SSCHA
Stochastic Self-Consistent Harmonic Approximation

Theory of the electron-phonon interaction and superconductivity

Giovanni Marini

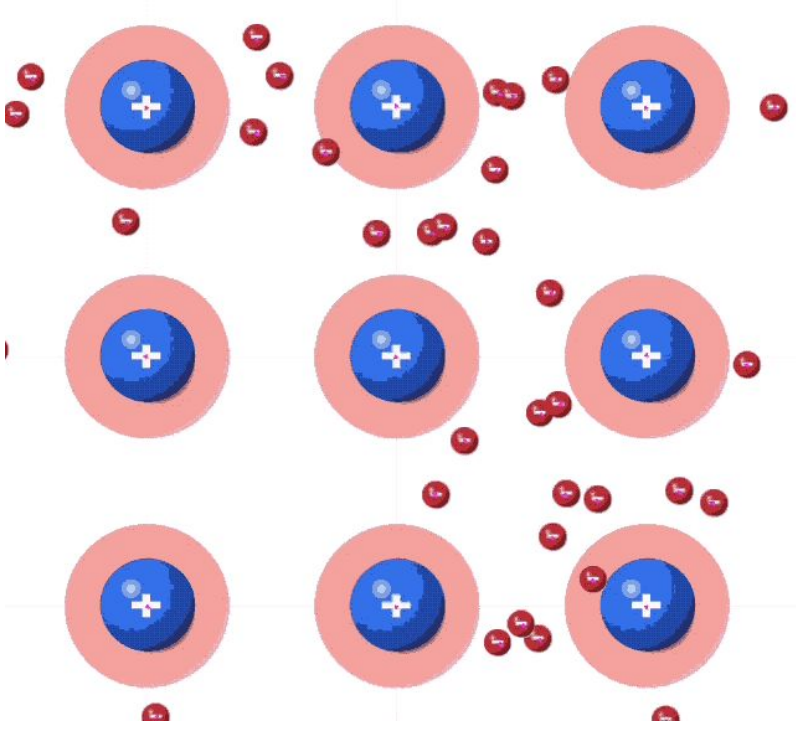
Istituto Italiano di Tecnologia

ISTITUTO ITALIANO DI TECNOLOGIA

SSCHA School 2023

What is electron-phonon interaction ?

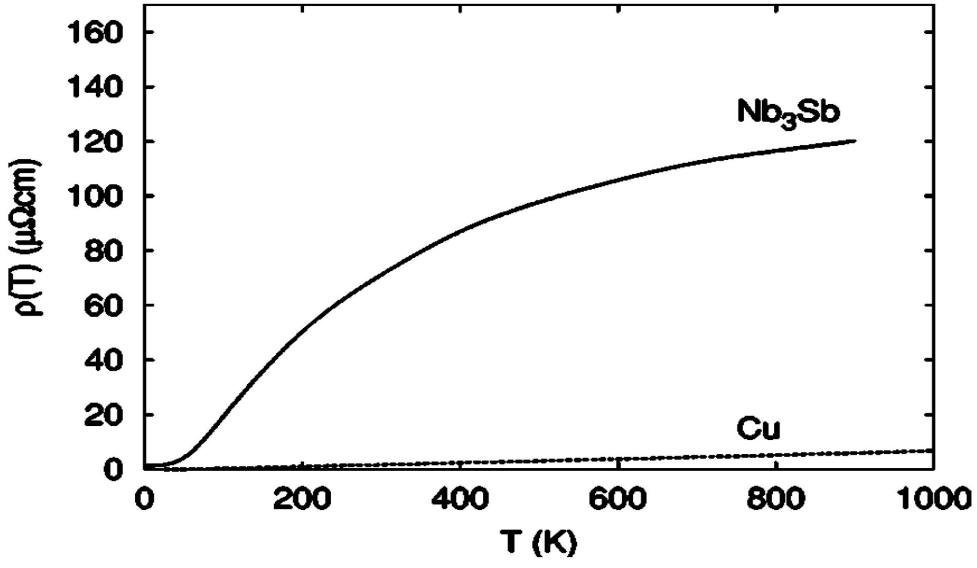
Electron-phonon interaction characterizes the interaction between electrons and the motion of nuclei.



How is el-ph. interaction relevant? What quantities does it affect?

First example: the intrinsic resistivity of metals

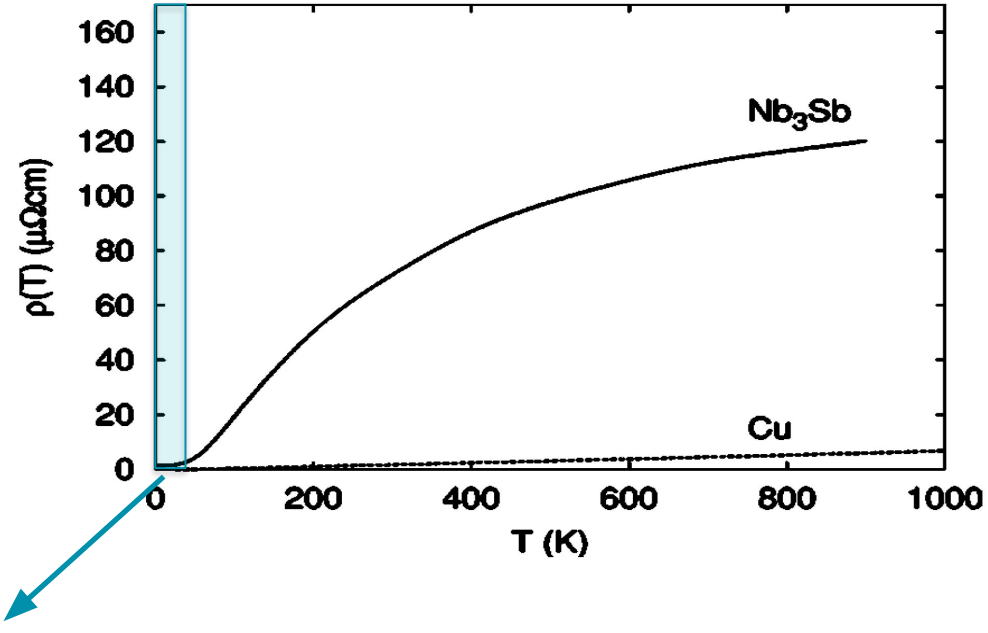
mostly due to the electron-phonon interaction for $k_B T \gtrsim \hbar\omega$



See O. Gunnarsson, M. Calandra, and J. E. Han
Rev. Mod. Phys. **75**, 1085 (2003)

First example: the intrinsic resistivity of metals

mostly due to the electron-phonon interaction for $k_B T \gtrsim \hbar\omega$

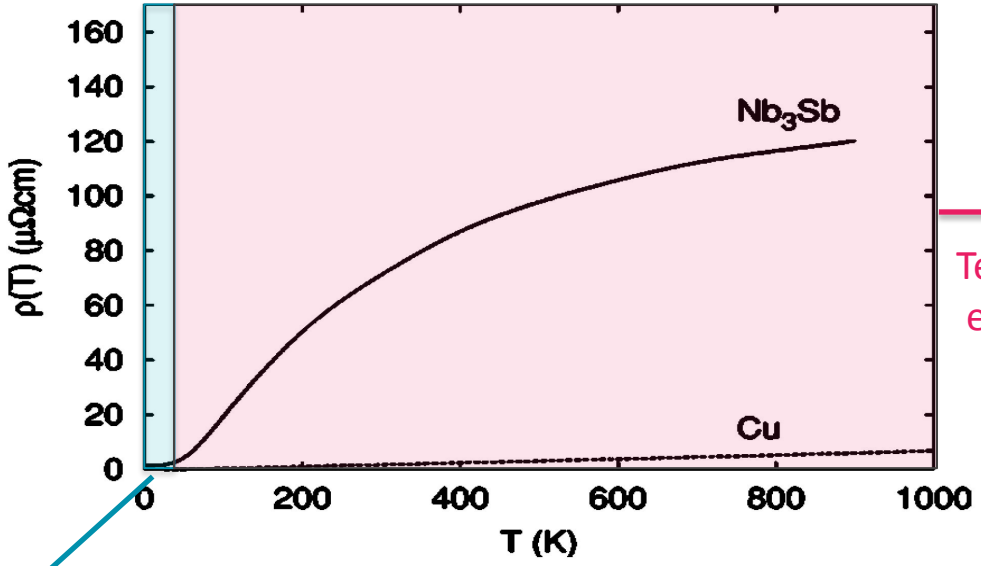


Temperature region where the el-el scattering is relevant

See O. Gunnarsson, M. Calandra, and J. E. Han
Rev. Mod. Phys. **75**, 1085 (2003)

First example: the intrinsic resistivity of metals

mostly due to the electron-phonon interaction for $k_B T \gtrsim \hbar\omega$



Temperature range where the el-ph scattering is dominant!

Temperature region where the el-el scattering is relevant

See O. Gunnarsson, M. Calandra, and J. E. Han
Rev. Mod. Phys. **75**, 1085 (2003)

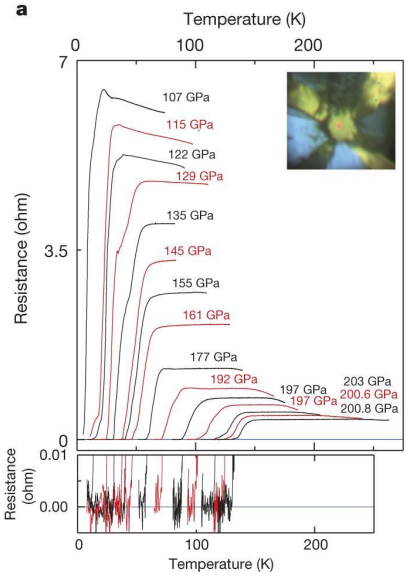
Second example: electron-phonon mediated superconductivity

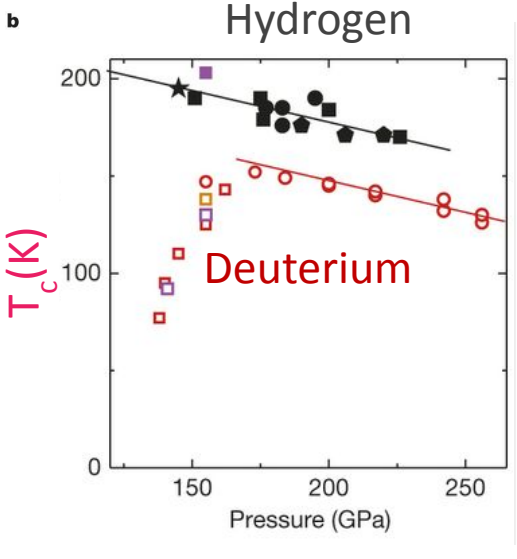
LETTER

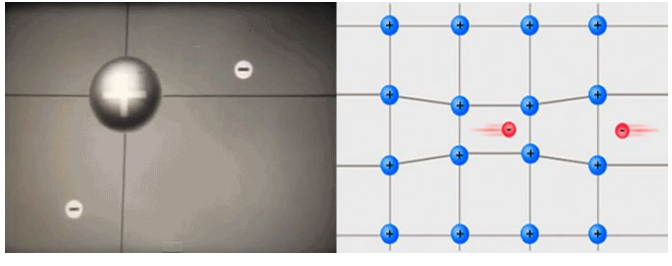
doi:10.1038/nature14964

Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system

A. P. Drozdov[1]*, M. I. Eremets[1]*, I. A. Troyan[1], V. Ksenofontov[2] & S. I. Shylin[2]

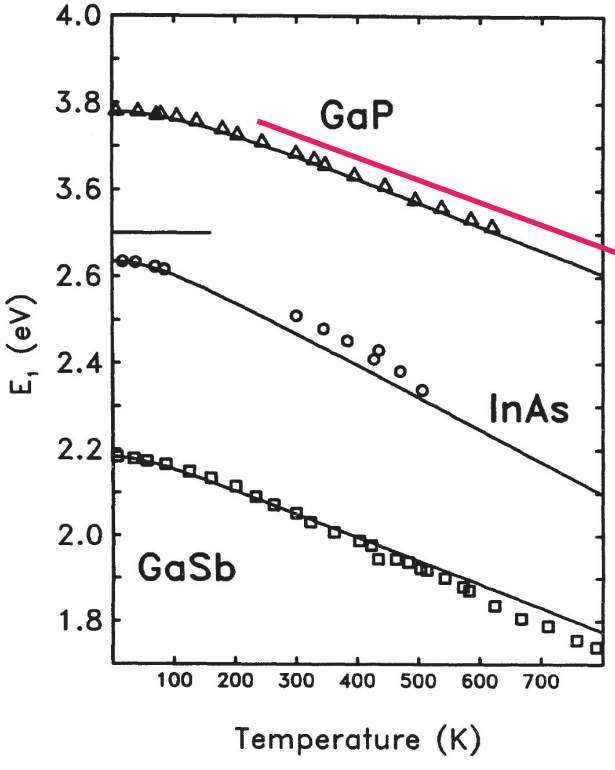






Conventional superconductivity is due to the electron-phonon interaction

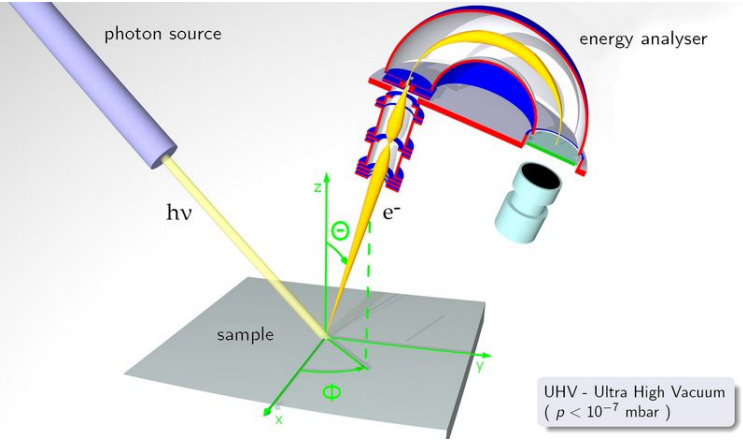
Third example: temperature dependence of band gaps in semiconductors

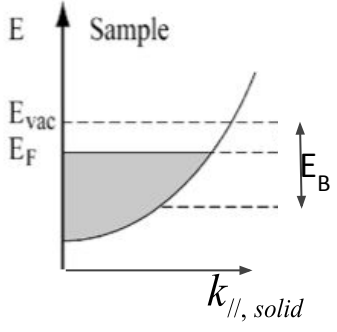


Electron-phonon interaction

M. Cardona, S. Gopalan, Progress in Electron Properties of Solids pp 51-64
P.B. Allen and M. Cardona Phys. Rev. B 27 4760 (1983)
G. Antonius, *et al.*, Phys. Rev. Lett. 112, 215501 (2014).

Fourth example: angle-resolved photoemission spectroscopy (ARPES)





Initial state (incident photon)

$$p_i = \hbar k_i \quad E_{in} = \hbar\omega$$

Final state (extracted electron)

$$p_f = \hbar k_f \quad E_{kin} = \frac{\hbar^2 k_f^2}{2m}$$

Energy conservation:

$$E_{in} = E_{kin} + E_B(k_{//,\,\mathrm{solid}})$$

E_B = Binding Energy

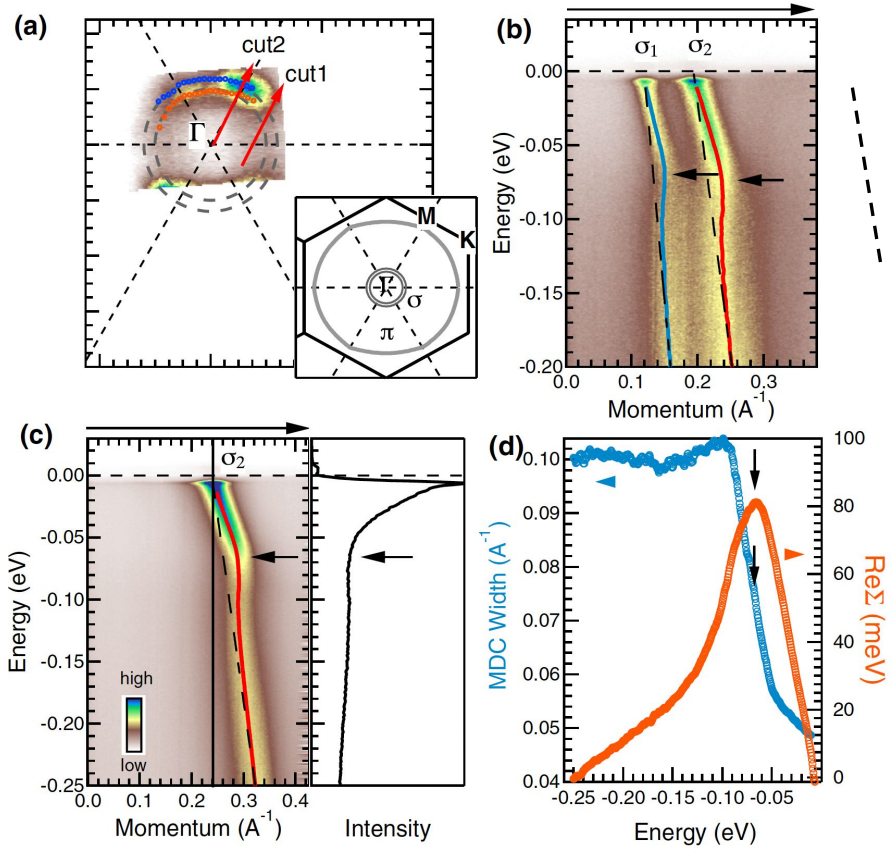
Momentum conservation

$$k_{//,i} = k_{//,f}$$

$$k_{\parallel,f} = \frac{1}{\hbar}\sqrt{2mE_{kin}}\,\sin(\theta)$$

We measure E_{kin}, ϑ to obtain $E_B, k_{//,\,solid}$

ARPES: kinks in electronic structure due to the electron-phonon interaction

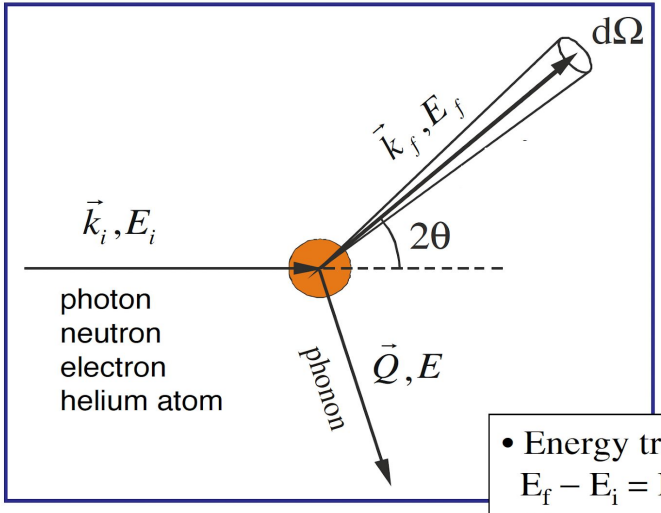


DFT bands

$$\Sigma(k = k_0, E)$$

Mou *et al.* Phys. Rev. B **91**, 140502(R)

Inelastic X-ray scattering to measure phonons



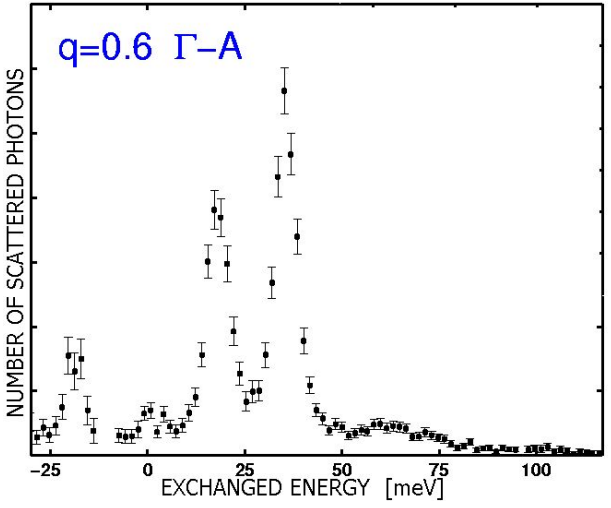
- Energy transfer:
  $E_f - E_i = E$ (0.001 – 1 eV)
- Momentum transfer:
  $\vec{k}_f - \vec{k}_i = \vec{Q}$ (0.0001 – 100 nm^{-1})

$$\mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i$$
$$E = E_f - E_i$$
$$E_f = ck_f$$
$$E_i = ck_i$$
$$E << E_f$$
$$E << E_i$$

$$Q = \sqrt{(\mathbf{k}_f - \mathbf{k}_i)^2} = \frac{1}{c^2}\sqrt{E_f^1 + E_i^2 - 2E_iE_f\cos(2\theta)} \approx \frac{2E_i}{c^2}\sqrt{\frac{1-\cos(2\theta)}{2}}$$

$$Q \approx 2k_i \sin(\theta)$$

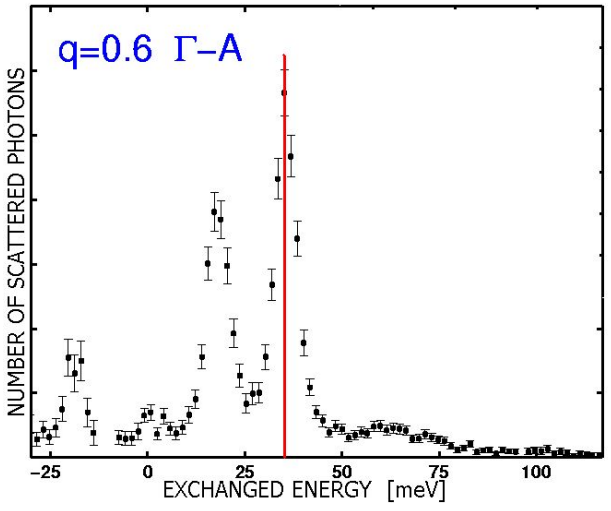
Fifth example: inelastic X-ray scattering spectra



Fifth example: inelastic X-ray scattering spectra

Energy of the phonon line :

