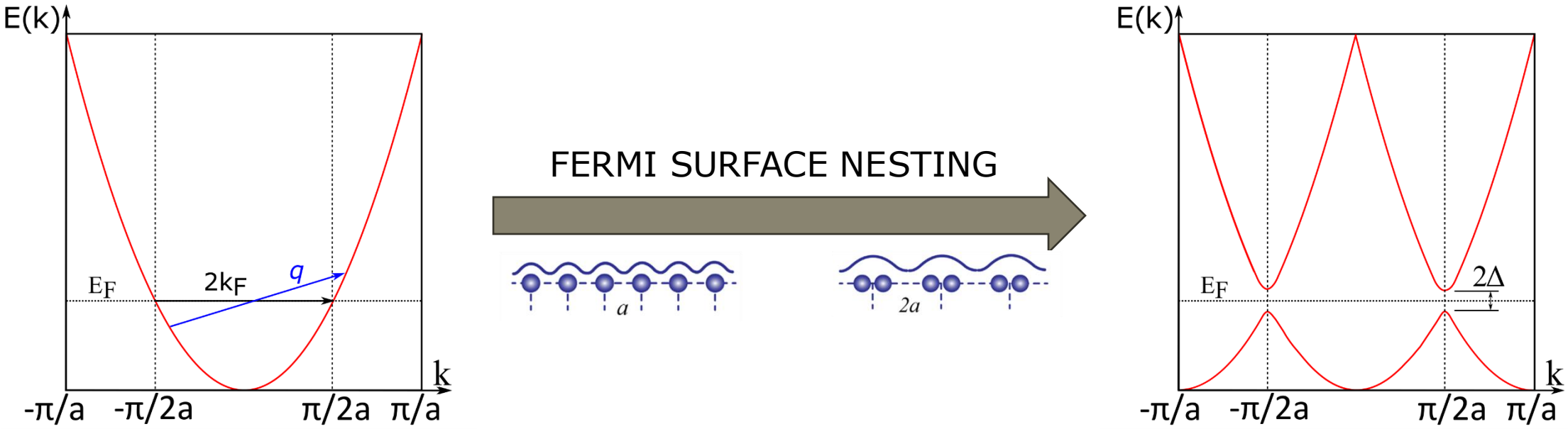
Keywords – **lindhard < siesta.fdf**

- Lindhard.Temperature 10 K # Controls the temperature of the FD distribution
- Lindhard.firstband 1 # Meaningful for the first band intersecting the FS
- Lindhard.lastband 2 # Meaningful for the last band intersecting the FS

- Lindhard.ngridx 122 # Interpolating on a much denser grid
- Lindhard.ngridy 243 # of k-points than the one used
- Lindhard.ngridz 88 # in the single-point DFT calculation

- Lindhard.nq1 n # Print in the siesta.lindhard every n^{th} point
- Lindhard.nq2 m # from the interpolated series of points

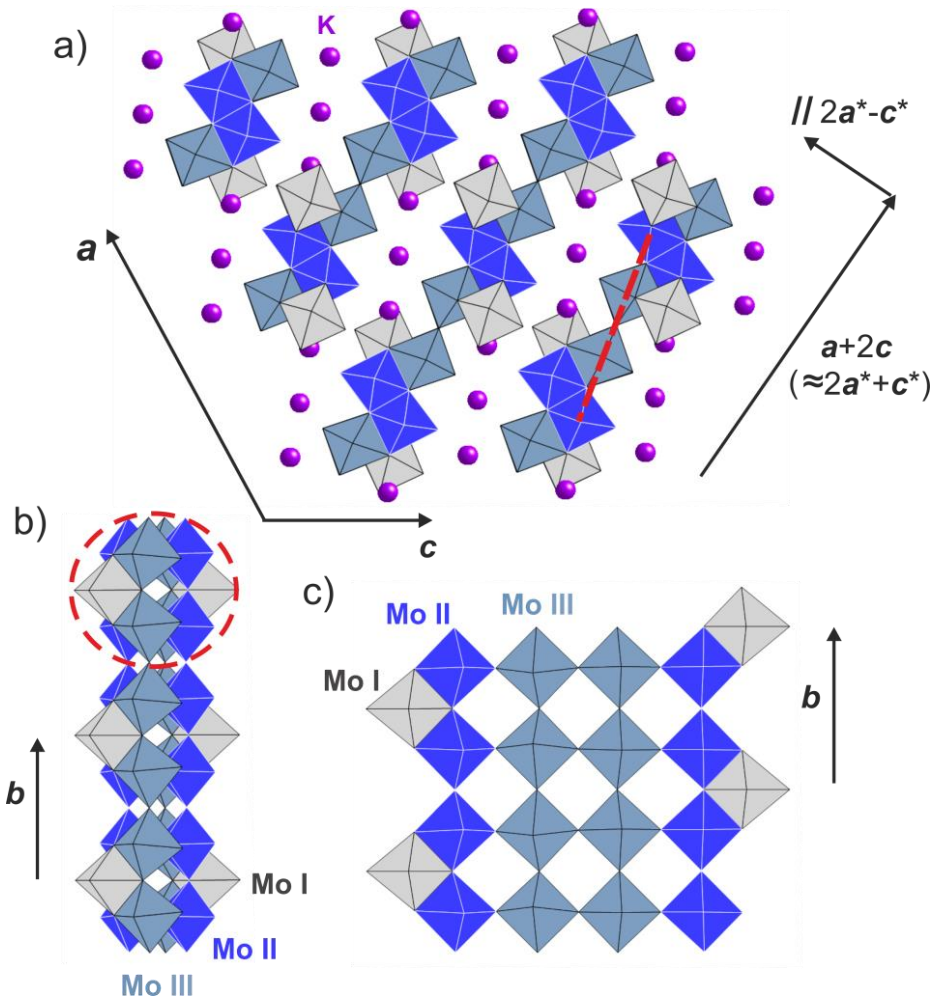
Very simple example – H chain (Ex 1)



