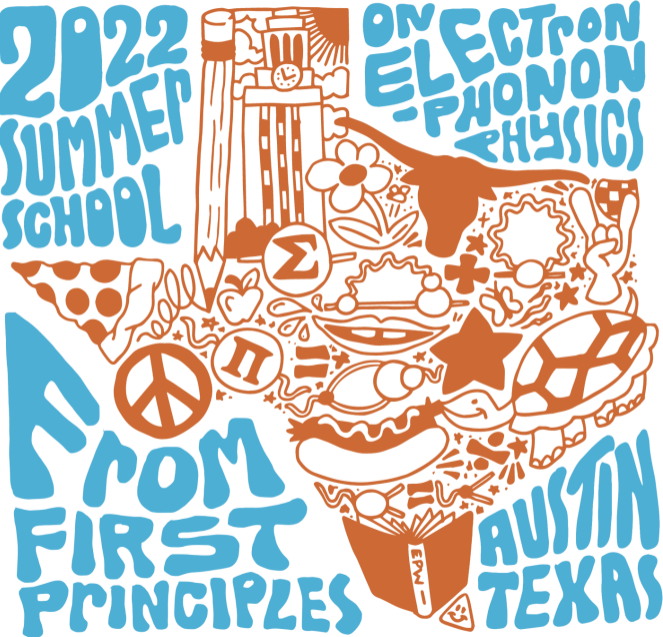


2022
SUMMER
SCHOOL

ON ELECTRON
-PHONON
PHYSICS



FROM
FIRST
PRINCIPLES

AUSTIN
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ENERGY

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Lecture Tue.2

Many-body methods for electron-phonon interactions

Feliciano Giustino

Oden Institute & Department of Physics

The University of Texas at Austin

- Limitations of Rayleigh-Schrödinger perturbation theory
- Many-body Hamiltonian
- Green's function and the spectral function
- Electron-phonon self-energy
- Mass enhancement and electron lifetimes

Kohn-Sham equations again

$$-\frac{\hbar^2}{2m_e} \nabla^2 \psi_n(\mathbf{r}) + V_{\text{SCF}}(\mathbf{r}; \boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \dots) \psi_n(\mathbf{r}) = \varepsilon_n \psi_n(\mathbf{r})$$

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- Adiabatic Born-Oppenheimer approximation

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- Adiabatic Born-Oppenheimer approximation
- Nuclei described as classical particles

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- Adiabatic Born-Oppenheimer approximation
- Nuclei described as classical particles
- Electron-phonon interactions depend on the XC functional

Breakdown of Rayleigh-Schrödinger perturbation theory

Polaron liquid at the SrTiO₃(001) surface

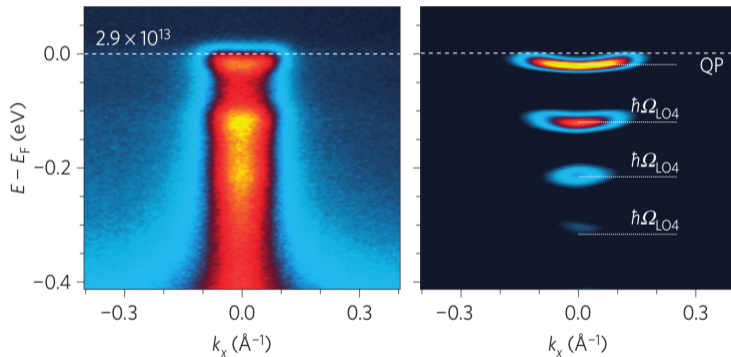
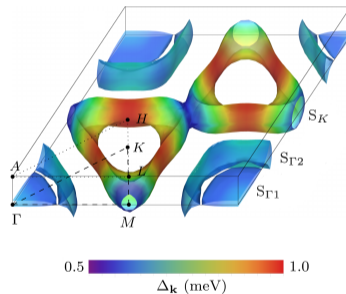
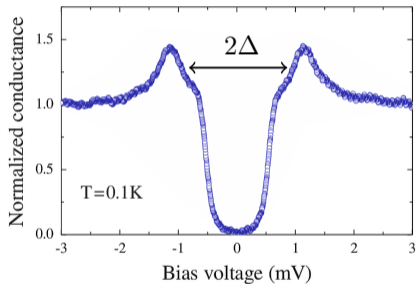


