2023 Virtual School on Many-Body Calculations using **EPW** and **BerkeleyGW**

5-9 June 2023

Lecture Mon.1

Many-body theory of electron-phonon interactions

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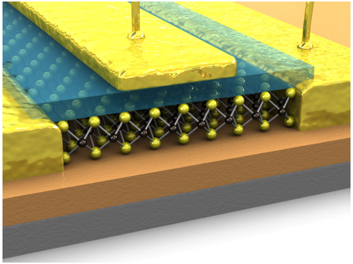
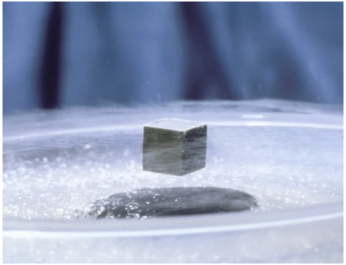
Lecture Summary

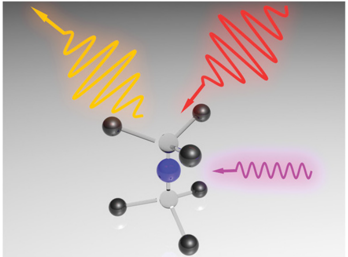
- Introduction to electron-phonon interactions
- How phonons influence electrons
- How electrons influence phonons

Manifestations of electron-phonon interactions



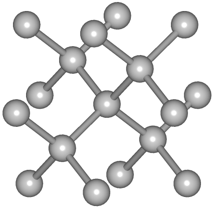
Radisavljevic et al, Nature Mater 2013



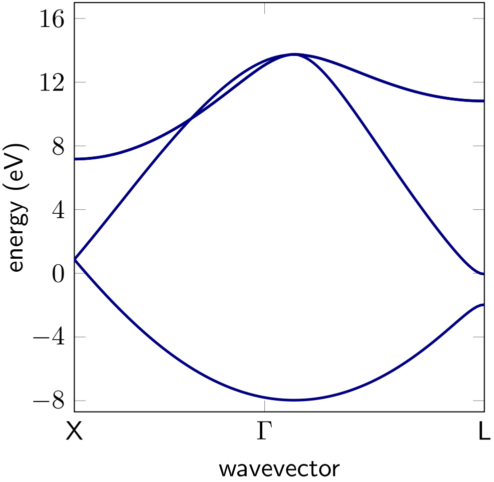


Tran et al, Sci. Adv. 2019

Heuristic notion of electron-phonon interactions



diamond



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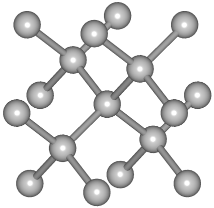

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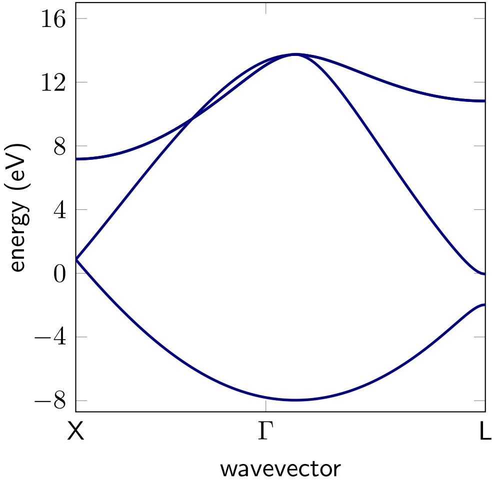
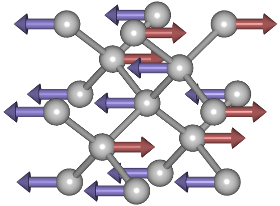
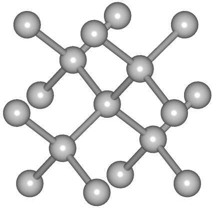




