ICTP/Psi-k/CECAM School on Electron-Phonon Physics from First Principles

Trieste, 19-23 March 2018

ICTP

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Centre Européen de Calcul Atomique et Moléculaire

Lecture Wed.1

Many-body theory of electron-phonon interactions

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Lecture Summary

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

Limitations of Rayleigh-Schrödinger perturbation theory

Kohn-Sham equations again

$$-\frac{\hbar^2}{2m_{\rm e}}\nabla^2\,\psi_n(\mathbf{r}) + V_{\rm SCF}(\mathbf{r};\boldsymbol{\tau}_1,\boldsymbol{\tau}_2,\cdots)\,\psi_n(\mathbf{r}) = E_n\,\psi_n(\mathbf{r})$$

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- Adiabatic Born-Oppenheimer approximation
- Nuclei described as classical particles
- Electron-phonon interactions depend on the XC functional
- Phonons are calculated from static displacements or DFPT

Breakdown of Rayleigh-Schrödinger perturbation theory

- Polaron liquid at the $SrTiO_3(001)$ surface

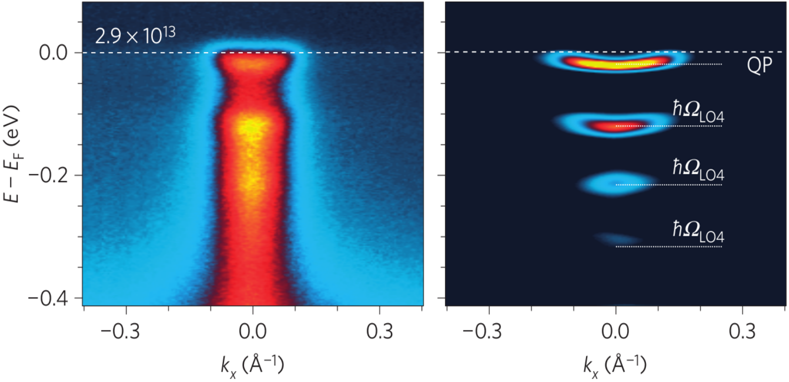
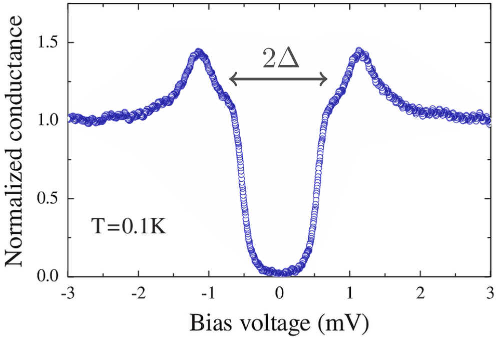
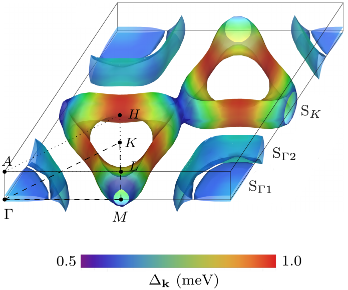


Figure from Wang et al, Nature Mater. 15, 835 (2016)

Breakdown of Rayleigh-Schrödinger perturbation theory

- Scanning tunneling spectra of 2H-NbS_2



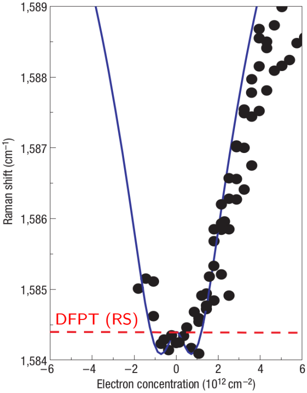


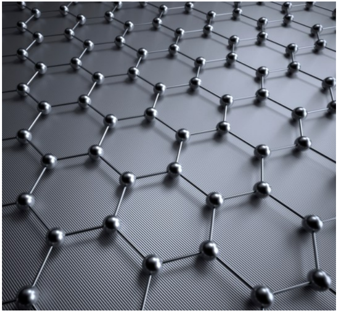
Figures from Guillamón et al, Phys. Rev. Lett. 101, 166407 (2008)

and Heil et al, Phys. Rev. Lett. 119, 087003 (2017)

Breakdown of Rayleigh-Schrödinger perturbation theory

- Raman G peak of gated graphene





Left figure from Pisana et al, Nat. Mater. 6, 198 (2007)