Figure from Wang et al, Nature Mater. 15, 835 (2016)

Breakdown of Rayleigh-Schrödinger perturbation theory

cf. Lec. Wed.2 Margine

Scanning tunneling spectra of superconducting 2H-NbS₂



Figures from Guillamón et al, Phys. Rev. Lett. 101, 166407 (2008)
and Heil et al, Phys. Rev. Lett. 119, 087003 (2017)

Many-body Schrödinger equation for electrons and nuclei

$$\left[-\frac{\hbar^2}{2m_e} \sum_i \nabla_i^2 - \frac{\hbar^2}{2M_\kappa} \sum_\kappa \nabla_\kappa^2 - \sum_{i,\kappa} Z_\kappa v(\mathbf{r}_i, \boldsymbol{\tau}_\kappa) + \sum_{\kappa > \kappa'} Z_\kappa Z_{\kappa'} v(\boldsymbol{\tau}_\kappa, \boldsymbol{\tau}_{\kappa'}) + \sum_{i > j} v(\mathbf{r}_i, \mathbf{r}_j) \right] \Psi = E_{\text{tot}} \Psi$$

$$\mathbf{r}_i \text{ electron, } \boldsymbol{\tau}_\kappa \text{ nucleus, } v(\mathbf{r}, \mathbf{r}') = \frac{e^2}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|}$$

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- Electrons and vibrations must be described on the same footing
- The many-body Schrödinger equation is impractical for calculations or EPIs

Many-electron wavefunction as a linear combination of Slater determinants

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots) = \sum_{mn} A_{mn} \hat{c}_m^\dagger \hat{c}_n |0_{\text{KS}}\rangle + \sum_{mnpq} B_{mnpq} \hat{c}_m^\dagger \hat{c}_n^\dagger \hat{c}_p \hat{c}_q |0_{\text{KS}}\rangle + \dots$$

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Operators in second quantization

$$\sum_i V(\mathbf{r}_i) \longrightarrow \sum_{mn} V_{mn} \hat{c}_m^\dagger \hat{c}_n$$

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Field operators

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Field operators

$$\hat{\psi}^\dagger(\mathbf{r}) \stackrel{\text{def}}{=} \sum_m \psi_m^*(\mathbf{r}) \hat{c}_m^\dagger \quad \hat{\psi}(\mathbf{r}) \stackrel{\text{def}}{=} \sum_n \psi_n(\mathbf{r}) \hat{c}_n$$

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Electron-nucleus interaction

$$\hat{U}_{en} = \int d\mathbf{r} d\mathbf{r}' \hat{n}_e(\mathbf{r}) \hat{n}_n(\mathbf{r}') v(\mathbf{r}, \mathbf{r}')$$

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$$\hat{U}_{ee} = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \hat{n}_e(\mathbf{r}) [\hat{n}_e(\mathbf{r}') - \delta(\mathbf{r} - \mathbf{r}')] v(\mathbf{r}, \mathbf{r}')$$

Time evolution of field operators and Dyson orbitals

Ground state of N -electron system

$$\hat{H}|N\rangle = E_N|N\rangle$$

Time evolution of field operators and Dyson orbitals

Ground state of N -electron system $\hat{H}|N\rangle = E_N|N\rangle$

s -th excited state of $N+1$ -electron system $\hat{H}|N+1, s\rangle = E_{N+1, s}|N+1, s\rangle$

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Exercise

$$\langle N | \hat{\psi}(\mathbf{x}, t) | N + 1, s \rangle$$

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$f_s(\mathbf{x})$ Dyson orbital

The Green's function at zero temperature

Time-ordered
Green's function

Wick's time-ordering operator

$$G(\mathbf{x}t, \mathbf{x}'t') = -\frac{i}{\hbar} \langle N | \hat{T} \hat{\psi}(\mathbf{x}t) \hat{\psi}^\dagger(\mathbf{x}'t') | N \rangle$$

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Consider $t > t'$ (electron added to ground state)

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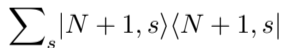
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$$\sum_s |N+1, s\rangle \langle N+1, s|$$

