2021 Virtual School on Electron-Phonon Physics and the EPW code

June 14-18 2021

Lecture Tue.2

Many-body methods for electron-phonon interactions

Feliciano Giustino

Oden Institute & Department of Physics

The University of Texas at Austin

Lecture Summary

- 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

Limitations of Rayleigh-Schrödinger perturbation theory

Kohn-Sham equations again

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

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

Breakdown of Rayleigh-Schrödinger perturbation theory

Polaron liquid at the $SrTiO_3(001)$ surface

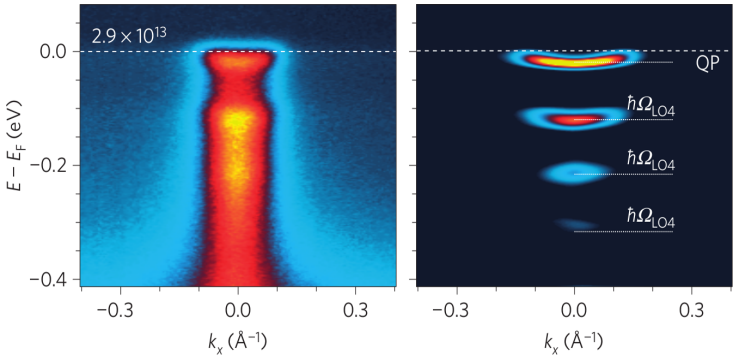
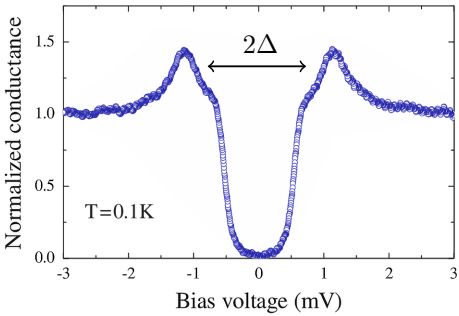
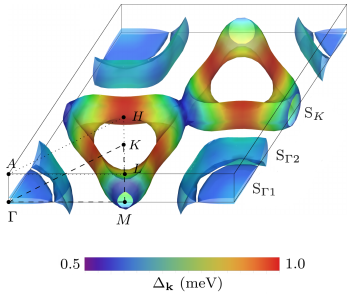


Figure from Wang et al, Nature Mater. 15, 835 (2016)

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)

Many-body Schrödinger equation

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

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

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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

Field operators

Many-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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Many-body Hamiltonian in second quantization

Non-relativistic Hamiltonian of coupled electrons and nuclei

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

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

Time evolution of field operators

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

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Heisenberg time evolution

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The Green's function at zero temperature

Time-ordered Green's function

Wick's time-ordering operator

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$\left|\right.$ electron in $\mathbf{x}'$ at time t' $\left.\right\rangle$

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&= -\frac{i}{\hbar}\sum\nolimits_s f_s(\mathbf{x}) f_s^*(\mathbf{x}') e^{-i\varepsilon_s(t-t')/\hbar}
\end{aligned}
$$

The spectral function

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

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

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

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

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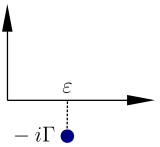
The spectral function is the many-body (local) density of states

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

The spectral function: Broadening

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



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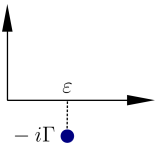

$$G(\mathbf{x},\mathbf{x},t-t') = -\frac{i}{\hbar}\left|f_s(\mathbf{x})\right|^2 e^{-i\varepsilon(t-t')/\hbar} e^{-\Gamma(t-t')/\hbar}$$

The spectral function: Broadening

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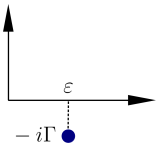

$$G(\mathbf{x},\mathbf{x},t-t') = -\frac{i}{\hbar}\left|f_s(\mathbf{x})\right|^2 e^{-i\varepsilon(t-t')/\hbar} e^{-\Gamma(t-t')/\hbar}$$

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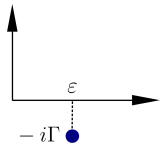

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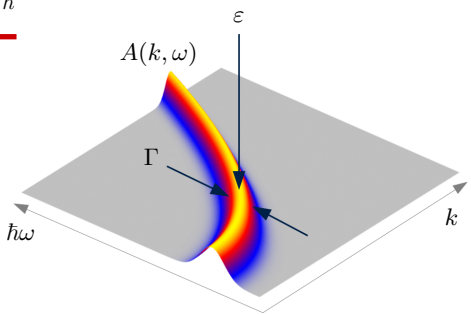