- Harmonic phonon frequency
- Anharmonic shift



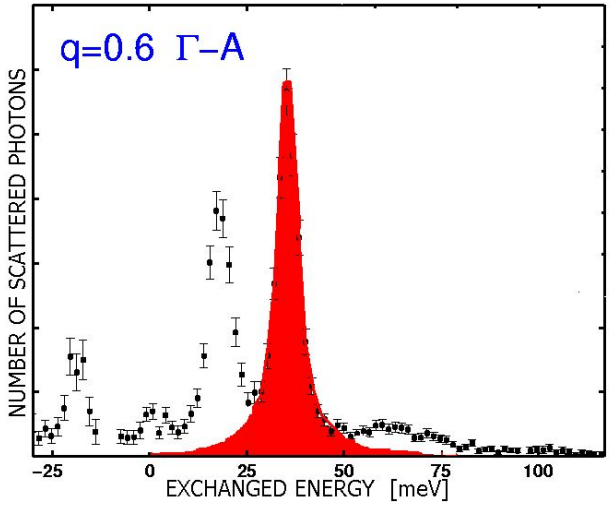
Fifth example: inelastic X-ray scattering spectra

Energy of the phonon line :

- Harmonic phonon frequency
- Anharmonic shift

Intensity of the phonon line :

- Phonon eigenvectors



Fifth example: inelastic X-ray scattering spectra

Energy of the phonon line :

- Harmonic phonon frequency
- Anharmonic shift

Intensity of the phonon line :

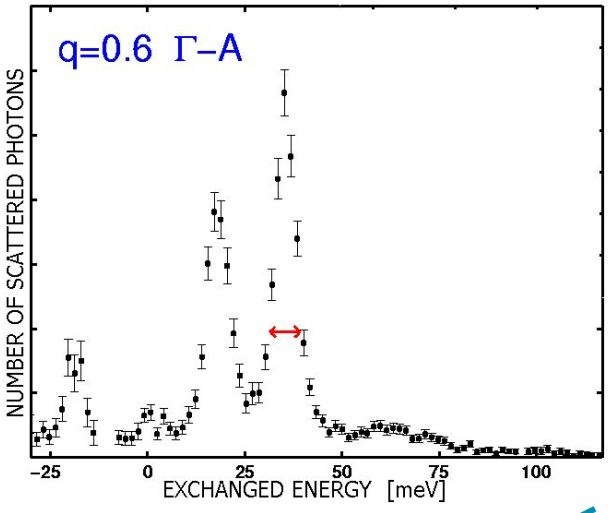
- Phonon eigenvectors

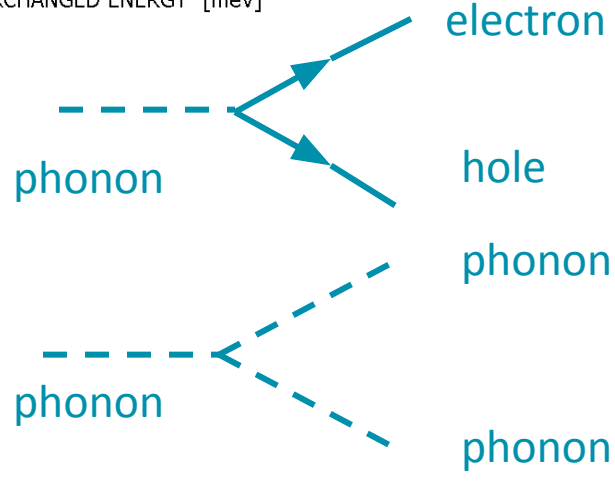
Phonon linewidth :

- Decay of a phonon in an electron-hole pair due to the electron-phonon coupling

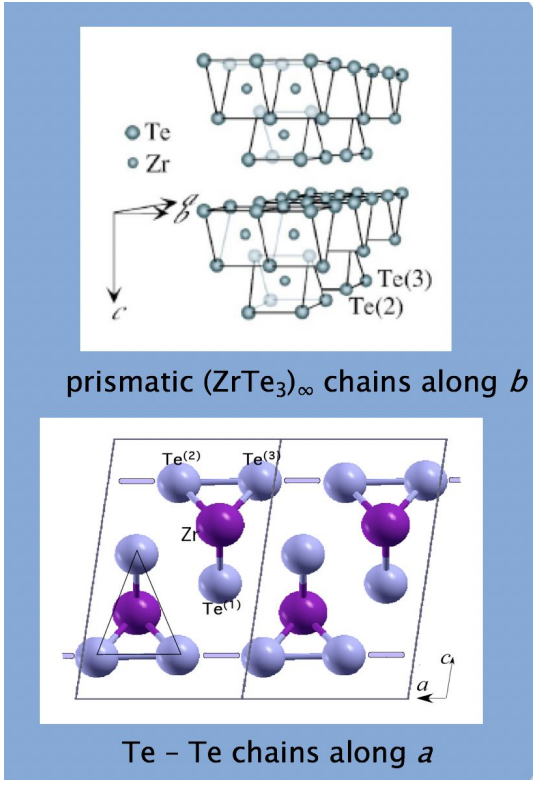
+

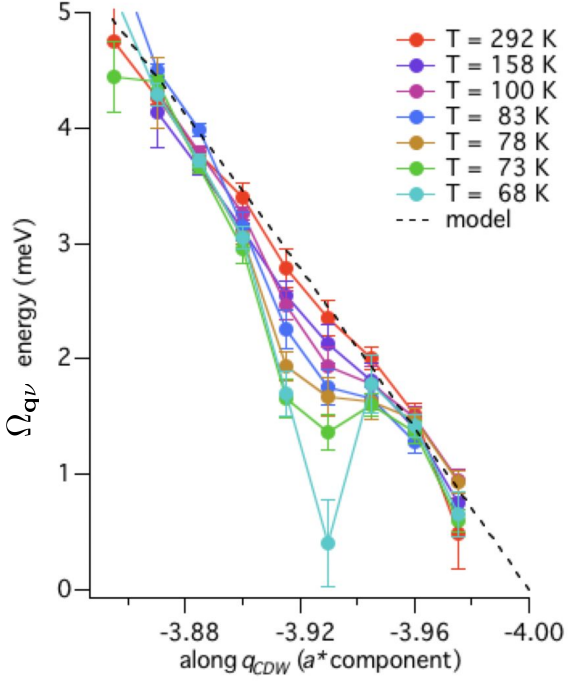
- Anharmonicity: decay of a phonon in two phonons conserving energy and momentum

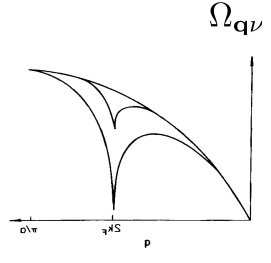




Sixth example: $ZrTe_3$ 1D metal, charge-density wave phase seen in IXS

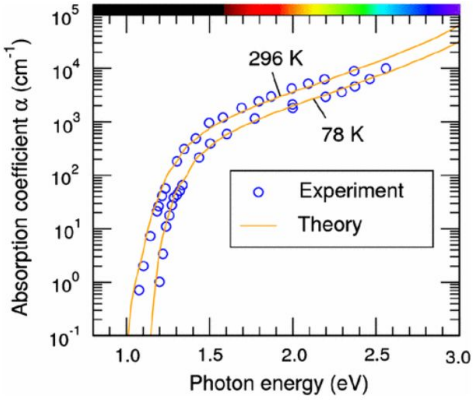


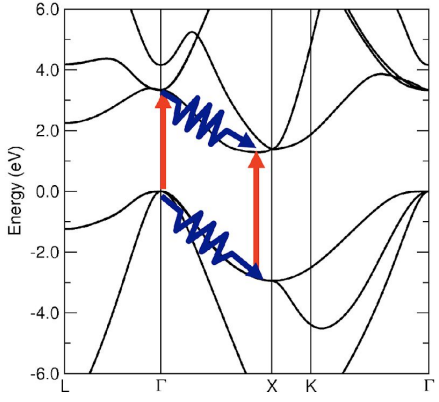




Hoesch, *et al.* Phys. Rev. Lett. **102**, 086402 (2009)

Seventh example: electron-phonon mediated optical absorption





Deslippe *et al. Comput. Phys. Commun.* **183**, 1269 (2012)

Gap of silicon is indirect (1.2 eV), minimum direct gap is 3.4 eV.
Direct optical absorption impossible in the visible.
Absorption in the visible is phonon-assisted, enables silicon solar cells.

Silicon captures photons above 1.1 eV

PRL **108,** 167402 (2012) PHYSICAL REVIEW LETTERS week ending 20 APRIL 2012

Phonon-Assisted Optical Absorption in Silicon from First Principles

Jesse Noffsinger,[1,2] Emmanouil Kioupakis,[3,4] Chris G. Van de Walle,[3] Steven G. Louie,[1,2] and Marvin L. Cohen[1,2]

Electron-phonon mediated optical absorption

Fermi golden rule @ first order

$$\mathscr{P}_{i\to f} = \frac{2\pi}{\hbar} |\langle f|\mathscr{L}|i\rangle|^2 \delta(E_f - E_i \mp \hbar\omega)$$

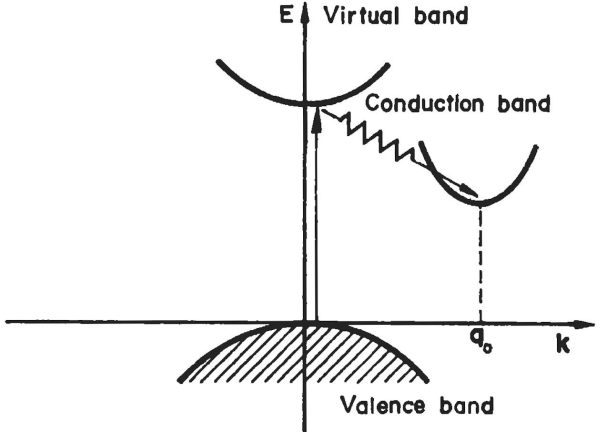
No absorption below the gap

Electron-phonon mediated optical absorption

Fermi golden rule @ second order

$$\mathscr{P}_{v\mathbf{k}_1 s \to c\mathbf{k}_2 s} = \frac{2\pi}{\hbar}\left(\frac{eA_0}{mc}\right)^2 \left| \frac{\langle \psi_{c\mathbf{k}_2} | V_p(\mathbf{q}, \mathbf{r}) | \psi_{\beta\mathbf{k}_1} \rangle n_{\mathbf{q}}^{1/2} \langle \psi_{\beta\mathbf{k}_1} | \mathbf{e} \cdot \mathbf{p} | \psi_{v\mathbf{k}_1} \rangle}{E_\beta(\mathbf{k}_1) - E_v(\mathbf{k}_1) - \hbar\omega} \right|^2$$

$$\times \delta(E_c(\mathbf{k}_2) - E_v(\mathbf{k}_1) - \hbar\omega + \hbar\omega_{\mathbf{q}}). \qquad (5\text{-}42)$$



Absorption below gap possible via electron-phonon scattering

Outline

- Born Oppenheimer (BO) and exact factorization
- Electron-phonon matrix elements
- Second quantization of the electron-phonon Hamiltonian
- Effects on the electrons
- Effects on the phonons
- Electron-phonon driven superconductivity

Outline

- Born Oppenheimer (BO) and exact factorization
- Electron-phonon matrix elements
- Second quantization of the electron-phonon Hamiltonian
- Effects on the electrons
- Effects on the phonons
- Electron-phonon driven superconductivity

Cystalline systems: notation

$\vec{a}_1, \vec{a}_2, \vec{a}_3$ direct lattice vectors.

The coordinate of each atom is identified by

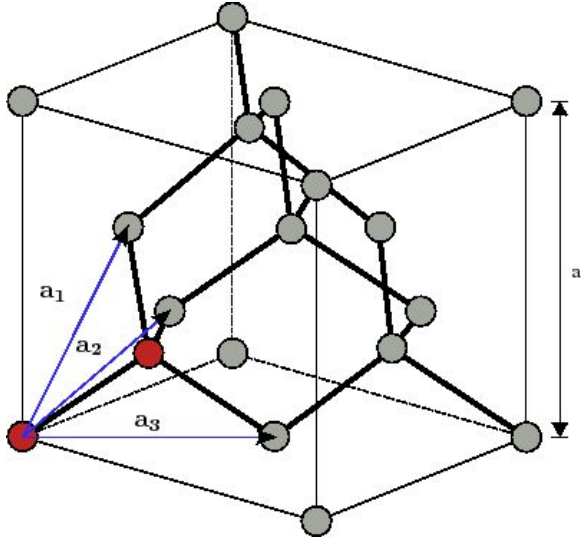
$$\mathbf{R}_{LA} = \mathbf{R}_L + \tau_A$$

Cell index

Atom in the cell

$$\mathbf{R}_L = i\mathbf{a}_1 + j\mathbf{a}_2 + l\mathbf{a}_3$$

$$L = (i, j, l)$$



Crystal Hamiltonian

$$\mathcal{H} = \sum_{L,A} \frac{\mathbf{P}_{LA}^2}{2M_A} + V_i(\mathbf{R}) + \sum_i \frac{\mathbf{p}_i^2}{2m} + V_e(\mathbf{r}) + V_{ie}(\mathbf{r}, \mathbf{R})$$

Crystal Hamiltonian

$$\mathcal{H} = \sum_{L,A} \frac{\mathbf{P}_{LA}^2}{2M_A} + V_i(\mathbf{R}) + \sum_i \frac{\mathbf{p}_i^2}{2m} + V_e(\mathbf{r}) + V_{ie}(\mathbf{r},\mathbf{R})$$

Purely Ionic part

$$V_i(\mathbf{R}) = \frac{e^2}{2} \sum_{\substack{LA,LB \\ (L,A)\neq(L,B)}} \frac{Z_A Z_B}{|\mathbf{R}_{LA} - \mathbf{R}_{MB}|}$$

Z_A atomic number

Crystal Hamiltonian

$$\mathcal{H} = \sum_{L,A} \frac{\mathbf{P}_{LA}^2}{2M_A} + V_i(\mathbf{R}) + \sum_i \frac{\mathbf{p}_i^2}{2m} + V_e(\mathbf{r}) + V_{ie}(\mathbf{r},\mathbf{R})$$

Purely Ionic part

Electronic part

$$V_i(\mathbf{R}) = \frac{e^2}{2} \sum_{\substack{LA,LB \\ (L,A)\neq(L,B)}} \frac{Z_A Z_B}{|\mathbf{R}_{LA} - \mathbf{R}_{MB}|}$$

Z_A atomic number

$$V_e(\mathbf{r},\mathbf{R}) = \frac{e^2}{2} \sum_{\substack{i,j \\ i\neq j}} \frac{1}{|\mathbf{r_i} - \mathbf{r_j}|}$$

$\mathbf{r}_i$ electronic coordinate

Crystal Hamiltonian

$$\mathcal{H} = \sum_{L,A} \frac{\mathbf{P}_{LA}^2}{2M_A} + V_i(\mathbf{R}) + \sum_i \frac{\mathbf{p}_i^2}{2m} + V_e(\mathbf{r}) + V_{ie}(\mathbf{r},\mathbf{R})$$

Purely Ionic part

Electronic part

$$V_i(\mathbf{R}) = \frac{e^2}{2} \sum_{\substack{LA,LB \\ (L,A)\neq(L,B)}} \frac{Z_A Z_B}{|\mathbf{R}_{LA} - \mathbf{R}_{MB}|}$$

Z_A atomic number

$$V_e(\mathbf{r},\mathbf{R}) = \frac{e^2}{2} \sum_{\substack{i,j \\ i\neq j}} \frac{1}{|\mathbf{r_i} - \mathbf{r_j}|}$$

$\mathbf{r}_i$ electronic coordinate

$$V_{ie}(\mathbf{r},\mathbf{R}) = -\sum_{i,LA} \frac{Z_A e^2}{|\mathbf{R}_{LA} - \mathbf{r_i}|}$$

« Bare » electron-ion interaction

Crystal Hamiltonian

$$\mathcal{H} = \sum_{L,A} \frac{\mathbf{P}_{LA}^2}{2M_A} + V_i(\mathbf{R}) + \sum_i \frac{\mathbf{p}_i^2}{2m} + V_e(\mathbf{r}) + V_{ie}(\mathbf{r},\mathbf{R})$$

Electronic Hamiltonian

$$H_{el} = \sum_i \frac{\mathbf{p}_i^2}{2m} + V_e(\mathbf{r}) + V_{ext}(\mathbf{r},\mathbf{R})$$

Exact factorization

$$\mathcal{H} = \sum_{L,A} \frac{\mathbf{P}_{LA}^2}{2M_A} + V_i(\mathbf{R}) + \sum_i \frac{\mathbf{p}_i^2}{2m} + V_e(\mathbf{r}) + V_{ie}(\mathbf{r},\mathbf{R})$$

$$\left[\mathcal{H} - i\hbar\frac{\partial}{\partial t}\right]\Phi(\mathbf{r},\mathbf{R},t) = 0$$

The exact solution of this equation is written as

1. $$\Phi(\mathbf{r},\mathbf{R},t) = \chi(\mathbf{R},t)\psi(\mathbf{r},\mathbf{R},t)$$

where for any t and any fixed ionic configuration **R**

2. $$\int d\mathbf{r}\,|\psi(\mathbf{r},\mathbf{R},t)|^2 = 1$$

Hunter, J. Quantum Chem., 9: 237-242 (1975)
Abedi et al. Phys. Rev. Lett. 105 123002 (2010)

Recasting the problem in terms of the ionic eigenvector

We can apply the Hamiltonian to the product of the functions:

$$\mathcal{H}\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R}) = \sum_I \frac{\mathbf{P}_I^2}{2M_I}\left[\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R})\right] + \chi(\mathbf{R})H_{el}\psi(\mathbf{r},\mathbf{R}) = \mathcal{E}\,\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R})$$

Recasting the problem in terms of the ionic eigenvector

We can apply the Hamiltonian to the product of the functions:

$$\mathcal{H}\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R}) = \sum_I \frac{\mathbf{P}_I^2}{2M_I}\left[\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R})\right] + \chi(\mathbf{R})H_{el}\psi(\mathbf{r},\mathbf{R}) = \mathcal{E}\,\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R})$$

This leads to:

$$\mathcal{H}\chi\psi = \sum_I \psi\frac{\mathbf{P}_I^2}{2M_I}\chi + \sum_I \frac{1}{2M_I}\left[2(\mathbf{P}_I\chi)\mathbf{P}_I + \chi\left(\mathbf{P}_I^2 + H_{el}\right)\right]\psi = \mathcal{E}\,\chi\psi$$

Recasting the problem in terms of the ionic eigenvector

We can apply the Hamiltonian to the product of the functions:

$$\mathcal{H}\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R}) = \sum_I \frac{\mathbf{P}_I^2}{2M_I}\left[\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R})\right] + \chi(\mathbf{R})H_{el}\psi(\mathbf{r},\mathbf{R}) = \mathcal{E}\,\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R})$$

This leads to:

$$\mathcal{H}\chi\psi = \sum_I \psi\frac{\mathbf{P}_I^2}{2M_I}\chi + \sum_I \frac{1}{2M_I}\left[2(\mathbf{P}_I\chi)\mathbf{P}_I + \chi\left(\mathbf{P}_I^2 + H_{el}\right)\right]\psi = \mathcal{E}\,\chi\psi$$

$\int d\mathbf{r}\,\psi^*$

$\int d\mathbf{r}\,\psi^*$

Recasting the problem in terms of the ionic eigenvector

We can apply the Hamiltonian to the product of the functions:

$$\mathcal{H}\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R}) = \sum_I \frac{\mathbf{P}_I^2}{2M_I}\left[\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R})\right] + \chi(\mathbf{R})H_{el}\psi(\mathbf{r},\mathbf{R}) = \mathcal{E}\,\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R})$$

This leads to:

$$\mathcal{H}\chi\psi = \sum_I \psi\frac{\mathbf{P}_I^2}{2M_I}\chi + \sum_I \frac{1}{2M_I}\left[2(\mathbf{P}_I\chi)\mathbf{P}_I + \chi\left(\mathbf{P}_I^2 + H_{el}\right)\right]\psi = \mathcal{E}\,\chi\psi$$

$\int d\mathbf{r}\,\psi^*$ $\int d\mathbf{r}\,\psi^*$

This leads to:

$$\sum_I \frac{\mathbf{P}_I^2}{2M_I}\chi + \sum_I \frac{1}{2M_I}\left[2(\mathbf{P}_I\chi)\langle\psi|\mathbf{P}_I|\psi\rangle + \chi\langle\psi|\mathbf{P}_I^2|\psi\rangle\right] + \chi\langle\psi|H_{el}|\psi\rangle = \mathcal{E}\,\chi$$

Recasting the problem in terms of the ionic eigenvector

We can apply the Hamiltonian to the product of the functions:

$$\mathcal{H}\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R}) = \sum_I \frac{\mathbf{P}_I^2}{2M_I}\left[\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R})\right] + \chi(\mathbf{R})H_{el}\psi(\mathbf{r},\mathbf{R}) = \mathcal{E}\,\chi(\mathbf{R})\psi(\mathbf{r},\mathbf{R})$$

This leads to:

$$\mathcal{H}\chi\psi = \sum_I \psi\frac{\mathbf{P}_I^2}{2M_I}\chi + \sum_I \frac{1}{2M_I}\left[2(\mathbf{P}_I\chi)\mathbf{P}_I + \chi\left(\mathbf{P}_I^2 + H_{el}\right)\right]\psi = \mathcal{E}\,\chi\psi$$

$\int d\mathbf{r}\,\psi^*$ $\int d\mathbf{r}\,\psi^*$

This leads to:

$$\sum_I \frac{\mathbf{P}_I^2}{2M_I}\chi + \sum_I \frac{1}{2M_I}\left[2(\mathbf{P}_I\chi)\langle\psi|\mathbf{P}_I|\psi\rangle + \chi\langle\psi|\mathbf{P}_I^2|\psi\rangle\right] + \chi\langle\psi|H_{el}|\psi\rangle = \mathcal{E}\,\chi$$

So that:

$$\left[\sum_I \frac{\mathbf{P}_I^2}{2M_I} + \sum_I \frac{1}{M_I}\langle\psi|\mathbf{P}_I|\psi\rangle\mathbf{P}_I + \sum_I \frac{1}{2M_I}\langle\psi|\mathbf{P}_I^2|\psi\rangle + E(\mathbf{R})\right]\chi = \mathcal{E}\,\chi$$

with:

$$E(\mathbf{R}) = \langle\psi|H_{el}|\psi\rangle$$

EXACT EQUATION

Born-Oppenheimer approximation

$$\left[\sum_I \frac{\mathbf{P}_I^2}{2M_I} + \sum_I \frac{1}{M_I}\langle\psi|\mathbf{P}_I|\psi\rangle\mathbf{P}_I + \sum_I \frac{1}{2M_I}\langle\psi|\mathbf{P}_I^2|\psi\rangle + E(\mathbf{R})\right]\chi = \mathcal{E}\,\chi$$

$$E(\mathbf{R}) = \langle\psi|H_{el}|\psi\rangle$$

Born-Oppenheimer approximation

$$\left[\sum_I \frac{\mathbf{P}_I^2}{2M_I} + \sum_I \frac{1}{M_I}\langle\psi|\mathbf{P}_I|\psi\rangle\mathbf{P}_I + \sum_I \frac{1}{2M_I}\langle\psi|\mathbf{P}_I^2|\psi\rangle + E(\mathbf{R})\right]\chi = \mathcal{E}\,\chi$$

$$E(\mathbf{R}) = \langle\psi|H_{el}|\psi\rangle$$

Born-Oppenheimer approximation


$$\left[\sum_I \frac{\mathbf{P}_I^2}{2M_I} + \sum_I \frac{1}{M_I}\langle\psi|\mathbf{P}_I|\psi\rangle\mathbf{P}_I + \sum_I \frac{1}{2M_I}\langle\psi|\mathbf{P}_I^2|\psi\rangle + E(\mathbf{R})\right]\chi = \mathcal{E}\,\chi$$

$$E(\mathbf{R}) = \langle\psi|H_{el}|\psi\rangle$$

- Electron and ions completely decoupled; no terms left coupling electrons and phonons.
- Eigenfunctions of the electronic problem $\psi_n(\mathbf{r},\mathbf{R})$
- Eigenfunctions of the ionic problem (harmonic) $\chi_\xi(\mathbf{R})$

$$H_{vib} = \sum_I \frac{\mathbf{P}_I^2}{2M_I} + E(\mathbf{R})$$

We now want to treat the neglected terms in perturbation theory.