Γ-point optical mode
0.015 Å C-displacement

Heuristic notion of electron-phonon interactions



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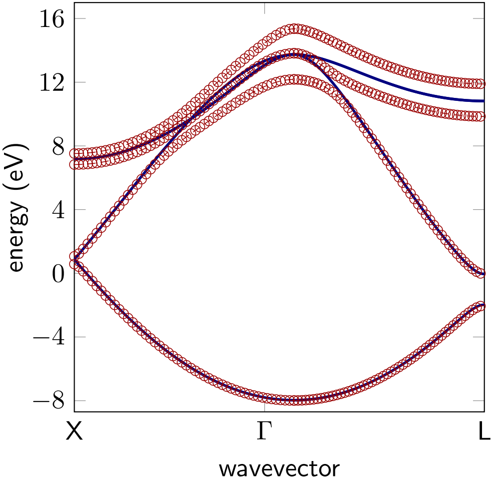

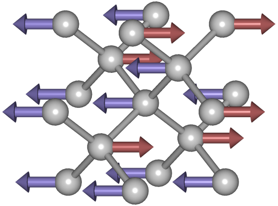

Γ-point optical mode

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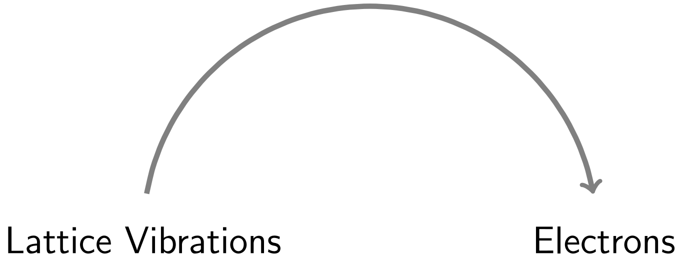
Mutual interactions between electrons and vibrations

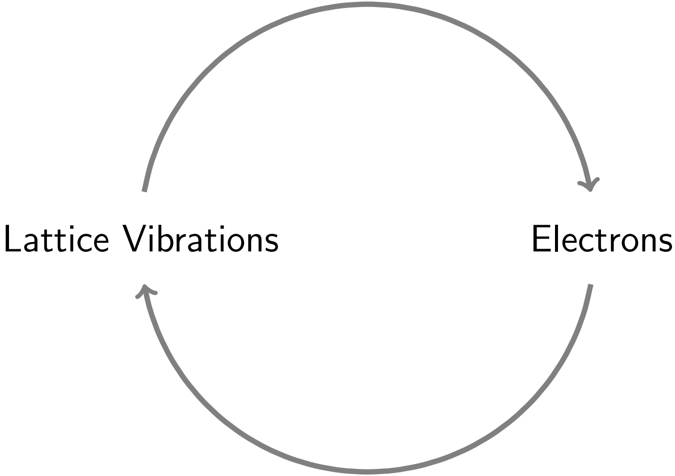
Lattice Vibrations

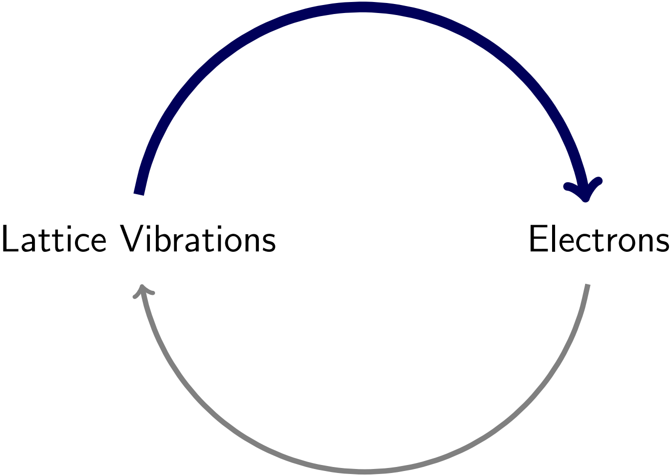
Electrons

Mutual interactions between electrons and vibrations



Mutual interactions between electrons and vibrations




Lattice Vibrations
Electrons

Many-body Schrödinger equation for electrons and nuclei

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

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

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- Electrons and vibrations must be described on the same footing