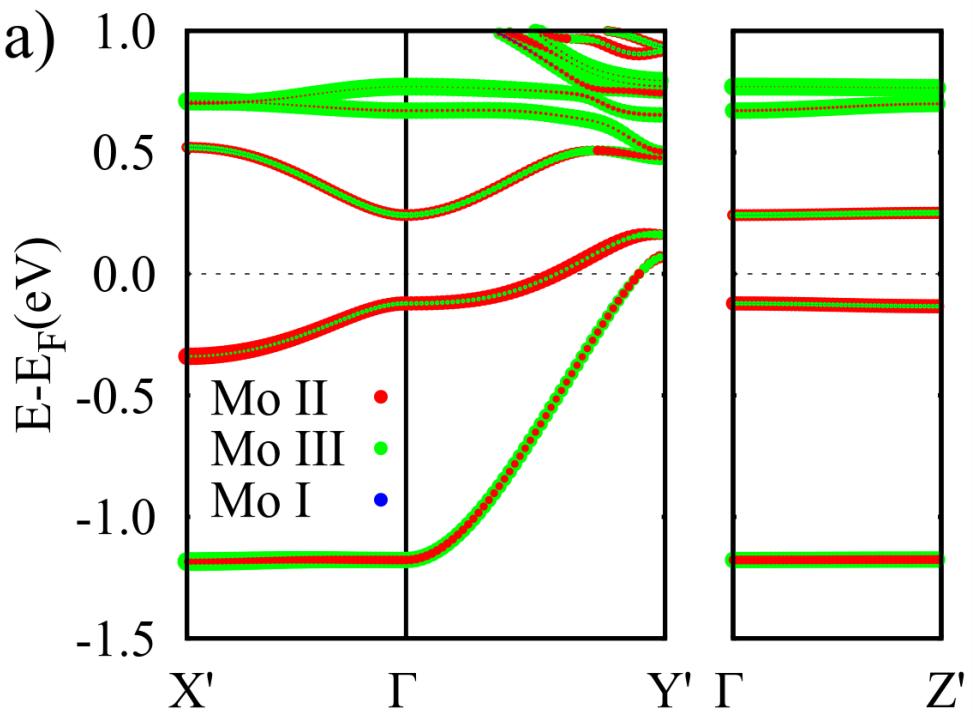
Lindhard response function can account for this metal to insulator phase transition

Real case scenario – $K_{0.3}MoO_3$ (Ex 2)