Outline

- Born Oppenheimer (BO) and exact factorization
- Electron-phonon matrix elements
- Second quantization of the electron-phonon Hamiltonian
- Effects on the electrons
- Effects on the phonons
- Electron-phonon driven superconductivity

Neglected terms in the BO

$$\langle \chi_\rho \psi_m | \mathcal{H} | \chi_\xi \psi_n \rangle = \langle \chi_\xi | \left[\sum_I \frac{\mathbf{P}_I^2}{2M_I} + E(\mathbf{R}) \right] | \chi_\xi \rangle \delta_{\xi,\rho} \delta_{n,m} + \sum_I \frac{1}{M_I} \langle \chi_\rho | \mathbf{P}_I | \chi_\xi \rangle \langle \psi_m | \mathbf{P}_I \psi_n \rangle + \sum_I \frac{1}{2M_I} \langle \psi_m | \mathbf{P}_I^2 | \psi_n \rangle \delta_{\rho,\xi}$$

$$\Delta H^1 = \sum_I \frac{1}{M_I} \langle \chi_\rho | \mathbf{P}_I | \chi_\xi \rangle \langle \psi_m | \mathbf{P}_I \psi_n \rangle$$

$$\Delta H^2 = \sum_I \frac{1}{2M_I} \langle \psi_m | \mathbf{P}_I^2 | \psi_n \rangle \delta_{\rho,\xi}$$

Expansion around equilibrium position

Equilibrium position $\mathbf{R}_0$ $\psi_n(\mathbf{r}, \mathbf{R}^0) = \psi_n^0$

We expand $\psi_n(\mathbf{r}, \mathbf{R}) = \psi_n$ as:

$$\psi_n = \psi_n^0 + \delta\psi_n = \psi_n^0 + \delta\psi_n^1 + \delta\psi_n^2 + \ldots =$$

$$= \psi_n^0 + \sum_{n' \neq n} \frac{\langle \psi_{n'}^0 | \Delta H_e | \psi_n^0 \rangle}{\epsilon_n^0 - \epsilon_{n'}^0} \psi_{n'}^0 + \sum_{n' \neq n} \sum_{m' \neq n} \frac{\langle \psi_{n'}^0 | \Delta H_e | \psi_{m'}^0 \rangle}{\epsilon_n^0 - \epsilon_{m'}^0} \frac{\langle \psi_{m'}^0 | \Delta H_e | \psi_{n'}^0 \rangle}{\epsilon_n^0 - \epsilon_{n'}^0} \psi_{n'}^0 + \ldots$$

Perturbation theory with

$$\Delta H_e = H_e(\mathbf{R}) - H_e(\mathbf{R}^0) \approx \sum_J \boldsymbol{\nabla}_{\mathbf{u}_J} H_e \cdot \mathbf{u}_J + \frac{1}{2} \sum_{I,J} \boldsymbol{\nabla}_{\mathbf{u}_J} \boldsymbol{\nabla}_{\mathbf{u}_I} H_e \mathbf{u}_J \mathbf{u}_I + \ldots$$

Expansion around equilibrium position

Equilibrium position $\mathbf{R_0}$ $\psi_n(\mathbf{r}, \mathbf{R}^0) = \psi_n^0$

We expand $\psi_n(\mathbf{r}, \mathbf{R}) = \psi_n$ as:

$$\psi_n = \psi_n^0 + \delta\psi_n = \psi_n^0 + \delta\psi_n^1 + \delta\psi_n^2 + \ldots =$$

$$= \psi_n^0 + \sum_{n' \neq n} \frac{\langle \psi_{n'}^0 | \Delta H_e | \psi_n^0 \rangle}{\epsilon_n^0 - \epsilon_{n'}^0} \psi_{n'}^0 + \sum_{n' \neq n} \sum_{m' \neq n} \frac{\langle \psi_{n'}^0 | \Delta H_e | \psi_{m'}^0 \rangle}{\epsilon_n^0 - \epsilon_{m'}^0} \frac{\langle \psi_{m'}^0 | \Delta H_e | \psi_{n'}^0 \rangle}{\epsilon_n^0 - \epsilon_{n'}^0} \psi_{n'}^0 + \ldots$$

Perturbation theory with

$$\Delta H_e = H_e(\mathbf{R}) - H_e(\mathbf{R}^0) \approx \sum_J \boldsymbol{\nabla}_{\mathbf{u}_J} H_e \cdot \mathbf{u}_J + \frac{1}{2} \sum_{I,J} \boldsymbol{\nabla}_{\mathbf{u}_J} \boldsymbol{\nabla}_{\mathbf{u}_I} H_e \mathbf{u}_J \mathbf{u}_I + \ldots$$

Then we have to replace ψ_n in

$$\Delta H^1 = \sum_I \frac{1}{M_I} \langle \chi_\rho | \mathbf{P}_I | \chi_\xi \rangle \langle \psi_m | \mathbf{P}_I \psi_n \rangle$$

$$\Delta H^2 = \sum_I \frac{1}{2M_I} \langle \psi_m | \mathbf{P}_I^2 | \psi_n \rangle \delta_{\rho,\xi}$$

Expansion around equilibrium position: Linear order in $\mathbf{R}$-$\mathbf{R}_0$

$$\Delta H^1 = \sum_I \frac{1}{M_I} \langle \chi_\rho | \mathbf{P}_I | \chi_\xi \rangle \langle \psi_m | \mathbf{P}_I \psi_n \rangle$$

$$\langle \psi_m | \mathbf{P}_I \psi_n \rangle = \int_v [d\mathbf{r}] \, (\psi_m^0 + \delta\psi_m)^* \mathbf{P}_I (\psi_n^0 + \delta\psi_n) \approx \int [d\mathbf{r}] \, (\psi_m^0)^* \mathbf{P}_I \delta\psi_n$$

Expansion around equilibrium position: Linear order in $\mathbf{R}$-$\mathbf{R}_0$

$$\Delta H^1 = \sum_I \frac{1}{M_I} \langle \chi_\rho | \mathbf{P}_I | \chi_\xi \rangle \langle \psi_m | \mathbf{P}_I \psi_n \rangle$$

$$\langle \psi_m | \mathbf{P}_I \psi_n \rangle = \int_v [d\mathbf{r}] \, (\psi_m^0 + \delta\psi_m)^* \mathbf{P}_I (\psi_n^0 + \delta\psi_n) \approx \int [d\mathbf{r}] \, (\psi_m^0)^* \mathbf{P}_I \delta\psi_n$$

$$\begin{aligned}
\langle \psi_m | \mathbf{P}_I \psi_n \rangle &\approx \langle \psi_m | \mathbf{P}_I \delta\psi_n \rangle = \\
&= \sum_{n' \neq n} \langle \psi_m^0 | \mathbf{P}_I \left[|\psi_{n'}^0\rangle \frac{\langle \psi_{n'}^0 | \Delta H_e | \psi_n^0 \rangle}{\epsilon_n^0 - \epsilon_{n'}^0} \right] = \\
&= \sum_{n' \neq n} \langle \psi_m^0 | \psi_{n'}^0 \rangle \frac{\langle \psi_{n'}^0 | \mathbf{P}_I \Delta H_e | \psi_n^0 \rangle}{\epsilon_n^0 - \epsilon_{n'}^0} = \\
&= -i\hbar \frac{\langle \psi_m^0 | \boldsymbol{\nabla}_{\mathbf{u}_I} H_e | \psi_n^0 \rangle}{\epsilon_n^0 - \epsilon_m^0} (1 - \delta_{mn})
\end{aligned}$$

Expansion around equilibrium position: Linear order in $\mathbf{R}$-$\mathbf{R}_0$

$$\Delta H^1 = \sum_I \frac{1}{M_I} \langle \chi_\rho | \mathbf{P}_I | \chi_\xi \rangle \langle \psi_m | \mathbf{P}_I \psi_n \rangle$$

$$\langle \psi_m | \mathbf{P}_I \psi_n \rangle = \int_v [d\mathbf{r}] \, (\psi_m^0 + \delta\psi_m)^* \mathbf{P}_I (\psi_n^0 + \delta\psi_n) \approx \int [d\mathbf{r}] \, (\psi_m^0)^* \mathbf{P}_I \delta\psi_n$$

$$\Delta H^1 = -i\hbar \sum_I \frac{1}{M_I} \langle \chi_\rho | \mathbf{P}_I | \chi_\xi \rangle \frac{\langle \psi_m^0 | \nabla_{\mathbf{u}_I} H_e | \psi_n^0 \rangle}{\epsilon_n^0 - \epsilon_m^0} (1 - \delta_{mn})$$

Expansion around equilibrium position: Linear order in $\mathbf{R}$-$\mathbf{R}_0$

The terms $\Delta H^2 = \sum_I \frac{1}{2M_I} \langle \psi_m | \mathbf{P}_I^2 | \psi_n \rangle \delta_{\rho,\xi}$ are

$$\langle \psi_m | \mathbf{P}_I^2 | \psi_n \rangle = \int [d\mathbf{r}]\, \psi_m^*(\mathbf{r},\mathbf{R}) \mathbf{P}_I^2 \psi_n(\mathbf{r},\mathbf{R}) \approx \int [d\mathbf{r}]\, (\psi_m^0 + \delta\psi_m^1)^* \mathbf{P}_I^2 (\psi_n^0 + \delta\psi_n^1)$$

$$\text{As } \delta\psi_n^1 \text{ is linear in } \mathbf{u}_I, \text{ then } \mathbf{P}_I^2 \mathbf{u}_I = 0 \text{ and } \Delta H^2 = 0.$$

P.S. At second order they are non-zero (nonlinear electron-phonon coupling).

Expansion around equilibrium position: Linear order in $\mathbf{R}$-$\mathbf{R}_0$

$$\langle \chi_\rho \psi_m | \mathcal{H} | \chi_\xi \psi_n \rangle \approx \underbrace{\langle \chi_\xi | \left[\sum_I \frac{\mathbf{P}_I^2}{2M_I} + E(\mathbf{R}) \right] | \chi_\xi \rangle \delta_{\xi,\rho} \delta_{n,m}}_{H_{vib}}$$

$$-i\hbar \sum_I \frac{1}{M_I} \langle \chi_\rho | \mathbf{P}_I | \chi_\xi \rangle \frac{\langle \psi_m^0 | \nabla_{\mathbf{u}_I} H_e | \psi_n^0 \rangle}{\epsilon_n^0 - \epsilon_m^0} (1 - \delta_{mn})$$

We rearrange these terms to obtain the linear electron-phonon coupling.

Linear electron-phonon coupling

We note that:

$$[H_{vib}, \mathbf{R}_I] = [H_{vib}, \mathbf{u}_I] = -i\hbar \frac{\mathbf{P}_I}{M_I}$$

meaning

$$-i\hbar \sum_I \frac{1}{M_I} \langle \chi_\rho | \mathbf{P}_I | \chi_\xi \rangle = \sum_I \langle \chi_\rho | [H_{vib}, \mathbf{u}_I] | \chi_\xi \rangle = (\mathcal{E}_\rho - \mathcal{E}_\xi) \sum_I \langle \chi_\rho | \mathbf{u}_I | \chi_\xi \rangle$$

We impose that the scattering among electrons and phonons conserves energy:

$$\mathcal{E}_\rho - \mathcal{E}_\xi = \epsilon^0_n - \epsilon^0_m$$

Linear electron-phonon coupling

We note that:

$$[H_{vib}, \mathbf{R}_I] = [H_{vib}, \mathbf{u}_I] = -i\hbar \frac{\mathbf{P}_I}{M_I}$$

meaning

$$-i\hbar \sum_I \frac{1}{M_I} \langle \chi_\rho | \mathbf{P}_I | \chi_\xi \rangle = \sum_I \langle \chi_\rho | [H_{vib}, \mathbf{u}_I] | \chi_\xi \rangle = (\mathcal{E}_\rho - \mathcal{E}_\xi) \sum_I \langle \chi_\rho | \mathbf{u}_I | \chi_\xi \rangle$$

So that $\mathcal{E}_\rho - \mathcal{E}_\xi = \epsilon_n^0 - \epsilon_m^0$

$$\Delta H^1 = -i\hbar \sum_I \frac{1}{M_I} \langle \chi_\rho | \mathbf{P}_I | \chi_\xi \rangle \frac{\langle \psi_m^0 | \nabla_{\mathbf{u}_I} H_e | \psi_n^0 \rangle}{\epsilon_n^0 - \epsilon_m^0} (1 - \delta_{mn})$$

becomes

$$\Delta H^1 = \sum_I \langle \chi_\rho | \mathbf{u}_I | \chi_\xi \rangle \langle \psi_m^0 | \nabla_{\mathbf{u}_I} H_e | \psi_n^0 \rangle = \sum_{La\alpha} \langle \chi_\rho | u_{La\alpha} | \chi_\xi \rangle \langle \psi_m^0 | \frac{\partial H_e}{\partial u_{La\alpha}} | \psi_n^0 \rangle$$

Linear electron-phonon coupling

$$\Delta H^1 = \sum_I \langle \chi_\rho | \mathbf{u}_I | \chi_\xi \rangle \langle \psi^0_m | \nabla_{\mathbf{u}_I} H_e | \psi^0_n \rangle = \sum_{La\alpha} \langle \chi_\rho | u_{La\alpha} | \chi_\xi \rangle \langle \psi^0_m | \frac{\partial H_e}{\partial u_{La\alpha}} | \psi^0_n \rangle$$

Deformation Potential
(real space)

$$\mathbf{u}_{La\alpha} = \sqrt{\frac{\hbar}{2N}} \sum_{\nu\mathbf{q}} \frac{(e^{a\alpha}_{\mathbf{q}\nu})^*}{\sqrt{M_a \omega_{\mathbf{q}\nu}}} e^{i\mathbf{q}\mathbf{R}_L} (a_{\mathbf{q}\nu} + a^\dagger_{-\mathbf{q}\nu})$$ (Harmonic approx.)

$$\Delta H^1 = \sqrt{\frac{\hbar}{2N}} \sum_{\nu\mathbf{q}} \sum_{La\alpha} \frac{(e^{a\alpha}_{\mathbf{q}\nu})^*}{\sqrt{M_a \omega_{\mathbf{q}\nu}}} e^{i\mathbf{q}\mathbf{R}_L} \langle \chi_\rho | a_{\mathbf{q}\nu} + a^\dagger_{-\mathbf{q}\nu} | \chi_\xi \rangle \langle \psi^0_m | \frac{\partial H_e}{\partial u_{La\alpha}} | \psi^0_n \rangle$$

Linear electron-phonon coupling

$$\Delta H^1 = \sqrt{\frac{\hbar}{2N}} \sum_{\nu\mathbf{q}} \sum_{La\alpha} \frac{(e^{a\alpha}_{\mathbf{q}\nu})^*}{\sqrt{M_a \omega_{\mathbf{q}\nu}}} e^{i\mathbf{q}\mathbf{R}_L} \langle \chi_\rho | a_{\mathbf{q}\nu} + a^\dagger_{-\mathbf{q}\nu} | \chi_\xi \rangle \langle \psi^0_m | \frac{\partial H_e}{\partial u_{La\alpha}} | \psi^0_n \rangle$$

Using

$$\frac{\partial}{\partial u_{La\alpha}} = \sum_{\mathbf{q}} \frac{\partial u_{\mathbf{q}a\alpha}}{\partial u_{La\alpha}} \frac{\partial}{\partial u_{\mathbf{q}a\alpha}} = \frac{1}{N} \sum_{\mathbf{q}} e^{-i\mathbf{q}\mathbf{R}_L} \frac{\partial}{\partial u_{\mathbf{q}a\alpha}}$$

We have

$$\Delta H^1 = \sum_{\nu\mathbf{q}} \sum_{a\alpha} \sqrt{\frac{\hbar}{2N M_a \omega_{\mathbf{q}\nu}}} (e^{a\alpha}_{\mathbf{q}\nu})^* \langle \chi_\rho | a_{\mathbf{q}\nu} + a^\dagger_{-\mathbf{q}\nu} | \chi_\xi \rangle \langle \psi^0_m | \frac{\partial H_e}{\partial u_{\mathbf{q}a\alpha}} | \psi^0_n \rangle$$

Outline

- Born Oppenheimer (BO) and exact factorization
- Electron-phonon matrix elements
- Second quantization of the electron-phonon Hamiltonian
- Effects on the electrons
- Effects on the phonons
- Electron-phonon driven superconductivity

Second quantization

Consider $$\Delta H^1 = \sum_{\nu\mathbf{q}}\sum_{a\alpha}\sqrt{\frac{\hbar}{2NM_a\omega_{\mathbf{q}\nu}}}(e^{a\alpha}_{\mathbf{q}\nu})^*\langle\chi_\rho|a_{\mathbf{q}\nu}+a^\dagger_{-\mathbf{q}\nu}|\chi_\xi\rangle\langle\psi^0_m|\frac{\partial H_e}{\partial u_{\mathbf{q}a\alpha}}|\psi^0_n\rangle$$

One body operators are written in second quantization as:

$$\mathcal{O} = \sum_{s,s'}\langle\phi_s|\mathcal{O}|\phi_{s'}\rangle c^\dagger_s c_{s'}$$

where $\{|\phi_s\rangle\}$ is any chosen single particle basis.