Many-body Schrödinger equation for electrons and nuclei

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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

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots) = \sum_{mn} A_{mn}\, \hat{c}^\dagger_m \hat{c}_n |0_{\rm KS}\rangle + \sum_{mnpq} B_{mnpq}\, \hat{c}^\dagger_m \hat{c}^\dagger_n \hat{c}_p \hat{c}_q |0_{\rm KS}\rangle + \cdots$$

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Operators in second quantization

$$\textstyle\sum_i V(\mathbf{r}_i) \quad \longrightarrow \quad \sum_{mn} V_{mn}\, \hat{c}^\dagger_m \hat{c}_n$$

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Field operators

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Hamiltonian in field-theoretic formulation

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

$$\hat{n}_{\rm e}(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$$

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Electron-nucleus interaction $\quad \hat{U}_{\rm en} = \int d\mathbf{r}\, d\mathbf{r}'\, \hat{n}_{\rm e}(\mathbf{r})\hat{n}_{\rm n}(\mathbf{r}')v(\mathbf{r},\mathbf{r}')$

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

Time evolution of field operators and Dyson orbitals

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

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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Excitation energy	$\varepsilon_s = E_{N+1,s} - E_N$

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

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Exercise

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

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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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$$\begin{aligned} \langle N|\hat{\psi}(\mathbf{x},t)|N+1,s\rangle &= \langle N|e^{i\hat{H}t/\hbar}\,\hat{\psi}(\mathbf{x})\,e^{-i\hat{H}t/\hbar}|N+1,s\rangle \\ &= \langle N|e^{iE_N t/\hbar}\,\hat{\psi}(\mathbf{x})\,e^{-iE_{N+1,s}t/\hbar}|N+1,s\rangle \end{aligned}$$

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

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

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

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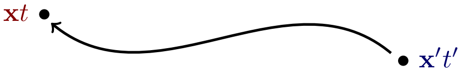

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Consider $t > t'$ (electron added to ground state)

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

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

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

The spectral function

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

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

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

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

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

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

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

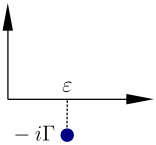
The poles of the Green's function represent the electron addition/removal energies of the interacting many-body system

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

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

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

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



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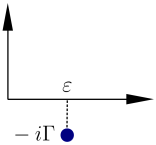

$$G(\mathbf{x},\mathbf{x},t-t') = -\frac{i}{\hbar}\,|f_s(\mathbf{x})|^2\, e^{-i\varepsilon(t-t')/\hbar} e^{-\Gamma(t-t')/\hbar}$$

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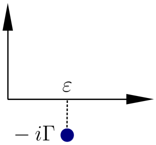

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$$A(\mathbf{x},\mathbf{x},\omega) = \frac{1}{\pi}\frac{\Gamma}{(\hbar\omega-\varepsilon)^2+\Gamma^2}\,|f_s(\mathbf{x})|^2$$

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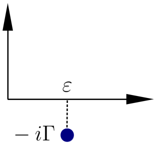

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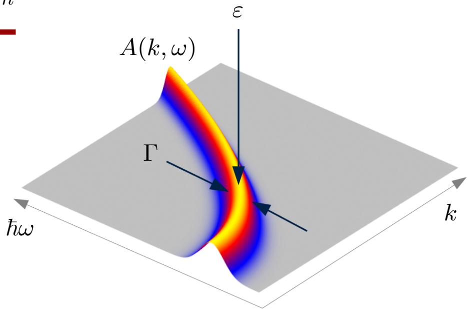

$$A(\mathbf{k},\omega) = \frac{1}{\pi}\,|\mathrm{Im}\,G(\mathbf{k},\omega)|$$

The spectral function: Coherent and incoherent structures

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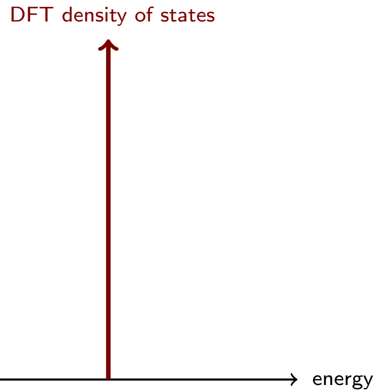