Many-body Schrödinger's equation

$$-\frac{\hbar^2}{2m_e}\sum\nolimits_i \nabla_i^2\,\Psi - \frac{\hbar^2}{2M_\kappa}\sum\nolimits_\kappa \nabla_\kappa^2\,\Psi - \sum\nolimits_{i,\kappa} Z_\kappa v(\mathbf{r}_i,\boldsymbol{\tau}_\kappa)\,\Psi$$

$$+\sum\nolimits_{\kappa>\kappa'} Z_\kappa Z_{\kappa'} v(\boldsymbol{\tau}_\kappa,\boldsymbol{\tau}_{\kappa'})\,\Psi + \sum\nolimits_{i>j} v(\mathbf{r}_i,\mathbf{r}_j)\,\Psi = E_{\text{tot}}\,\Psi$$

$$v(\mathbf{r},\mathbf{r}') = \frac{e^2}{4\pi\epsilon_0|\mathbf{r}-\mathbf{r}'|}$$

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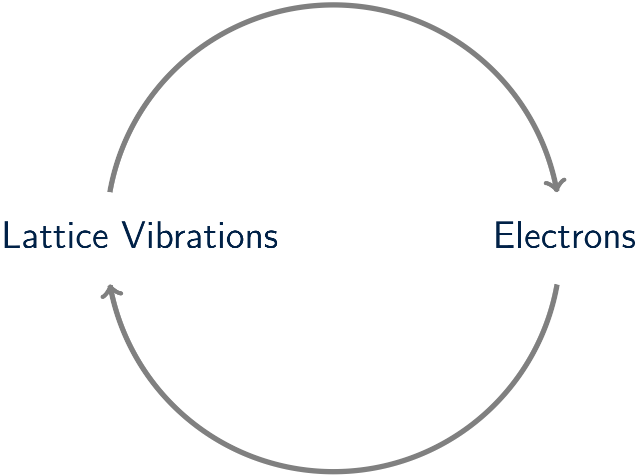
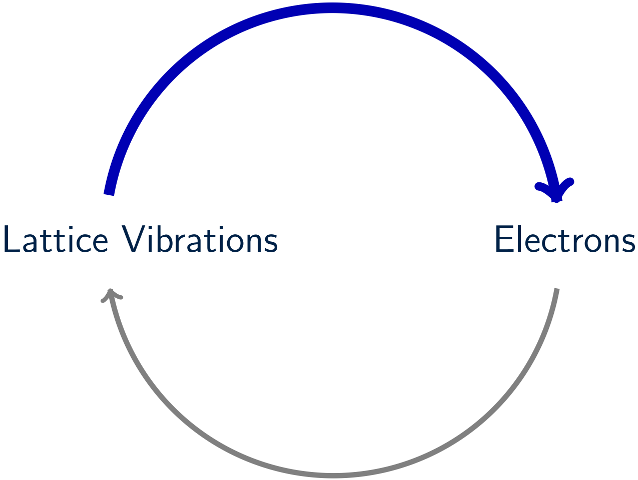
- We need to describe electrons and vibrations on the same footing
- The many-body Schrödinger equation is impractical for calculations


Lattice Vibrations
Electrons


Lattice Vibrations
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Field operators

N-electron wavefunction as a linear combination of Slater determinants

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \cdots) = \sum_{mn} a_{mn}\, \hat{c}_m^\dagger \hat{c}_n |0_{\mathrm{KS}}\rangle + \sum_{mnpq} b_{mnpq}\, \hat{c}_m^\dagger \hat{c}_n^\dagger \hat{c}_p \hat{c}_q |0_{\mathrm{KS}}\rangle + \cdots$$

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Operators in second quantization

$$V(\mathbf{x}_1) + V(\mathbf{x}_2) + \cdots \longrightarrow \sum_{mn} V_{mn} \hat{c}^\dagger_m \hat{c}_n$$

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Many-body Hamiltonian in second quantization

Non-relativistic Hamiltonian of coupled electrons and nuclei

$$\hat{H} = \hat{T}_{\rm e} + \hat{T}_{\rm n} + \hat{U}_{\rm en} + \hat{U}_{\rm ee} + \hat{U}_{\rm nn}$$

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Electron kinetic energy

$$\hat{T}_{\mathrm{e}} = -\frac{\hbar^2}{2m_{\mathrm{e}}} \int d\mathbf{x}\, \hat{\psi}^\dagger(\mathbf{x})\, \nabla^2\, \hat{\psi}(\mathbf{x})$$