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The spectral function

Carry out the same operation for $t < t'$ and Fourier transform

$$G(\mathbf{x}, \mathbf{x}', \omega) = \sum_s \frac{f_s(\mathbf{x}) f_s^*(\mathbf{x}')}{\hbar\omega - \varepsilon_s \mp i0^+} \quad \mp \text{ occ/unocc}$$

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The poles of the Green's function represent the electron addition/removal energies of the interacting many-body system

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From the Green's function we can obtain the **spectral (density) function**

$$A(\mathbf{x}, \omega) = \frac{1}{\pi} |\text{Im} G(\mathbf{x}, \mathbf{x}, \omega)| = \sum_s |f_s(\mathbf{x})|^2 \delta(\hbar\omega - \varepsilon_s)$$

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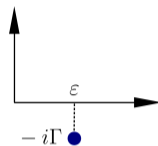
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The spectral function is the many-body (local) density of states

Usually presented as momentum-resolved $A(\mathbf{k}, \omega)$

The spectral function: Broadening

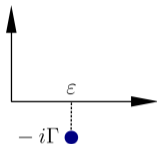
Example: a single complex pole $\varepsilon_s = \varepsilon - i\Gamma$



The spectral function: Broadening

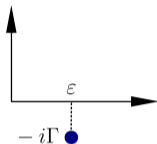
Example: a single complex pole $\varepsilon_s = \varepsilon - i\Gamma$

$$G(\mathbf{x}, \mathbf{x}, t-t') = -\frac{i}{\hbar} |f_s(\mathbf{x})|^2 e^{-i\varepsilon(t-t')/\hbar} \underline{e^{-\Gamma(t-t')/\hbar}}$$



The spectral function: Broadening

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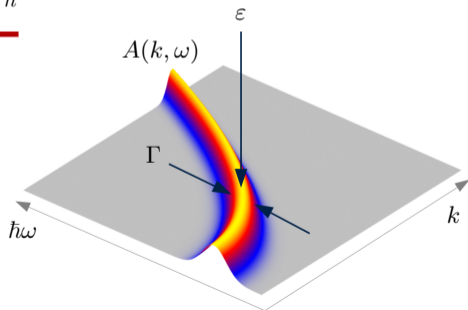
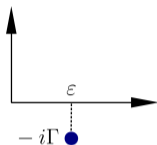
$$A(\mathbf{x}, \mathbf{x}, \omega) = \frac{1}{\pi} \frac{\Gamma}{(\hbar\omega - \varepsilon)^2 + \Gamma^2} |f_s(\mathbf{x})|^2$$

The spectral function: Broadening

Example: a single complex pole $\varepsilon_s = \varepsilon - i\Gamma$

$$G(\mathbf{x}, \mathbf{x}, t-t') = -\frac{i}{\hbar} |f_s(\mathbf{x})|^2 e^{-i\varepsilon(t-t')/\hbar} \underline{e^{-\Gamma(t-t')/\hbar}}$$

$$A(\mathbf{x}, \mathbf{x}, \omega) = \frac{1}{\pi} \frac{\Gamma}{(\hbar\omega - \varepsilon)^2 + \Gamma^2} |f_s(\mathbf{x})|^2$$



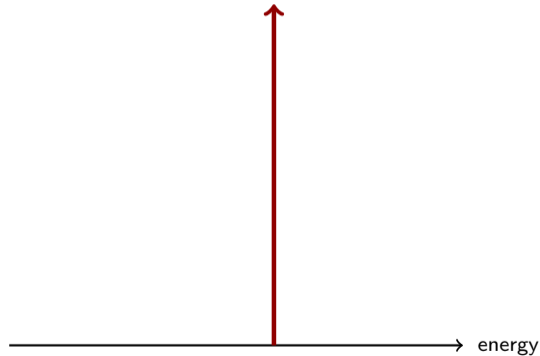
The spectral function: Coherent and incoherent structures

$$A(\mathbf{k}, \omega) = \frac{1}{\pi} |\operatorname{Im} G(\mathbf{k}, \omega)|$$