The spectral function: Coherent and incoherent structures

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

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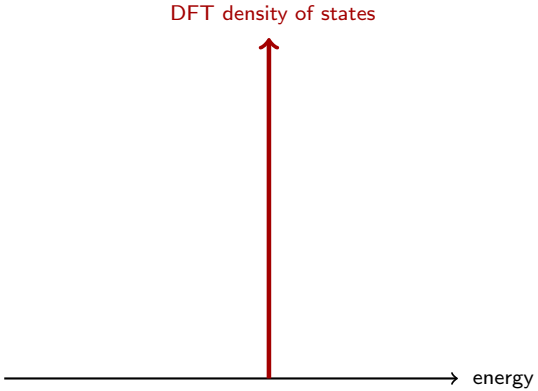

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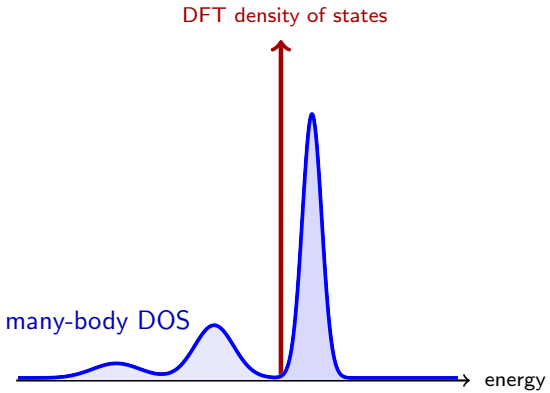

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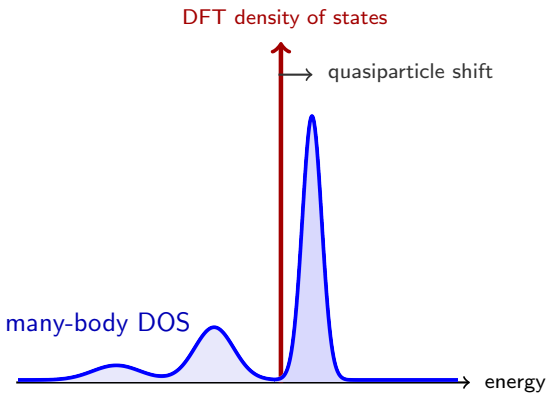

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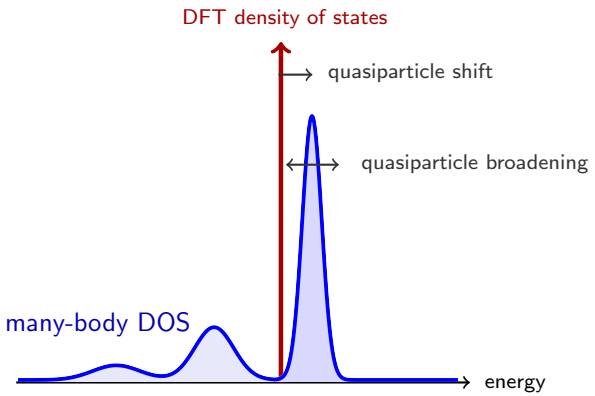

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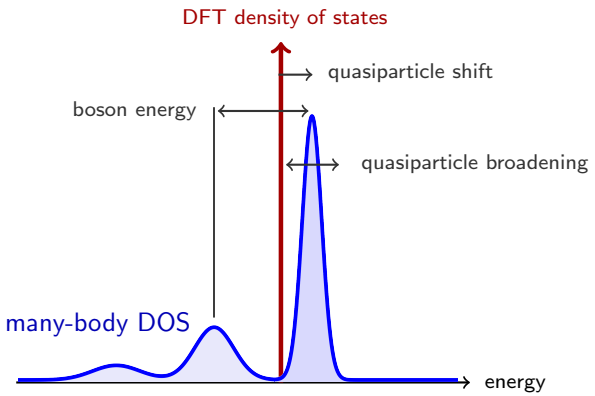

How to calculate the Green's function

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

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4 field operators

Hartree+Fock+2-particle Green's function

How to calculate the Green's function

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

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

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

How to calculate the Green's function

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

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

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

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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

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$G(13)$: Green's function

$\Gamma(324)$: Vertex

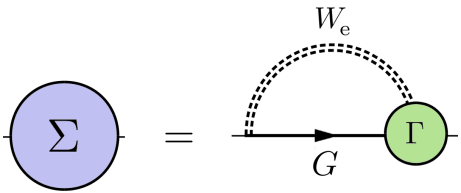
$W(41^+)$: Screened Coulomb interaction

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

$$W_{\mathrm{e}}(12) = \int d3\, \epsilon_{\mathrm{e}}^{-1}(13) v(32)$$

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)