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Electron-nucleus interaction

$$\hat{U}_{\rm en} = \int d\mathbf{r} \int d\mathbf{r}'\, \hat{n}_{\rm e}(\mathbf{r}) \hat{n}_{\rm n}(\mathbf{r}') v(\mathbf{r}, \mathbf{r}'), \quad \hat{n}_{\rm e}(\mathbf{r}) = \sum\nolimits_\sigma \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x})$$

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Electron-electron interaction

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

Time evolution of field operators

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

Time evolution of field operators

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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Heisenberg time evolution

$$\hat{\psi}(\mathbf{x}, t) = e^{i\hat{H}t/\hbar}\,\hat{\psi}(\mathbf{x})\,e^{-i\hat{H}t/\hbar} \qquad i\hbar\frac{\partial}{\partial t}\hat{\psi}(\mathbf{x}, t) = \left[\hat{\psi}(\mathbf{x}, t), \hat{H}\right]$$

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Exercise

$$\langle N|\psi(\mathbf{x},t)|N+1,s\rangle \quad = \quad \langle N|e^{i\hat{H}t/\hbar}\,\hat{\psi}(\mathbf{x})\,e^{-i\hat{H}t/\hbar}|N+1,s\rangle$$

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&= \underbrace{\langle N|\,\hat{\psi}(\mathbf{x})|N+1,s\rangle}_{f_s(\mathbf{x})\ \text{Dyson orbital}}\,e^{-i\varepsilon_s t/\hbar}
\end{aligned}$$

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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$\Big|$ electron in $\mathbf{x}'$ at time t' $\Big\rangle$

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Consider $t > t'$ (electron injection)

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&= -\frac{i}{\hbar}\langle N|\,\hat{\psi}(\mathbf{x})\,e^{-i(\hat{H}-E_N)(t-t')/\hbar}\;\;\hat{\psi}^\dagger(\mathbf{x}')|N\rangle
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$$\sum\nolimits_s |N+1,s\rangle\langle N+1,s|$$

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\end{aligned}
$$

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

$$= -\frac{i}{\hbar} \sum_s f_s(\mathbf{x}) f_s^*(\mathbf{x}') e^{-i\varepsilon_s(t-t')/\hbar}$$

The spectral function

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

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

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

The spectral function

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

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

The spectral function

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

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

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

The spectral function

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

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

The spectral function

Example: a single complex pole

$$\varepsilon_s = \varepsilon - i\Gamma$$

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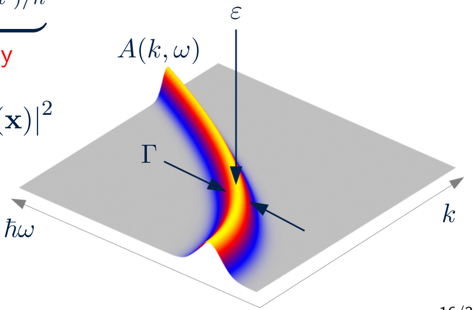

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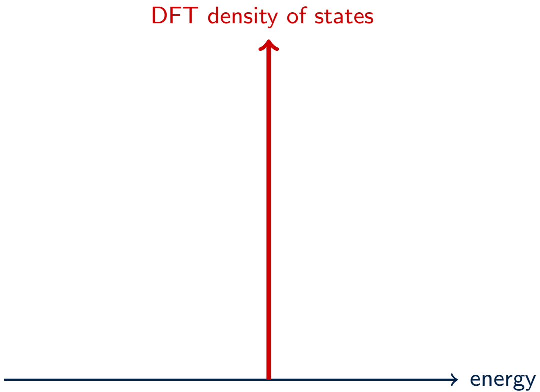

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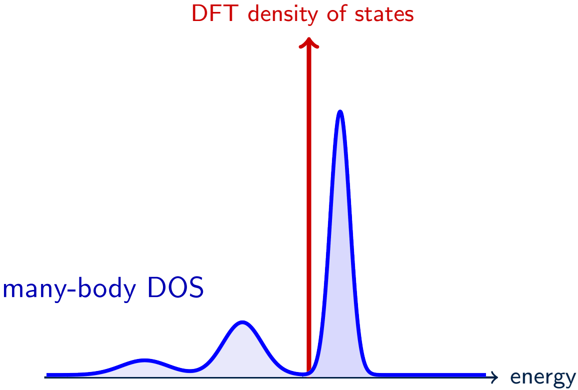