The spectral function: Coherent and incoherent structures

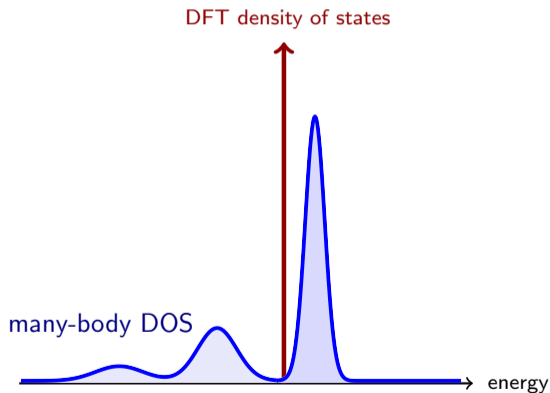
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DFT density of states



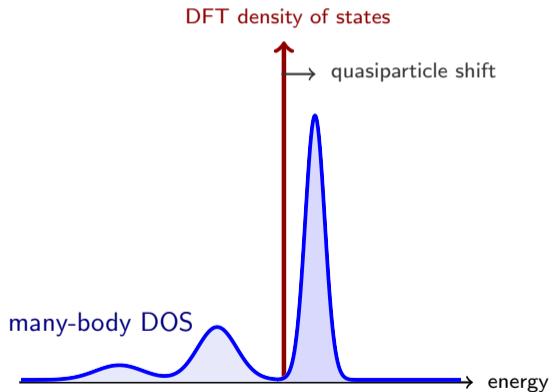
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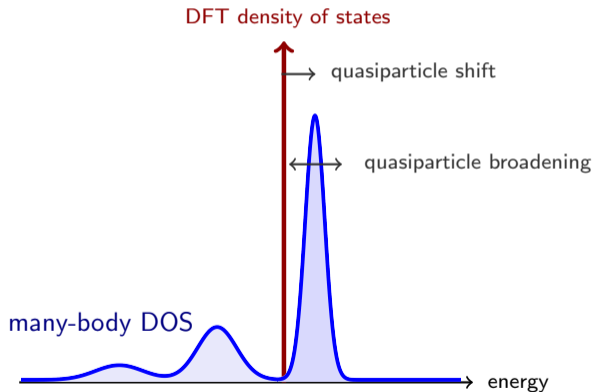
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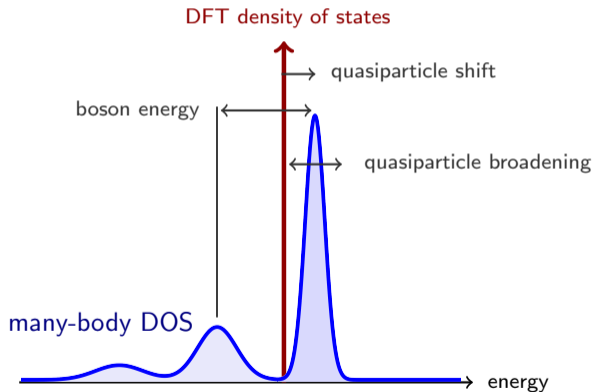
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How to calculate the Green's function

Heisenberg time evolution

$$\hat{\psi}(\mathbf{x}, t) = e^{i\hat{H}t/\hbar} \hat{\psi}(\mathbf{x}) e^{-i\hat{H}t/\hbar}$$

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Equation of motion for **field operators**

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total charge, electrons & nuclei \longrightarrow

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total charge, electrons & nuclei \longleftarrow

Equation of motion for **Green's function**

$$\left[i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m_e} \nabla_1^2 \right] G(12) + \frac{i}{\hbar} \int d3 v(13) \langle \hat{T} \hat{n}(3) \psi(1) \psi^\dagger(2) \rangle = \delta(12)$$

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4 field operators

Hartree+Fock+2-particle Green's function

Dyson equation

$$V_{\text{tot}}(1) = \int d2 v(12) \langle \hat{n}(2) \rangle$$

2-particle Green's function
rewritten using self-energy Σ

$$\left[i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m_e} \nabla_1^2 - V_{\text{tot}}(1) \right] G(12) - \int d3 \Sigma(13) G(32) = \delta(12)$$

