

Theory of the electron-phonon interaction and superconductivity in anharmonic crystals

Giovanni Marini

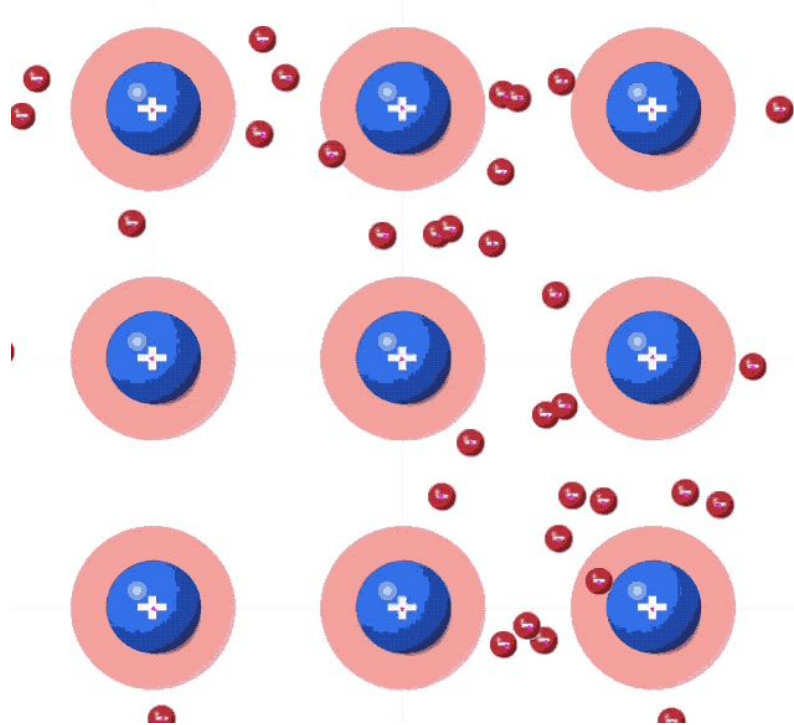
University of Trento

SSCHA School 2026



What is electron-phonon interaction ?

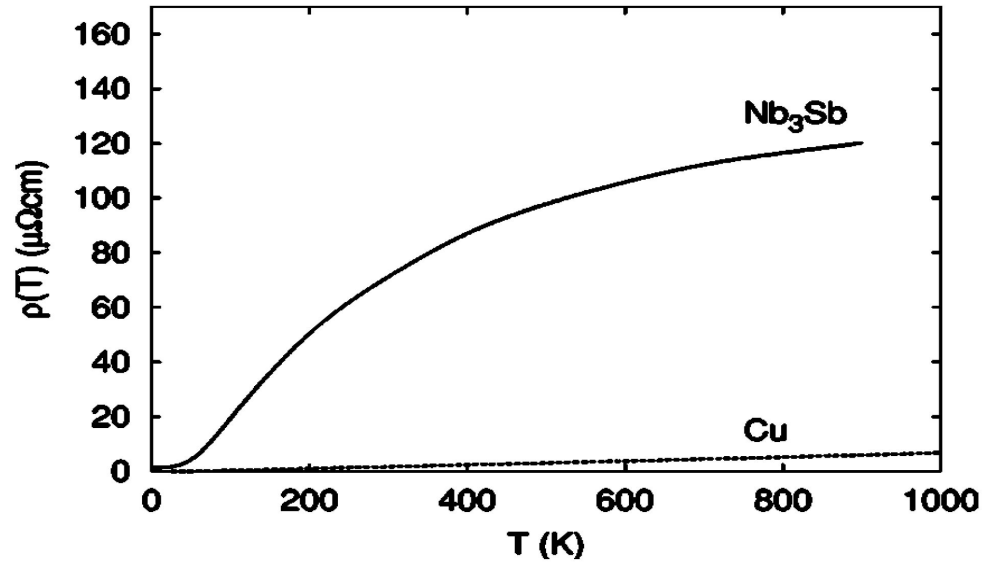
Electron-phonon interaction characterizes the interaction between electrons and the motion of nuclei.



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

First example: the intrinsic resistivity of metals

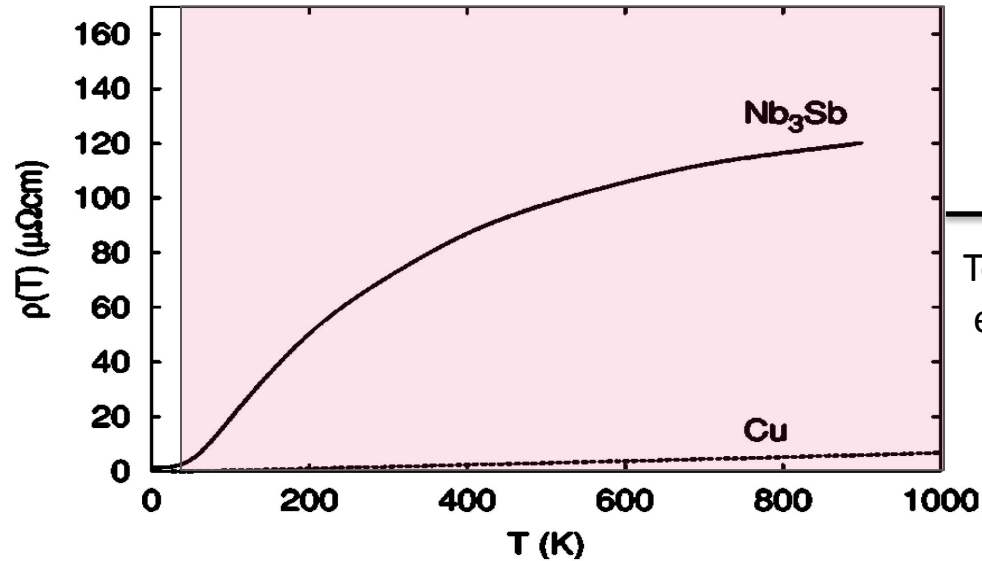
mostly due to the electron-phonon interaction for $k_B T \gtrsim \hbar \omega$



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

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

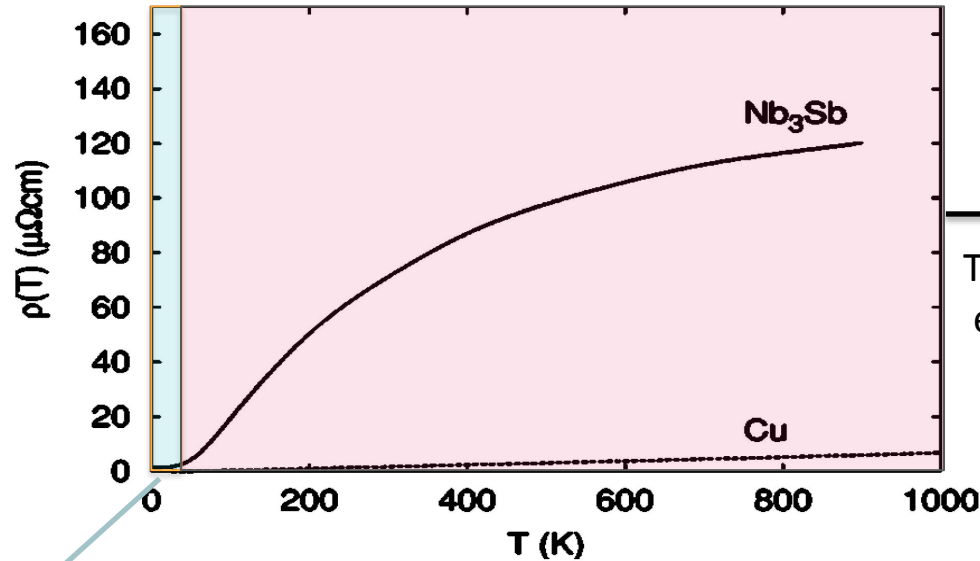


Temperature range where the el-ph scattering is dominant!

See O. Gunnarsson, M. Calandra, and J. E. Han
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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
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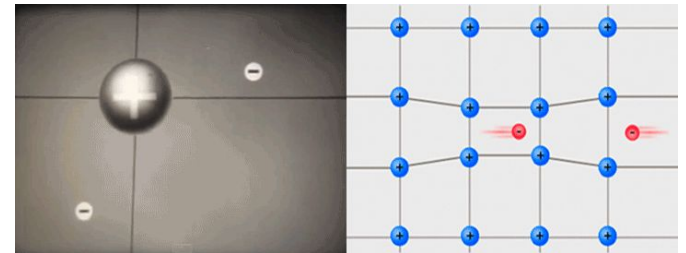
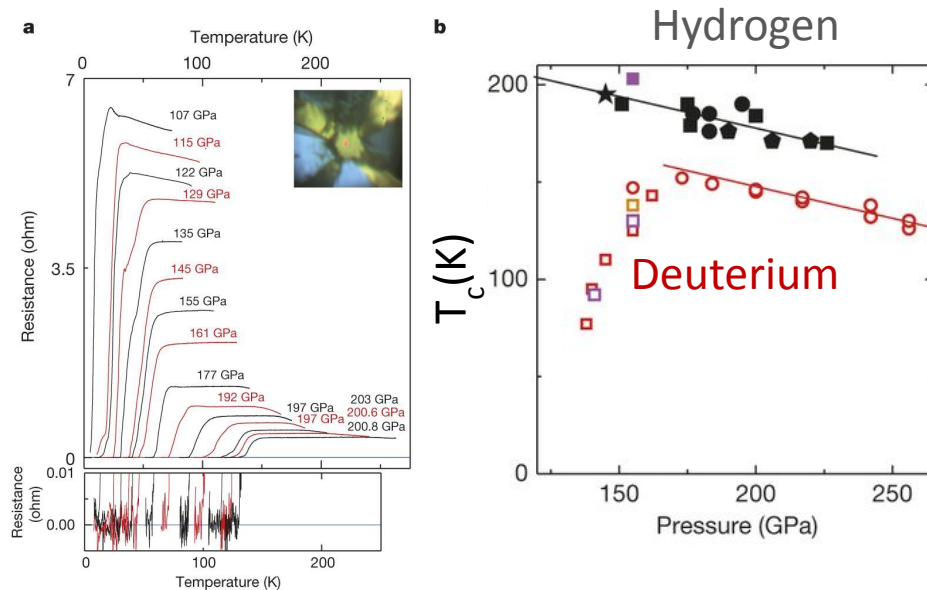
Second example: electron-phonon mediated superconductivity

LETTER

doi:10.1038/nature14964

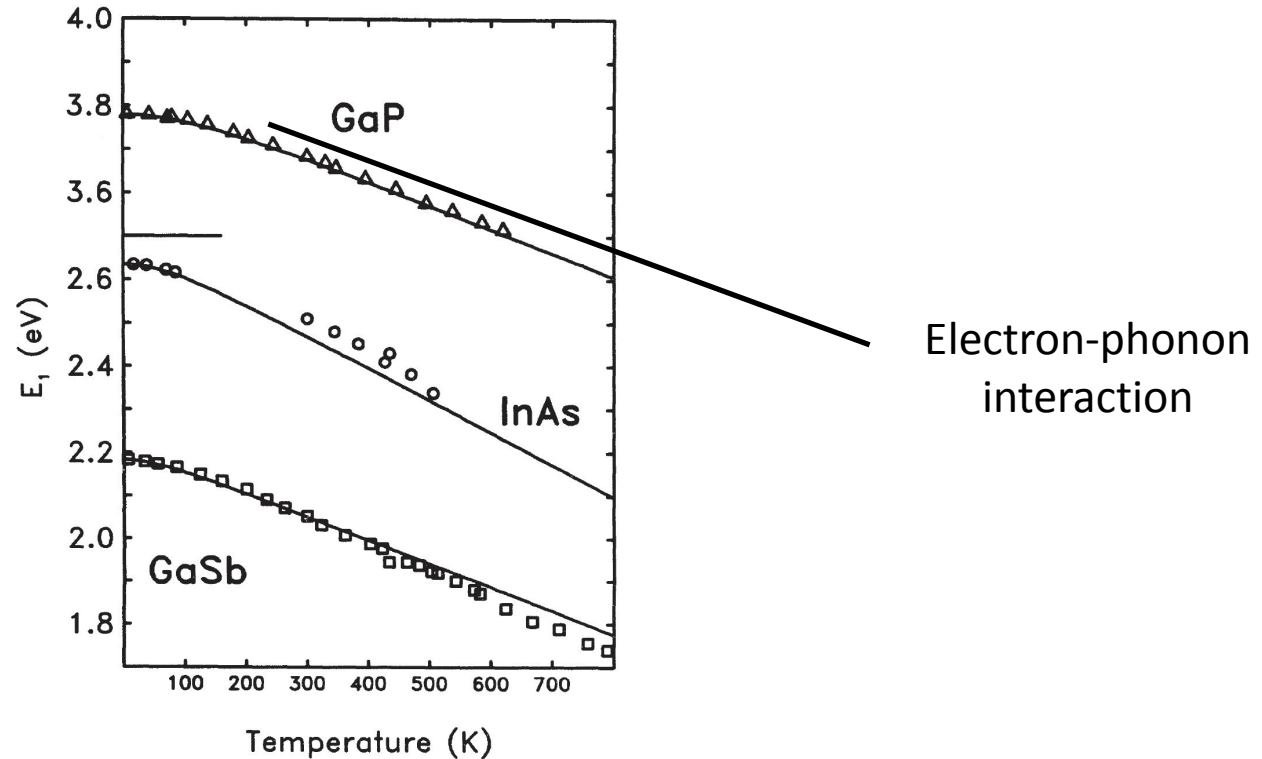
Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system