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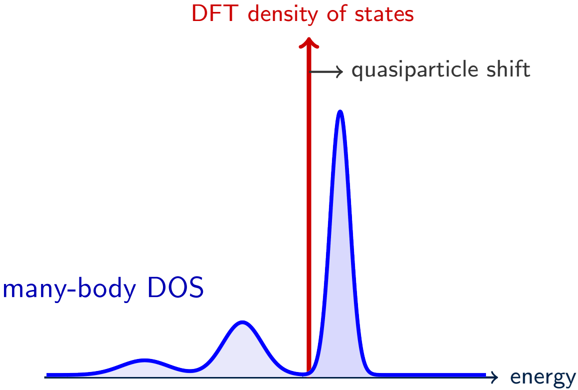

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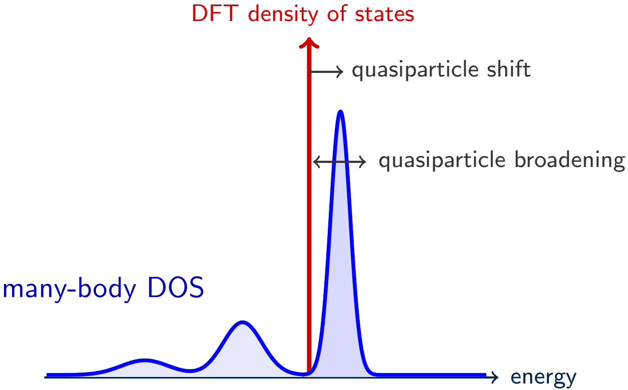

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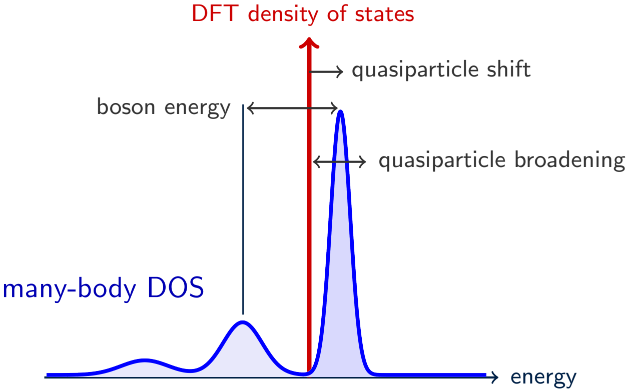

How to calculate the Green's function

Equation of motion for field operators

$$i\hbar \frac{\partial}{\partial t}\hat{\psi}(\mathbf{x}t) = \left[\hat{\psi}(\mathbf{x},t), \hat{H}\right]$$

How to calculate the Green's function

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total charge, electrons & nuclei → $\hat{n}(\mathbf{r}'t)$

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4 field operators → 2-particle Green's function

$$\langle \hat{T}\psi^\dagger(3)\psi(3)\psi(1)\psi^\dagger(2)\rangle = [\text{Hartree}] + [\text{Fock}] + G_2(31,32)$$

How to calculate the Green's function

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

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

↑ rewrite 2-particle Green's function using self-energy Σ

How to calculate the Green's function

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

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Sources of electron-phonon interaction

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Sources of electron-phonon interaction

How to calculate the self-energy

Electron self-energy from Hedin-Baym's equations

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

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$$W = W_\mathrm{e} + W_\mathrm{ph}$$

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Basically the standard GW method + screening from nuclei

How to calculate the self-energy

Screened Coulomb interaction from the nuclei

$$W_{\rm ph}(12) = \sum_{\kappa\kappa'} \int d(34)\, \epsilon_{\rm e}^{-1}(13) \frac{\partial V_\kappa(\mathbf{r}_3)}{\partial \boldsymbol{\tau}_\kappa} \cdot \mathbf{D}_{\kappa\kappa'}(t_3 t_4) \cdot \epsilon_{\rm e}^{-1}(24) \frac{\partial V_{\kappa'}(\mathbf{r}_4)}{\partial \boldsymbol{\tau}_{\kappa'}}$$

How to calculate the self-energy

Screened Coulomb interaction from the nuclei

"electron-phonon matrix elements"