For a crystal we choose $$\phi_n \mapsto \psi_{\mathbf{k}n}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}}u_{\mathbf{k}n}(\mathbf{r})/\sqrt{N}$$

Second quantization

If we define the screened Kohn-Sham potential as $V_{KS}(\mathbf{r}) = H_{el} - T_{el}$

and perform a monochromatic perturbation $V_{KS}(\mathbf{r}) = e^{i\mathbf{qr}} v_{KS}(\mathbf{r})$

We have

$$\begin{aligned}
\langle \psi^0_{\mathbf{k}m} | \frac{\partial H_e}{\partial u_{a\alpha}} | \psi^0_{\mathbf{k}'n} \rangle &= \frac{1}{N} \int_V d\mathbf{r} e^{-i\mathbf{kr}} u^*_{\mathbf{k}m}(\mathbf{r}) e^{i\mathbf{qr}} \frac{\partial v_{KS}(\mathbf{r})}{\partial u_{a\alpha}} e^{i\mathbf{k}'\mathbf{r}} u_{\mathbf{k}'m}(\mathbf{r}) = \\
&= \frac{1}{N} \sum_R e^{i(\mathbf{k}'-\mathbf{k}+\mathbf{q})\mathbf{R}} \int_\Omega d\mathbf{r} e^{-i\mathbf{kr}} u^*_{\mathbf{k}m}(\mathbf{r}) e^{i\mathbf{qr}} \frac{\partial v_{KS}(\mathbf{r})}{\partial u_{a\alpha}} e^{i\mathbf{k}'\mathbf{r}} u_{\mathbf{k}'m}(\mathbf{r}) = \\
&= \delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}} \left\langle u_{\mathbf{k}m} \left| \frac{\partial v_{KS}(\mathbf{r})}{\partial u_{a\alpha}} \right| u_{\mathbf{k}+\mathbf{q}n} \right\rangle
\end{aligned}$$

Defining the electron-phonon matrix element as

$$g^{\nu}_{\mathbf{k}m,\mathbf{k}+\mathbf{q}n} = \sqrt{\frac{\hbar}{2N}} \sum_{a\alpha} \frac{(e^{a\alpha}_{\mathbf{q}\nu})^*}{\sqrt{M_a \omega_{\mathbf{q}\nu}}} \left\langle u_{\mathbf{k}m} \left| \frac{\partial v_{KS}(\mathbf{r})}{\partial u_{a\alpha}} \right| u_{\mathbf{k}+\mathbf{q}n} \right\rangle$$

Hamiltonian in second quantization (Frölich)

We obtain the electron-phonon Hamiltonian in second quantization:

$$\hat{H}_{e-ph} = \sum_{\mathbf{k}n} \epsilon_{\mathbf{k}n} c^{\dagger}_{\mathbf{k}n} c_{\mathbf{k}n} + \sum_{\mathbf{q}\nu} \hbar\omega_{\mathbf{q}\nu} \left(a^{\dagger}_{\mathbf{q}\nu} a_{\mathbf{q}\nu} + \frac{1}{2} \right) + \sum_{\mathbf{k},\mathbf{q}} \sum_{n,m} \sum_{\nu} g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} c^{\dagger}_{\mathbf{k}n} c_{\mathbf{k}+\mathbf{q}m} (a_{\mathbf{q}\nu} + a^{\dagger}_{-\mathbf{q}\nu})$$

with

$$\epsilon_{\mathbf{k}n} = \langle \psi_{\mathbf{k}n} | H_{KS} | \psi_{\mathbf{k}+\mathbf{q},m} \rangle - \epsilon_F$$

and

$$g^{\nu}_{\mathbf{k}m,\mathbf{k}+\mathbf{q}n} = \sqrt{\frac{\hbar}{2N}} \sum_{a\alpha} \frac{(e^{a\alpha}_{\mathbf{q}\nu})^*}{\sqrt{M_a \omega_{\mathbf{q}\nu}}} \left\langle u_{\mathbf{k}m} \left| \frac{\partial v_{KS}(\mathbf{r})}{\partial u_{a\alpha}} \right| u_{\mathbf{k}+\mathbf{q}n} \right\rangle$$

Outline

- Born Oppenheimer (BO) and exact factorization
- Electron-phonon matrix elements
- Second quantization of the electron-phonon Hamiltonian
- Effects on the electrons
- Effects on the phonons
- Electron-phonon driven superconductivity

Perturbation Theory

$$\hat{H}_{e-ph} = \sum_{\mathbf{k}n} \epsilon_{\mathbf{k}n} c^{\dagger}_{\mathbf{k}n} c_{\mathbf{k}n} + \sum_{\mathbf{q}\nu} \hbar\omega_{\mathbf{q}\nu} \left(a^{\dagger}_{\mathbf{q}\nu} a_{\mathbf{q}\nu} + \frac{1}{2} \right) + \sum_{\mathbf{k},\mathbf{q}} \sum_{n,m} \sum_{\nu} g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} c^{\dagger}_{\mathbf{k}n} c_{\mathbf{k}+\mathbf{q}m} (a_{\mathbf{q}\nu} + a^{\dagger}_{-\mathbf{q}\nu})$$

Green functions

$G_0(kn, \omega)$

$G(kn, \omega)$

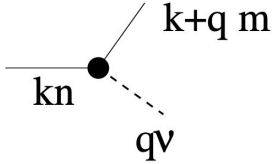
$D_0(q\,\nu, \omega)$

$D(q\,\nu, \omega)$

Free/bare

Interacting/dressed

electron-phonon vertex



- $g^{\nu}_{kn,k+q\,m}$

Perturbation Theory

Electrons

Phonons

$$G_0(\mathbf{k}n,\omega) = \frac{1}{\hbar\omega - \epsilon_{\mathbf{k}n} + i\eta}$$

non-interacting

$$D_0(\mathbf{q}\nu,\omega) = \frac{2\hbar\omega_{\mathbf{q}\nu}}{(\hbar\omega)^2 - (\hbar\omega_{\mathbf{q}\nu})^2 + i\eta}$$

$$G(\mathbf{k}n,\omega) = \frac{1}{\hbar\omega - \epsilon_{\mathbf{k}n} - \Sigma(\mathbf{k}n,\omega)}$$

interacting

$$D(\mathbf{q}\nu,\omega) = \frac{2\hbar\omega_{\mathbf{q}\nu}}{(\hbar\omega)^2 - (\hbar\omega_{\mathbf{q}\nu})^2 + i\eta - 2\hbar\omega_{\mathbf{q}\nu}\Pi(\mathbf{q}\nu,\omega)}$$

Electron self energy

$$\Sigma(\mathbf{k}n,\omega) = G_0^{-1}(\mathbf{k}n,\omega) - G^{-1}(\mathbf{k}n,\omega)$$

Phonon self-energy

$$\Pi(\mathbf{q}\nu,\omega) = D_0^{-1}(\mathbf{q}\nu,\omega) - D^{-1}(\mathbf{q}\nu,\omega)$$

What is the effect of the self-energy (i.e. interactions) on the spectrum ?

Effect on the electrons: spectral function

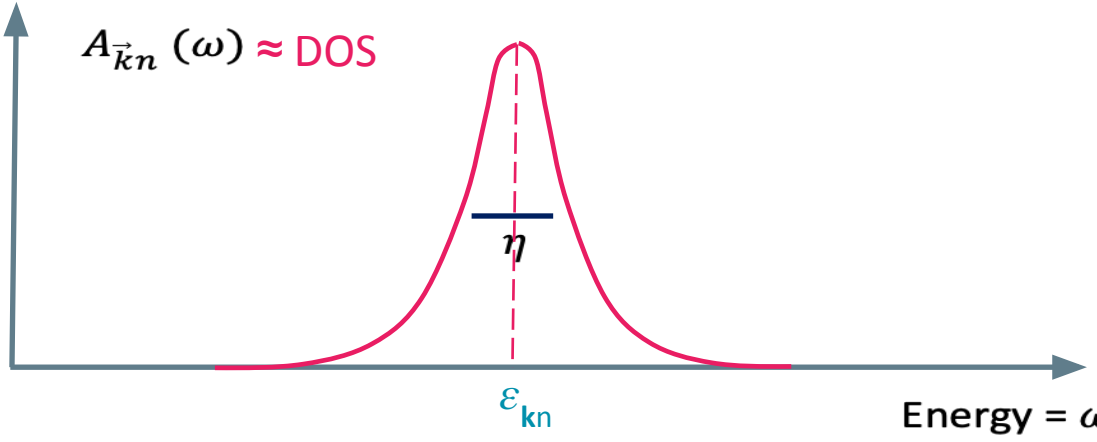
Spectral function

$$A_{\mathbf{k}n}(\omega) = -\operatorname{Im} G(\mathbf{k}n,\omega) = -\frac{\operatorname{Im}\Sigma(\mathbf{k}n,\omega)}{\left(\hbar\omega - \epsilon_{\mathbf{k}n} - \operatorname{Re}\Sigma(\mathbf{k}n,\omega)\right)^2 + \left(\operatorname{Im}\Sigma(\mathbf{k}n,\omega)\right)^2}$$

In the absence of interaction,

$$\operatorname{Re}\Sigma(\mathbf{k}n,\omega) \quad \to 0$$
$$\operatorname{Im}\Sigma(\mathbf{k}n,\omega) \quad \to \eta$$

the spectral weight has simple poles at the energies ε_{kn}



Fixed k

(Lorentzian)

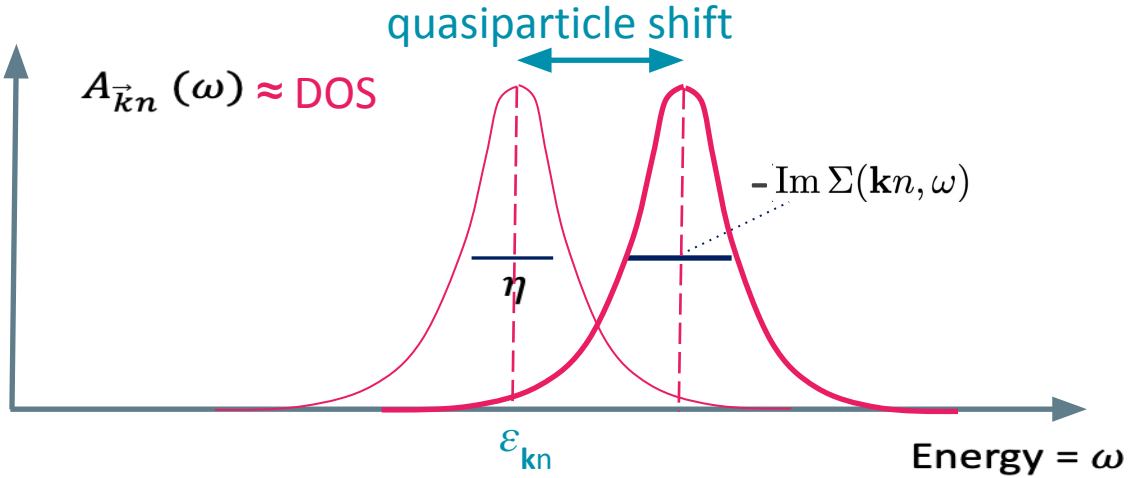
Effect on the electrons: spectral function

Spectral function

$$A_{\mathbf{k}n}(\omega) = -\operatorname{Im} G(\mathbf{k}n,\omega) = -\frac{\operatorname{Im}\Sigma(\mathbf{k}n,\omega)}{\left(\hbar\omega - \epsilon_{\mathbf{k}n} - \operatorname{Re}\Sigma(\mathbf{k}n,\omega)\right)^2 + \left(\operatorname{Im}\Sigma(\mathbf{k}n,\omega)\right)^2}$$

In the presence of interaction if $\operatorname{Im}\Sigma(\mathbf{k}n,\omega) \ll \operatorname{Re}\Sigma(\mathbf{k}n,\omega)$

THE QUASIPARTICLE PICTURE IS PRESERVED



Fixed k

(Lorentzian)

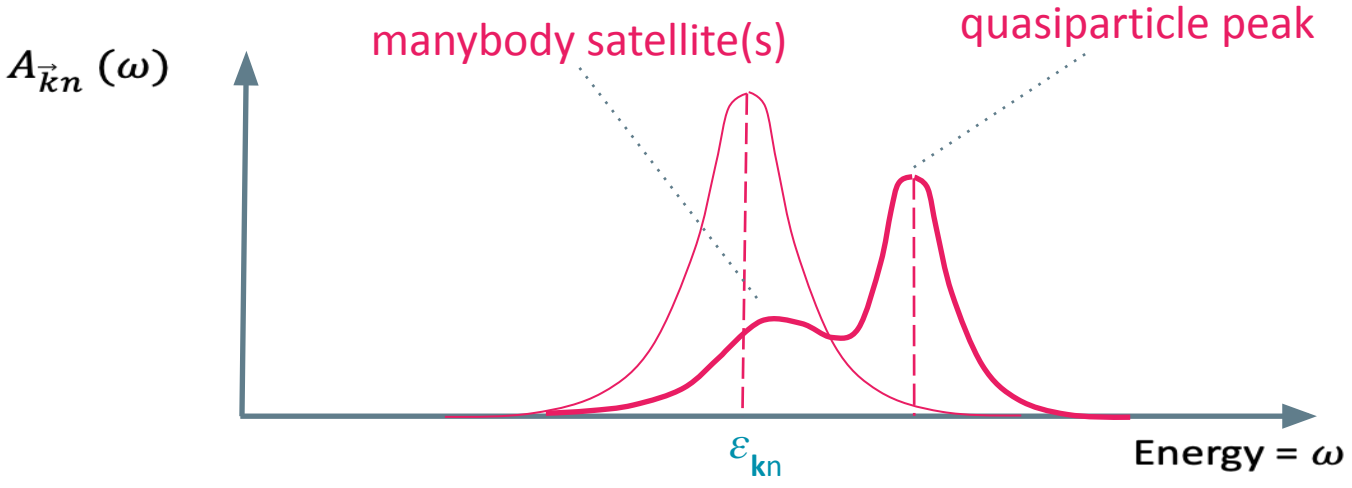
Effect on the electrons: spectral function

Spectral function

$$A_{\mathbf{k}n}(\omega) = -\operatorname{Im} G(\mathbf{k}n,\omega) = -\frac{\operatorname{Im}\Sigma(\mathbf{k}n,\omega)}{\left(\hbar\omega - \epsilon_{\mathbf{k}n} - \operatorname{Re}\Sigma(\mathbf{k}n,\omega)\right)^2 + \left(\operatorname{Im}\Sigma(\mathbf{k}n,\omega)\right)^2}$$

In the presence of interaction if $\operatorname{Im}\Sigma(\mathbf{k}n,\omega)$ is large

THE QUASIPARTICLE PICTURE IS BROKEN



Fixed k

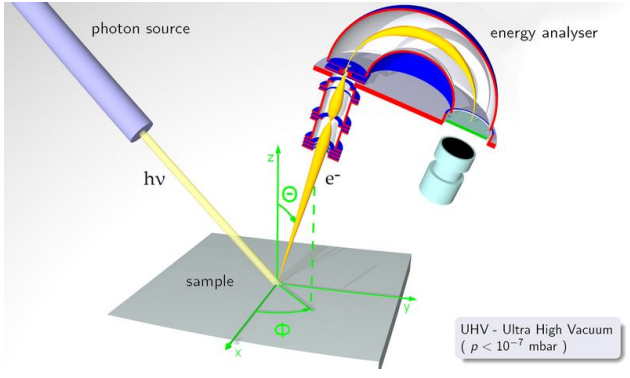
(non Lorentzian)

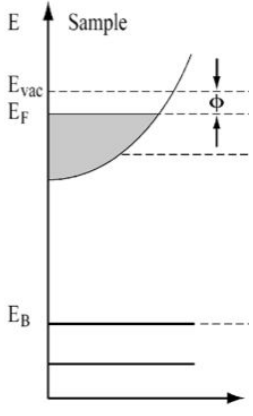
Effect on the electrons: spectral function

Spectral function

$$A_{\mathbf{k}n}(\omega) = -\operatorname{Im} G(\mathbf{k}n,\omega) = -\frac{\operatorname{Im}\Sigma(\mathbf{k}n,\omega)}{\left(\hbar\omega - \epsilon_{\mathbf{k}n} - \operatorname{Re}\Sigma(\mathbf{k}n,\omega)\right)^2 + \left(\operatorname{Im}\Sigma(\mathbf{k}n,\omega)\right)^2}$$

Angle-resolved photoemission experiments essentially measure the spectral weight of the occupied electronic states (times a matrix element)





Quasiparticle picture

$$\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) \;<<\; \mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)$$

We can expand around the quasiparticle peak $E_{\mathbf{k}n}$

$$\Sigma(\mathbf{k}n,\omega) \approx \Sigma(\mathbf{k}n,E_{\mathbf{k}n}) + \frac{1}{\hbar}\left.\frac{\partial\Sigma(\mathbf{k}n,\omega)}{\partial\omega}\right|_{\omega=E_{\mathbf{k}n}/\hbar}(\hbar\omega - E_{\mathbf{k}n})$$

Quasiparticle picture

$$\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) \;<<\; \mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)$$

We can expand around the quasiparticle peak $E_{\mathbf{k}n}$

$$\Sigma(\mathbf{k}n,\omega) \approx \Sigma(\mathbf{k}n,E_{\mathbf{k}n}) + \frac{1}{\hbar}\left.\frac{\partial\Sigma(\mathbf{k}n,\omega)}{\partial\omega}\right|_{\omega=E_{\mathbf{k}n}/\hbar}(\hbar\omega - E_{\mathbf{k}n})$$

Assuming also that $\frac{\partial\,\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega)}{\partial\omega} << \frac{\partial\,\mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)}{\partial\omega}$ we obtain:

Quasiparticle picture

$$\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) \;<<\; \mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)$$

We can expand around the quasiparticle peak E_{kn}

$$\Sigma(\mathbf{k}n,\omega) \approx \Sigma(\mathbf{k}n,E_{\mathbf{k}n}) + \frac{1}{\hbar}\left.\frac{\partial\Sigma(\mathbf{k}n,\omega)}{\partial\omega}\right|_{\omega=E_{\mathbf{k}n}/\hbar}(\hbar\omega - E_{\mathbf{k}n})$$

Assuming also that $\frac{\partial\,\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega)}{\partial\omega} << \frac{\partial\,\mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)}{\partial\omega}$ we obtain:

$$A_{\mathbf{k}n}(\omega) = -\frac{\mathrm{Im}\,\Sigma(\mathbf{k}n,E_{\mathbf{k}n})}{\left(\hbar\omega - \epsilon_{\mathbf{k}n} - \mathrm{Re}\,\Sigma(\mathbf{k}n,E_{\mathbf{k}n}) - \frac{1}{\hbar}\left.\frac{\partial\,\mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)}{\partial\omega}\right|_{\omega=E_{\mathbf{k}n}/\hbar}(\hbar\omega - E_{\mathbf{k}n})\right)^2 + (\mathrm{Im}\,\Sigma(\mathbf{k}n,E_{\mathbf{k}n}))^2}$$

The quasiparticles are shifted by an amount

$$\epsilon_{\mathbf{k}n} \longmapsto E_{\mathbf{k}n} \quad = \quad \epsilon_{\mathbf{k}n} + \mathrm{Re}\,\Sigma(\mathbf{k}n,E_{\mathbf{k}n}) + \lambda_{\mathbf{k}n}(\hbar\omega - E_{\mathbf{k}n})$$

Where $\lambda_{\mathbf{k}n} = \frac{1}{\hbar}\left.\frac{\partial\,\mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)}{\partial\omega}\right|_{\omega=E_{\mathbf{k}n}/\hbar}$ Is called the mass enhancement parameter.

Quasiparticle picture

$$\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) \;<<\; \mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)$$

The quasiparticles are shifted by an amount

$$\epsilon_{\mathbf{k}n} \longmapsto E_{\mathbf{k}n} \;=\; \epsilon_{\mathbf{k}n} + \mathrm{Re}\,\Sigma(\mathbf{k}n, E_{\mathbf{k}n}) + \lambda_{\mathbf{k}n}(\hbar\omega - E_{\mathbf{k}n})$$

Where $$\lambda_{\mathbf{k}n} = \frac{1}{\hbar}\left.\frac{\partial\,\mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)}{\partial\omega}\right|_{\omega=E_{\mathbf{k}n}/\hbar}$$ Is called the mass enhancement parameter.

Taking the gradient with respect to **k** we get

$$\mathbf{V}_{\mathbf{k}n} = \mathbf{v}_{\mathbf{k}n} - \lambda_{\mathbf{k}n}\mathbf{V}_{\mathbf{k}n}$$

Dressed velocity

Bare velocity

Quasiparticle picture

$$\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) \;<<\; \mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)$$

The quasiparticles are shifted by an amount

$$\epsilon_{\mathbf{k}n} \longmapsto E_{\mathbf{k}n} \;=\; \epsilon_{\mathbf{k}n} + \mathrm{Re}\,\Sigma(\mathbf{k}n, E_{\mathbf{k}n}) + \lambda_{\mathbf{k}n}(\hbar\omega - E_{\mathbf{k}n})$$

Where $\lambda_{\mathbf{k}n} = \frac{1}{\hbar}\left.\frac{\partial\,\mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)}{\partial\omega}\right|_{\omega=E_{\mathbf{k}n}/\hbar}$ Is called the mass enhancement parameter.

Taking the gradient with respect to **k** we get*

$$\mathbf{V}_{\mathbf{k}n} = \mathbf{v}_{\mathbf{k}n} - \lambda_{\mathbf{k}n}\mathbf{V}_{\mathbf{k}n}$$

Dressed velocity — Bare velocity

$\mathbf{V}_{\mathbf{k}n} = \frac{\mathbf{v}_{\mathbf{k}n}}{1+\lambda_{\mathbf{k}n}}$ Velocity renormalization due to the electron-phonon coupling

As $\lambda_{\mathbf{k}n} > 0$ The velocity is always reduced by the electron-phonon coupling

Quasiparticle picture

$\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) \;<<\; \mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)$

$$\mathbf{V}_{\mathbf{k}n} = \frac{\mathbf{v}_{\mathbf{k}n}}{1+\lambda_{\mathbf{k}n}}$$

or, equivalently, a renormalized effective mass (v=p/m):

$$M^*_{\mathbf{k}n} = (1+\lambda_{\mathbf{k}n}) m^*_{\mathbf{k}n}$$

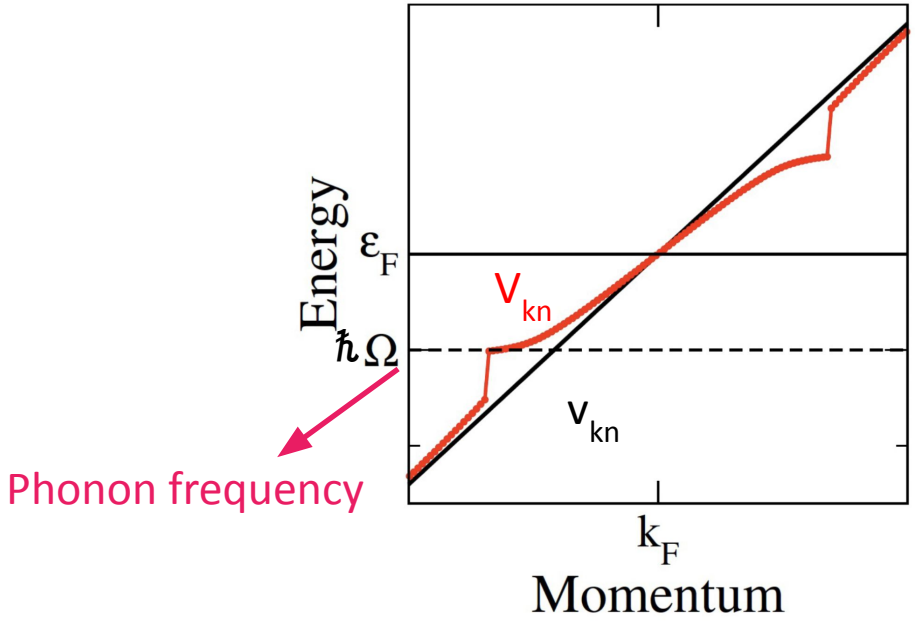
$\lambda_{\mathbf{k}n} > 0$ → The effective mass is always enhanced by the electron-phonon coupling

That is why $\lambda_{\mathbf{k}n}$ is called the mass enhancement parameter.