A. P. Drozdov¹*, M. I. Erements¹*, I. A. Troyan¹, V. Ksenofontov² & S. I. Shylin²



Conventional superconductivity is due to the electron-phonon interaction

Third example: temperature dependence of band gaps in semiconductors

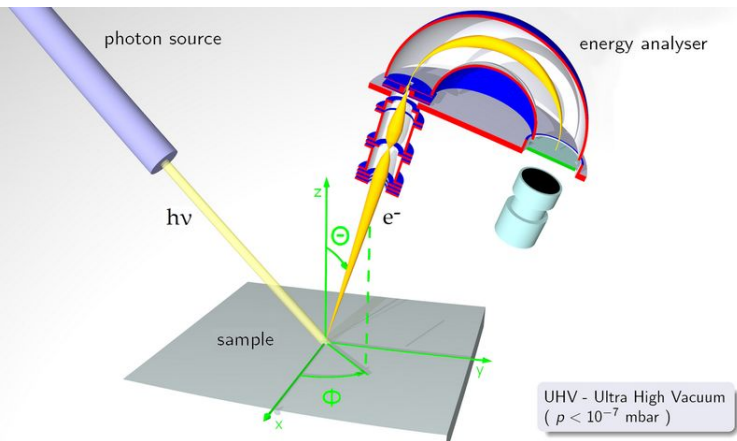


M. Cardona, S. Gopalan, Progress in Electron Properties of Solids pp 51-64

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)



Energy conservation:

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

E_B = Binding Energy

We measure E_{kin}, ϑ

to obtain $E_B, k_{//, solid}$

Initial state (incident photon)

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

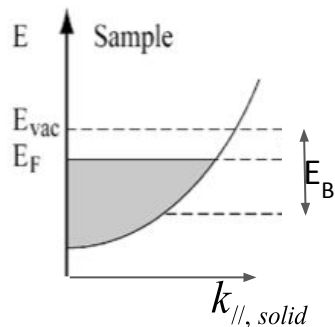
Final state (extracted electron)

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

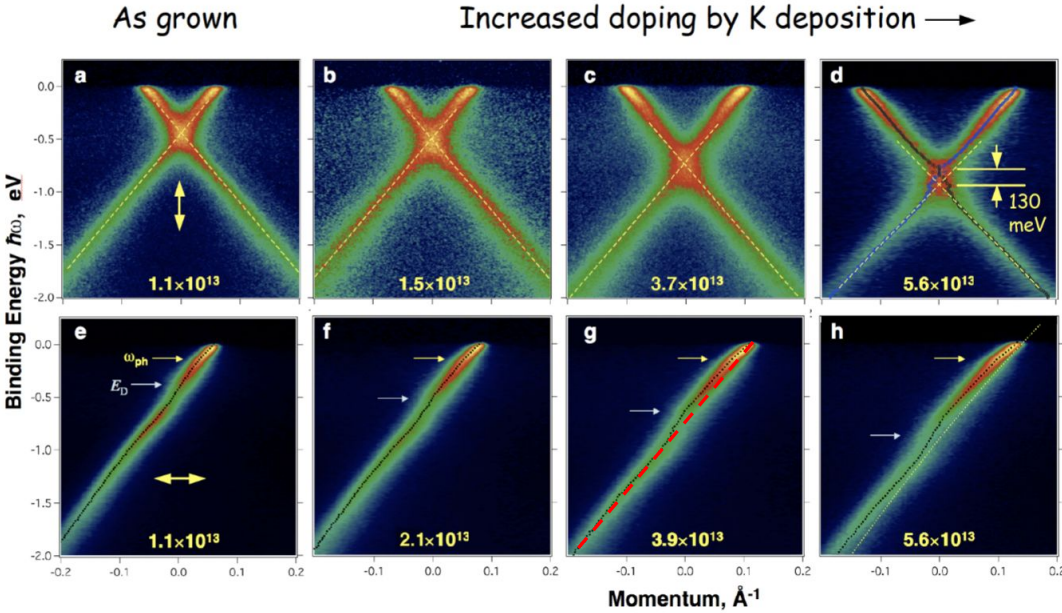
Momentum conservation

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

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



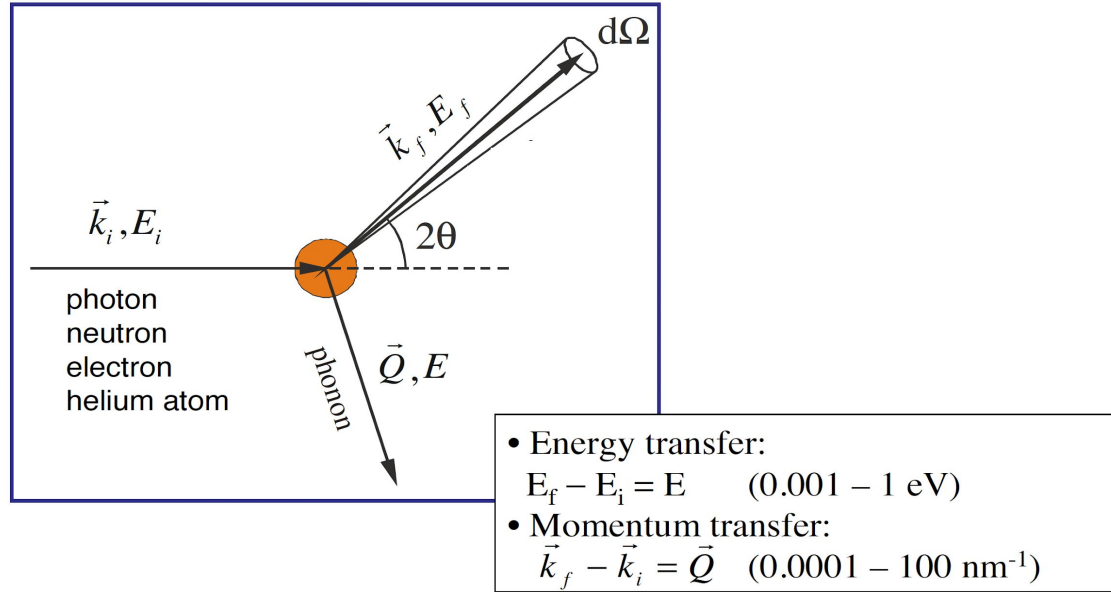
ARPES: kinks in electronic structure due to the electron-phonon interaction



DFT bands

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

Inelastic X-ray scattering to measure phonons



$$\mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i$$

$$E = E_f - E_i$$

$$E_f = ck_f$$

$$E_i = ck_i$$

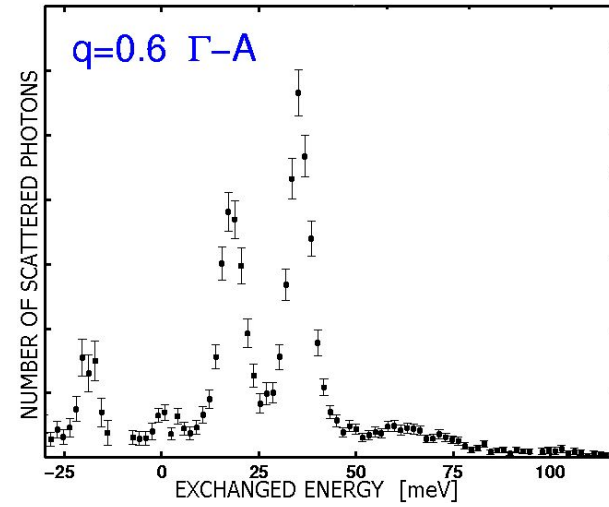
$$E \ll E_f$$

$$E \ll E_i$$

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

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

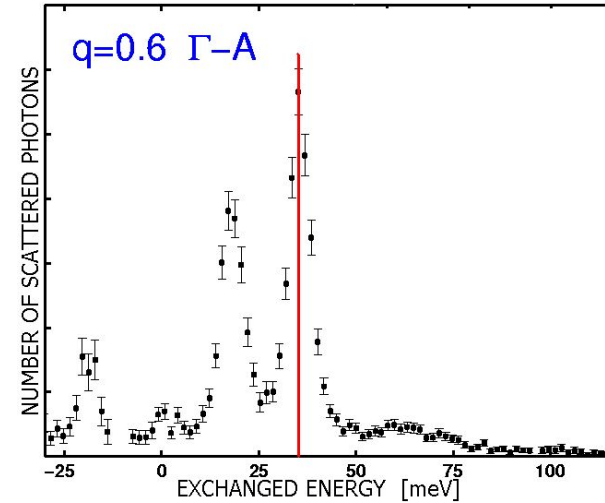
Fifth example: inelastic X-ray scattering spectra



Fifth example: inelastic X-ray scattering spectra

Energy of the phonon line :

- ➔ Harmonic phonon frequency
- ➔ Anharmonic shift



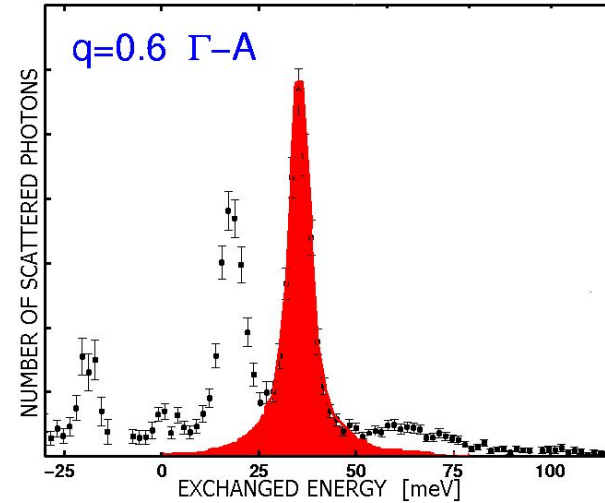
Fifth example: inelastic X-ray scattering spectra

Energy of the phonon line :

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Intensity of the phonon line :

- Phonon eigenvectors



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Energy of the phonon line :

- Harmonic phonon frequency
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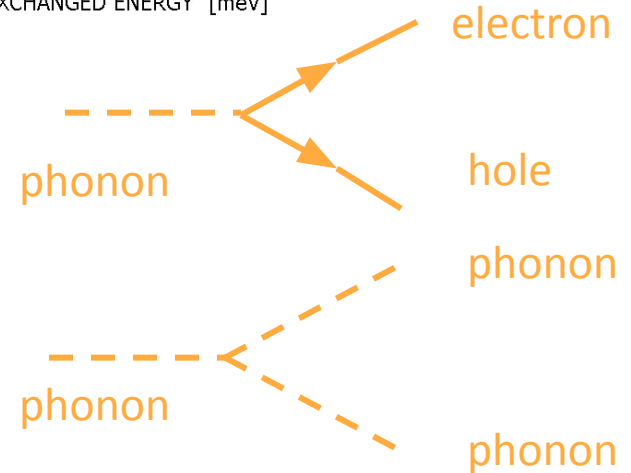
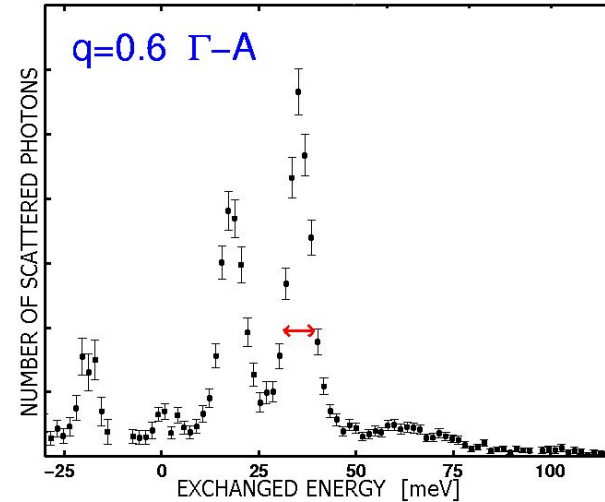
- Phonon eigenvectors

Phonon linewidth :

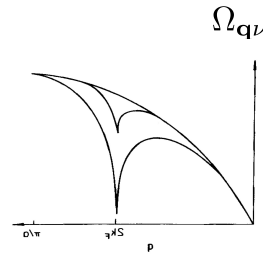
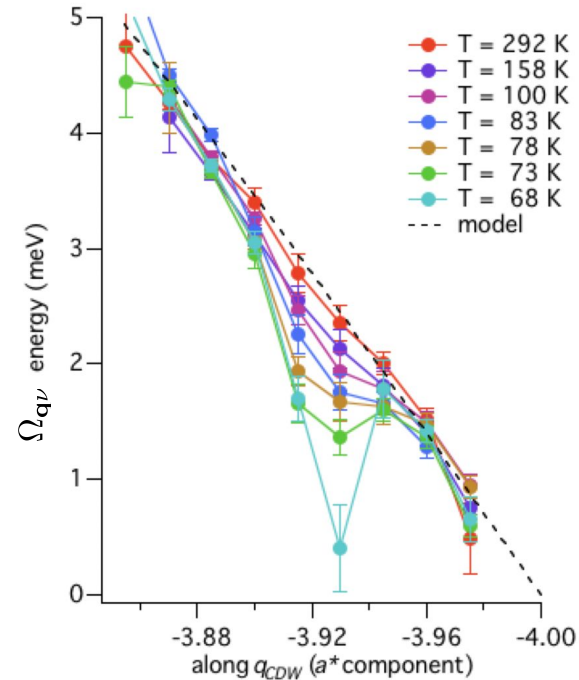
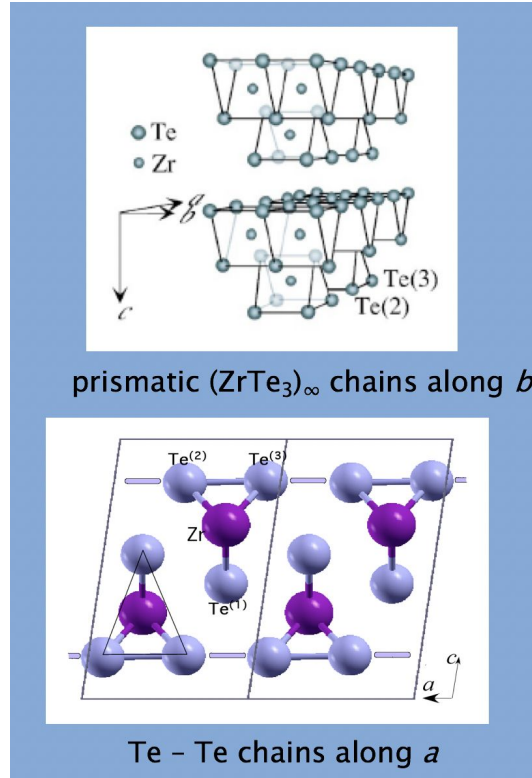
- Decay of a phonon in an electron-hole pair due to the electron-phonon coupling