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Express the Green's function in terms of Dyson's orbitals

$$\left[-\frac{\hbar^2}{2m_e} \nabla^2 + V_{\text{tot}}(\mathbf{r}) \right] f_s(\mathbf{x}) + \int d\mathbf{x}' \Sigma(\mathbf{x}, \mathbf{x}', \varepsilon_s / \hbar) f_s(\mathbf{x}') = \varepsilon_s f_s(\mathbf{x})$$

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Sources of **electron-phonon** interaction

How to calculate the electron-phonon self-energy

Electron self-energy from Hedin-Baym's equations

$$\Sigma(12) = i\hbar \int d(34) G(13) \Gamma(324) W(41^+)$$

Green's function

Vertex

Screened Coulomb interaction

How to calculate the electron-phonon self-energy

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Vertex

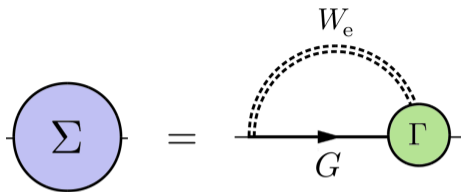
Screened Coulomb interaction

$$W = W_e + W_{\text{ph}}$$

$$W_e(12) = \int d3 \epsilon_e^{-1}(13) v(32)$$

Reduces to the standard GW method + screening from nuclei

Diagrammatic representation of the self-energy



Standard GW self-energy
(we will ignore this from now on)

Figure from
FG, Rev. Mod. Phys. 89, 015003 (2017)

Diagrammatic representation of the self-energy

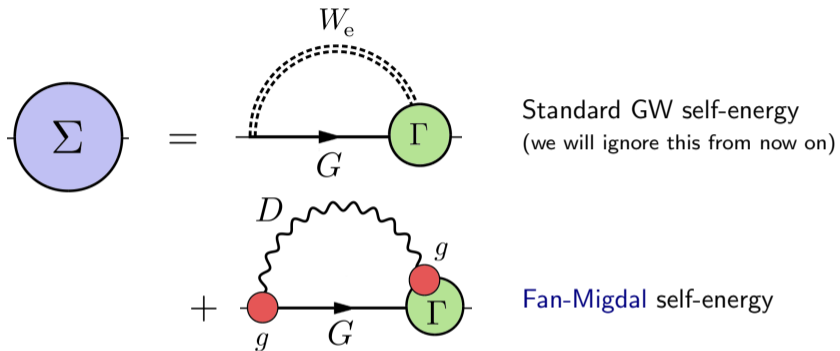
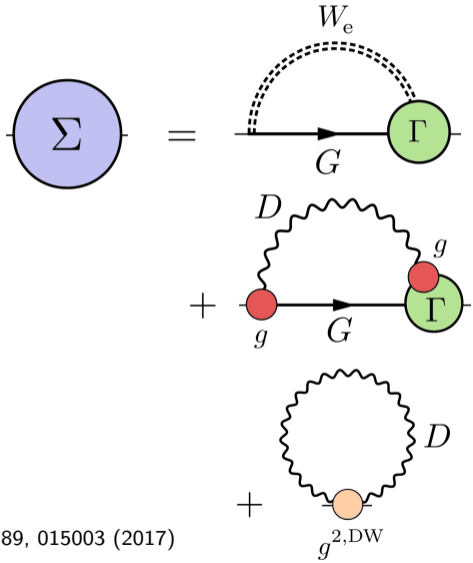


Figure from
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Diagrammatic representation of the self-energy



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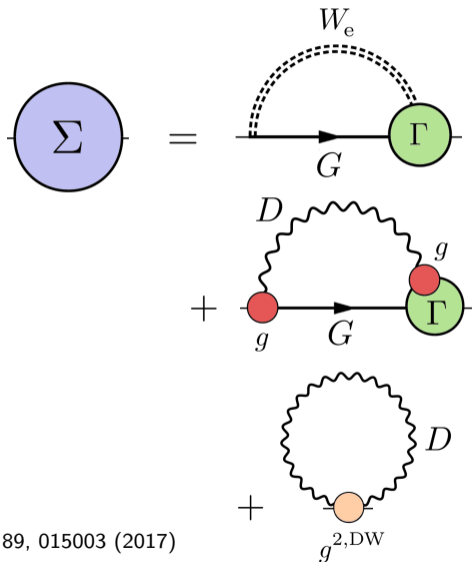
Fan-Migdal self-energy