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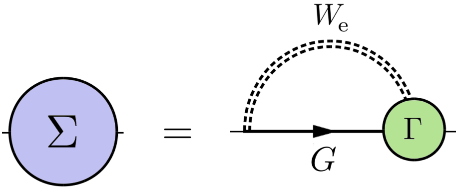
Displacement-displacement correlation function of the nuclei,

a.k.a. the phonon Green's function

$$\mathbf{D}_{\kappa\kappa'}(tt') = -\frac{i}{\hbar} \langle\, \hat{T}\, \Delta\hat{\boldsymbol{\tau}}_\kappa(t)\, \Delta\hat{\boldsymbol{\tau}}^T_{\kappa'}(t')\, \rangle$$

Diagrammatic representation of the self-energy



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

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

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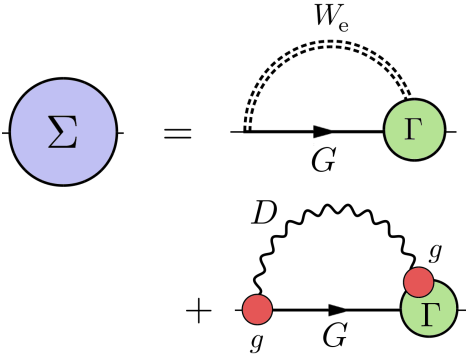

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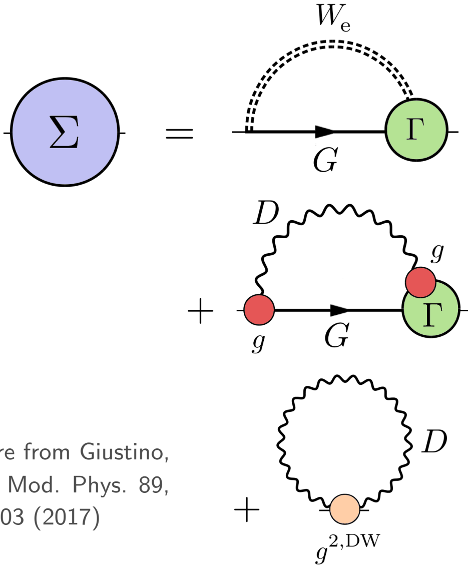

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Debye-Waller self-energy
(Lecture Thu.2)
Improper self-energy: comes form
$V_{tot}(1) = \int d2\, v(12)\langle\hat{n}(2)\rangle$ term

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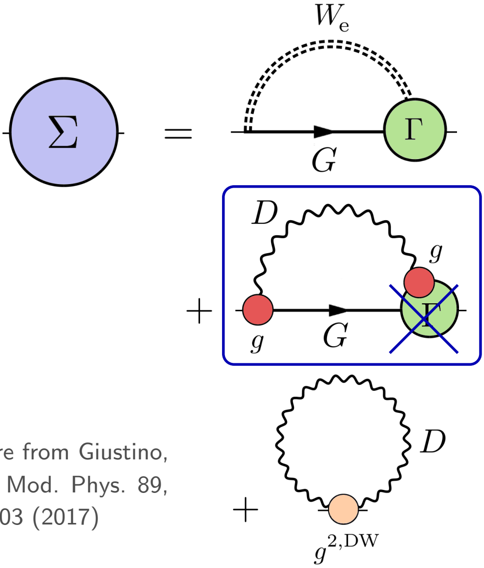

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Fan-Migdal self-energy

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

$$\Sigma^{\rm FM}_{n\mathbf{k}}(\omega) = \frac{1}{\hbar}\sum_{m\nu}\int\frac{d\mathbf{q}}{\Omega_{\rm BZ}}\,|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$$

$$\times\left[\frac{1-f_{m\mathbf{k}+\mathbf{q}}}{\omega-\varepsilon_{m\mathbf{k}+\mathbf{q}}/\hbar-\omega_{\mathbf{q}\nu}+i\eta}+\frac{f_{m\mathbf{k}+\mathbf{q}}}{\omega-\varepsilon_{m\mathbf{k}+\mathbf{q}}/\hbar+\omega_{\mathbf{q}\nu}+i\eta}\right]$$

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Dynamical structure on the scale of the phonon energy

Fan-Migdal self-energy

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

Summation over all phonon branches and wavevectors

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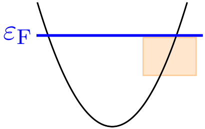
Extension to finite temperature

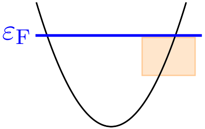
Dynamical structure on the scale of the phonon energy

Fan-Migdal self-energy



Example: A single dispersionless phonon (Holstein model)