+

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

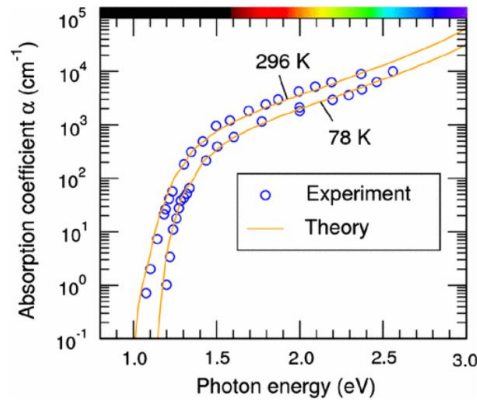


Sixth example: ZrTe_3 1D metal, charge-density wave phase seen in IXS

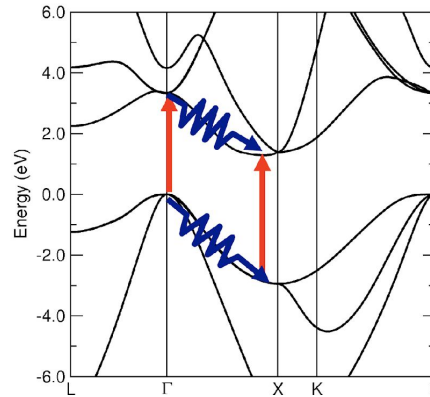


Hoesch, *et al.* Phys. Rev. Lett. **102**, 086402 (2009)

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

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

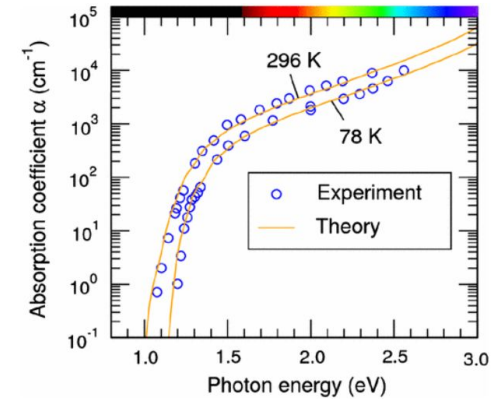
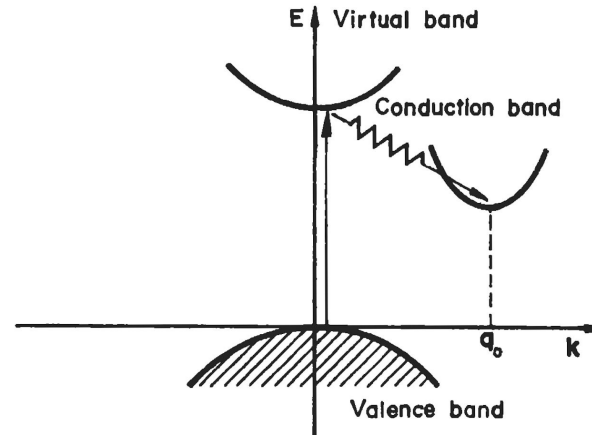
No absorption below the gap

Electron-phonon mediated optical absorption

Fermi golden rule @ second order

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

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



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

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Crystalline systems: notation

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

The coordinate of each atom is identified by

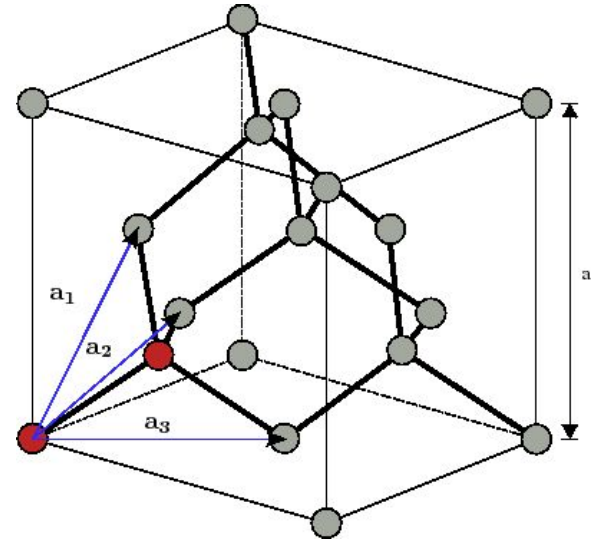
$$\mathbf{R}_{LA} = \mathbf{R}_L + \tau_A$$

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

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

Crystal Hamiltonian

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

Purely Ionic part

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

Z_A atomic number

Crystal Hamiltonian

$$\mathcal{H} = \underbrace{\sum_{L,A} \frac{\mathbf{P}_{LA}^2}{2M_A}}_{\text{Purely Ionic part}} + V(\mathbf{R}) + \underbrace{\sum_i \frac{\mathbf{p}_i^2}{2m}}_{\text{Electronic part}} + V_e(\mathbf{r}) + V_{ie}(\mathbf{r}, \mathbf{R})$$

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Electronic part

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

$\mathbf{r}_i$ electronic coordinate

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$\mathbf{r}_i$ 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

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



We call this H_{el}

Exact factorization

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

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

The exact solution of this equation is written as

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

where for any t and any fixed ionic configuration $\mathbf{R}$

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

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:

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

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This leads to:

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

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This leads to:

$$\int d\mathbf{r} \psi^* \mathcal{H} \chi \psi = \sum_I \psi \frac{\mathbf{P}_I^2}{2M_I} \chi + \sum_I \frac{1}{2M_I} [2(\mathbf{P}_I \chi) \mathbf{P}_I + \chi (\mathbf{P}_I^2 + H_{el})] \psi = \mathcal{E} \chi \psi \int d\mathbf{r} \psi^*$$

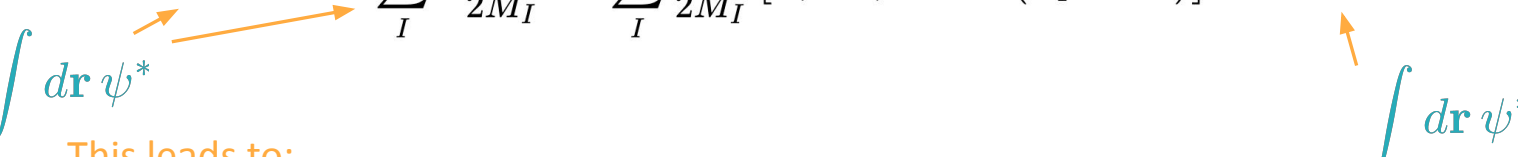
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$$\sum_I \frac{\mathbf{P}_I^2}{2M_I} \chi + \sum_I \frac{1}{2M_I} [2(\mathbf{P}_I \chi) \langle \psi | \mathbf{P}_I | \psi \rangle + \chi \langle \psi | \mathbf{P}_I^2 | \psi \rangle] + \chi \langle \psi | H_{el} | \psi \rangle = \mathcal{E} \chi$$

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

This leads to:

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

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



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

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Born-Oppenheimer approximation



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Born-Oppenheimer approximation



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

- 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.

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- Electron-phonon matrix elements
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Neglected terms in the BO

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

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

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

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:

$$\begin{aligned}\psi_n &= \psi_n^0 + \delta\psi_n = \psi_n^0 + \delta\psi_n^1 + \delta\psi_n^2 + \dots = \\ &= \psi_n^0 + \sum_{n' \neq n} \frac{\langle \psi_{n'}^0 | \Delta H_e | \psi_n^0 \rangle}{\epsilon_n^0 - \epsilon_{n'}^0} \psi_{n'}^0 + \sum_{n' \neq n} \sum_{m' \neq n} \frac{\langle \psi_{n'}^0 | \Delta H_e | \psi_{m'}^0 \rangle}{\epsilon_n^0 - \epsilon_{m'}^0} \frac{\langle \psi_{m'}^0 | \Delta H_e | \psi_{n'}^0 \rangle}{\epsilon_{n'}^0 - \epsilon_{n'}^0} \psi_{n'}^0 + \dots\end{aligned}$$

Perturbation theory with

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

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:

$$\begin{aligned}\psi_n &= \psi_n^0 + \delta\psi_n = \psi_n^0 + \delta\psi_n^1 + \delta\psi_n^2 + \dots = \\ &= \psi_n^0 + \sum_{n' \neq n} \frac{\langle \psi_{n'}^0 | \Delta H_e | \psi_n^0 \rangle}{\epsilon_n^0 - \epsilon_{n'}^0} \psi_{n'}^0 + \sum_{n' \neq n} \sum_{m' \neq n} \frac{\langle \psi_{n'}^0 | \Delta H_e | \psi_{m'}^0 \rangle}{\epsilon_n^0 - \epsilon_{m'}^0} \frac{\langle \psi_{m'}^0 | \Delta H_e | \psi_{n'}^0 \rangle}{\epsilon_n^0 - \epsilon_{n'}^0} \psi_{n'}^0 + \dots\end{aligned}$$

Perturbation theory with

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

Then we have to replace ψ_n in

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

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 $\mathbf{R}-\mathbf{R}_0$

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

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

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

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

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

As $\delta\psi_n^1$ is linear in $\mathbf{u}_I$, then $\mathbf{P}_I^2 \mathbf{u}_I = 0$ 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 $\mathbf{R}-\mathbf{R}_0$

$$\begin{aligned} \langle \chi_\rho \psi_m | \mathcal{H} | \chi_\xi \psi_n \rangle \approx & \langle \chi_\xi | \left[\sum_I \frac{\mathbf{P}_I^2}{2M_I} + E(\mathbf{R}) \right] | \chi_\xi \rangle \delta_{\xi,\rho} \delta_{n,m} \\ & - i\hbar \sum_I \frac{1}{M_I} \langle \chi_\rho | \mathbf{P}_I | \chi_\xi \rangle \frac{\langle \psi_m^0 | \nabla_{\mathbf{u}_I} H_e | \psi_n^0 \rangle}{\epsilon_n^0 - \epsilon_m^0} (1 - \delta_{mn}) \end{aligned}$$

We focus on the linear order and manipulate this term 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 energy conservation:

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

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

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

Deformation Potential
(real space)

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

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

Linear electron-phonon coupling

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

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

$$\Delta H^1 = \sum_{\nu \mathbf{q}} \sum_{a\alpha} \sqrt{\frac{\hbar}{2NM_a \omega_{\mathbf{q}\nu}}} (e_{\mathbf{q}\nu}^{a\alpha})^* \langle \chi_\rho | a_{\mathbf{q}\nu} + a_{-\mathbf{q}\nu}^\dagger | \chi_\xi \rangle \langle \psi_m^0 | \frac{\partial H_e}{\partial u_{\mathbf{q}a\alpha}} | \psi_n^0 \rangle$$

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

$$\Delta H^1 = \sum_{\nu \mathbf{q}} \sum_{a\alpha} \sqrt{\frac{\hbar}{2NM_a\omega_{\mathbf{q}\nu}}} (e_{\mathbf{q}\nu}^{a\alpha})^* \langle \chi_\rho | a_{\mathbf{q}\nu} + a_{-\mathbf{q}\nu}^\dagger | \chi_\xi \rangle \langle \psi_m^0 | \frac{\partial H_e}{\partial u_{\mathbf{q}a\alpha}} | \psi_n^0 \rangle$$

One-body operators are written in second quantization as:

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

where $\{|\phi_s\rangle\}$ is a 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

We introduce the Kohn-Sham potential:

$$V_{KS}(\mathbf{r}) = H_{el} - T_{el}$$

and apply a monochromatic perturbation

$$V_{KS}(\mathbf{r}) = e^{i\mathbf{q}\mathbf{r}} v_{KS}(\mathbf{r})$$

We have

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

Defining the electron-phonon matrix element as

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

Hamiltonian in second quantization (Frölich)



We obtain the electron-phonon Hamiltonian in second quantization:

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

with

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

and

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

Outline

- Born Oppenheimer (BO) and exact factorization
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- Effects on the phonons
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Perturbation Theory