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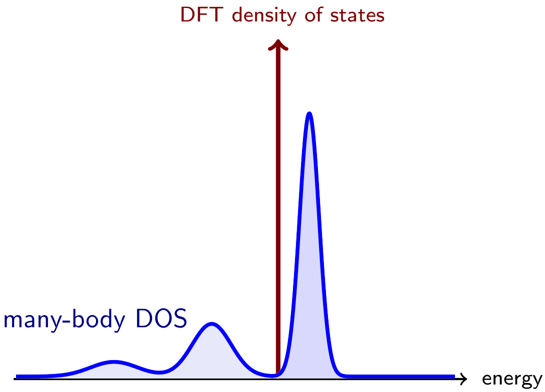

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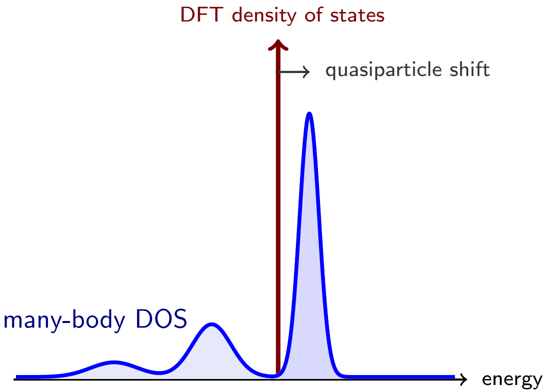

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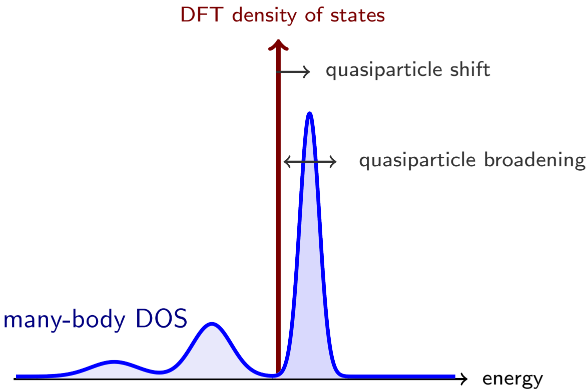

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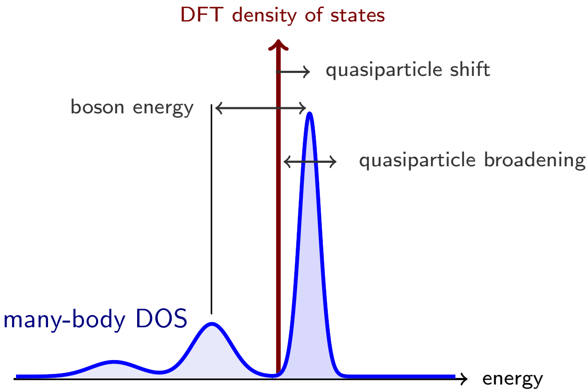

How to calculate the Green's function

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

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

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

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Equation of motion for Green's function

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

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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

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

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

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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

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

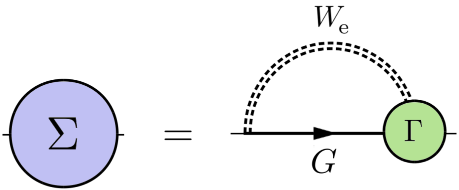
Screened Coulomb interaction

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

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

Reduces to the standard GW method + screening from nuclei

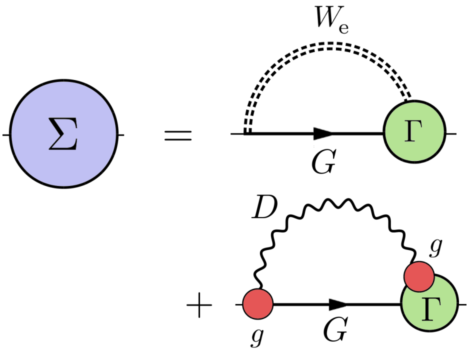
Diagrammatic representation of the self-energy