Fan-Migdal self-energy



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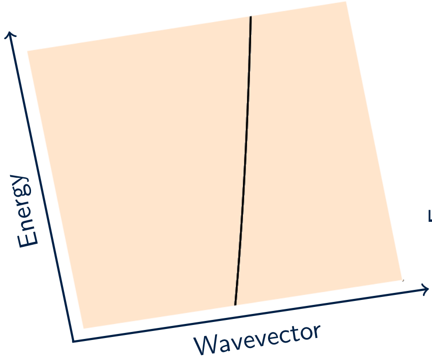
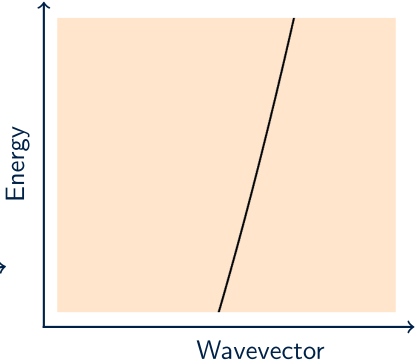
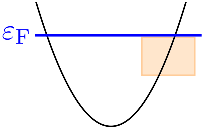




Fan-Migdal self-energy



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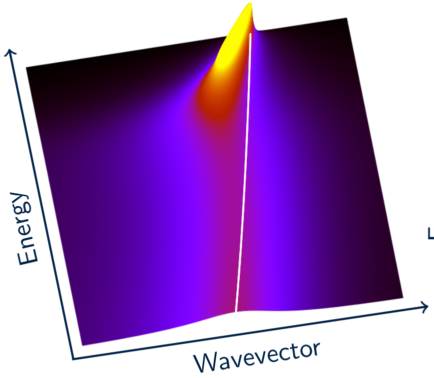

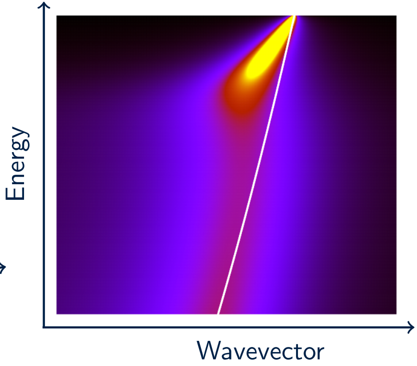

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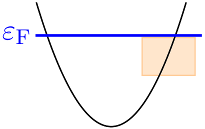

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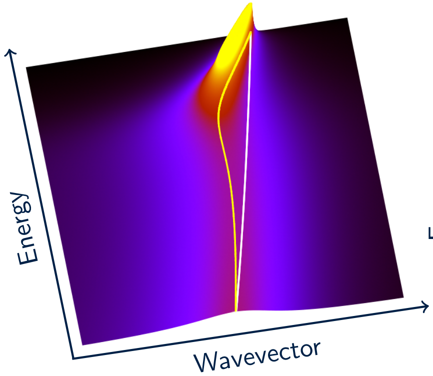

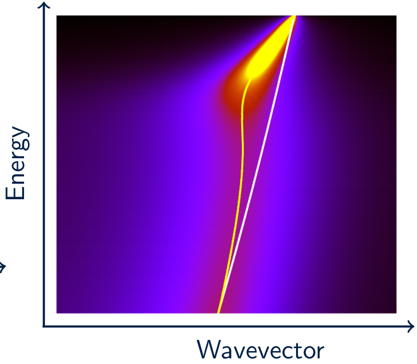

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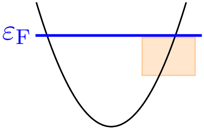

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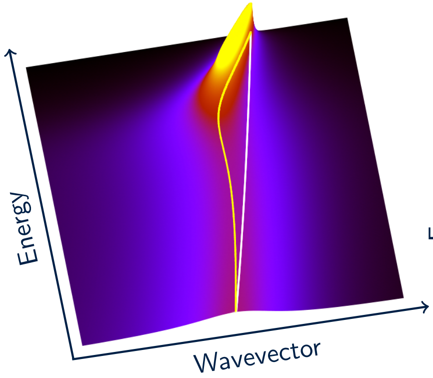
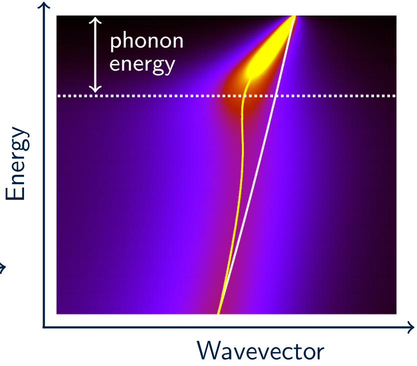
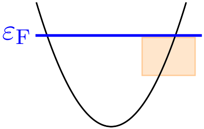
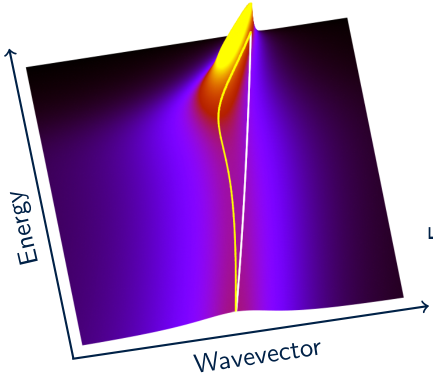