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

Green's function

$$\underline{G_0(\mathbf{k}n, \omega)}$$

$$\underline{G(\mathbf{k}n, \omega)}$$

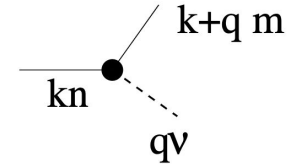
$$\cdots D_0(\mathbf{q}\nu, \omega) \cdots$$

$$\cdots D(\mathbf{q}\nu, \omega) \cdots$$

Free/bare

Interacting/dressed

electron-phonon vertex



$$\bullet g_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}^\nu$$

Perturbation Theory

Electrons

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

non-interacting

Phonons

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

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

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

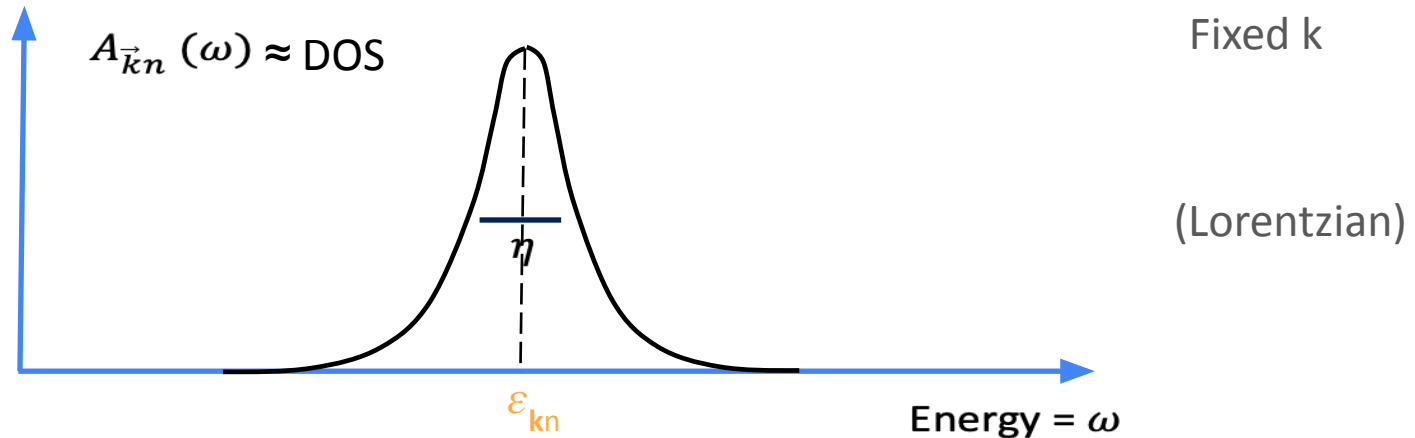
Spectral function

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

In the absence of interaction,

$$\begin{aligned}\text{Re } \Sigma(\mathbf{k}n, \omega) &\rightarrow 0 \\ \text{Im } \Sigma(\mathbf{k}n, \omega) &\rightarrow \eta\end{aligned}$$

the spectral weight has simple poles at the energies $\epsilon_{\mathbf{k}n}$



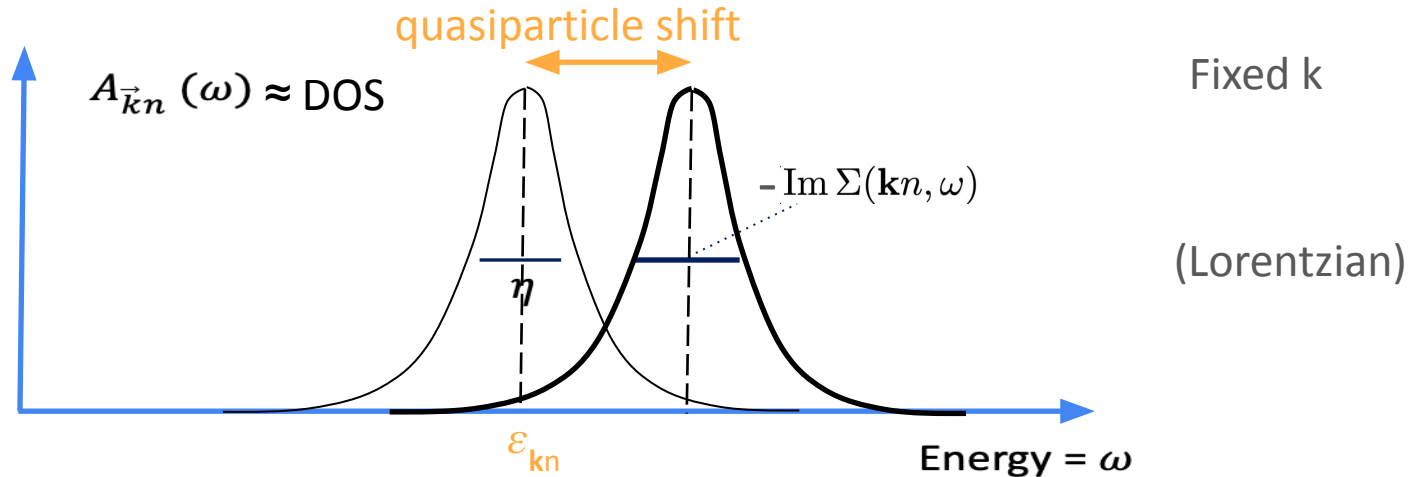
Effect on the electrons: spectral function

Spectral function

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

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

THE QUASIPARTICLE PICTURE IS PRESERVED



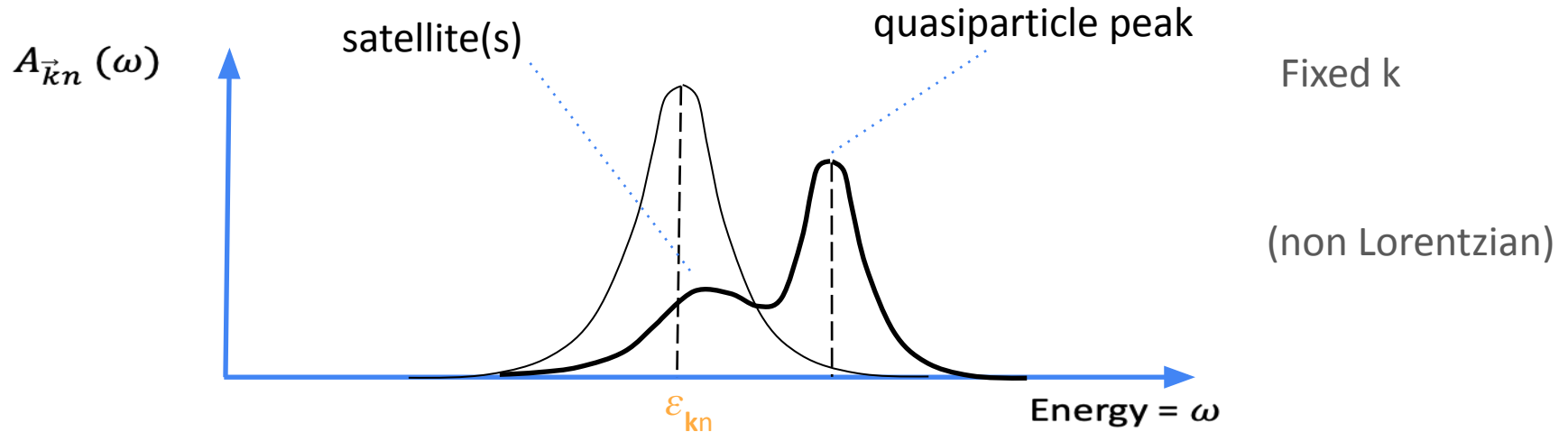
Effect on the electrons: spectral function

Spectral function

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

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

THE QUASIPARTICLE PICTURE IS BROKEN

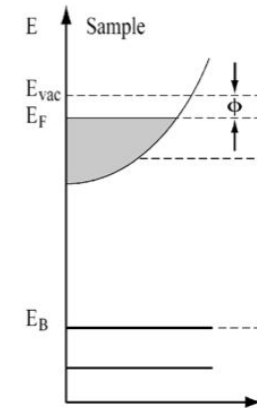
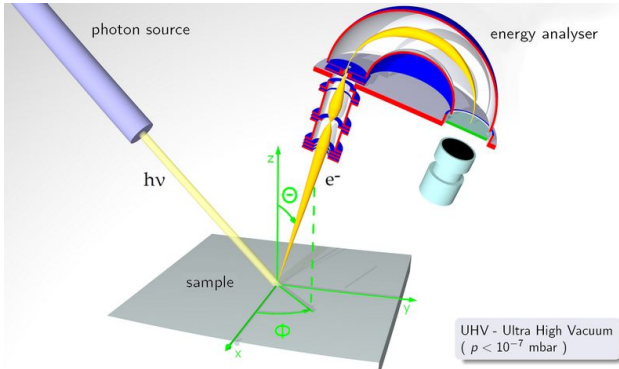


Effect on the electrons: spectral function

Spectral function

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

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



Quasiparticle picture $\text{Im } \Sigma(\mathbf{k}n, \omega) \ll \text{Re } \Sigma(\mathbf{k}n, \omega)$

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

$$\text{Im } \Sigma(\mathbf{k}n, \omega) \ll \text{Re } \Sigma(\mathbf{k}n, \omega)$$

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 $\frac{\partial \text{Im } \Sigma(\mathbf{k}n, \omega)}{\partial \omega} \ll \frac{\partial \text{Re } \Sigma(\mathbf{k}n, \omega)}{\partial \omega}$ we obtain:

Quasiparticle picture $\text{Im } \Sigma(\mathbf{k}n, \omega) \ll \text{Re } \Sigma(\mathbf{k}n, \omega)$

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 $\frac{\partial \text{Im } \Sigma(\mathbf{k}n, \omega)}{\partial \omega} \ll \frac{\partial \text{Re } \Sigma(\mathbf{k}n, \omega)}{\partial \omega}$ we obtain:

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

The quasiparticles are shifted by an amount

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

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

Quasiparticle picture $\text{Im } \Sigma(\mathbf{k}n, \omega) \ll \text{Re } \Sigma(\mathbf{k}n, \omega)$

The quasiparticles are shifted by an amount

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

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

Is called the mass enhancement parameter.

Taking the gradient with respect to $\mathbf{k}$ 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 $\text{Im } \Sigma(\mathbf{k}n, \omega) \ll \text{Re } \Sigma(\mathbf{k}n, \omega)$

The quasiparticles are shifted by an amount

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

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

Is called the mass enhancement parameter.

Taking the gradient with respect to $\mathbf{k}$ 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

$$\text{Im } \Sigma(\mathbf{k}n, \omega) \ll \text{Re } \Sigma(\mathbf{k}n, \omega)$$

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

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.

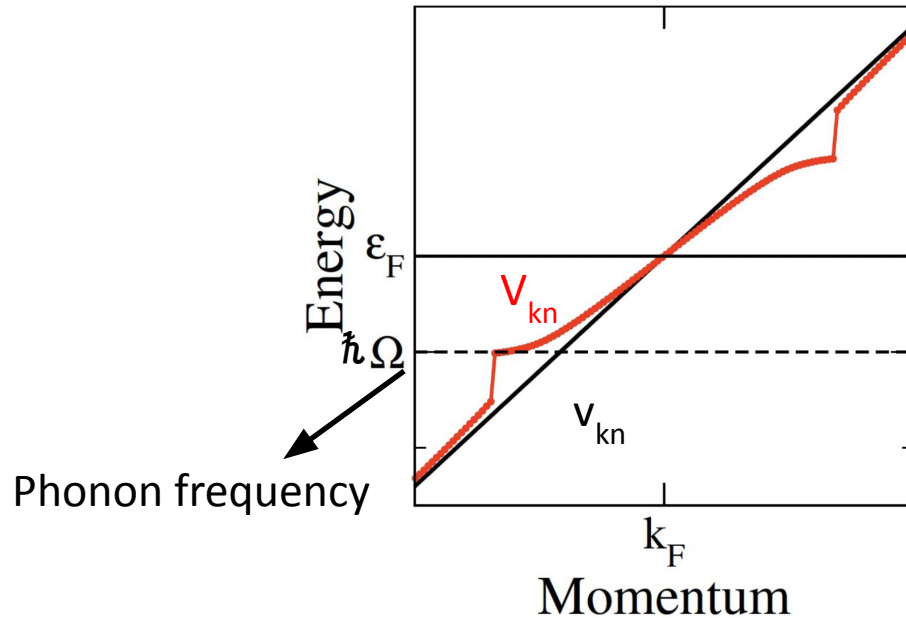
Velocity and mass renormalization

$$V_{kn} = \frac{v_{kn}}{1 + \lambda_{kn}}$$

Velocity renormalization due to the electron-phonon coupling

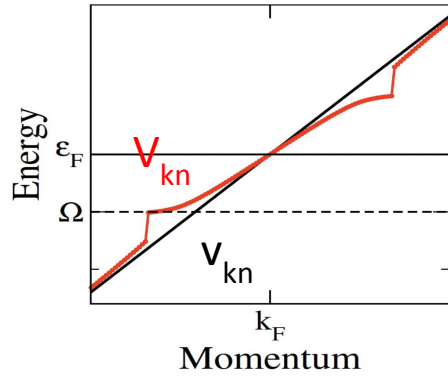
$$M_{kn}^* = (1 + \lambda_{kn})m_{kn}^*$$