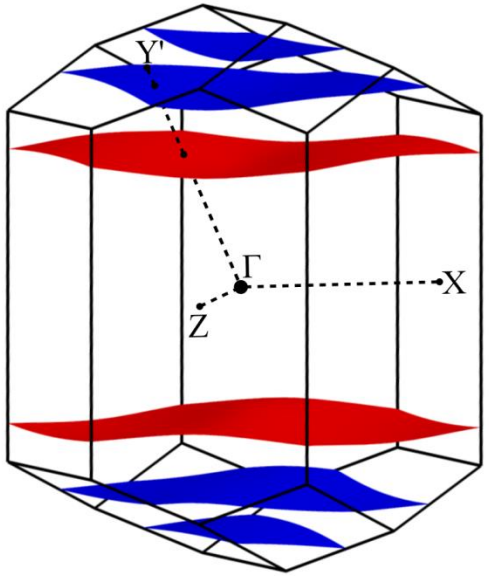
Crystal structure



Electronic band structure

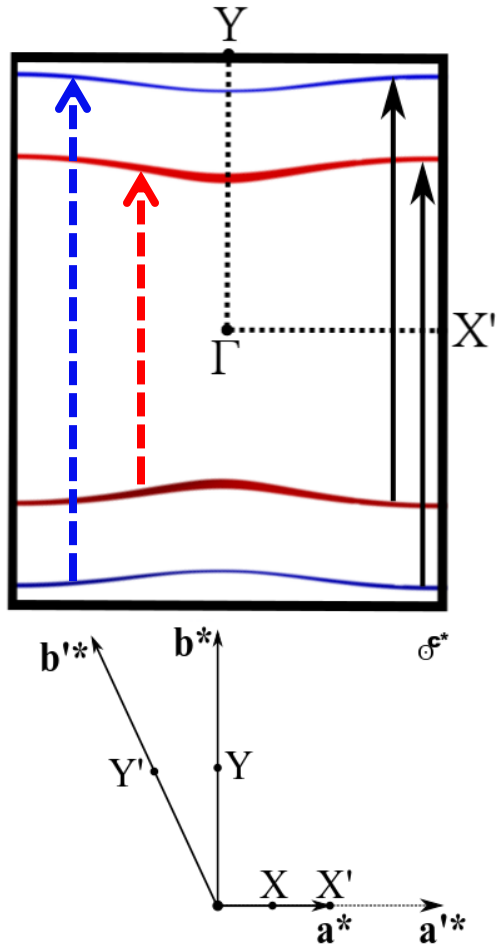


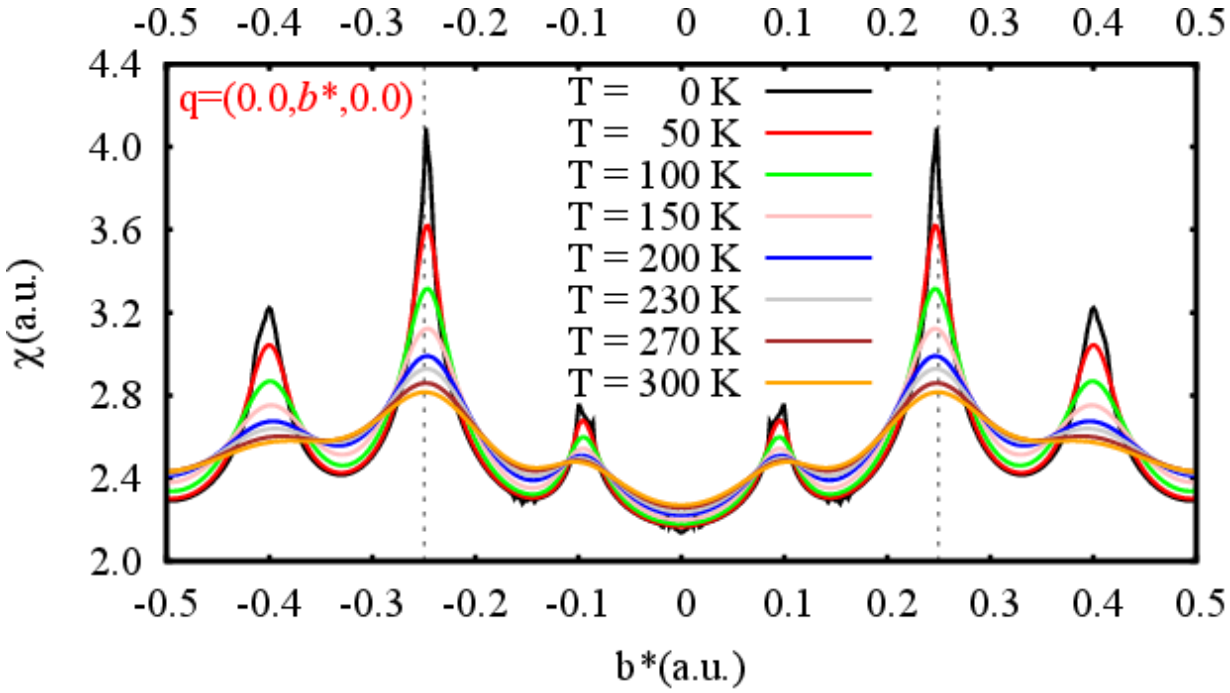
Real case scenario – $K_{0.3}MoO_3$



3D View of the FS

Section of the FS along c*





Real case scenario – $K_{0.3}MoO_3$