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

Figure from FG, RMP2017

Diagrammatic representation of the self-energy



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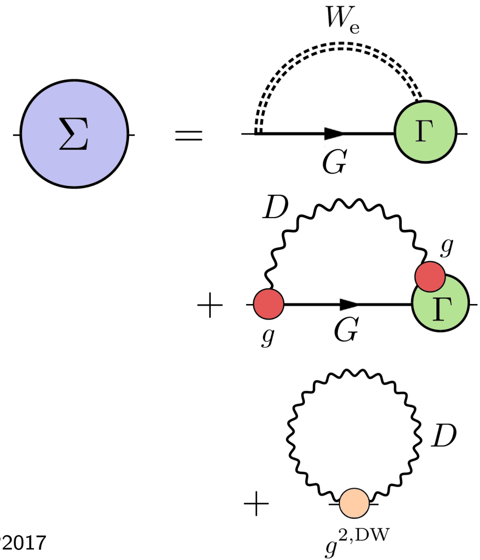
Fan-Migdal self-energy

Figure from FG, RMP2017

Diagrammatic representation of the self-energy



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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

Figure from FG, RMP2017

Diagrammatic representation of the self-energy

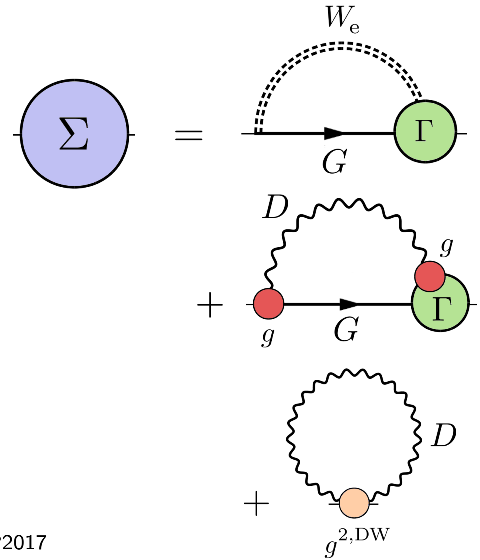

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Figure from FG, RMP2017

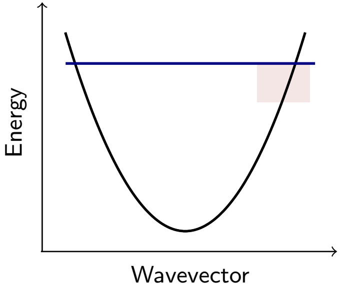
Fan-Migdal self-energy

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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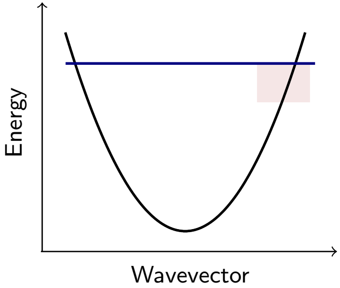
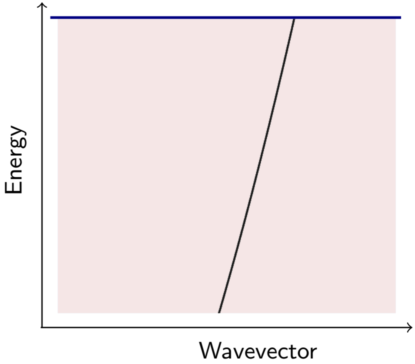
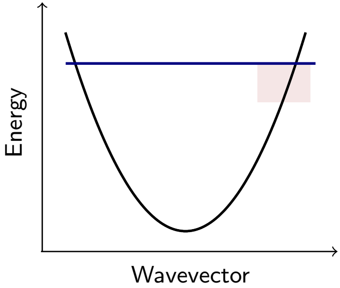
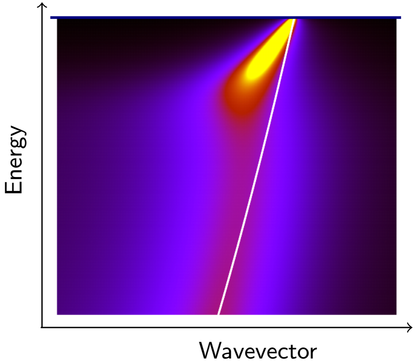