Mass renormalization due to the electron-phonon coupling



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

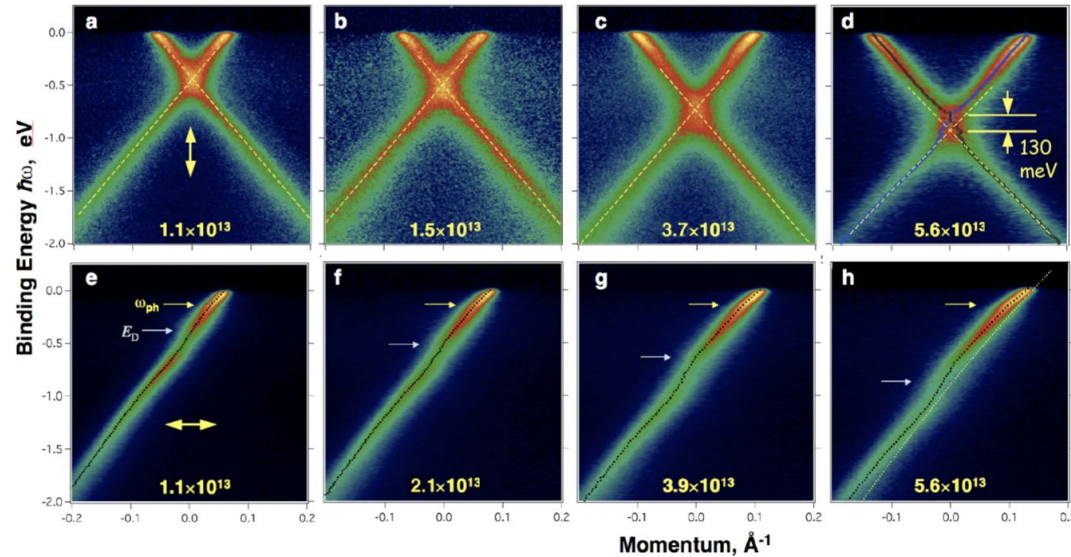
Velocity and mass renormalization – Experiments (K-covered Graphene)



As grown

Increased doping by K deposition →

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



Quasiparticle picture $\text{Im } \Sigma(\mathbf{k}n, \omega) \ll \text{Re } \Sigma(\mathbf{k}n, \omega)$

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 $\frac{\partial \text{Im } \Sigma(\mathbf{k}n, \omega)}{\partial \omega} \ll \frac{\partial \text{Re } \Sigma(\mathbf{k}n, \omega)}{\partial \omega}$ we obtain:

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

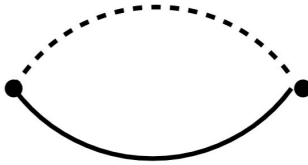
We finally note that the width of the Lorentzian is $\Gamma_{\mathbf{k}n} = -\text{Im } \Sigma(\mathbf{k}n, \omega)$

The electron scattering time for an electron of momentum $\mathbf{k}$ in the n^{th} band is

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

Electron self-energy

The lowest energy diagram is

$$\Sigma(\mathbf{k}, \omega) =$$


The diagram shows two vertices (black dots) connected by a solid line (electron) and a dashed line (photon), representing the lowest-order electron self-energy.

Electron self-energy

The lowest energy diagram is

$$\Sigma(\mathbf{k}n, \omega) = \text{[Diagram: A fermion line with two vertices connected by a dashed loop and a solid loop.]}$$

Leading to:

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

with:

$$n_{\mathbf{q}\nu} = \frac{1}{\exp(\beta\hbar\omega_{\mathbf{q}\nu}) - 1}$$

$$f_{\mathbf{k}n} = \frac{1}{\exp(\beta(\epsilon_{\mathbf{k}n} - \mu)) + 1}$$

Real part of the electron self-energy

The real part is

Principal value

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

Real part of the electron self-energy

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The quasiparticles are:

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

Imaginary part of the electron self-energy

The imaginary part is

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

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

Imaginary part of the electron self-energy

The imaginary part is

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

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

At low temperature the Bose functions can be neglected and

$$-\text{Im } \Sigma(\mathbf{k}n, \omega) = \frac{\pi}{N_q} \sum_{\mathbf{q}m} \sum_{\nu} |g_{\mathbf{k}n, \mathbf{k}+\mathbf{q}m}^{\nu}|^2 [f_{\mathbf{k}+\mathbf{q}m} \delta(\hbar\omega + \hbar\omega_{\mathbf{q}\nu} - \epsilon_{\mathbf{k}+\mathbf{q}m}) + (1 - f_{\mathbf{k}+\mathbf{q}m}) \delta(\hbar\omega - \hbar\omega_{\mathbf{q}\nu} - \epsilon_{\mathbf{k}+\mathbf{q}m})] \propto \frac{1}{T}$$

Eliashberg function

The imaginary part is

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

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

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

Eliashberg function

The imaginary part is

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

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

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

Eliashberg function (approximation)

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

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)

$$\alpha^2 F_{\mathbf{kn}}^{\pm}(\omega, \Omega) = \frac{1}{N_q} \sum_{\mathbf{q}\nu} \delta(\hbar\Omega - \hbar\omega_{\mathbf{q}\nu}) \sum_m |g_{\mathbf{kn}, \mathbf{k}+\mathbf{q}m}^{\nu}|^2 \delta(\hbar\omega - \epsilon_{\mathbf{k}+\mathbf{q}m} \pm \hbar\omega_{\mathbf{q}\nu})$$

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:

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

$$\alpha^2 F_{\mathbf{kn}}(\omega, \Omega) = \alpha^2 F_{\mathbf{kn}}^+(\omega, \Omega) = \alpha^2 F_{\mathbf{kn}}^-(\omega, \Omega)$$

Eliashberg function (approximation)

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

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

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

To obtain:

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

Eliashberg function - zero temperature

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

At T=0 we have

$$n(\Omega) = 0$$

$$f(\omega) = 1 - \theta(\omega)$$

Eliashberg function - zero temperature

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

At T=0 we have

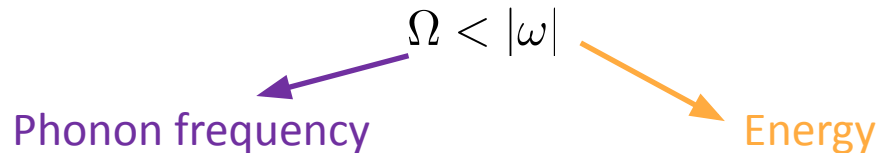
$$n(\Omega) = 0$$

$$f(\omega) = 1 - \theta(\omega)$$

So that

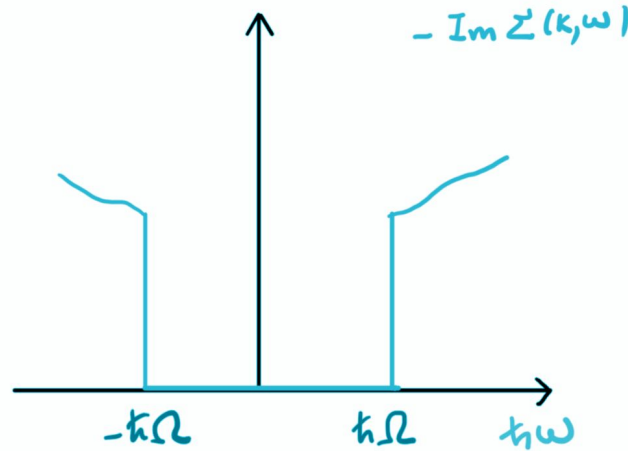
$$\text{Im } \Sigma(\mathbf{k}n, \omega) = -\pi \hbar \int_{-0}^\infty d\Omega [\alpha^2 F_{\mathbf{k}n}(\omega, \Omega) (2 - \theta(\omega + \Omega) - \theta(\Omega - \omega))]$$

This expression is zero if



Imaginary part of the electron self-energy at zero temperature

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



Finite temperature behaviour of the electronic linewidth

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

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

Finite temperature behaviour of the electronic linewidth

$$\begin{aligned}\Gamma_{\mathbf{k}n} &= -\text{Im} \Sigma(\mathbf{k}n, \omega = E_{\mathbf{k}n}) \\ &= \pi \int_0^\infty d\Omega \left[\alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n}, \Omega) (2n(\Omega) + f(\Omega + E_{\mathbf{k}n}) + f(\Omega - E_{\mathbf{k}n})) \right]\end{aligned}$$

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):

$$\begin{aligned}&\approx 2\pi \int_0^\infty d\Omega \alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n}, \Omega) + 2\pi k_B T \int_0^\infty \frac{\alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n}, \Omega)}{\hbar\Omega} d\Omega : \\ &= 2\pi \int_0^\infty d\Omega \alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n}, \Omega) + \pi k_B T \lambda_{\mathbf{k}n}\end{aligned}$$
$$\lambda_{\mathbf{k}n} = 2 \int_0^\infty \frac{\alpha^2 F_{\mathbf{k}n}(E_{\mathbf{k}n}, \Omega)}{\hbar\Omega} d\Omega$$

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.

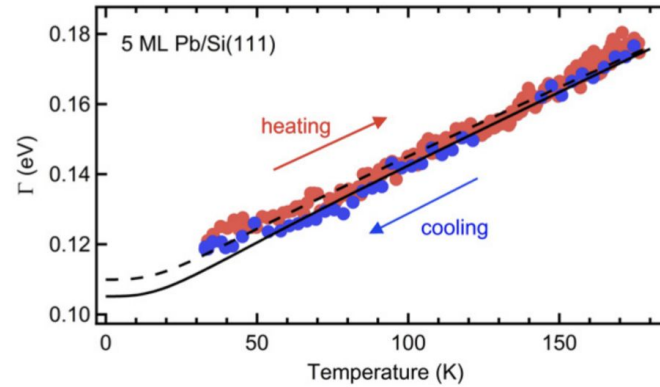
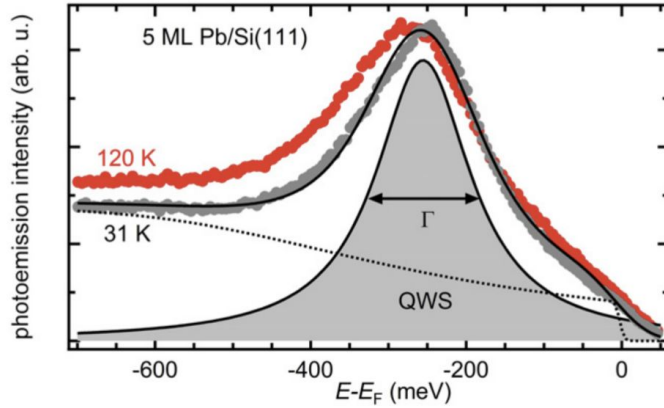
It is labeled exactly as the mass enhancement parameter:

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

as it is possible to show that they are the same quantity.

Electron-linewidth finite temperature behaviour - Experiments

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



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

=====

$D(\mathbf{q}\nu,\omega)$

Phonon interacting Green Function

The simplest approximation to the interacting phonon propagator is

$D(\mathbf{q}\nu,\omega)$

=====

=

$D_0(\mathbf{q}\nu,\omega)$

+

$D_0(\mathbf{q}\nu,\omega)$

$D_0(\mathbf{q}\nu,\omega)$

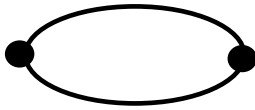
+

.....

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

$$\Pi(\mathbf{q}\nu, \omega) = \text{diagram}$$
A Feynman diagram representing the phonon self-energy at the lowest order. It consists of two black dots (vertices) connected by two curved lines (phonon lines) forming a horizontal loop or bubble.

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

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

$$\Pi(\mathbf{q}\nu, \omega) = \text{diagram of a bubble loop}$$

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

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.

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

Phonon self-energy at lowest order

$$\Pi(\mathbf{q}\nu, \omega) = \text{diagram of a bubble loop}$$

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

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.

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

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

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:

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

with

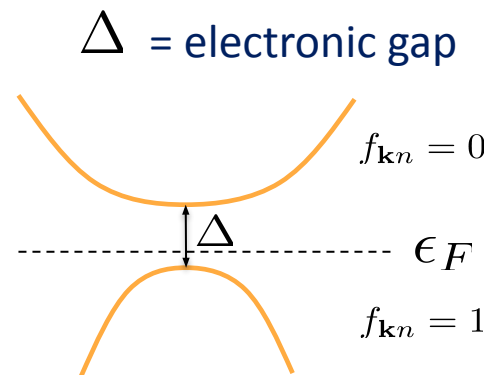
$$\operatorname{Re} \Pi(\mathbf{q}\nu, \omega) = -\frac{1}{N_{\mathbf{q}}} \mathcal{P} \sum_{\mathbf{k}} \sum_{n,m} |g_{\mathbf{k}n, \mathbf{k}+\mathbf{q}m}^{\nu}|^2 \frac{f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m}}{\hbar\omega + \epsilon_{\mathbf{k}n} - \epsilon_{\mathbf{k}+\mathbf{q}m}}$$

Phonon quasiparticle energies (insulators)

In an insulator (large gap), we have

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

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



We have

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

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

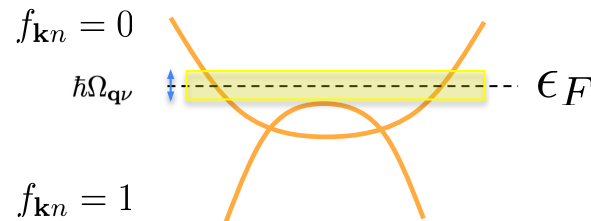
The fraction is dominated by the gap at the denominator and this term is small.

Phonon quasiparticle energies (metals)

In metals, we have

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

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



We have

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

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

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

with

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

It is a very accurate approximation in most cases.

Phonon quasiparticle energies in the adiabatic approximation

Thus we have

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

with

$$\operatorname{Re} \Pi(\mathbf{q}\nu, \Omega_{\mathbf{q}\nu}) = -\frac{1}{N_{\mathbf{q}}} \mathcal{P} \sum_{\mathbf{k}} \sum_{n,m} |g_{\mathbf{k}n, \mathbf{k}+\mathbf{q}m}^{\nu}|^2 \frac{f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m}}{\hbar\Omega_{\mathbf{q}\nu} + \epsilon_{\mathbf{k}n} - \epsilon_{\mathbf{k}+\mathbf{q}m}}$$

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

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

with

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

It can also be shown that due to causality

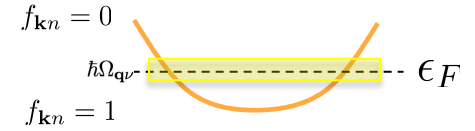
$$\operatorname{Re} \Pi(\mathbf{q}, 0) > 0$$

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

Example

One parabolic band.