Velocity and mass renormalization

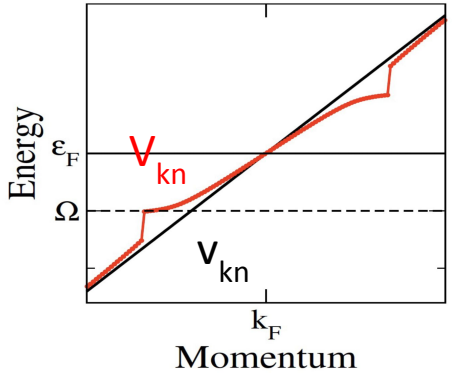
$\mathbf{V}_{\mathbf{k}n} = \dfrac{\mathbf{v}_{\mathbf{k}n}}{1+\lambda_{\mathbf{k}n}}$ Velocity renormalization due to the electron-phonon coupling

$M^*_{\mathbf{k}n} = (1+\lambda_{\mathbf{k}n})m^*_{\mathbf{k}n}$ Mass renormalization due to the electron-phonon coupling

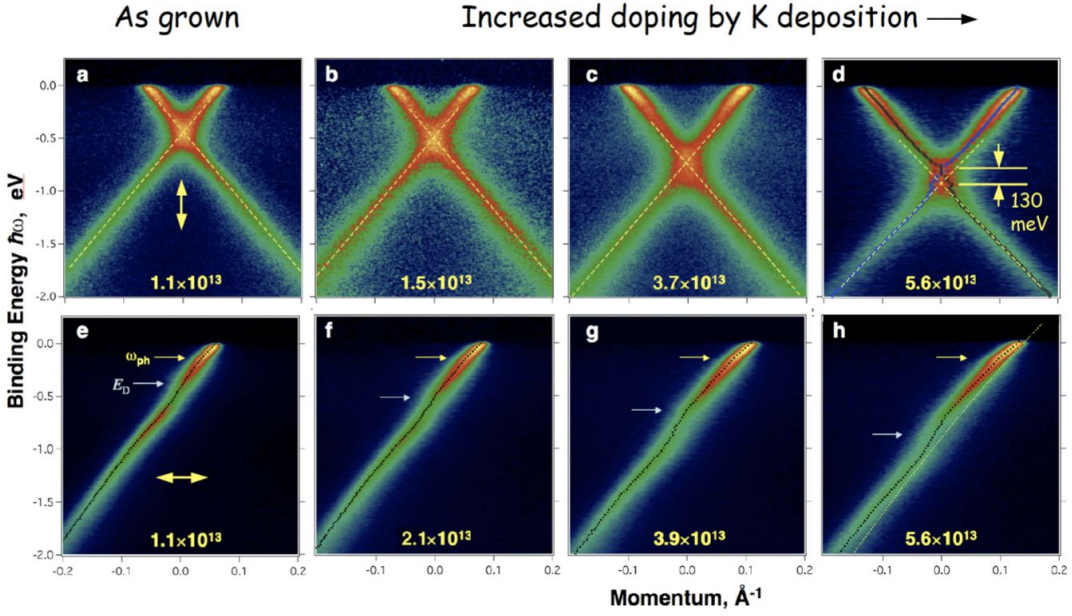


The red line has an enhanced mass with respect to the black one.

Velocity and mass renormalization – Experiments (K-covered Graphene)

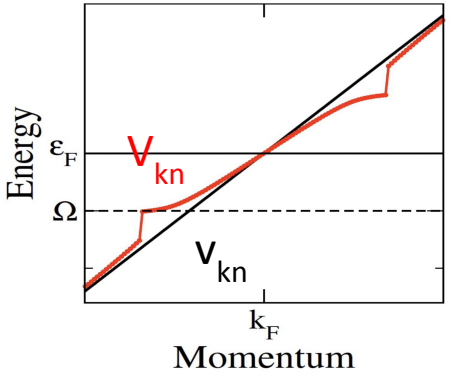


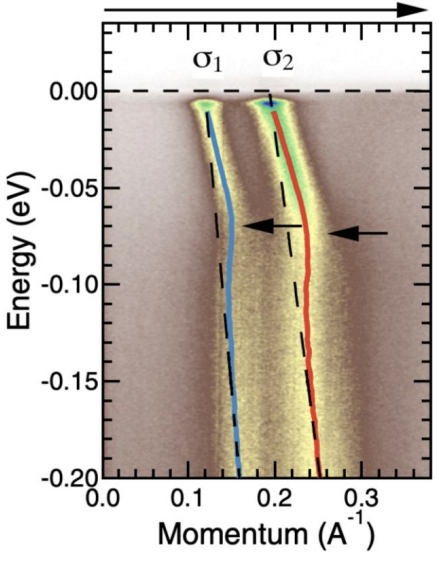
$A(\mathbf{k},\omega)$



A. Bostwick *et al.* Nature Physics (2007)

Velocity and mass renormalization – Experiments (MgB_2)





Quasiparticle picture $\quad \mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) \;<<\; \mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)$

We can expand around the quasiparticle peak $E_{\mathbf{k}n}$

$$\Sigma(\mathbf{k}n,\omega) \approx \Sigma(\mathbf{k}n,E_{\mathbf{k}n}) + \frac{1}{\hbar}\left.\frac{\partial\Sigma(\mathbf{k}n,\omega)}{\partial\omega}\right|_{\omega=E_{\mathbf{k}n}/\hbar}(\hbar\omega - E_{\mathbf{k}n})$$

Assuming also that $\frac{\partial\,\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega)}{\partial\omega} << \frac{\partial\,\mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)}{\partial\omega}$ we obtain:

$$A_{\mathbf{k}n}(\omega) = -\frac{\mathrm{Im}\,\Sigma(\mathbf{k}n,E_{\mathbf{k}n})}{\left(\hbar\omega - \epsilon_{\mathbf{k}n} - \mathrm{Re}\,\Sigma(\mathbf{k}n,E_{\mathbf{k}n}) - \frac{1}{\hbar}\left.\frac{\partial\,\mathrm{Re}\,\Sigma(\mathbf{k}n,\omega)}{\partial\omega}\right|_{\omega=E_{\mathbf{k}n}/\hbar}(\hbar\omega - E_{\mathbf{k}n})\right)^2 + (\mathrm{Im}\,\Sigma(\mathbf{k}n,E_{\mathbf{k}n}))^2}$$

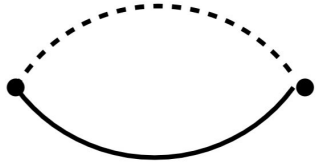
We finally note that the width of the Lorentzian is $\quad \Gamma_{\mathbf{k}n} = \quad -\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega)$

The electron scattering time for an electron of momentum **k** in the nth band is

$$\boxed{\frac{\Gamma_{\mathbf{k}n}}{2} = \frac{\hbar}{2\tau_{\mathbf{k}n}}}$$

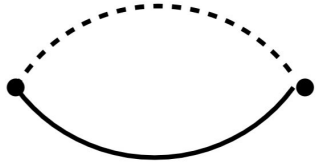
Electron self-energy

The lowest energy diagram is

$\Sigma(\mathrm{kn},\omega)=$ 

Electron self-energy

The lowest energy diagram is

$\Sigma(\mathrm{kn},\omega)=$ 

Leading to:

$$\Sigma(\mathbf{k}n,\omega)=\frac{1}{N_q}\sum_{\mathbf{q}m}\sum_{\nu}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2\left[\frac{n_{\mathbf{q}\nu}+f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega+\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m}+i\eta}+\frac{n_{\mathbf{q}\nu}+1-f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega-\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m}+i\eta}\right]$$

with:

$$n_{\mathbf{q}\nu}=\frac{1}{\exp(\beta\hbar\omega_{\mathbf{q}\nu})-1} \qquad f_{\mathbf{k}n}=\frac{1}{\exp(\beta(\epsilon_{\mathbf{k}n}-\mu))+1}$$

Real part of the electron self-energy

The real part is

Principal value

$$\mathrm{Re}\,\Sigma(\mathbf{k}n,\omega) = \frac{1}{N_q}\mathcal{P}\sum_{\mathbf{q}n}\sum_{\nu}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2\left[\frac{n_{\mathbf{q}\nu}+f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega+\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m}}+\frac{n_{\mathbf{q}\nu}+1-f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega-\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m}}\right]$$

Real part of the electron self-energy

The real part is

Principal value

$$\mathrm{Re}\,\Sigma(\mathbf{k}n,\omega) = \frac{1}{N_q}\mathcal{P}\sum_{\mathbf{q}n}\sum_{\nu}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2\left[\frac{n_{\mathbf{q}\nu}+f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega+\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m}}+\frac{n_{\mathbf{q}\nu}+1-f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega-\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m}}\right]$$

The quasiparticles are:

$$E_{\mathbf{k}n} = \epsilon_{\mathbf{k}n} + \mathrm{Re}\,\Sigma(\mathbf{k}n, \omega = E_{\mathbf{k}n}/\hbar)$$

Imaginary part of the electron self-energy

The imaginary part is

$$\begin{aligned}\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) &= -\frac{\pi}{N_q}\sum_{\mathbf{q}m}\sum_{\nu}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2\left[(n_{\mathbf{q}\nu}+f_{\mathbf{k}+\mathbf{q}m})\,\delta(\hbar\omega+\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m})\right.\\ &\left.+\,(n_{\mathbf{q}\nu}+1-f_{\mathbf{k}+\mathbf{q}m})\,\delta(\hbar\omega-\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m})\right]\end{aligned}$$

Note the similarity of this expression with the Fermi golden rule.

Imaginary part of the electron self-energy

The imaginary part is

$$\begin{aligned}\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) &= -\frac{\pi}{N_q}\sum_{\mathbf{q}m}\sum_{\nu}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2\left[(n_{\mathbf{q}\nu}+f_{\mathbf{k}+\mathbf{q}m})\,\delta(\hbar\omega+\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m})\right.\\ &\left.+\,(n_{\mathbf{q}\nu}+1-f_{\mathbf{k}+\mathbf{q}m})\,\delta(\hbar\omega-\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m})\right]\end{aligned}$$

Note the similarity of this expression with the Fermi golden rule.

At low temperature the Bose functions can be neglected and

$$-\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega)=\frac{\pi}{N_q}\sum_{\mathbf{q}m}\sum_{\nu}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2\left[f_{\mathbf{k}+\mathbf{q}m}\delta(\hbar\omega+\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m})+(1-f_{\mathbf{k}+\mathbf{q}m})\,\delta(\hbar\omega-\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m})\right]\quad\propto\frac{1}{\tau}$$

Eliashberg function

The imaginary part is

$$\begin{aligned}\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) &= -\frac{\pi}{N_q}\sum_{\mathbf{q}m}\sum_{\nu}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2\left[(n_{\mathbf{q}\nu}+f_{\mathbf{k}+\mathbf{q}m})\,\delta(\hbar\omega+\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m})\right.\\ &\left.+\,(n_{\mathbf{q}\nu}+1-f_{\mathbf{k}+\mathbf{q}m})\,\delta(\hbar\omega-\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m})\right]\end{aligned}$$

It is customary to rewrite it in terms of the Eliashberg functions

$$\alpha^2F^{\pm}_{\mathbf{k}n}(\omega,\Omega)=\frac{1}{N_q}\sum_{\mathbf{q}\nu}\delta(\hbar\Omega-\hbar\omega_{\mathbf{q}\nu})\sum_{m}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2\delta(\hbar\omega-\epsilon_{\mathbf{k}+\mathbf{q}m}\pm\hbar\omega_{\mathbf{q}\nu})$$

Eliashberg function

The imaginary part is

$$\begin{aligned}\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) &= -\frac{\pi}{N_q}\sum_{\mathbf{q}m}\sum_{\nu}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2\left[(n_{\mathbf{q}\nu}+f_{\mathbf{k}+\mathbf{q}m})\,\delta(\hbar\omega+\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m})\right.\\ &\left.+\,(n_{\mathbf{q}\nu}+1-f_{\mathbf{k}+\mathbf{q}m})\,\delta(\hbar\omega-\hbar\omega_{\mathbf{q}\nu}-\epsilon_{\mathbf{k}+\mathbf{q}m})\right]\end{aligned}$$

It is customary to rewrite it in terms of the Eliashberg functions

$$\alpha^2F^{\pm}_{\mathbf{k}n}(\omega,\Omega)=\frac{1}{N_q}\sum_{\mathbf{q}\nu}\delta(\hbar\Omega-\hbar\omega_{\mathbf{q}\nu})\sum_{m}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2\delta(\hbar\omega-\epsilon_{\mathbf{k}+\mathbf{q}m}\pm\hbar\omega_{\mathbf{q}\nu})$$

Substituting it in the self-energy we can write the textbook expression.

$$\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) = -\pi\hbar\int_0^{\infty}d\Omega\left[\alpha^2F^{+}_{\mathbf{k}n}(\omega,\Omega)\,(n(\Omega)+f(\omega+\Omega))+\alpha^2F^{-}_{\mathbf{k}n}(\omega,\Omega)\,(n(\Omega)+f(\Omega-\omega))\right]$$

Eliashberg function (approximation)

$$\alpha^2 F^{\pm}_{\mathbf{k}n}(\omega,\Omega) = \frac{1}{N_q}\sum_{\mathbf{q}\nu}\delta(\hbar\Omega-\hbar\omega_{\mathbf{q}\nu})\sum_{m}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2\delta(\hbar\omega-\epsilon_{\mathbf{k}+\mathbf{q}m}\pm\hbar\omega_{\mathbf{q}\nu})$$

The energy of electronic states is of the order of the eV.

The phonon frequencies are of the order of 0-0.15 eV.

Eliashberg function (approximation)

$$\alpha^2 F^{\pm}_{\mathbf{k}n}(\omega,\Omega) = \frac{1}{N_q}\sum_{\mathbf{q}\nu}\delta(\hbar\Omega - \hbar\omega_{\mathbf{q}\nu})\sum_m \left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 \delta(\hbar\omega - \epsilon_{\mathbf{k}+\mathbf{q}m} \pm \hbar\omega_{\mathbf{q}\nu})$$

The energy of electronic states is of the order of the eV.

The phonon frequencies are of the order of 0-0.15 eV.

We can approximate the Eliashberg function as:

$$\alpha^2 F_{\mathbf{k}n}(\omega,\Omega) = \frac{1}{N_q}\sum_{\mathbf{q}\nu}\delta(\hbar\Omega - \hbar\omega_{\mathbf{q}\nu})\sum_m \left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 \delta(\hbar\omega - \epsilon_{\mathbf{k}+\mathbf{q}m})$$

$$\alpha^2 F_{\mathbf{k}n}(\omega,\Omega) = \alpha^2 F^{+}_{\mathbf{k}n}(\omega,\Omega) = \alpha^2 F^{-}_{\mathbf{k}n}(\omega,\Omega)$$

Eliashberg function (approximation)

$$\alpha^2 F^{\pm}_{\mathbf{k}n}(\omega,\Omega) = \frac{1}{N_q}\sum_{\mathbf{q}\nu}\delta(\hbar\Omega - \hbar\omega_{\mathbf{q}\nu})\sum_m \left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 \delta(\hbar\omega - \epsilon_{\mathbf{k}+\mathbf{q}m} \pm \hbar\omega_{\mathbf{q}\nu})$$

The energy of electronic states is of the order of the eV.

The phonon frequencies are of the order of 0-0.15 eV.

We can approximate the Eliashberg function as:

$$\alpha^2 F_{\mathbf{k}n}(\omega,\Omega) = \frac{1}{N_q}\sum_{\mathbf{q}\nu}\delta(\hbar\Omega - \hbar\omega_{\mathbf{q}\nu})\sum_m \left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 \delta(\hbar\omega - \epsilon_{\mathbf{k}+\mathbf{q}m})$$

$$\alpha^2 F_{\mathbf{k}n}(\omega,\Omega) = \alpha^2 F^{+}_{\mathbf{k}n}(\omega,\Omega) = \alpha^2 F^{-}_{\mathbf{k}n}(\omega,\Omega)$$

To obtain:

$$\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) = -\pi\hbar\int_0^{\infty} d\Omega\left[\alpha^2 F_{\mathbf{k}n}(\omega,\Omega)\left(2n(\Omega) + f(\omega+\Omega) + f(\Omega-\omega)\right)\right]$$

Eliashberg function - zero temperature

$$\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) \;=\; -\pi\hbar\int_0^\infty d\Omega\,\left[\alpha^2F_{\mathbf{k}n}(\omega,\Omega)\,(2n(\Omega)+f(\omega+\Omega)+f(\Omega-\omega))\right]$$

At T=0 we have

$$n(\Omega)=0 \qquad\qquad f(\omega)=1-\theta(\omega)$$

Eliashberg function - zero temperature

$$\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) = -\pi\hbar\int_0^\infty d\Omega\,\left[\alpha^2F_{\mathbf{k}n}(\omega,\Omega)\,(2n(\Omega)+f(\omega+\Omega)+f(\Omega-\omega))\right]$$

At T=0 we have

$$n(\Omega)=0 \qquad\qquad f(\omega)=1-\theta(\omega)$$

So that

$$\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) = -\pi\hbar\int_{-0}^\infty d\Omega\,\left[\alpha^2F_{\mathbf{k}n}(\omega,\Omega)\,(2-\theta(\omega+\Omega)-\theta(\Omega-\omega))\right]$$

This expression is zero if

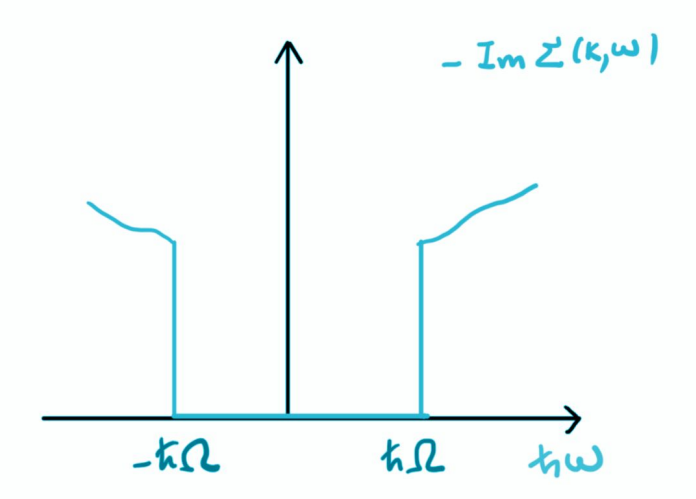
$$\Omega < |\omega|$$

Phonon frequency

Energy

Imaginary part of the electron self-energy at zero temperature

$$\mathrm{Im}\,\Sigma(\mathbf{k}n,\omega) \;=\; -\pi\hbar\int_{-0}^{\infty} d\Omega\,\left[\alpha^2 F_{\mathbf{k}n}(\omega,\Omega)\,(2-\theta(\omega+\Omega)-\theta(\Omega-\omega))\right]$$



Finite temperature behaviour of the electronic linewidth

$$\Gamma_{\mathbf{k}n} = -\operatorname{Im}\Sigma(\mathbf{k}n, \omega = E_{\mathbf{k}n})$$

$$= \pi \int_0^\infty d\Omega \left[\alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n}, \Omega)\,(2n(\Omega) + f(\Omega + E_{\mathbf{k}n}) + f(\Omega - E_{\mathbf{k}n}))\right]$$

Finite temperature behaviour of the electronic linewidth

$$\Gamma_{\mathbf{k}n} = -\operatorname{Im}\Sigma(\mathbf{k}n, \omega = E_{\mathbf{k}n})$$

$$= \pi \int_0^\infty d\Omega \left[\alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n}, \Omega)\,(2n(\Omega) + f(\Omega + E_{\mathbf{k}n}) + f(\Omega - E_{\mathbf{k}n}))\right]$$

Expanding at low T with the condition $k_B T > \hbar\Omega$ but negligible for the electronic energy scale (Fermi functions replaced by step functions):

$$\approx 2\pi \int_0^\infty d\Omega\, \alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n}, \Omega) + 2\pi k_B T \int_0^\infty \frac{\alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n}, \Omega)}{\hbar\Omega}\, d\Omega$$

$$= 2\pi \int_0^\infty d\Omega\, \alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n}, \Omega) + \pi k_B T\, \lambda_{\mathbf{k}n}$$

$$\lambda_{\mathbf{k}n} = 2 \int_0^\infty \frac{\alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n}, \Omega)}{\hbar\Omega}\, d\Omega$$

The electron linewidth should increase linearly with temperature.

Electron-coupling function

The quantity

$$\lambda_{\mathbf{k}n} = 2\int_0^\infty \frac{\alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n},\Omega)}{\hbar\Omega}\, d\Omega$$

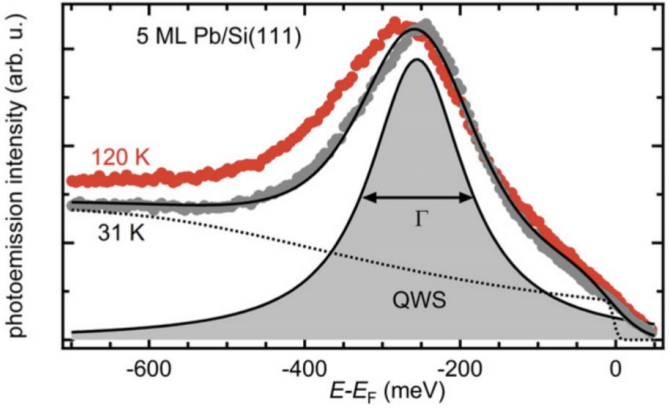
is named the electron-phonon coupling function.