Energy
Wavevector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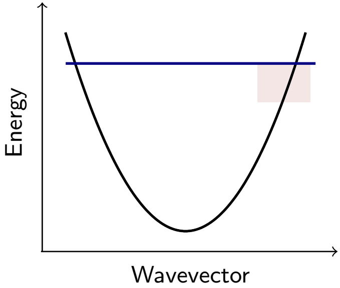

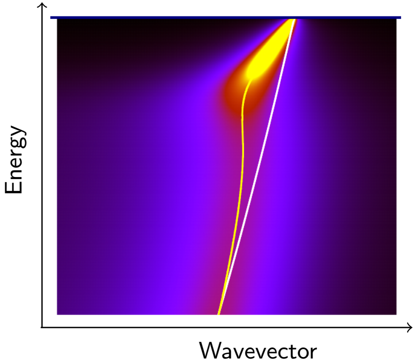

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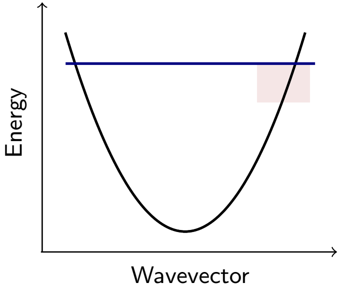
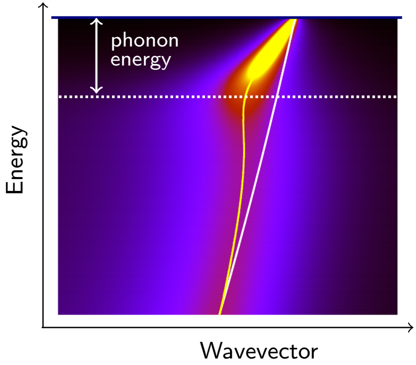
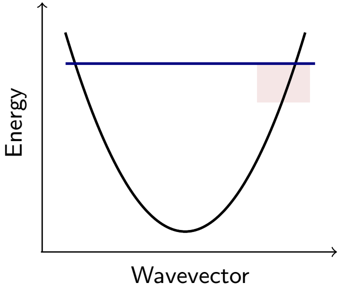
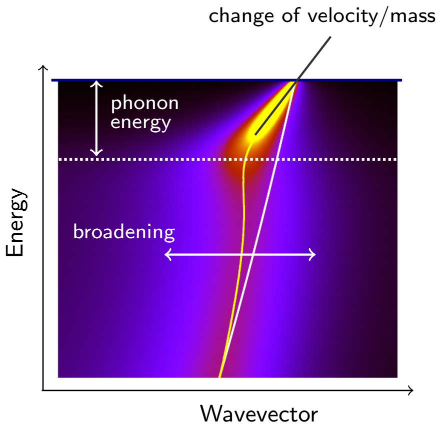
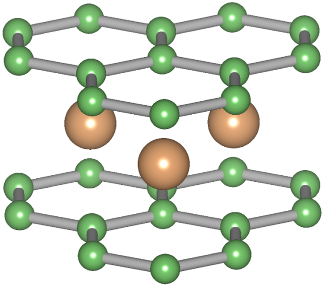