One phonon mode.



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

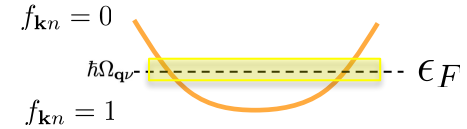
We have: $\text{Re } \Pi(\mathbf{q}, 0) = -g^2 \chi_0(\mathbf{q})$

$\chi_0(\mathbf{q})$ Lindhard function

Example

One parabolic band.

One phonon mode.

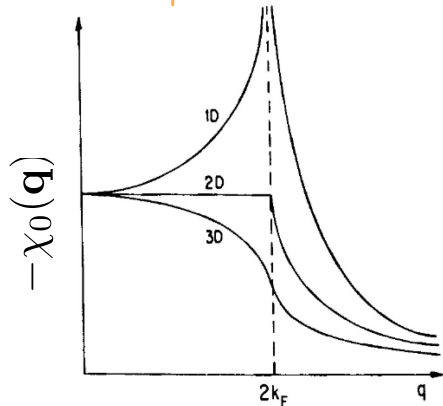


Constant electron-phonon matrix elements: $|g_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}^\nu|^2 = g^2$

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Lindhard function

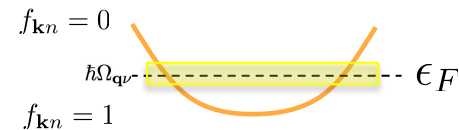
The self-energy diverges
At $2k_F$ in $D=1$



Example

One parabolic band.

One phonon mode.

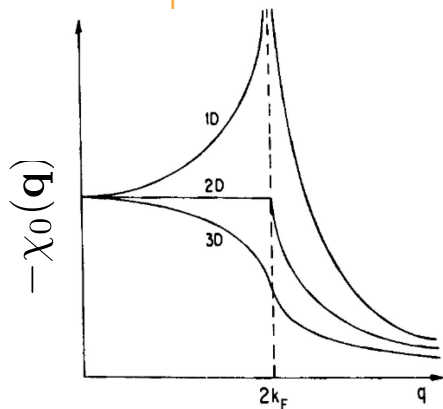


Constant electron-phonon matrix elements: $|g_{\mathbf{k}n, \mathbf{k}+\mathbf{q}m}^\nu|^2 = g^2$

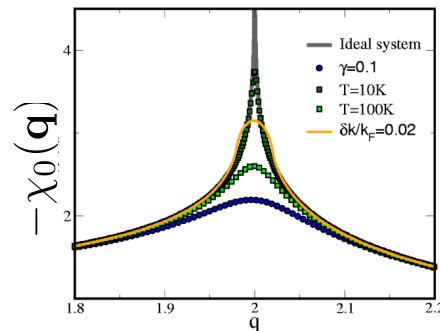
We have:

$$\text{Re } \Pi(\mathbf{q}, 0) = -g^2 \underbrace{\chi_0(\mathbf{q})}_{\text{Lindhard function}}$$

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



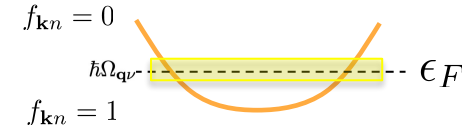
Temperature dependence



Example

One parabolic band.

One phonon mode.



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

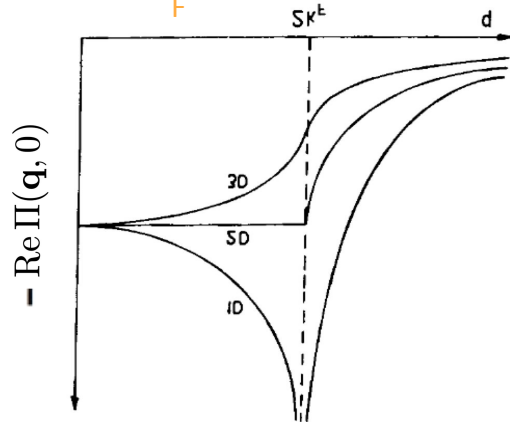
We have:

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

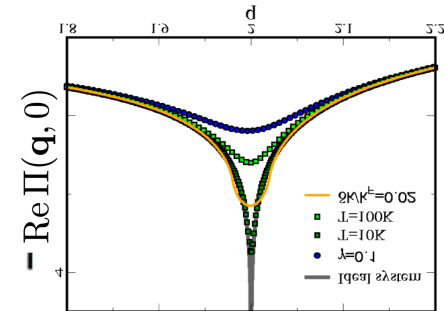
Lindhard function

The self-energy diverges

At $2k_F$ in $D=1$



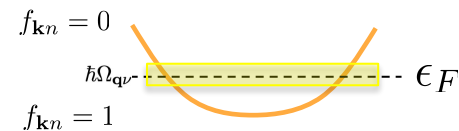
Temperature dependence



Example

One parabolic band.

One phonon mode.



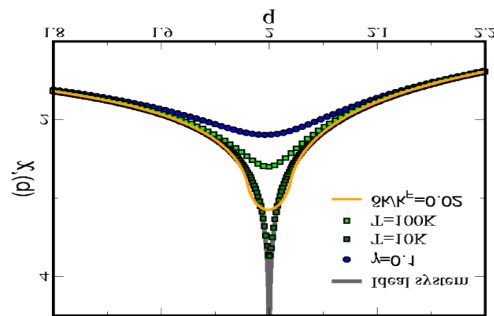
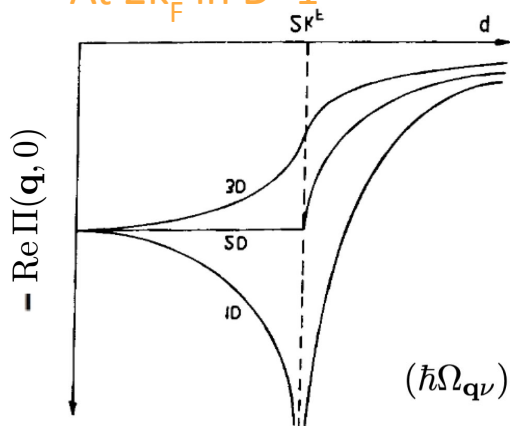
Constant electron-phonon matrix elements: $|g_{\mathbf{k}n, \mathbf{k}+\mathbf{q}m}^\nu|^2 = g^2$

We have:

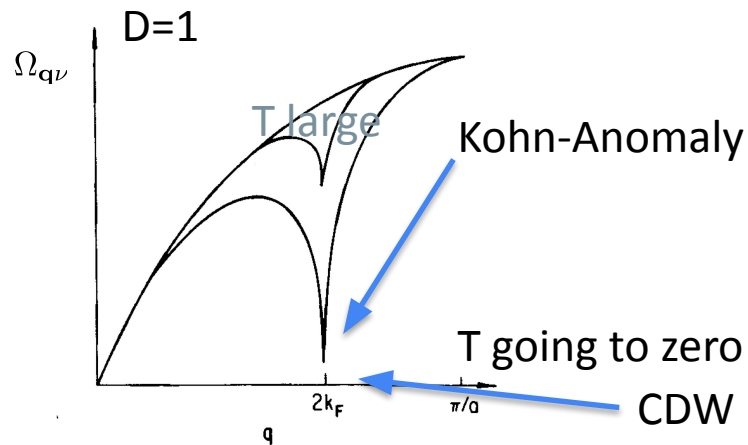
$$\text{Re } \Pi(\mathbf{q}, 0) = -g^2 \chi_0(\mathbf{q})$$

Lindhard function

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



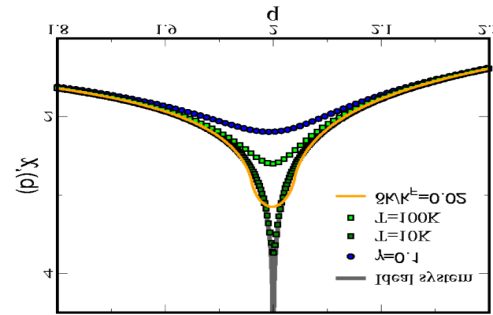
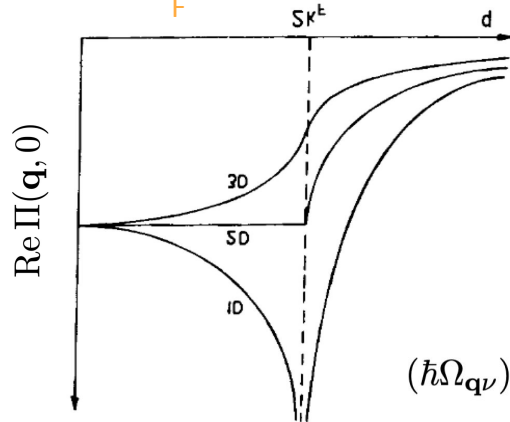
$$(\hbar\Omega_{q\nu})^2 = (\hbar\omega_{q\nu})^2 - 2\hbar\omega_{q\nu} \text{Re } \Pi(\mathbf{q}, 0)$$



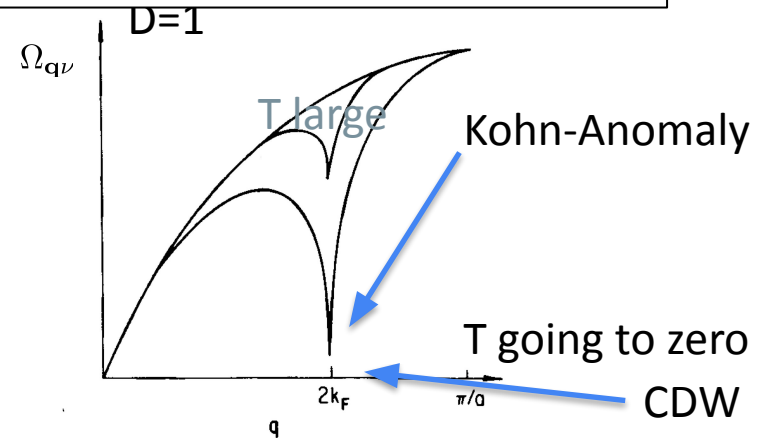
Exercise:

DFT Phonon frequencies already include this effect (with non constant g and non parabolic bands) !

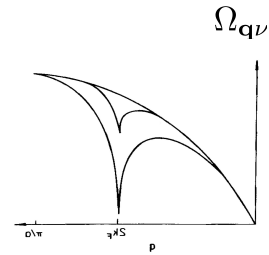
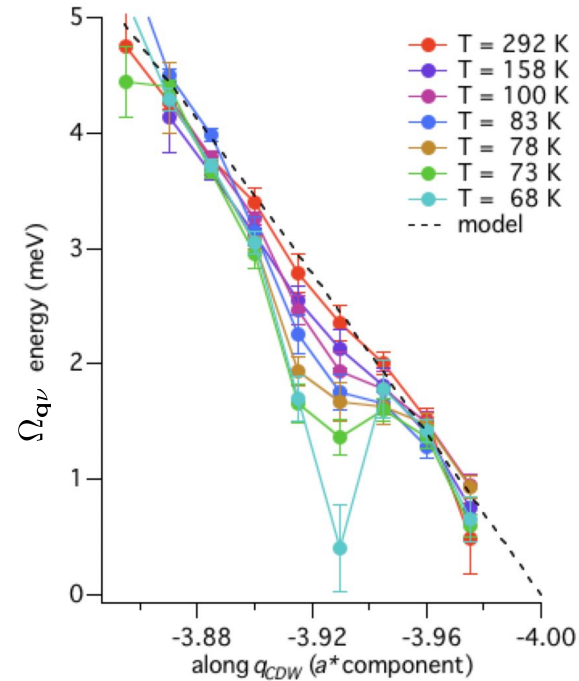
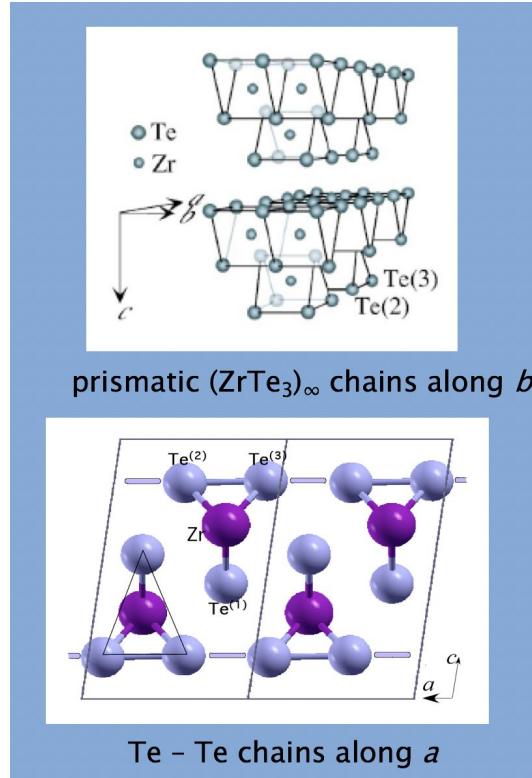
The self energy diverges
At $2k_F$ in D=1



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



ZrTe₃ 1D metal, CDW seen in IXS



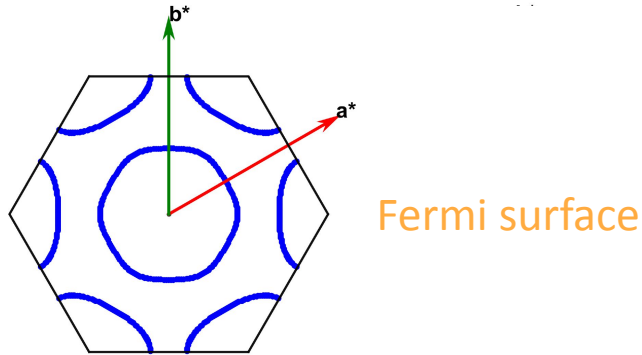
Hoesch, *et al.* Phys. Rev. Lett. **102**, 086402

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 $\mathbf{q}$ mapping one portion (not just a point) of the Fermi surface in another one.