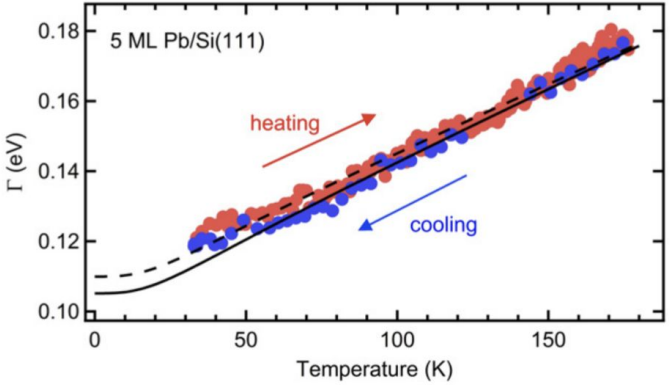
It is labeled exactly as the mass enhancement parameter:

$$\lambda_{\mathbf{k}n} = \frac{1}{\hbar}\left.\frac{\partial \operatorname{Re}\Sigma(\mathbf{k}n,\omega)}{\partial\omega}\right|_{\omega=E_{\mathbf{k}n}/\hbar}$$

Electron-linewidth finite temperature behaviour - Experiments

$$\Gamma_{\mathbf{k}n} = -\,\mathrm{Im}\,\Sigma(\mathbf{k}n, \omega = E_{\mathbf{k}n}) = 2\pi \int_0^\infty d\Omega\, \alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n}, \Omega) + \pi k_B T\, \lambda_{\mathbf{k}n}$$





Ligges *et al.* J. Phys. Cond. Mat. (2014)

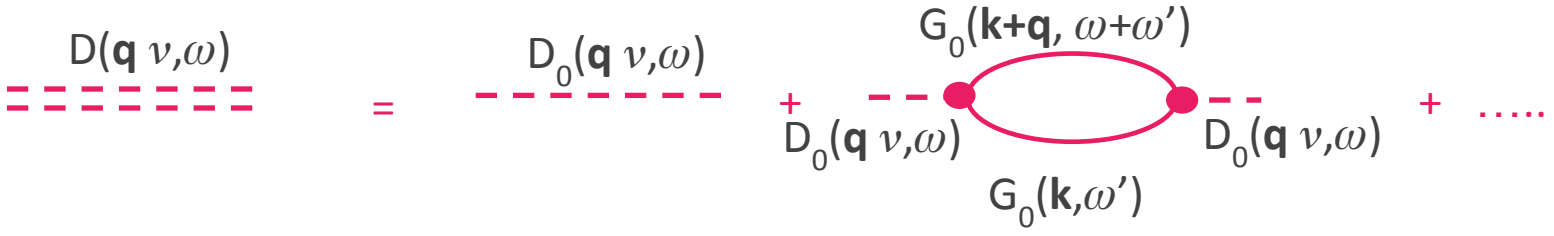
Outline

- Born Oppenheimer (BO) and exact factorization
- Electron-phonon matrix elements
- Second quantization of the electron-phonon Hamiltonian
- Effects on the electrons
- Effects on the phonons
- Electron-phonon driven superconductivity

Interacting phonon Green function

D(**q**ν,ω) Phonon interacting Green Function

The lowest order correction (Dyson equation) is the bubble diagram



The interacting Green function is written as:

$$D(\mathbf{q}\nu,\omega) = \frac{2\hbar\omega_{\mathbf{q}\nu}}{(\hbar\omega)^2 - (\hbar\omega_{\mathbf{q}\nu})^2 + i\eta - 2\hbar\omega_{\mathbf{q}\nu}\Pi(\mathbf{q}\nu,\omega)}$$

Phonon self-energy at lowest order

$$\Pi(\mathbf{q}\nu,\omega) \quad = \quad$$

$$= \frac{1}{N_{\mathbf{q}}} \sum_{\mathbf{k}} \sum_{n,m} \left| g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} \right|^2 \frac{f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m}}{\epsilon_{\mathbf{k}+\mathbf{q}m} - \epsilon_{\mathbf{k}n} - \hbar\omega - i\eta}$$

We note that this is non zero only if $f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m} \neq 0$

meaning $\epsilon_{\mathbf{k}n}$ occupied and $\epsilon_{\mathbf{k}+\mathbf{q}m}$ empty or vice versa.

Phonon self-energy at lowest order

$$\Pi(\mathbf{q}\nu,\omega) \quad = \quad$$ 

$$= \frac{1}{N_{\mathbf{q}}} \sum_{\mathbf{k}} \sum_{n,m} \left| g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} \right|^2 \frac{f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m}}{\epsilon_{\mathbf{k}+\mathbf{q}m} - \epsilon_{\mathbf{k}n} - \hbar\omega - i\eta}$$

We note that this is non zero only if $f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m} \neq 0$

meaning $\epsilon_{\mathbf{k}n}$ occupied and $\epsilon_{\mathbf{k}+\mathbf{q}m}$ empty or vice versa.

$$\mathrm{Re}\,\Pi(\mathbf{q}\nu,\omega) \quad = \quad -\frac{1}{N_{\mathbf{q}}} \mathcal{P} \sum_{\mathbf{k}} \sum_{n,m} \left| g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} \right|^2 \frac{f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega + \epsilon_{\mathbf{k}n} - \epsilon_{\mathbf{k}+\mathbf{q}m}}$$

Phonon self-energy at lowest order

$$\Pi(\mathbf{q}\nu,\omega) \quad = \quad$$

$$= \frac{1}{N_{\mathbf{q}}} \sum_{\mathbf{k}} \sum_{n,m} \left| g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} \right|^2 \frac{f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m}}{\epsilon_{\mathbf{k}+\mathbf{q}m} - \epsilon_{\mathbf{k}n} - \hbar\omega - i\eta}$$

We note that this is non zero only if $f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m} \neq 0$

meaning $\epsilon_{\mathbf{k}n}$ occupied and $\epsilon_{\mathbf{k}+\mathbf{q}m}$ empty or vice versa.

$$\mathrm{Re}\,\Pi(\mathbf{q}\nu,\omega) = -\frac{1}{N_{\mathbf{q}}} \mathcal{P} \sum_{\mathbf{k}} \sum_{n,m} \left| g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} \right|^2 \frac{f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega + \epsilon_{\mathbf{k}n} - \epsilon_{\mathbf{k}+\mathbf{q}m}}$$

$$\mathrm{Im}\,\Pi(\mathbf{q}\nu,\omega) = \frac{\pi}{N_{\mathbf{q}}} \sum_{\mathbf{k}} \sum_{n,m} \left| g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} \right|^2 (f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m})\, \delta(\epsilon_{\mathbf{k}+\mathbf{q}m} - \epsilon_{\mathbf{k}n} - \hbar\omega)$$

Phonon quasiparticle energies

The quasiparticle energies are obtained from the poles of the Green function

$$D(\mathbf{q}\nu,\omega) = \frac{2\hbar\omega_{\mathbf{q}\nu}}{(\hbar\omega)^2 - (\hbar\omega_{\mathbf{q}\nu})^2 + i\eta - 2\hbar\omega_{\mathbf{q}\nu}\Pi(\mathbf{q}\nu,\omega)}$$

Assuming a small imaginary part of the self-energy:

$$(\hbar\Omega_{\mathbf{q}\nu})^2 = (\hbar\omega_{\mathbf{q}\nu})^2 - 2\hbar\omega_{\mathbf{q}\nu}\,\mathrm{Re}\,\Pi(\mathbf{q}\nu,\Omega_{\mathbf{q}\nu})$$

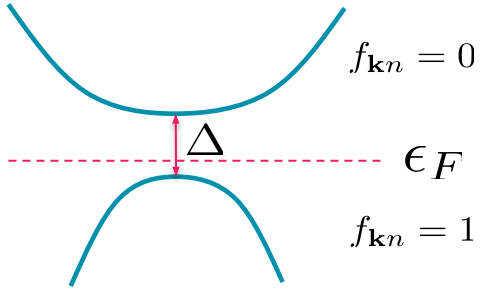
with

$$\mathrm{Re}\,\Pi(\mathbf{q}\nu,\omega) \;=\; -\frac{1}{N_{\mathbf{q}}}\mathcal{P}\sum_{\mathbf{k}}\sum_{n,m}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 \frac{f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega + \epsilon_{\mathbf{k}n} - \epsilon_{\mathbf{k}+\mathbf{q}m}}$$

Phonon quasiparticle energies (insulators)

In an insulator (large gap), we have

Δ = electronic gap



$$|\epsilon_{\mathbf{k}n} - \epsilon_{\mathbf{k}+\mathbf{q}}| \geq \Delta \qquad \approx 1eV$$

$$\hbar\Omega_{\mathbf{q}\nu} \qquad \approx 0 - 150\, meV \ll \Delta$$

We have

$$\mathrm{Re}\,\Pi(\mathbf{q}\nu,\omega) = -\frac{1}{N_{\mathbf{q}}}\mathcal{P}\sum_{\mathbf{k}}\sum_{n,m}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 \frac{f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega + \epsilon_{\mathbf{k}n} - \epsilon_{\mathbf{k}+\mathbf{q}m}} \qquad \sim g^2/\Delta$$

$\hbar\Omega_{\mathbf{q}\nu}$

$\geq \Delta$

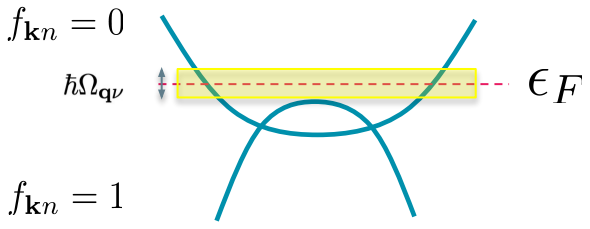
The fraction is dominated by the gap at the denominator and this term is small.

Phonon quasiparticle energies (metals)

In metals, we have

$$\left|\epsilon_{\mathbf{k}n} - \epsilon_{\mathbf{k}+\mathbf{q}m}\right| \qquad \text{as small as we like}$$

$$\hbar\Omega_{\mathbf{q}\nu} \approx \mathbf{0 - 150\ meV}$$



We have

$$\mathrm{Re}\,\Pi(\mathbf{q}\nu,\omega) = -\frac{1}{N_{\mathbf{q}}}\mathcal{P}\sum_{\mathbf{k}}\sum_{n,m}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 \frac{f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega + \epsilon_{\mathbf{k}n} - \epsilon_{\mathbf{k}+\mathbf{q}m}}$$

The real part of the self energy is dominated by the poles, namely

$$\hbar\omega = \epsilon_{\mathbf{k}+\mathbf{q}m} - \epsilon_{\mathbf{k}n}$$

Phonon quasiparticle energies in the adiabatic approximation

The adiabatic approximation consists in replacing

$$(\hbar\Omega_{\mathbf{q}\nu})^2 = (\hbar\omega_{\mathbf{q}\nu})^2 - 2\hbar\omega_{\mathbf{q}\nu}\,\mathrm{Re}\,\Pi(\mathbf{q}\nu, \Omega_{\mathbf{q}\nu})$$

with

$$(\hbar\Omega_{\mathbf{q}\nu})^2 = (\hbar\omega_{\mathbf{q}\nu})^2 - 2\hbar\omega_{\mathbf{q}\nu}\,\mathrm{Re}\,\Pi(\mathbf{q}\nu, 0)$$

It is a very accurate approximation in most cases.

Phonon quasiparticle energies in the adiabatic approximation

Thus we have

$$(\hbar\Omega_{\mathbf{q}\nu})^2 = (\hbar\omega_{\mathbf{q}\nu})^2 - 2\hbar\omega_{\mathbf{q}\nu}\,\mathrm{Re}\,\Pi(\mathbf{q}\nu, \Omega_{\mathbf{q}\nu})$$

with

$$\mathrm{Re}\,\Pi(\mathbf{q}\nu,\cancel{\omega}) = -\frac{1}{N_{\mathbf{q}}}\mathcal{P}\sum_{\mathbf{k}}\sum_{n,m}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 \frac{f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m}}{\cancel{\hbar\omega} + \epsilon_{\mathbf{k}n} - \epsilon_{\mathbf{k}+\mathbf{q}m}}$$

The real part is dominated by the nesting condition

$$\epsilon_{\mathbf{k}+\mathbf{q}m} = \epsilon_{\mathbf{k}n}$$

Phonon quasiparticle energies in the adiabatic approximation

Thus we have

$$(\hbar\Omega_{\mathbf{q}\nu})^2 = (\hbar\omega_{\mathbf{q}\nu})^2 - 2\hbar\omega_{\mathbf{q}\nu}\,\mathrm{Re}\,\Pi(\mathbf{q}\nu,\Omega_{\mathbf{q}\nu})$$

with

$$\mathrm{Re}\,\Pi(\mathbf{q}\nu,\cancel{\omega}) = -\frac{1}{N_{\mathbf{q}}}\mathcal{P}\sum_{\mathbf{k}}\sum_{n,m}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 \frac{f_{\mathbf{k}n}-f_{\mathbf{k}+\mathbf{q}m}}{\cancel{\hbar\omega}+\epsilon_{\mathbf{k}n}-\epsilon_{\mathbf{k}+\mathbf{q}m}}$$

It can also be shown that due to causality

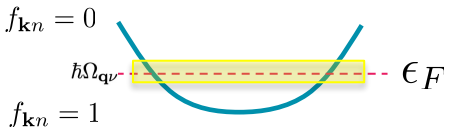
$$\mathrm{Re}\,\Pi(\mathbf{q},0) > 0$$

The electron-phonon coupling always softens the bare phonon frequencies!

Example

One parabolic band.

One phonon mode.



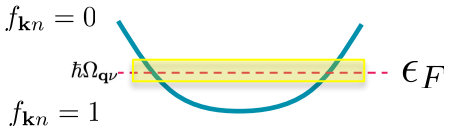
Constant electron-phonon matrix elements: $|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}|^2 = g^2$

We have:

$$\mathrm{Re}\,\Pi(\mathbf{q},0) = -g^2\chi_0(\mathbf{q})$$

Lindhardt function (electron-gas)

Example



One parabolic band.

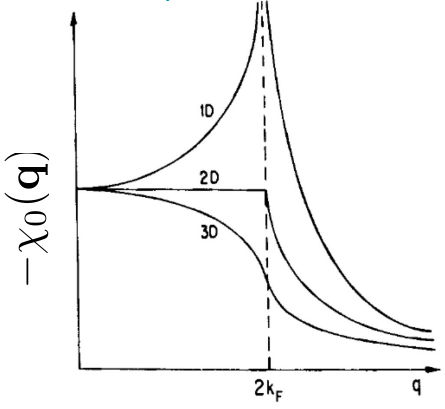
One phonon mode.

Constant electron-phonon matrix elements: $|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}|^2 = g^2$

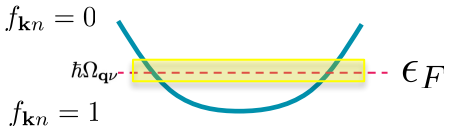
We have: $\mathrm{Re}\,\Pi(\mathbf{q},0) = -g^2\chi_0(\mathbf{q})$

Lindhardt function (electron-gas)

The self-energy diverges
At $2k_F$ in D=1



Example



One parabolic band.

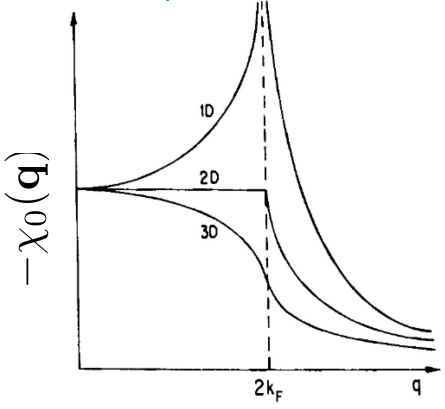
One phonon mode.

Constant electron-phonon matrix elements: $|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}|^2 = g^2$

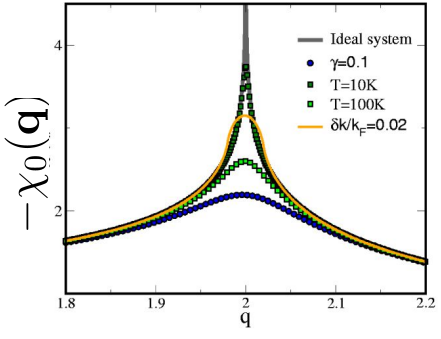
We have: $\mathrm{Re}\,\Pi(\mathbf{q},0) = -g^2\chi_0(\mathbf{q})$

Lindhardt function (electron-gas)

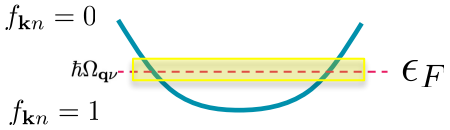
The self-energy diverges
At $2k_F$ in D=1



Temperature dependence



Example



One parabolic band.

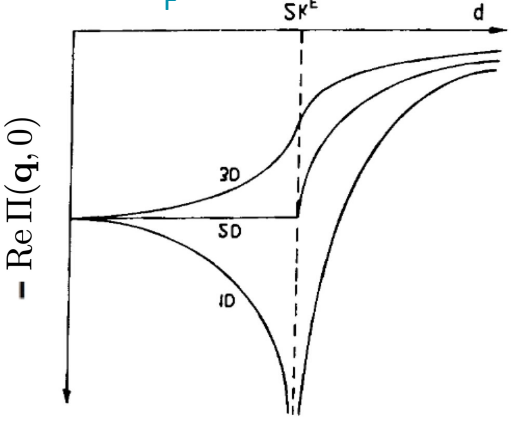
One phonon mode.

Constant electron-phonon matrix elements: $|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}|^2 = g^2$

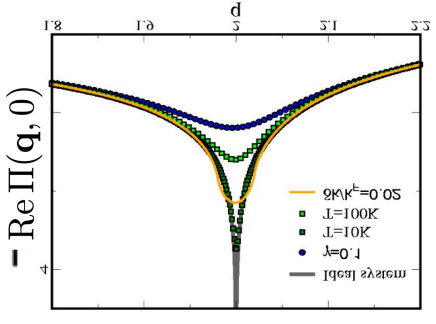
We have: $\mathrm{Re}\,\Pi(\mathbf{q},0) = -g^2\chi_0(\mathbf{q})$

Lindhardt function (electron-gas)

The self-energy diverges
At $2k_F$ in D=1



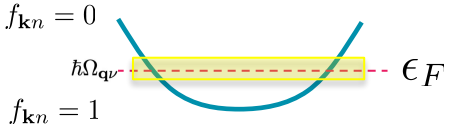
Temperature dependence



Example

One parabolic band.

One phonon mode.

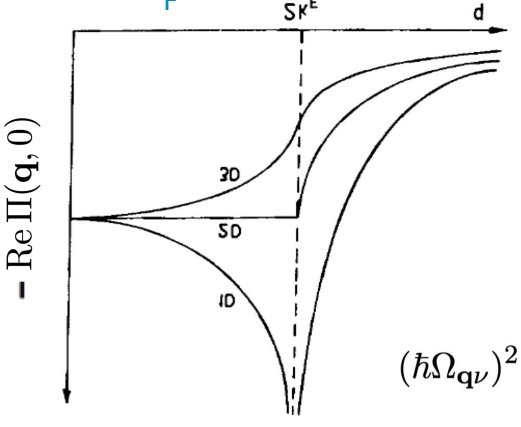


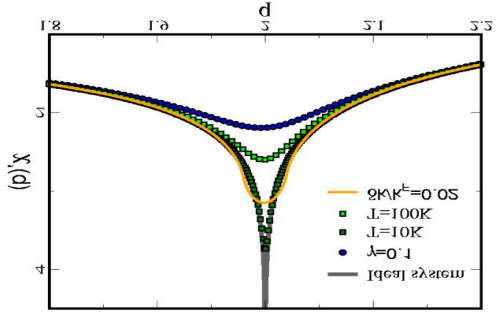
Constant electron-phonon matrix elements: $|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}|^2 = g^2$

We have: $\mathrm{Re}\,\Pi(\mathbf{q},0) = -g^2\chi_0(\mathbf{q})$

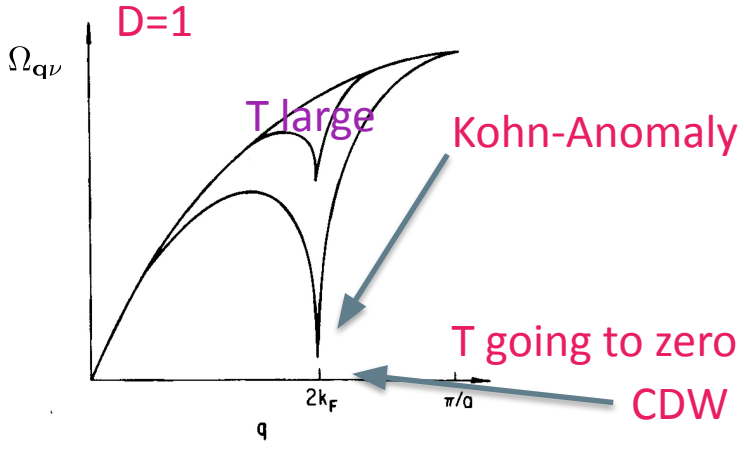
Lindhardt function (electron-gas)

The self-energy diverges
At $2k_F$ in D=1





$$(\hbar\Omega_{\mathbf{q}\nu})^2 = (\hbar\omega_{\mathbf{q}\nu})^2 - 2\hbar\omega_{\mathbf{q}\nu}\,\mathrm{Re}\,\Pi(\mathbf{q}\nu,0)$$



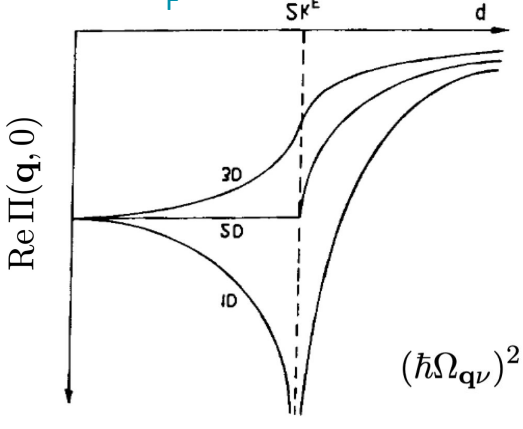
Exercise:

DFT Phonon frequencies already include this effect

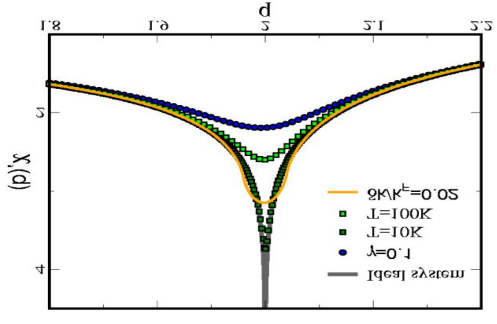
(with non constant g and non parabolic bands) !