Debye-Waller self-energy

Improper self-energy: comes from $V_{tot}(1) = \int d2 v(12) \langle \hat{n}(2) \rangle$ term

Figure from
FG, Rev. Mod. Phys. 89, 015003 (2017)

Diagrammatic representation of the self-energy



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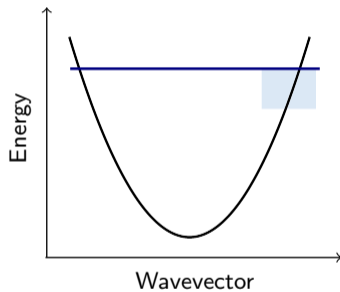
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Figure from
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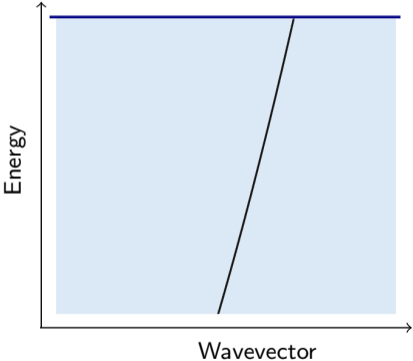
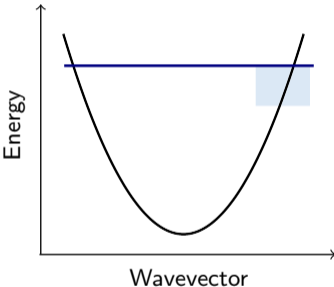
Fan-Migdal self-energy using Kohn-Sham states and DFPT phonons

$$\Sigma_{n\mathbf{k}}^{\text{FM}}(\omega) = \frac{1}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} |g_{m\nu}(\mathbf{k}, \mathbf{q})|^2$$
$$\times \left[\frac{1 - f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu}}{\omega - \varepsilon_{m\mathbf{k}+\mathbf{q}}/\hbar - \omega_{\mathbf{q}\nu} + i\eta} + \frac{f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu}}{\omega - \varepsilon_{m\mathbf{k}+\mathbf{q}}/\hbar + \omega_{\mathbf{q}\nu} + i\eta} \right]$$

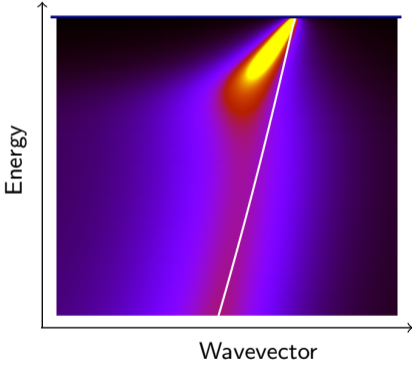
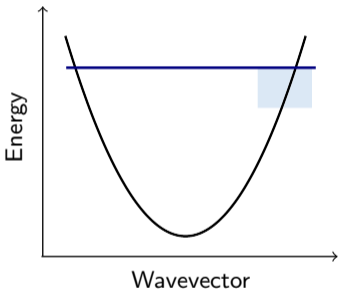
Example: Interaction with dispersionless phonon