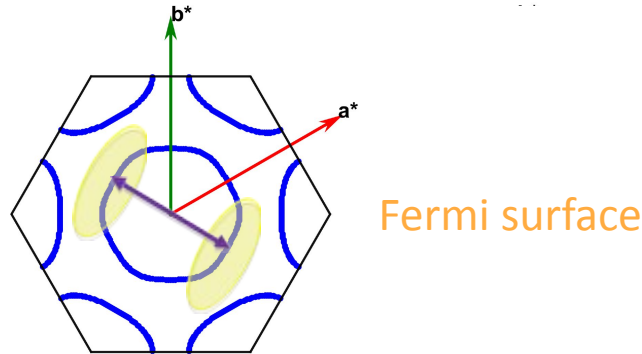


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is the nesting vector: we expect softening at (or close to) the nesting vector

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

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

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,

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

induces an electronic charge density

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

where

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

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

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

and

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

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 vec-

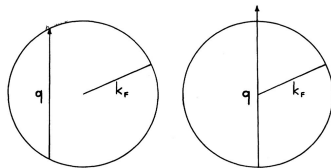


FIG. 1. Virtual excitations for $q < 2k_F$ and $q > 2k_F$.

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PHYSICAL REVIEW LETTERS

MAY 1, 1959

tor $\vec{q}$ produces a change of ionic charge density of the form

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

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 $\vec{K}_{\nu}$,

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

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

$$E(\vec{k}) = \epsilon. \quad (9)$$

Again one finds singularities of $\text{grad}_{\vec{q}} \omega$, 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

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

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

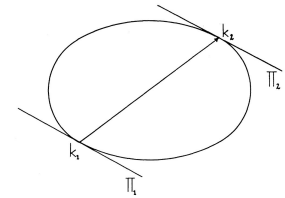


FIG. 2. Construction for the case of Bloch electrons.

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.

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.

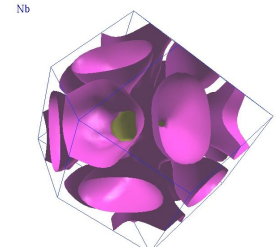
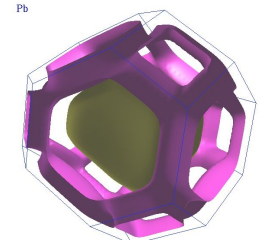
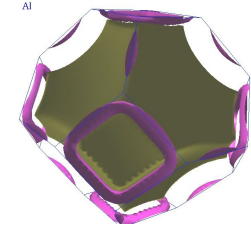
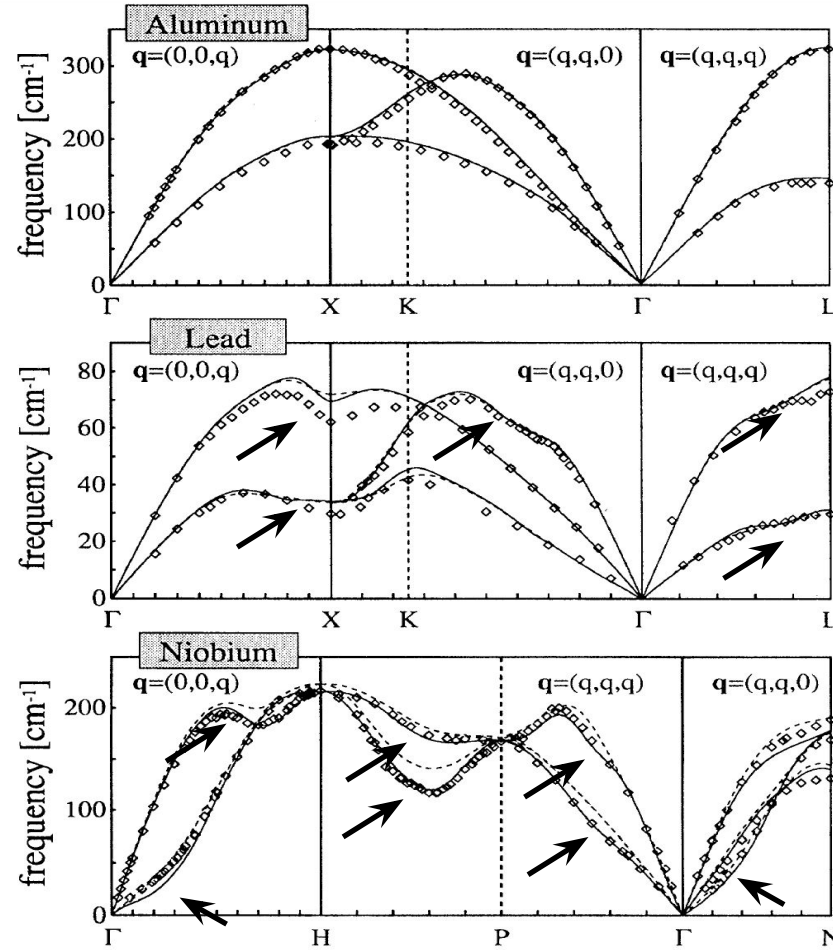
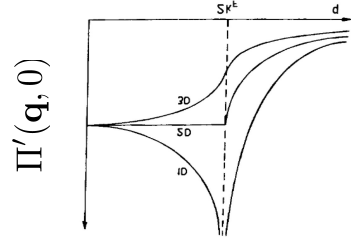
Similar "images" of the Fermi surface may be expected in spin wave spectra, when the interaction between localized spins is brought about by exchange with conduction electrons.

A detailed report is in preparation.

* Supported in part by the Office of Naval Research.

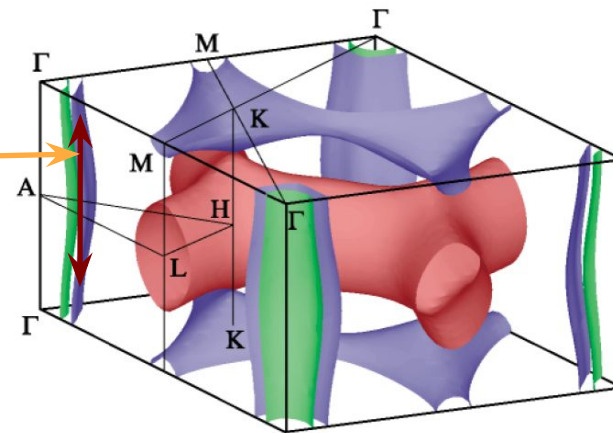
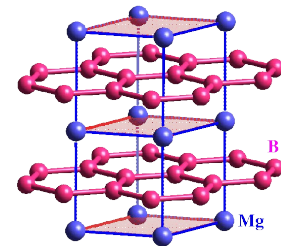
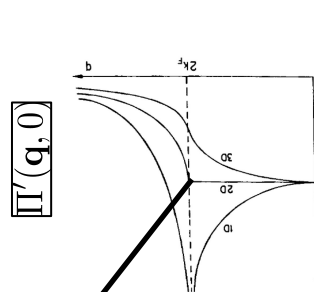
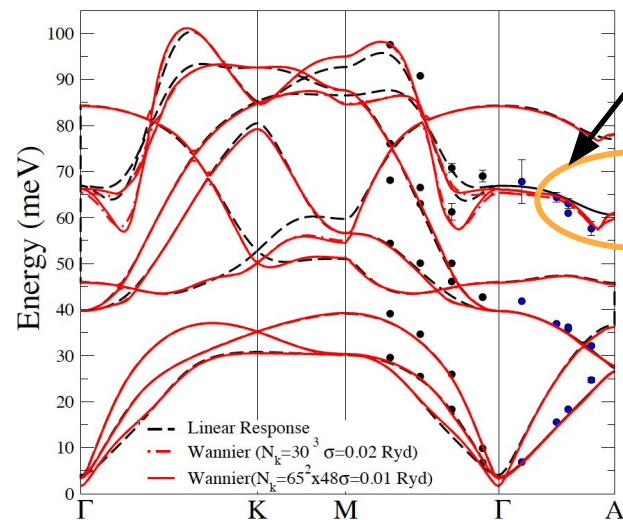
The Kohn-effect (Kohn-anomaly) – slightly more than 1 page.

Phonon dispersion in simple 3D metals



Arrows indicates Kohn Anomalies

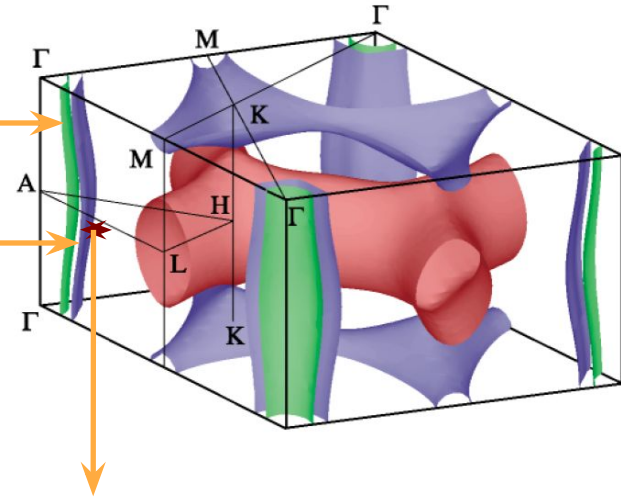
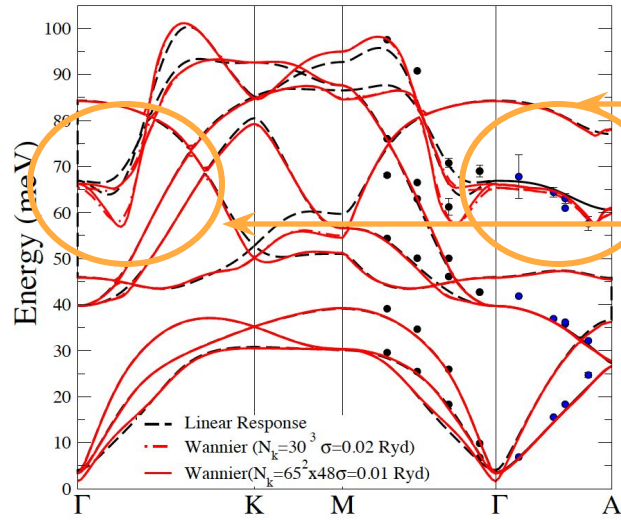
Kohn anomaly in MgB_2



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

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

Kohn anomaly in MgB_2



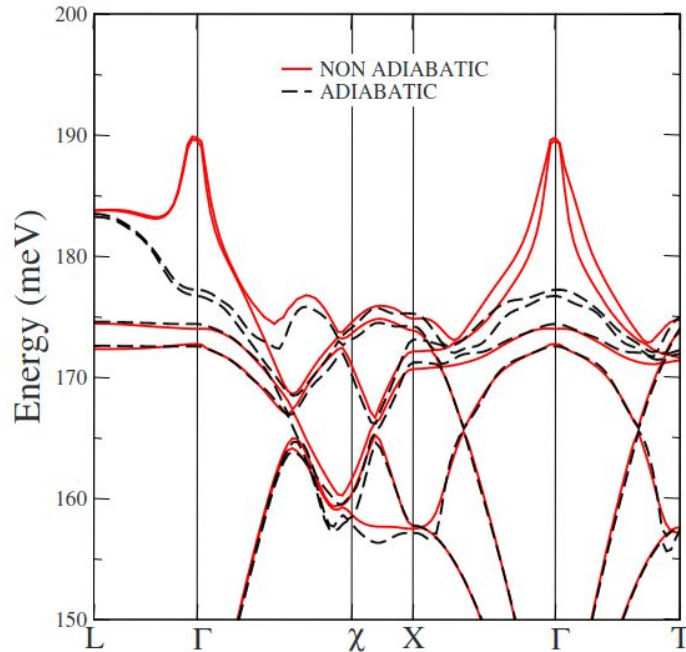
Nesting between cylinders

Dynamical effects (non-adiabatic)

$$\text{Re } \Pi(\mathbf{q}, \nu, \mathbf{x}) = -\frac{1}{N_{\mathbf{q}}} \mathcal{P} \sum_{\mathbf{k}} \sum_{n,m} |g_{\mathbf{k}n, \mathbf{k}+\mathbf{q}m}^{\nu}|^2 \frac{f_{\mathbf{k}n} - f_{\mathbf{k}+\mathbf{q}m}}{\hbar\nu + \epsilon_{\mathbf{k}n} - \epsilon_{\mathbf{k}+\mathbf{q}m}}$$

Dynamical effects (non-adiabatic)

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



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

DYNAMICAL (NON ADIABATIC) EFFECTS ARE IMPORTANT !