The self-energy diverges

At $2k_F$ in D=1

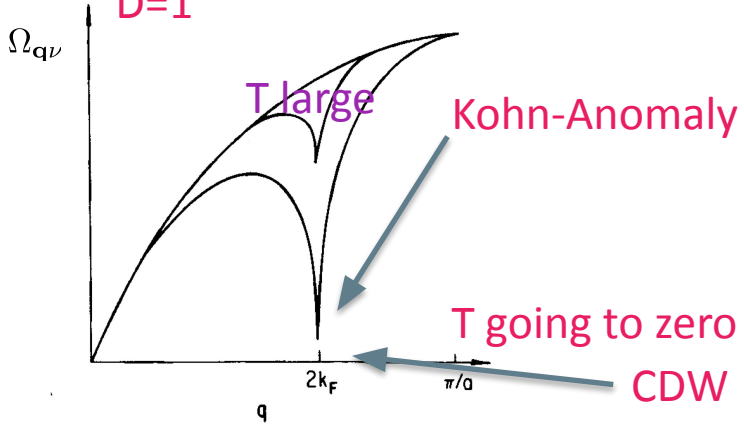


$\mathrm{Re}\,\Pi(\mathbf{q},0)$

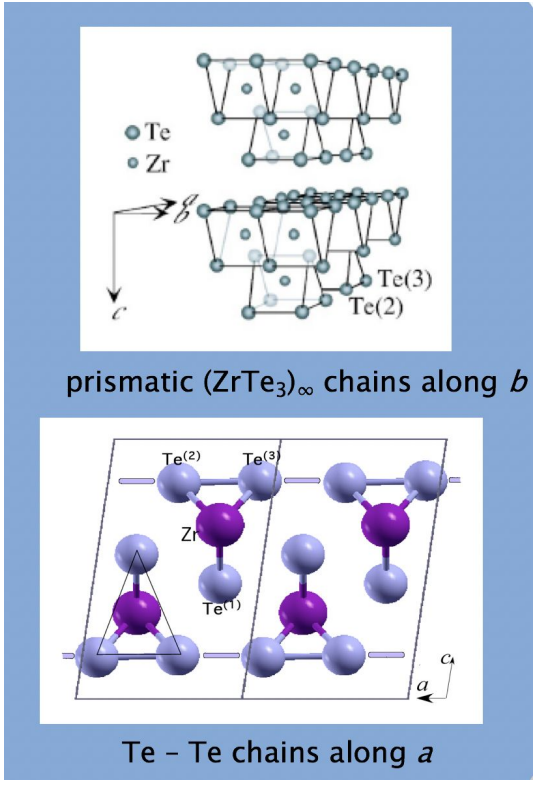


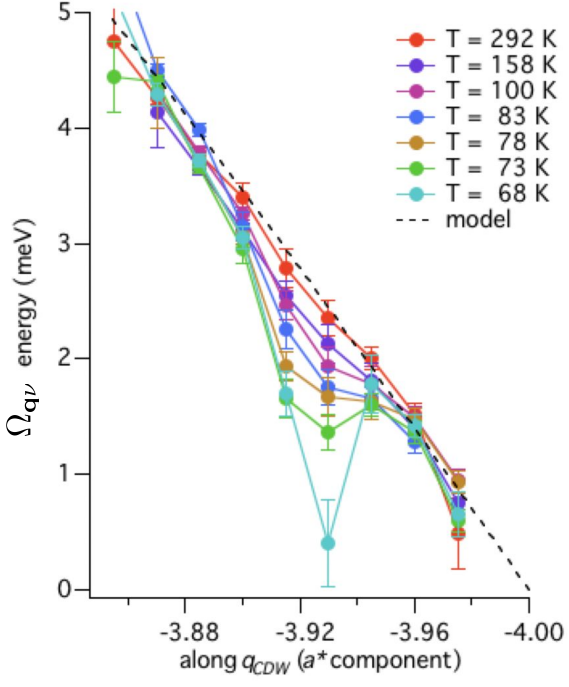
$$(\hbar\Omega_{\mathbf{q}\nu})^2 = (\hbar\omega_{\mathbf{q}\nu})^2 - 2\hbar\omega_{\mathbf{q}\nu}\,\mathrm{Re}\,\Pi(\mathbf{q}\nu,0)$$

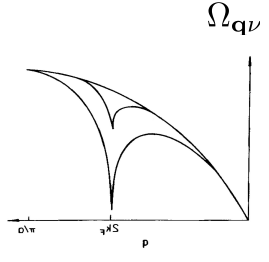
D=1



$ZrTe_3$ 1D metal, CDW seen in IXS







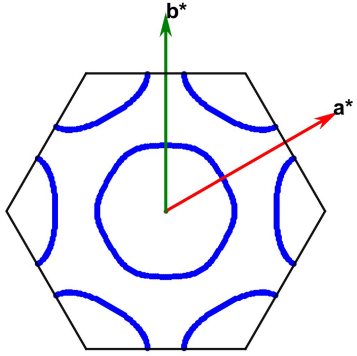
Hoesch, *et al.* Phys. Rev. Lett. **102**, 086402

What happens in 2D, 3D metals ?

The real part is dominated by the condition (nesting condition)

$$\epsilon_{\mathbf{k}+\mathbf{q}m} = \epsilon_{\mathbf{k}n}$$

We expect contributions in phonon spectra at the vector **q** mapping one portion (not just a point) of the Fermi surface in another one.



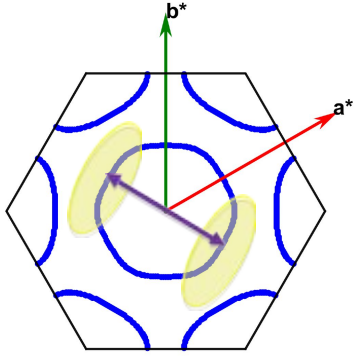
Fermi surface

What happens in 2D, 3D metals ?

The real part is dominated by the condition (nesting condition)

$$\epsilon_{\mathbf{k}+\mathbf{q}m} = \epsilon_{\mathbf{k}n}$$

We expect contributions in phonon spectra at the vector **q** mapping one portion (not just a point) of the Fermi surface in another one.



Fermi surface

is the nesting vector: we expect softening at the nesting vector!

IMAGE OF THE FERMI SURFACE IN THE VIBRATION SPECTRUM OF A METAL*

W. Kohn
Department of Physics, Carnegie Institute of Technology, Pittsburgh, Pennsylvania
(Received April 6, 1959)

The lattice vibrations of the ions in a metal are partly screened by the conduction electrons. We shall see that this screening changes rather rapidly on certain surfaces in the space of phonon $\vec{q}$-vectors and that therefore on these surfaces the frequencies ω vary abruptly with $\vec{q}$. The calculations we have done give the result that $\omega(\vec{q})$ is a continuous function of $\vec{q}$ but that on the surfaces in question

$$|\operatorname{grad}_{\vec{q}}\omega(\vec{q})| = \infty. \tag{1}$$

The location of these surfaces is entirely determined by the shape of the electronic Fermi surface, using a simple geometrical construction.

To explain the physical origin of this effect let us first describe the conduction electrons by a free electron gas, with Fermi wave number k_F. One then finds that an embedded charge distribution,

$$\rho_{\text{ext}}(\vec{r}) = \rho_0 e^{i\vec{q}\cdot\vec{r}}, \tag{2}$$

induces an electronic charge density

$$\rho_{\text{el}}(\vec{r}) = -F(q)\rho_0 e^{i\vec{q}\cdot\vec{r}}, \tag{3}$$

where

$$F(q) = \frac{1}{\pi a_0 q^2}\left[1 + \frac{k_F}{q}\left(1 - \frac{q^2}{4k_F^2}\right)\ln\left|\frac{q+2k_F}{q-2k_F}\right|\right]; \tag{4}$$

here a_0 is the Bohr radius. Note that near $q = 2k_F$,

$$F(q) = \frac{1}{2\pi a_0 k_F}\left(1 + \frac{1}{2k_F}(q - 2k_F)\ln|q - 2k_F|\right), \tag{5}$$

and

$$\frac{dF(q)}{dq} = \frac{1}{4\pi a_0 k_F^2}\ln|q - 2k_F| \approx -\infty. \tag{6}$$

The last equation shows an abrupt decrease of the ability of the electrons to screen the embedded charge distribution as soon as q exceeds $2k_F$. This is due to the fact that as long as $q < 2k_F$, $\rho_{\text{ext}}(\vec{r})$ causes virtual excitations of some electrons with conservation of energy while when $q > 2k_F$ such excitations are no longer possible (see Fig. 1). Now a lattice vibration of wave vector $\vec{q}$ produces a change of ionic charge density of the form

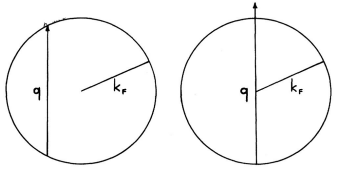


FIG. 1. Virtual excitations for $q < 2k_F$ and $q > 2k_F$.

$$\rho_{\text{ion}}(\vec{r}) = \textstyle\sum_\nu A_\nu \exp[i(\vec{q} + \vec{K}_\nu)\cdot\vec{r}], \tag{7}$$

where $\vec{K}_\nu$ are the reciprocal lattice vectors. Therefore we expect an abrupt change of the restoring force whenever $\vec{q}$ is such that, for some reciprocal lattice vector $\vec{K}_\nu$,

$$|\vec{q} + \vec{K}_\nu| = 2k_F. \tag{8}$$

On the surfaces in $\vec{q}$-space defined by (8), one finds the singularity (1) as a consequence of (6).

Next we consider noninteracting Bloch electrons with a Fermi surface given by

$$E(\vec{k}) = \zeta. \tag{9}$$

Again one finds singularities of $\operatorname{grad}_{\vec{q}}\omega$, whose locus is determined by the following construction (Fig. 2): Let Π_1 and Π_2 be two parallel planes in $\vec{k}$-space touching the Fermi surface at $\vec{k}_1$ and $\vec{k}_2$. Then there exists exactly one reciprocal lattice vector $\vec{K}_\nu$ such that the vector $\vec{q}$, defined by

$$\vec{q} = \vec{k}_2 - \vec{k}_1 + \vec{K}_\nu, \tag{10}$$

lies in the fundamental Brillouin zone. At this point $\vec{q}$, Eq. (1) holds. The totality of pairs of planes Π_1 and Π_2 generate the required locus of singularities of the vibration spectrum by means of Eq. (10).

Finally the question arises how the Coulomb interaction between the conduction electrons affects our conclusions. We have partly allowed for this interaction by regarding it as a perturbation and summing certain important terms in the resulting perturbation expansion of $\omega(\vec{q})$. These terms do not affect the nature of the singularities, but only their magnitude. It therefore appears unlikely that the Coulomb interactions can obliterate the effect we have discussed, which basically reflects the sharpness of the Fermi surface.

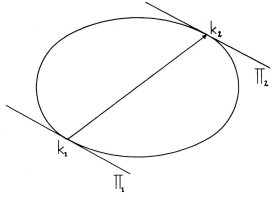


FIG. 2. Construction for the case of Bloch electrons.

The magnitude of the effect may be quite large (very roughly of the order of percent), and its observation in lattice vibration spectra would give rather direct information about the shape of the Fermi surface.

Similar "images" of the Fermi surface may be expected in spin wave spectra, when the interaction between localized spins is brought about by exchange with conduction electrons.

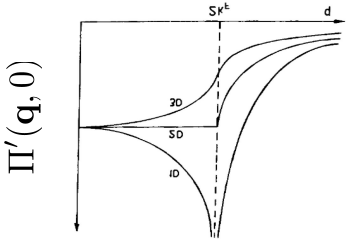
A detailed report is in preparation.

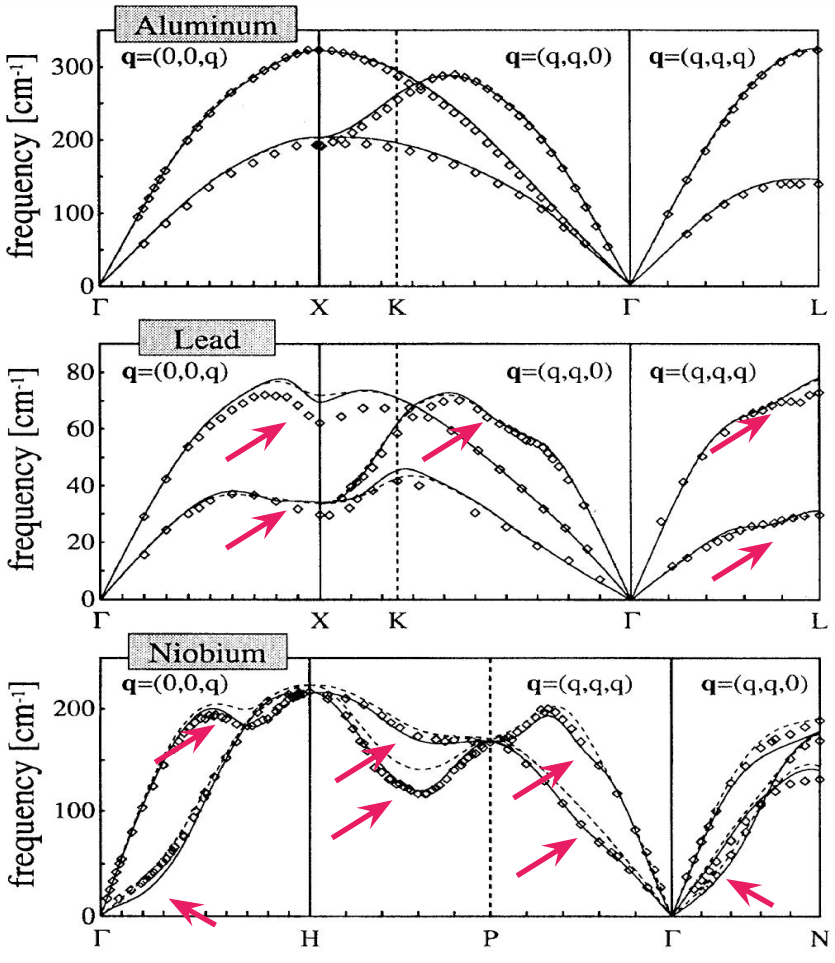
*Supported in part by the Office of Naval Research.

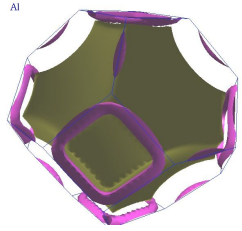
The Kohn-effect (Kohn-anomaly) – slightly more than 1 page.

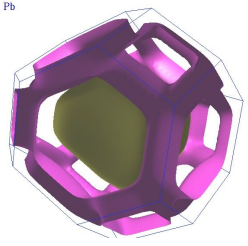
June 29, 2023 - Donostia/San Sebastián, Spain

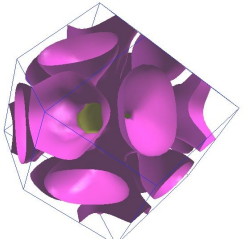
Phonon dispersion in simple 3D metals





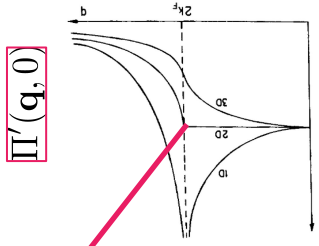


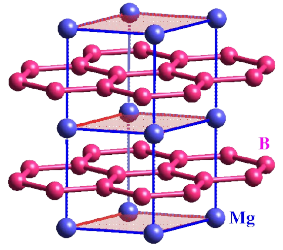


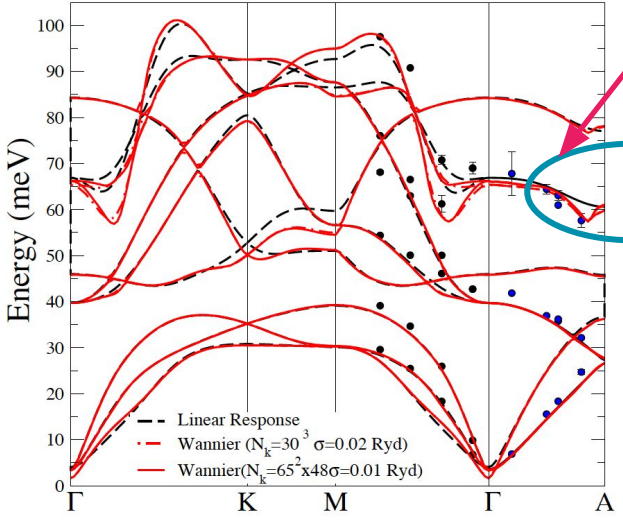


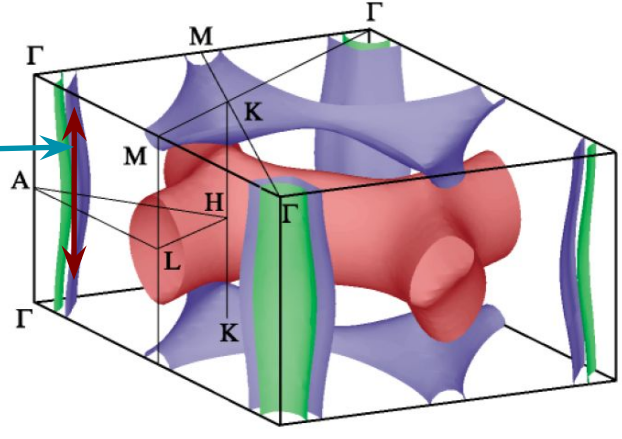
Arrows indicates Kohn Anomalies

Kohn anomaly in MgB_2





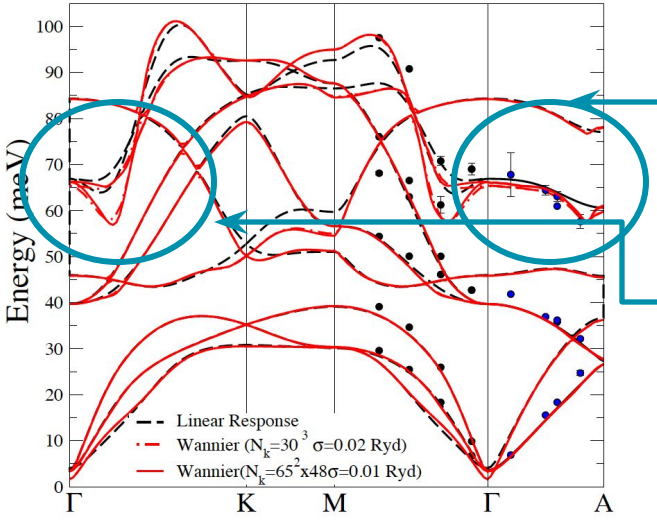


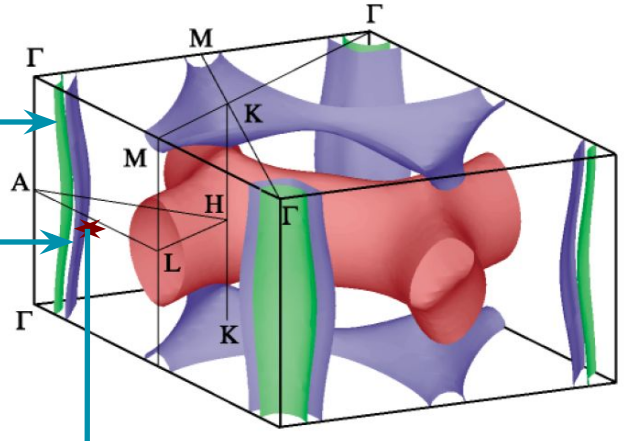


Kortus *et al.* PRL **86**, 4656 (2001)

Strong but irregular nesting along ΓA in warped cylinders formed by σ-bands results in softening of the full E_{2g} branch.

Kohn anomaly in MgB_2





Nesting between cylinders

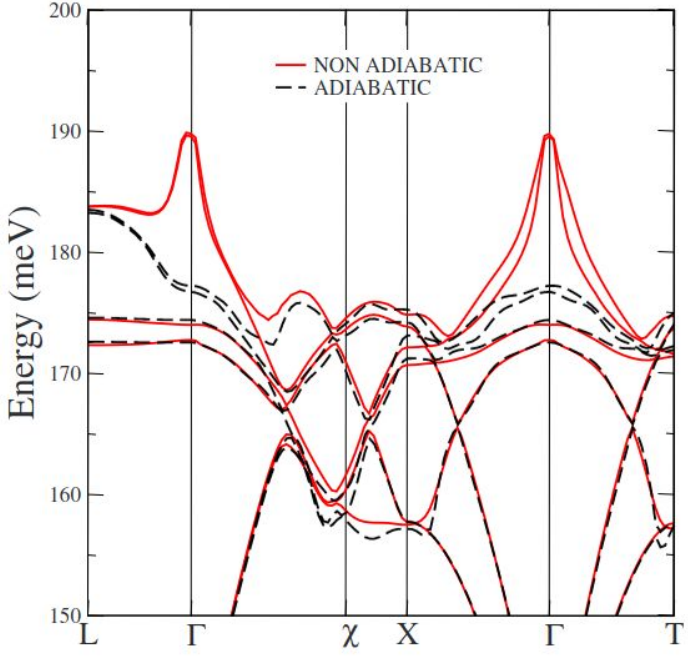
M. Calandra *et al.* PRB **82**, 165111 (2010)

Dynamical effects (non-adiabatic)

$$\mathrm{Re}\,\Pi(\mathbf{q}\nu,\cancel{\omega}) = -\frac{1}{N_{\mathbf{q}}}\mathcal{P}\sum_{\mathbf{k}}\sum_{n,m}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 \frac{f_{\mathbf{k}n}-f_{\mathbf{k}+\mathbf{q}m}}{\cancel{\hbar\omega}+\epsilon_{\mathbf{k}n}-\epsilon_{\mathbf{k}+\mathbf{q}m}}$$

Dynamical effects (non-adiabatic)

$$\mathrm{Re}\,\Pi(\mathbf{q}\nu,\omega) \;=\; -\frac{1}{N_{\mathbf{q}}}\mathcal{P}\sum_{\mathbf{k}}\sum_{n,m}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2\frac{f_{\mathbf{k}n}-f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega+\epsilon_{\mathbf{k}n}-\epsilon_{\mathbf{k}+\mathbf{q}m}}$$



- Carbon systems (and generally super-hard materials) are very peculiar in this respect as they have high energy phonon modes $\Omega_{q\upsilon}$ ~0.2 eV

DYNAMICAL (NON ADIABATIC) EFFECTS ARE IMPORTANT !

Imaginary part and phonon linewidth

$$\mathrm{Im}\,\Pi(\mathbf{q}\nu,\omega) = \frac{\pi}{N_{\mathbf{q}}}\sum_{\mathbf{k}}\sum_{n,m}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 (f_{\mathbf{k}n}-f_{\mathbf{k}+\mathbf{q}m})\,\delta(\epsilon_{\mathbf{k}+\mathbf{q}m}-\epsilon_{\mathbf{k}n}-\hbar\omega)$$

This is what you would obtain applying the Fermi Golden rule for a phonon scattering with electrons.

The phonon linewidth is the inverse of the phonon scattering time and it can be measured in neutron scattering or in inelastic X-ray scattering.