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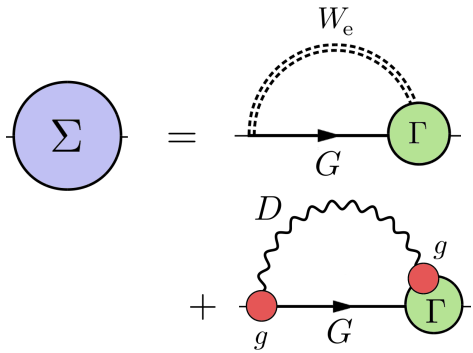

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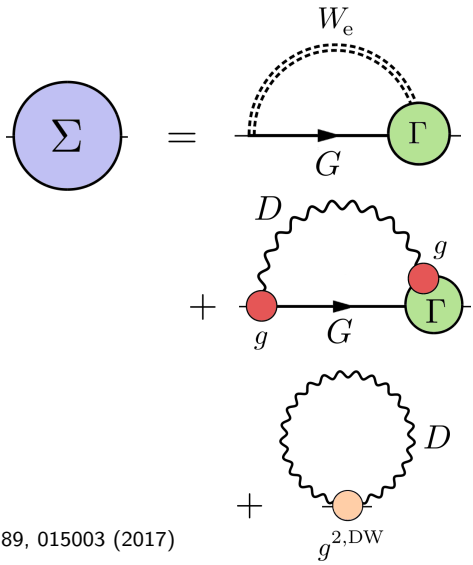

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Debye-Waller self-energy

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

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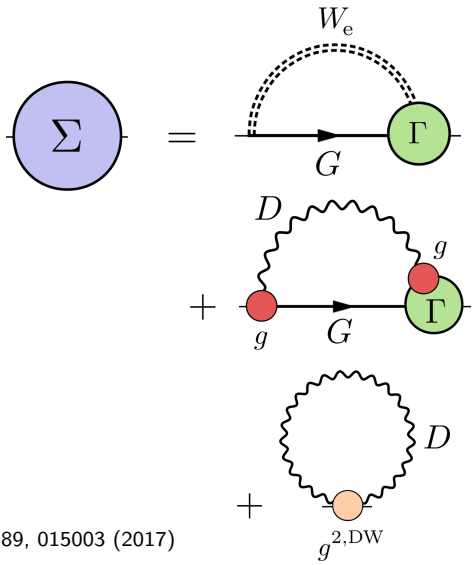

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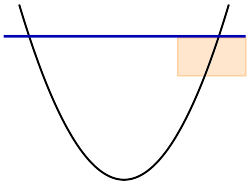
Fan-Migdal self-energy

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

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

Example: Interaction with dispersionless phonon



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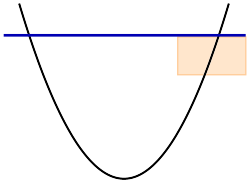

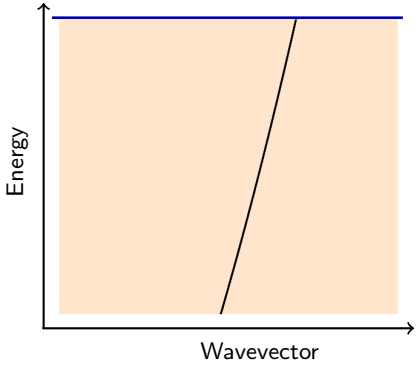

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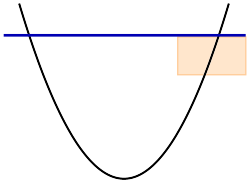

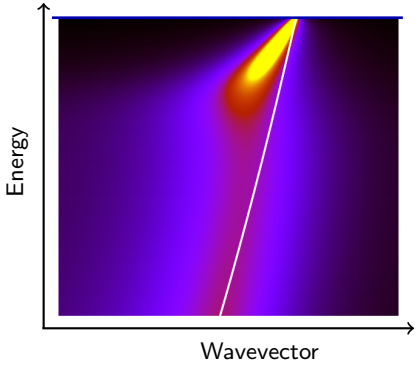

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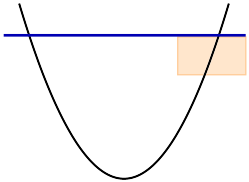

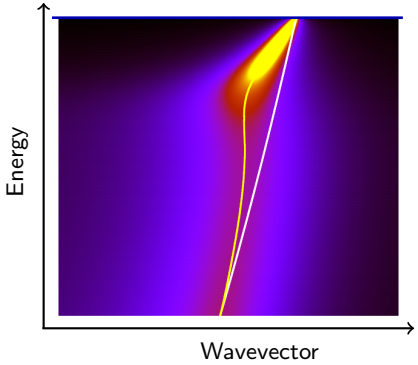

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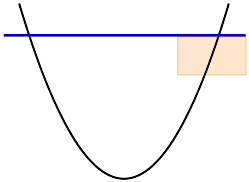