Imaginary part and phonon linewidth

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

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

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

Key points:

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

$$\gamma_{qv} = \frac{4\pi\omega_{qv}}{N_k} \sum_{k,n,m} |g_{\mathbf{k}n, \mathbf{k}+\mathbf{q}m}^v|^2 \frac{f(\epsilon_{\mathbf{k}n}) - f(\epsilon_{\mathbf{k}+\mathbf{q}m})}{\omega_{qv}} \delta(\epsilon_{\mathbf{k}+\mathbf{q}m} - \epsilon_{\mathbf{k}n} - \omega_{qv})$$

2 for spin and 2 for Full width half maximum

Allen formula (metals)



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

$$\gamma_{qv} = \frac{4\pi\omega_{qv}}{N_k} \sum_{k,n,m} |g_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}^v|^2 \frac{f(\varepsilon_{\mathbf{k}n}) - f(\varepsilon_{\mathbf{k}+\mathbf{q}m})}{\omega_{qv}} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}m} - \varepsilon_{\mathbf{k}n} - \omega_{qv})$$

If temperature dependence is weak:

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

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We have

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

Allen formula (metals)



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

$$\gamma_{q\nu} = \frac{4\pi\omega_{q\nu}}{N_k} \sum_{k,n,m} |g_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}^\nu|^2 \delta(\epsilon_{\mathbf{k}n}) \delta(\epsilon_{\mathbf{k}+\mathbf{q}m} - \epsilon_{\mathbf{k}n} - \omega_{q\nu})$$

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

$$\gamma_{q\nu} = \frac{4\pi\omega_{q\nu}}{N_k} \sum_{k,n,m} |g_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}^\nu|^2 \delta(\epsilon_{\mathbf{k}n}) \delta(\epsilon_{\mathbf{k}+\mathbf{q}m})$$

We have

Remember: electron energies measured from the Fermi Level

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

Electron-phonon coupling

DOS per spin at the Fermi level

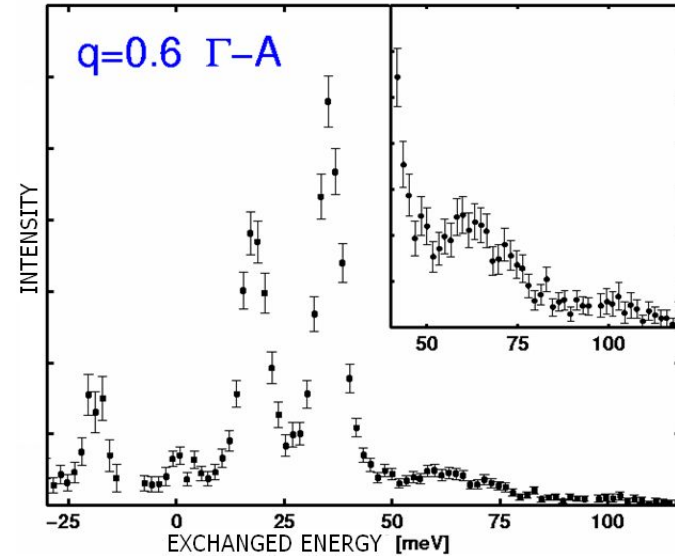
When anharmonicity is negligible, the phonon linewidth measures the electron-phonon coupling

Electron-phonon coupling and anharmonicity in real materials

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

 experiment

Both can contribute!



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

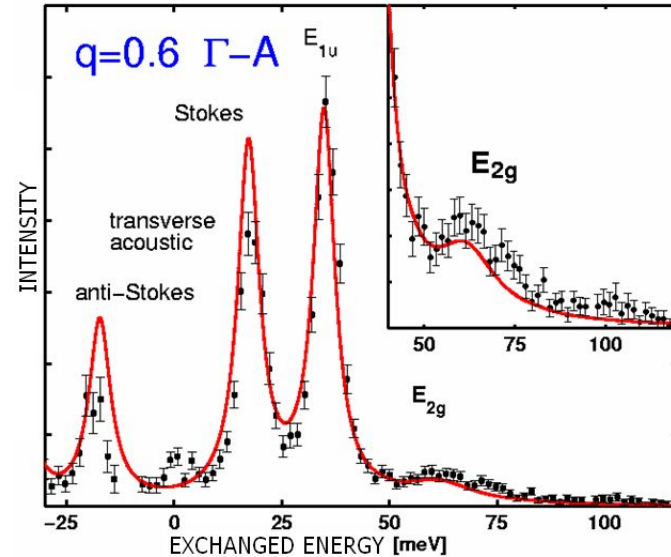
Electron-phonon coupling and anharmonicity in real materials

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Both can contribute!

First principles calculations can guide the interpretation.

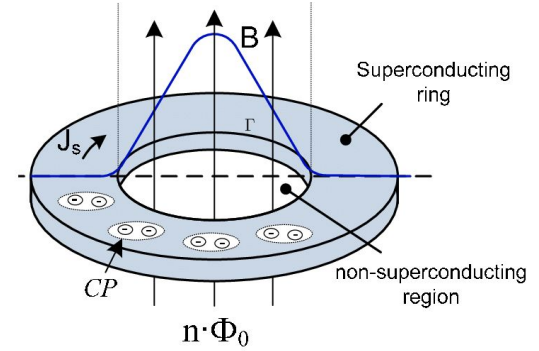
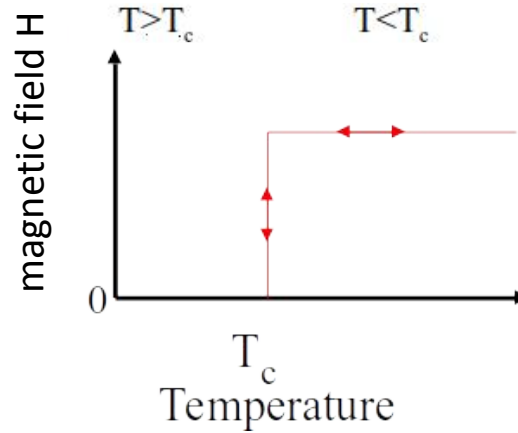
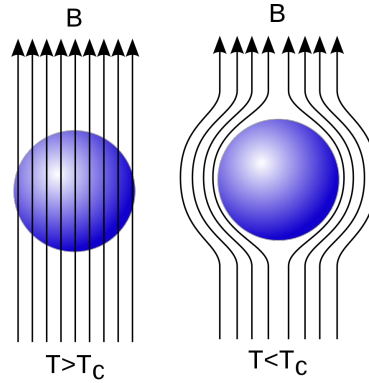
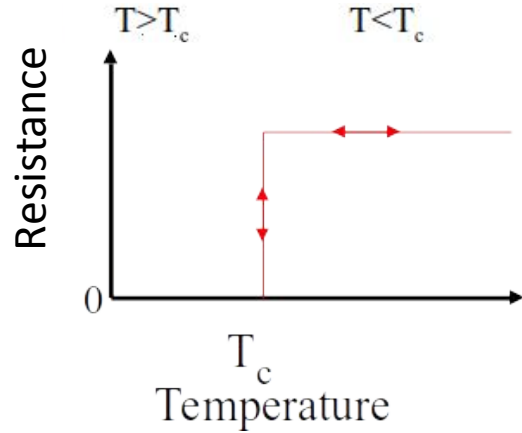
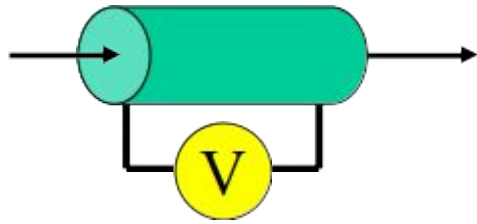


A. Shukla, *et al.* PRL **90**, 095506 (2003)

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

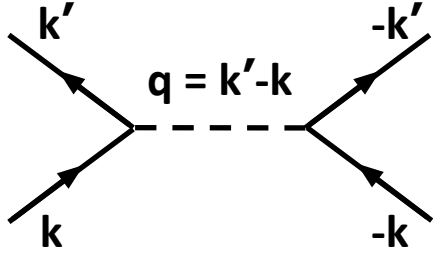
The superconducting phase



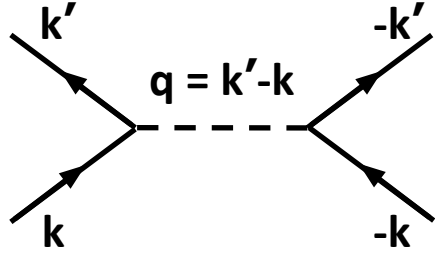
- macroscopic quantum effects
- magnetic flux quantization
 - Josephson effect

BCS theory

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



BCS theory

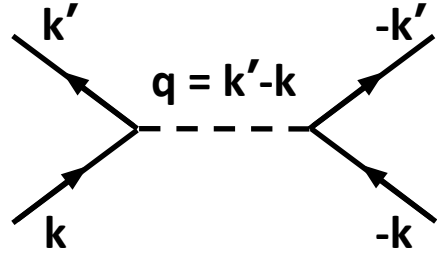


$$H_{\text{BCS}} = \underbrace{H_0}_{\text{circled}} + \underbrace{H_{\text{red}}}_{\text{circled}}$$

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

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

BCS theory



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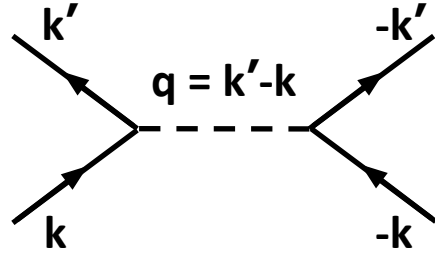
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$$\Delta_{n\mathbf{k}} = \sum_m \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \tanh\left(\frac{E_{m\mathbf{k}+\mathbf{q}}}{2k_{\text{B}}T}\right) \frac{V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} \Delta_{m\mathbf{k}+\mathbf{q}}}{2E_{m\mathbf{k}+\mathbf{q}}}$$

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

BCS theory



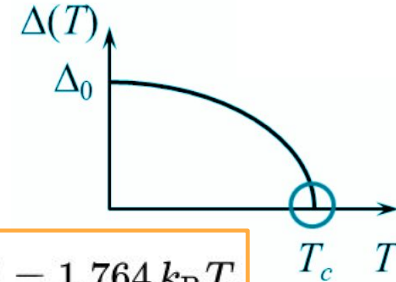
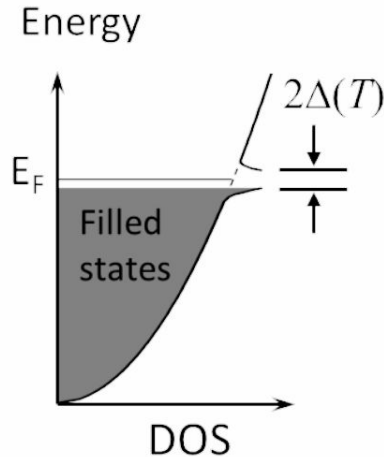
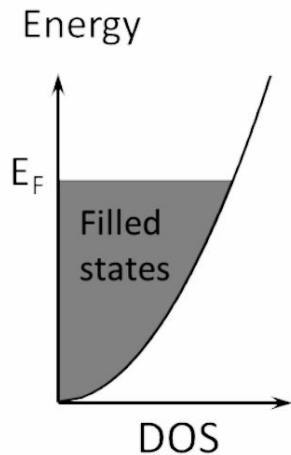
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$$E_{n\mathbf{k}} = \sqrt{(\epsilon_{n\mathbf{k}} - \epsilon_F)^2 + |\Delta_{n\mathbf{k}}|^2}$$



$$\Delta(T=0) = 1.764 k_B T_c$$

$$\Delta(T \rightarrow T_c) \approx 3.06 k_B T_c \sqrt{1 - (T/T_c)}$$

Migdal-Eliashberg (isotropic)

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

Nambu notation

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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

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

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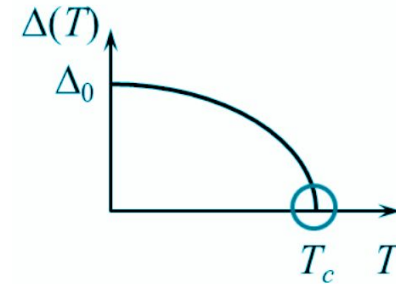
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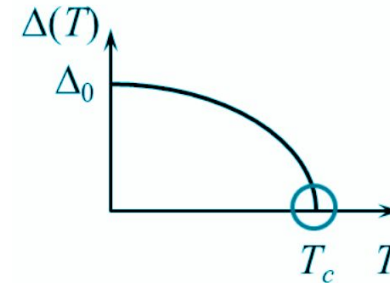
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Allen-Dynes-modified McMillan formula

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

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



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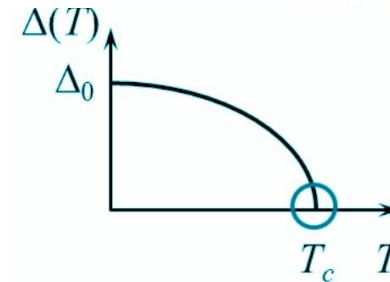
$$\lambda = 2 \int \frac{\alpha^2 F(\omega)}{\omega} d\omega = \sum_{\mathbf{q}\nu} \lambda_{\mathbf{q}\nu},$$

$$\lambda_{\mathbf{q}\nu} = \frac{2}{N(\varepsilon_F) \omega_{\mathbf{q}\nu}} \sum_{mn} \sum_{\mathbf{k}} |g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{\mathbf{q}\nu,mn}|^2 \times \delta(\varepsilon_{\mathbf{k}+\mathbf{q},m} - \varepsilon_F) \delta(\varepsilon_{\mathbf{k},n} - \varepsilon_F).$$

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Take-home messages

- 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.

How do we integrate anharmonic effects and electron-phonon coupling in a fully *ab initio* calculation?

It will be shown in the hands-on session.

We will learn to use SSCHA and EPIq together



+