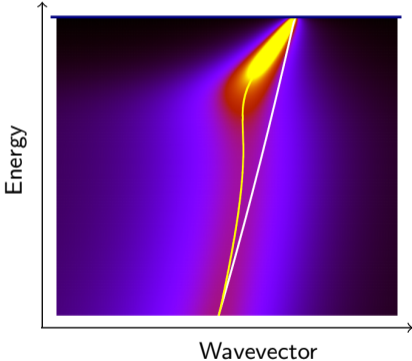
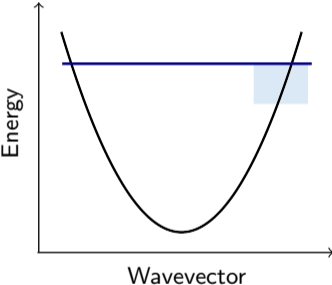
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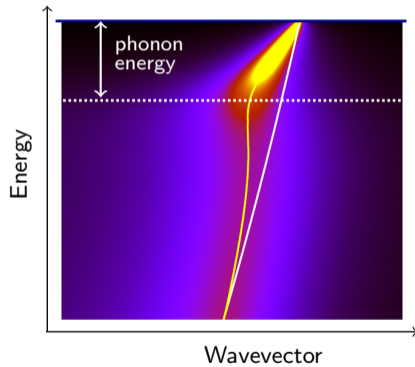
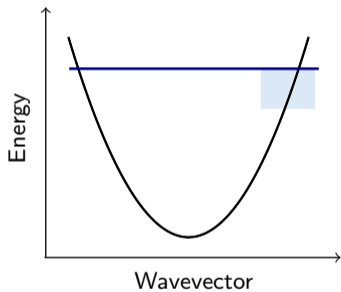
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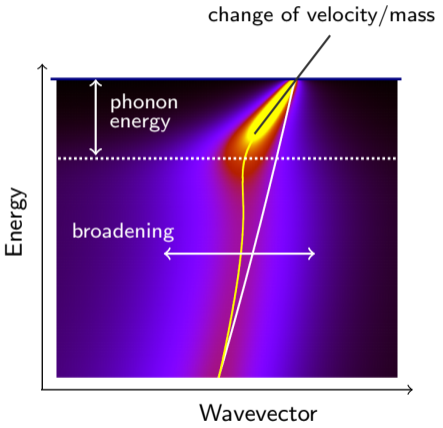
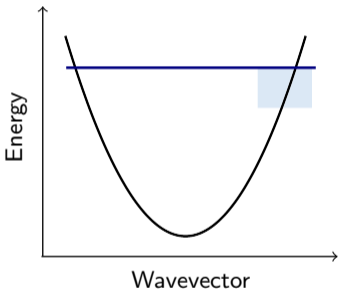
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Example: Interaction with dispersionless phonon



Example from experiments: Velocity renormalization in MgB_2

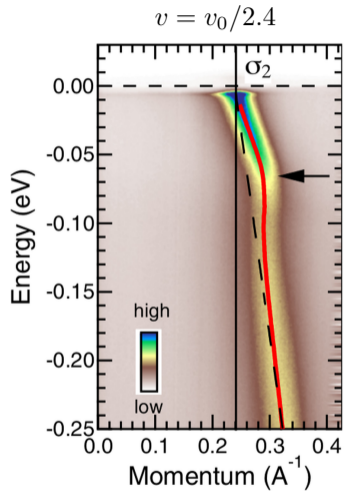
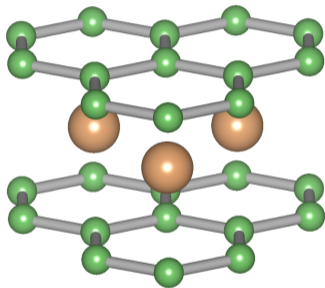


Figure from Mou et al, Phys. Rev. B 91, 140502(R) (2015)

Spectral function from the self-energy

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} \sum_n \frac{1}{\hbar\omega - \varepsilon_{n\mathbf{k}} - \Sigma_{n\mathbf{k}}(\omega)}$$

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Quasiparticle approximation: assume simple poles in the complex plane

$$\Sigma_{n\mathbf{k}}(\omega) = \Sigma_{n\mathbf{k}}(z) + \frac{1}{\hbar} \left. \frac{\partial \text{Re} \Sigma_{n\mathbf{k}}}{\partial \omega} \right|_{\omega=z/\hbar} (\hbar\omega - z) + \dots$$

Quasiparticle shift and broadening

Replace the Taylor expansion inside the spectral function and rearrange:

$$A(\mathbf{k}, \omega) = \sum_n Z_{n\mathbf{k}} \frac{1}{\pi} \frac{\Gamma_{n\mathbf{k}}}{(\hbar\omega - E_{n\mathbf{k}})^2 + \Gamma_{n\mathbf{k}}^2}$$

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$$E_{n\mathbf{k}} = \varepsilon_{n\mathbf{k}} + \text{Re} \Sigma_{n\mathbf{k}}(E_{n\mathbf{k}}/\hbar) \quad \text{quasiparticle energy}$$