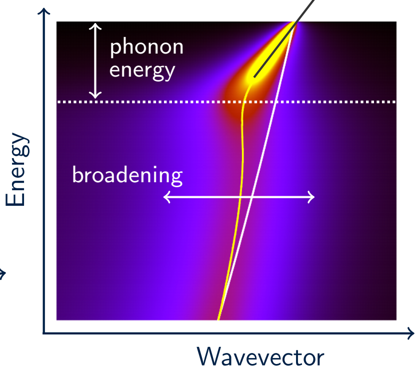


Fan-Migdal self-energy



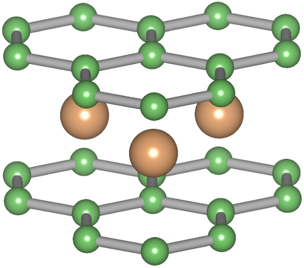
Example: A single dispersionless phonon
(Holstein model)



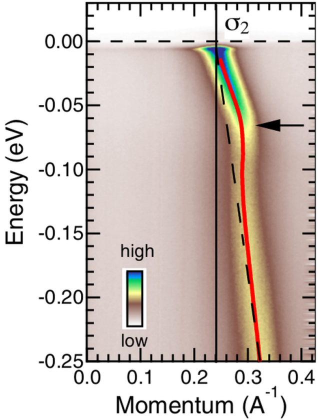


Examples from experiments

- Velocity renormalization in MgB_2



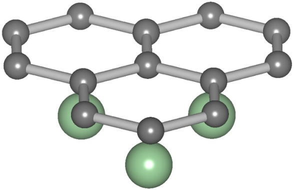
$$v = v_0/2.4$$

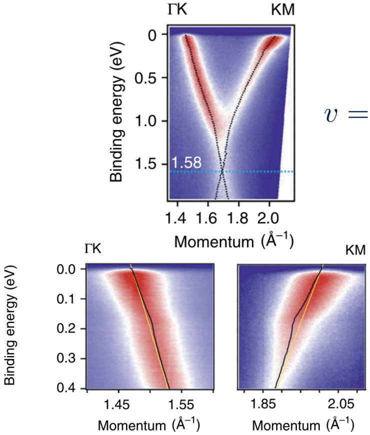


Right figure from Mou et al, Phys. Rev. B 91, 140502(R) (2015)

Examples from experiments

- Velocity renormalization in Ca-decorated graphene on Au





$$v = v_0/1.25$$

Right figure adapted from Fedorov et al, Nat. Commun. 5, 3257 (2014)

Examples from calculations

- Velocity renormalization in C_6CaC_6 (EPW)

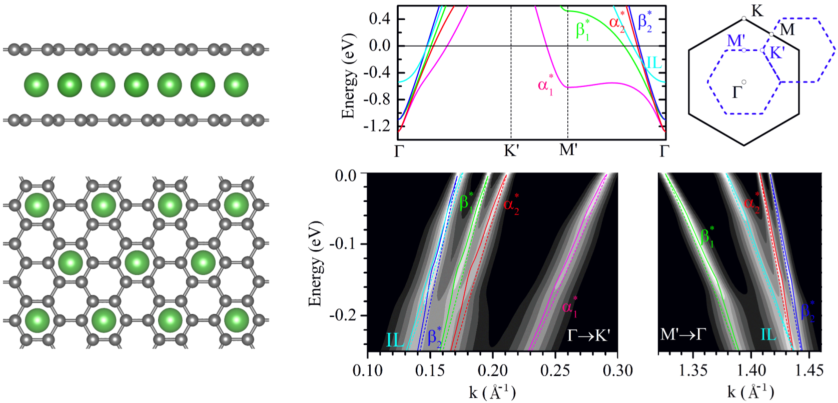


Figure adapted from Margine et al, Sci Rep. 6, 21414 (2016)