Imaginary part and phonon linewidth

$$\mathrm{Im}\,\Pi(\mathbf{q}\nu,\omega) = \frac{\pi}{N_{\mathbf{q}}}\sum_{\mathbf{k}}\sum_{n,m}\left|g^{\nu}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 (f_{\mathbf{k}n}-f_{\mathbf{k}+\mathbf{q}m})\,\delta(\epsilon_{\mathbf{k}+\mathbf{q}m}-\epsilon_{\mathbf{k}n}-\hbar\omega)$$

Key points:

- Imaginary part is positive definite.
- As in insulators $\hbar\omega \ll \Delta(gap)$ the imaginary part is zero.
- In metals the phonon linewidth is dominated by Fermi-surface effects
- The phonon linewidth (inverse of phonon lifetime) is:

$$\gamma_{q\nu} = \frac{4\pi\omega_{q\upsilon}}{N_k}\sum_{k,n,m}\left|g^{\upsilon}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}\right|^2 \frac{f(\varepsilon_{\mathbf{k}n})-f(\varepsilon_{\mathbf{k}+\mathbf{q}m})}{\omega_{q\upsilon}}\delta(\varepsilon_{\mathbf{k}+\mathbf{q}m}-\varepsilon_{\mathbf{k}n}-\omega_{q\upsilon})$$

2 for spin and 2 for Full width half maximum

Allen formula (metals)

P. B. Allen, PRB **6**, 2577 (1972)

$$\gamma_{q\nu} = \frac{4\pi\omega_{q\upsilon}}{N_k} \sum_{k,n,m} \left| g^{\upsilon}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} \right|^2 \frac{f(\varepsilon_{\mathbf{k}n}) - f(\varepsilon_{\mathbf{k}+\mathbf{q}m})}{\omega_{q\upsilon}} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}m} - \varepsilon_{\mathbf{k}n} - \omega_{q\upsilon})$$

If temperature dependence is weak:

$$\frac{f(\varepsilon_{\mathbf{k}+\mathbf{q}m}) - f(\varepsilon_{\mathbf{k}n})}{\omega_{q\upsilon}} \rightarrow \left. \frac{\partial f}{\partial \varepsilon} \right|_{\varepsilon=\varepsilon_{\mathbf{k}n}} \xrightarrow{\text{no T dep.}} \delta(\varepsilon_{\mathbf{k}n})$$

Allen formula (metals)

P. B. Allen, PRB **6**, 2577 (1972)

$$\gamma_{q\nu} = \frac{4\pi\omega_{q\upsilon}}{N_k} \sum_{k,n,m} \left| g^{\upsilon}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} \right|^2 \frac{f(\varepsilon_{\mathbf{k}n}) - f(\varepsilon_{\mathbf{k}+\mathbf{q}m})}{\omega_{q\upsilon}} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}m} - \varepsilon_{\mathbf{k}n} - \omega_{q\upsilon})$$

If temperature dependence is weak:

$$\frac{f(\varepsilon_{\mathbf{k}+\mathbf{q}m}) - f(\varepsilon_{\mathbf{k}n})}{\omega_{q\upsilon}} \rightarrow \left. \frac{\partial f}{\partial \varepsilon} \right|_{\varepsilon=\varepsilon_{\mathbf{k}n}} \xrightarrow{\text{no T dep.}} \delta(\varepsilon_{\mathbf{k}n})$$

We have

$$\gamma_{q\nu} = \frac{4\pi\omega_{q\upsilon}}{N_k} \sum_{k,n,m} \left| g^{\upsilon}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} \right|^2 \delta(\varepsilon_{\mathbf{k}n}) \delta(\varepsilon_{\mathbf{k}+\mathbf{q}m} - \varepsilon_{\mathbf{k}n} - \omega_{q\upsilon})$$

Allen formula (metals)

P. B. Allen, PRB **6**, 2577 (1972)

$$\gamma_{q\nu} = \frac{4\pi\omega_{q\upsilon}}{N_k} \sum_{k,n,m} \left| g^{\upsilon}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} \right|^2 \delta(\varepsilon_{\mathbf{k}n}) \delta(\varepsilon_{\mathbf{k}+\mathbf{q}m} - \varepsilon_{\mathbf{k}n} - \omega_{q\upsilon})$$

Neglecting the phonon frequency in the double delta (not always justified)

$$\gamma_{q\nu} = \frac{4\pi\omega_{q\upsilon}}{N_k} \sum_{k,n,m} \left| g^{\upsilon}_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m} \right|^2 \delta(\varepsilon_{\mathbf{k}n}) \delta(\varepsilon_{\mathbf{k}+\mathbf{q}m})$$

We have

Remember: electron energies measured from the Fermi Level

$$\lambda_{\mathbf{q}\nu} = \frac{\gamma_{\mathbf{q}\nu}}{2\pi N(\epsilon_F)\omega^2_{\mathbf{q}\nu}}$$

Electron-phonon coupling

DOS per spin at the Fermi level

When anharmonicity is negligible, the phonon linewidth measures the electron-phonon coupling

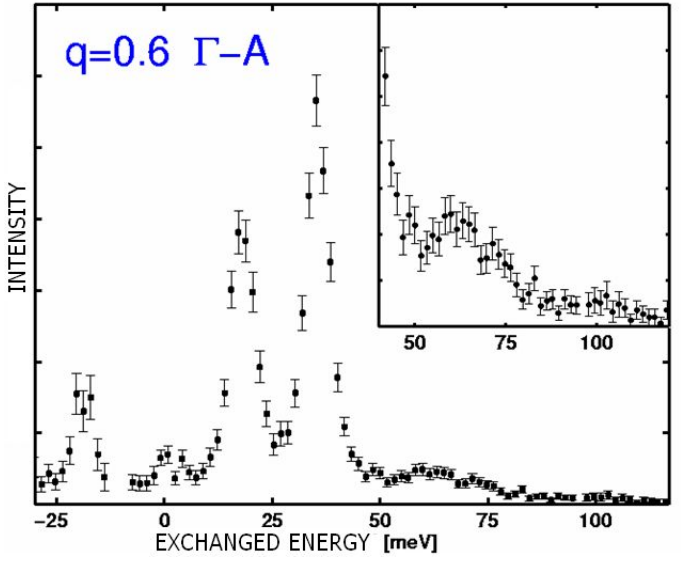
MgB_2 Measure of the electron-phonon coupling

Problem: Origin of the ≈20 meV linewidth of the E_{2g} modes:
Anharmonicity or strong electron-phonon coupling ?

experiment

Impossible to distinguish

the two contributions !



MgB_2 Measure of the electron-phonon coupling

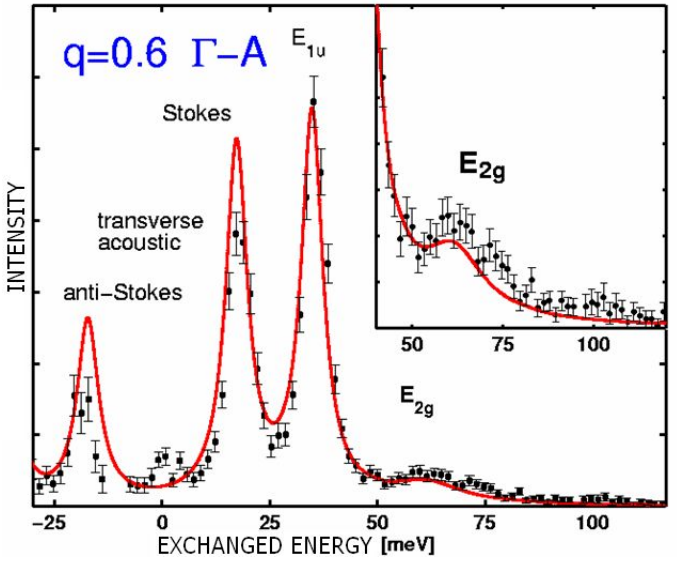
Problem: Origin of the ≈20 meV linewidth of the E_{2g} modes:
Anharmonicity or strong electron-phonon coupling ?

— Theoretical calculation

(including only the electron-phonon contribution to the linewidth)

↓

Good agreement with experiments
-> Weak anharmonicity.



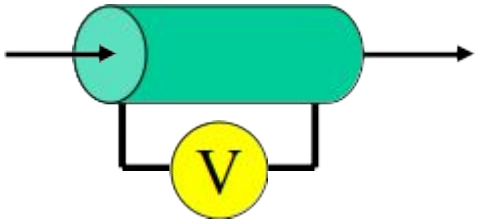
Linewidth = measure of the electron-phonon coupling

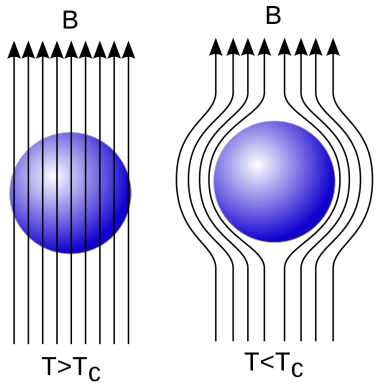
A. Shukla, *et al.* PRL **90**, 095506 (2003)

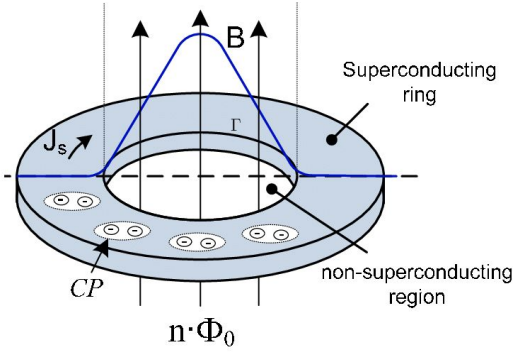
Outline

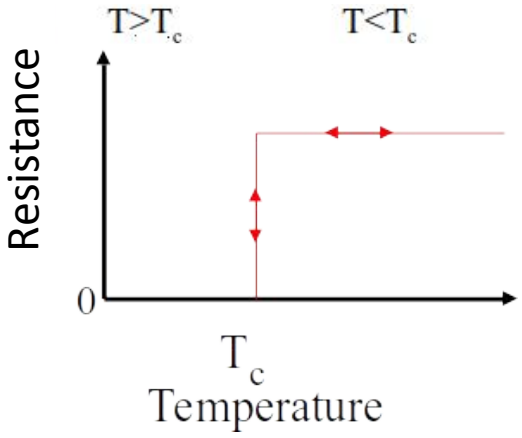
- Born Oppenheimer (BO) and exact factorization
- Electron-phonon matrix elements
- Second quantization of the electron-phonon Hamiltonian
- Effects on the electrons
- Effects on the phonons
- Electron-phonon driven superconductivity

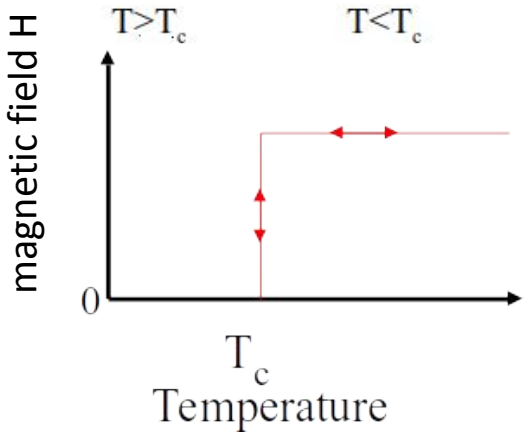
The superconducting phase









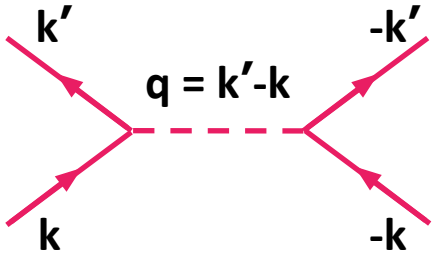


macroscopic quantum effects

- magnetic flux quantization
- Josephson effect

BCS theory

$$H_{BCS} = H_0 + H_{red}$$

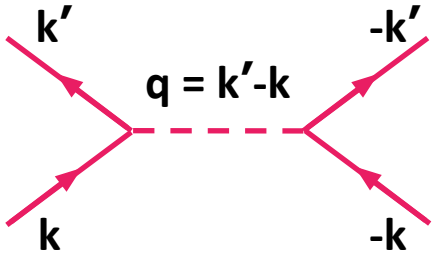


BCS theory

$H_{BCS} = H_0 + H_{red}$

$$\mathcal{H}_0 = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma},$$

$$\mathcal{H}_{\text{red}} = -\sum_{kk'} V_{k'k} (c^\dagger_{-k'\downarrow} c^\dagger_{k'\uparrow})(c_{k\uparrow} c_{-k\downarrow}).$$

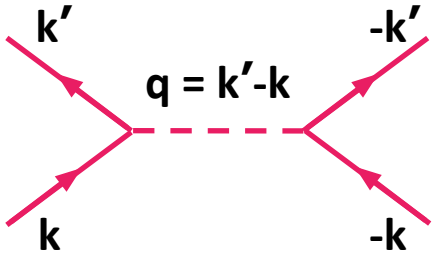


BCS theory

$H_{BCS} = H_0 + H_{red}$

$$\mathscr{H}_0 = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma},$$

$$\mathscr{H}_{\mathrm{red}} = -\sum_{kk'} V_{k'k} (c^\dagger_{-k'\downarrow} c^\dagger_{k'\uparrow})(c_{k\uparrow} c_{-k\downarrow}).$$



$$\Delta_{n\mathbf{k}} = \sum_m \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \tanh\left(\frac{E_{m\mathbf{k}+\mathbf{q}}}{2k_{\mathrm{B}}T}\right) \frac{V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} \Delta_{m\mathbf{k}+\mathbf{q}}}{2E_{m\mathbf{k}+\mathbf{q}}}$$

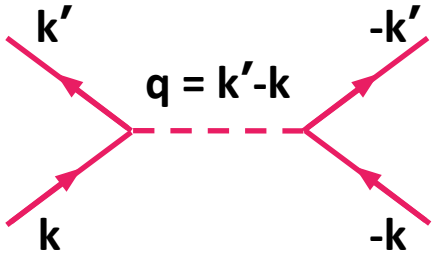
$$E_{n\mathbf{k}} = \sqrt{(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})^2 + |\Delta_{n\mathbf{k}}|^2}$$

BCS theory

$H_{BCS} = H_0 + H_{red}$

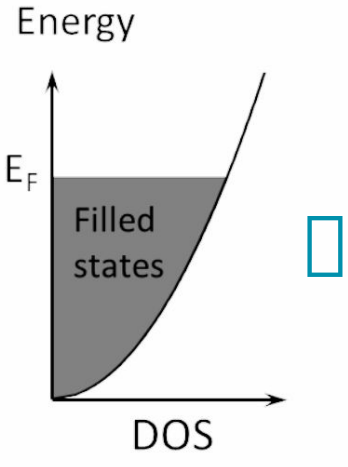
$$\mathcal{H}_0 = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma},$$

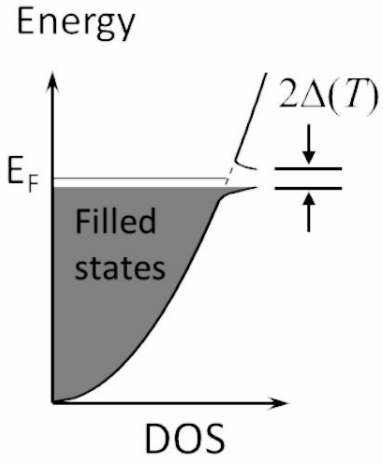
$$\mathcal{H}_{\text{red}} = -\sum_{kk'} V_{k'k} (c^\dagger_{-k'\downarrow} c^\dagger_{k'\uparrow})(c_{k\uparrow} c_{-k\downarrow}).$$

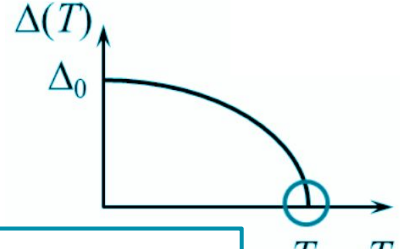


$$\Delta_{n\mathbf{k}} = \sum_m \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \tanh\left(\frac{E_{m\mathbf{k}+\mathbf{q}}}{2k_{\text{B}}T}\right) \frac{V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} \Delta_{m\mathbf{k}+\mathbf{q}}}{2E_{m\mathbf{k}+\mathbf{q}}}$$

$$E_{n\mathbf{k}} = \sqrt{(\epsilon_{n\mathbf{k}} - \epsilon_{\text{F}})^2 + |\Delta_{n\mathbf{k}}|^2}$$







$$\Delta(T=0) = 1.764\, k_{\text{B}} T_{\text{c}}$$

$$\Delta(T \to T_{\text{c}}) \approx 3.06\, k_{\text{B}} T_{\text{c}} \sqrt{1 - (T/T_{\text{c}})}$$

Migdal-Eliashberg (isotropic)

$$\hat{G}(k,\tau) = -\langle T_\tau \Psi_k(\tau)\Psi_k^\dagger(0)\rangle$$
$$= -\begin{pmatrix} \langle T_\tau c_{k\uparrow}(\tau)c_{k\uparrow}^\dagger(0)\rangle & \langle T_\tau c_{k\uparrow}(\tau)c_{-k\downarrow}(0)\rangle \\ \langle T_\tau c_{-k\downarrow}^\dagger(\tau)c_{k\uparrow}^\dagger(0)\rangle & \langle T_\tau c_{-k\downarrow}^\dagger(\tau)c_{-k\downarrow}(0)\rangle \end{pmatrix}$$

Nambu notation

Migdal-Eliashberg (isotropic)

$$\hat{G}(k,\tau) = -\langle T_\tau \Psi_k(\tau)\Psi_k^\dagger(0)\rangle = -\begin{pmatrix} \langle T_\tau c_{k\uparrow}(\tau)c_{k\uparrow}^\dagger(0)\rangle & \langle T_\tau c_{k\uparrow}(\tau)c_{-k\downarrow}(0)\rangle \\ \langle T_\tau c_{-k\downarrow}^\dagger(\tau)c_{k\uparrow}^\dagger(0)\rangle & \langle T_\tau c_{-k\downarrow}^\dagger(\tau)c_{-k\downarrow}(0)\rangle \end{pmatrix}$$

Nambu notation

$$Z(i\omega_n) = 1 + \frac{\pi}{\beta\omega_n}\sum_{n'}\frac{\omega_{n'}}{\sqrt{\omega_{n'}^2 + \Delta^2(i\omega_{n'})}}\lambda(n-n'),$$

$$Z(i\omega_n)\Delta(i\omega_n) = \sum_{n'}\frac{\Delta(i\omega_{n'})}{\sqrt{\omega_{n'}^2 + \Delta^2(i\omega_{n'})}}[\lambda(n-n') - \mu^*]$$

where

$$\lambda(n-n') = \int_0^\infty d\Omega \frac{2\Omega\,\alpha^2F(\Omega)}{(\omega_n - \omega_{n'})^2 + \Omega^2}$$

Migdal-Eliashberg (isotropic)

$$\hat{G}(k,\tau) = -\langle T_\tau \Psi_k(\tau)\Psi_k^\dagger(0)\rangle = -\begin{pmatrix} \langle T_\tau c_{k\uparrow}(\tau)c_{k\uparrow}^\dagger(0)\rangle & \langle T_\tau c_{k\uparrow}(\tau)c_{-k\downarrow}(0)\rangle \\ \langle T_\tau c_{-k\downarrow}^\dagger(\tau)c_{k\uparrow}^\dagger(0)\rangle & \langle T_\tau c_{-k\downarrow}^\dagger(\tau)c_{-k\downarrow}(0)\rangle \end{pmatrix}$$

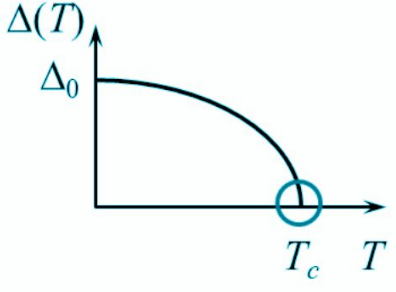
Nambu notation

$$Z(i\omega_n) = 1 + \frac{\pi}{\beta\omega_n}\sum_{n'}\frac{\omega_{n'}}{\sqrt{\omega_{n'}^2 + \Delta^2(i\omega_{n'})}}\lambda(n-n'),$$

$$Z(i\omega_n)\Delta(i\omega_n) = \sum_{n'}\frac{\Delta(i\omega_{n'})}{\sqrt{\omega_{n'}^2 + \Delta^2(i\omega_{n'})}}[\lambda(n-n') - \mu^*]$$

where

$$\lambda(n-n') = \int_0^\infty d\Omega \frac{2\Omega\,\alpha^2F(\Omega)}{(\omega_n - \omega_{n'})^2 + \Omega^2}$$



Migdal-Eliashberg (isotropic)

$$\hat{G}(k,\tau) = -\langle T_\tau \Psi_k(\tau)\Psi_k^\dagger(0)\rangle = -\begin{pmatrix} \langle T_\tau c_{k\uparrow}(\tau)c_{k\uparrow}^\dagger(0)\rangle & \langle T_\tau c_{k\uparrow}(\tau)c_{-k\downarrow}(0)\rangle \\ \langle T_\tau c_{-k\downarrow}^\dagger(\tau)c_{k\uparrow}^\dagger(0)\rangle & \langle T_\tau c_{-k\downarrow}^\dagger(\tau)c_{-k\downarrow}(0)\rangle \end{pmatrix}$$

Nambu notation

$$Z(i\omega_n) = 1 + \frac{\pi}{\beta\omega_n}\sum_{n'}\frac{\omega_{n'}}{\sqrt{\omega_{n'}^2 + \Delta^2(i\omega_{n'})}}\lambda(n-n'),$$

$$Z(i\omega_n)\Delta(i\omega_n) = \sum_{n'}\frac{\Delta(i\omega_{n'})}{\sqrt{\omega_{n'}^2 + \Delta^2(i\omega_{n'})}}[\lambda(n-n') - \mu^*]$$

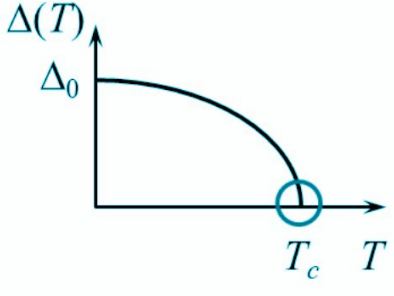
where

$$\lambda(n-n') = \int_0^\infty d\Omega \frac{2\Omega\,\alpha^2F(\Omega)}{(\omega_n - \omega_{n'})^2 + \Omega^2}$$

Allen-Dynes-modified McMillan formula

$$T_c = \frac{\omega_{\log}}{1.2}\exp\left(\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right)$$

The superconducting critical temperature is well approximated by the Allen-Dynes formula for moderate λ values in most systems.



Take-home message

- Electron-phonon coupling is involved in many quantities of interest.
- It affects both electronic and phononic spectral functions.
- It is the driving mechanism of conventional superconductivity.
- It is relevant for many technological applications.