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$$Z_{n\mathbf{k}} = \frac{1}{1 - \frac{1}{\hbar} \left. \frac{\partial \text{Re} \Sigma_{n\mathbf{k}}(\omega)}{\partial \omega} \right|_{\omega = E_{n\mathbf{k}}/\hbar}}$$

quasiparticle strength

The mass enhancement parameter

Take \mathbf{k} -derivatives of the quasiparticle energy $E_{n\mathbf{k}}$
to find **velocity** and **mass** renormalization[†]

$$V_{n\mathbf{k}} = \frac{v_{n\mathbf{k}}}{1 + \lambda_{n\mathbf{k}}} \quad M_{n\mathbf{k}}^* = (1 + \lambda_{n\mathbf{k}}) m_{n\mathbf{k}}^*$$

[†]These expressions are for the electron gas; more complex expressions are needed in other cases

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$\lambda_{n\mathbf{k}}$ is the **mass enhancement parameter**

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

[†]These expressions are for the electron gas; more complex expressions are needed in other cases

$$\tau_{n\mathbf{k}} = \frac{\hbar}{2\Gamma_{n\mathbf{k}}} = \frac{\hbar}{2|Z_{n\mathbf{k}}\text{Im}\Sigma_{n\mathbf{k}}(E_{n\mathbf{k}}/\hbar)|}$$

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Common **approximation**: replace $E_{n\mathbf{k}}$ by $\varepsilon_{n\mathbf{k}}$ and set $Z_{n\mathbf{k}} = 1$

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$$\frac{1}{\tau_{n\mathbf{k}}} = \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} |g_{nm\nu}(\mathbf{k}, \mathbf{q})|^2$$

$\times [(1 - f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu})\delta(\varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu} - \varepsilon_{m\mathbf{k}+\mathbf{q}}) \quad \text{phonon emission}$
 $+ (f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu})\delta(\varepsilon_{n\mathbf{k}} + \hbar\omega_{\mathbf{q}\nu} - \varepsilon_{m\mathbf{k}+\mathbf{q}})] \quad \text{phonon absorption}$

Identical to Fermi Golden rule formula discussed in Lec. Mon.1

Example: Mass enhancement and lifetimes in MAPbI₃

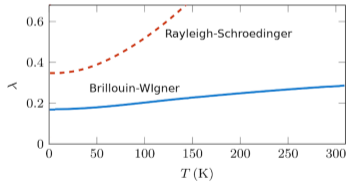
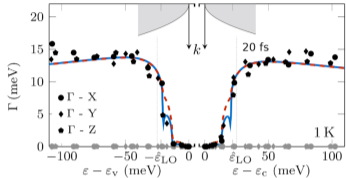
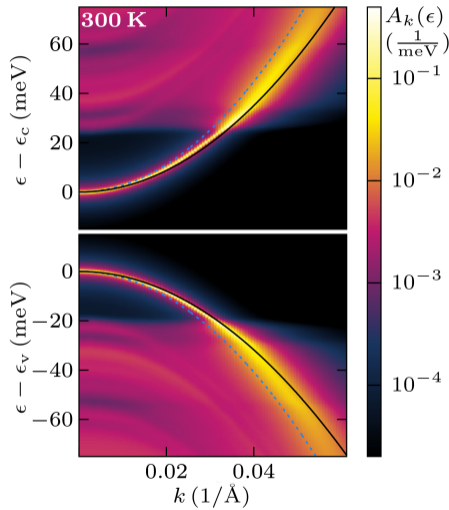
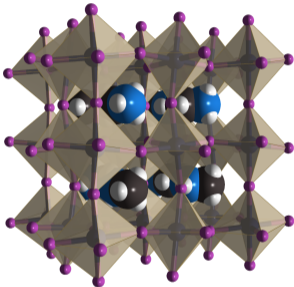


Figure adapted from Schlipf et al, Phys. Rev. Lett. 121, 086402 (2018)

- Field theory provides a rigorous and systematic framework for studying electron-phonon physics
- The electron-phonon self-energy yields the mass enhancement and the lifetimes resulting from EPIs
- Many-body formulas are similar but not identical to elementary perturbation theory

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