Examples from calculations

- Velocity renormalization and broadening in MgB_2

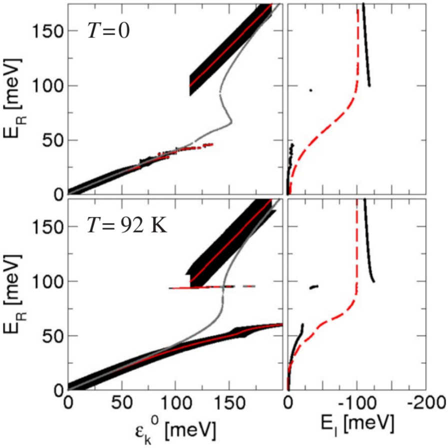


Figure from Eiguren et al, Phys. Rev. B 79. 245103 (2009)

Quasiparticle shift and broadening

Spectral function from the self-energy

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

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Quasiparticle approximation:

assume Lorentzian peaks centered near $\hbar\omega = E_{n\mathbf{k}}$

$$\Sigma_{n\mathbf{k}}(\omega) = \Sigma_{n\mathbf{k}}(E_{n\mathbf{k}}) + \frac{1}{\hbar}\,\frac{\partial \mathrm{Re}\Sigma_{n\mathbf{k}}}{\partial\omega}\bigg|_{\omega=E_{n\mathbf{k}}/\hbar} (\hbar\omega - E_{n\mathbf{k}}) + \cdots$$

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Define the quasiparticle strength

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

Quasiparticle shift and broadening

Replace the Taylor expansion inside the spectral function

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

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After rearranging(*):

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

(*) Requires the additional approximation $|\partial \mathrm{Im}\Sigma_{n\mathbf{k}}/\partial\omega| \ll |\partial \mathrm{Re}\Sigma_{n\mathbf{k}}/\partial\omega|$

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The mass enhancement parameter

Taking the $\mathbf{k}$-derivatives of the quasiparticle energy $E_{n\mathbf{k}}$
we find the velocity and mass renormalization

$$V_{n\mathbf{k}} = \frac{v_{n\mathbf{k}}}{1+\lambda_{n\mathbf{k}}}$$

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

(valid only for simple metals)

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(Cauchy-Riemann condition)

Electron lifetimes

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

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$$\frac{1}{\tau_{n\mathbf{k}}} = \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} |g_{nm\nu}(\mathbf{k},\mathbf{q})|^2 \times \left[(1 - f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu}) \delta(\varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu} - \varepsilon_{m\mathbf{k}+\mathbf{q}}) + (f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu}) \delta(\varepsilon_{n\mathbf{k}} + \hbar\omega_{\mathbf{q}\nu} - \varepsilon_{m\mathbf{k}+\mathbf{q}}) \right]$$

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

$$+\,(f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu})\delta(\varepsilon_{n\mathbf{k}} + \hbar\omega_{\mathbf{q}\nu} - \varepsilon_{m\mathbf{k}+\mathbf{q}})]$$ phonon absorption

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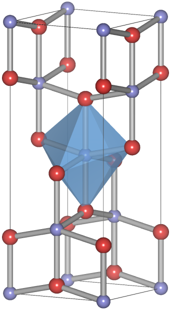
Standard Fermi Golden rule expression for lifetimes

Example from calculations

- Electron lifetimes in anatase TiO_2 (EPW)



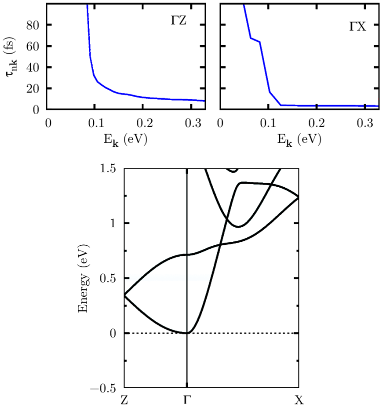


Figure adapted from Verdi et al, Phys. Rev. Lett. 115, 176401 (2015)

Take-home messages

- Quantum field theory is extremely useful in the study of electron-phonon physics
- The electron-phonon self-energy works as in the GW method, but on much smaller energy scales
- We can calculate the change of the effective mass and band velocity induced by EPIs
- We can calculate electron lifetimes arising from EPIs

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