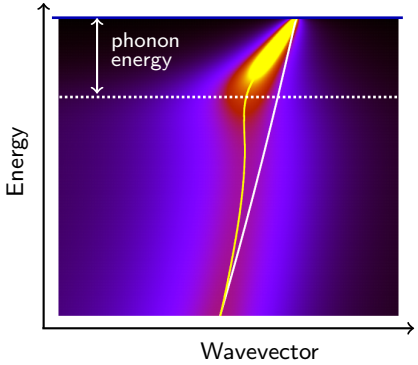

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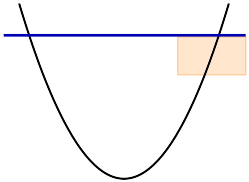
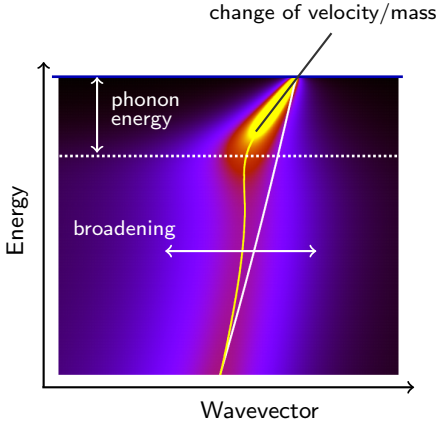
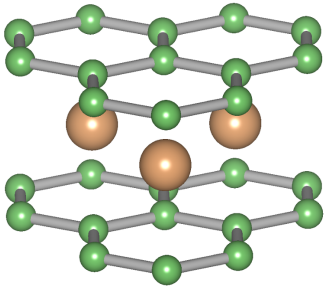
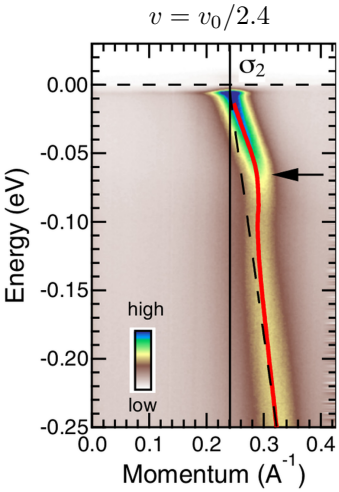




Example from experiments: Velocity renormalization in MgB_2





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

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 simple poles in the complex plane

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

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

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The mass enhancement parameter

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

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

(valid only for simple metals)

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

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

Electron lifetimes

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

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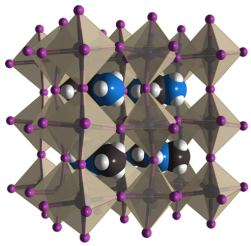
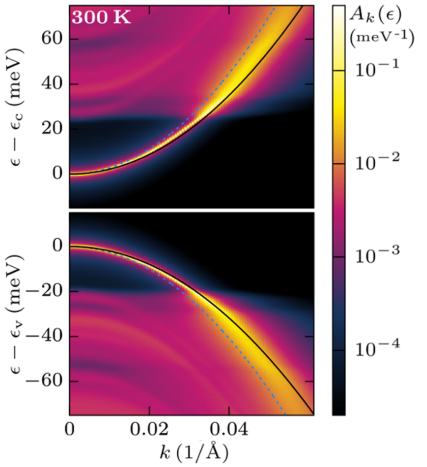
$$\frac{1}{\tau_{n\mathbf{k}}} = \frac{2\pi}{\hbar}\sum_{m\nu}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2$$
$$\times\,[(1 - f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu})\delta(\varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu} - \varepsilon_{m\mathbf{k}+\mathbf{q}})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

Standard Fermi Golden rule expression for lifetimes

Example: Mass enhancement and lifetimes in $MAPbI_3$





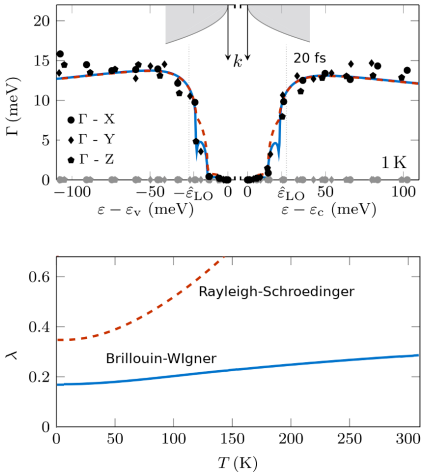


Figure adapted from Schlipf et al, Phys. Rev. Lett. 121, 086402 (2018)

Take-home messages

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

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