Energy
Wavevector


change of velocity/mass
phonon
energy
broadening
Energy
Wavevector



$$v = v_0/2.4$$

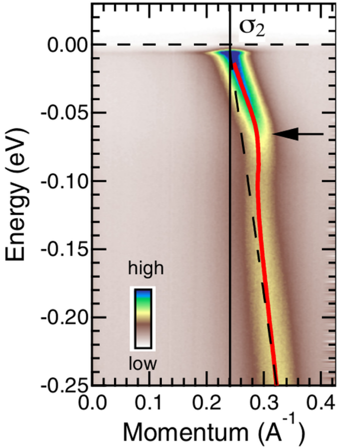


Figure from Mou et al, Phys. Rev. B 91, 140502(R) (2015)

Spectral function from the self-energy

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

Quasiparticle shift and broadening

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

The mass enhancement parameter

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

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

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

The mass enhancement parameter

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

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

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

Electron lifetimes

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

Electron lifetimes

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

Identical to Fermi Golden rule formula

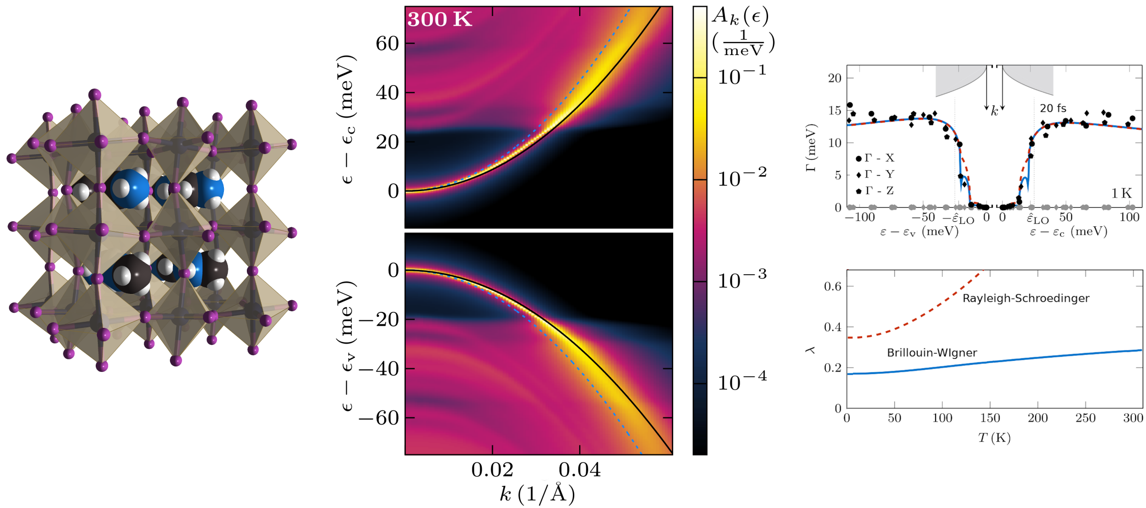
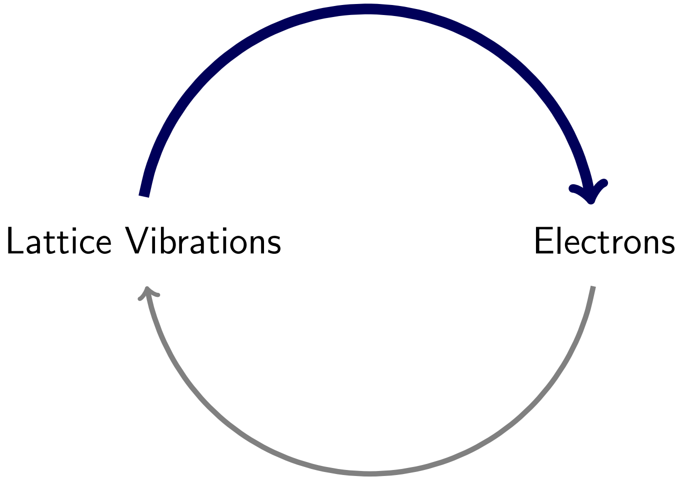
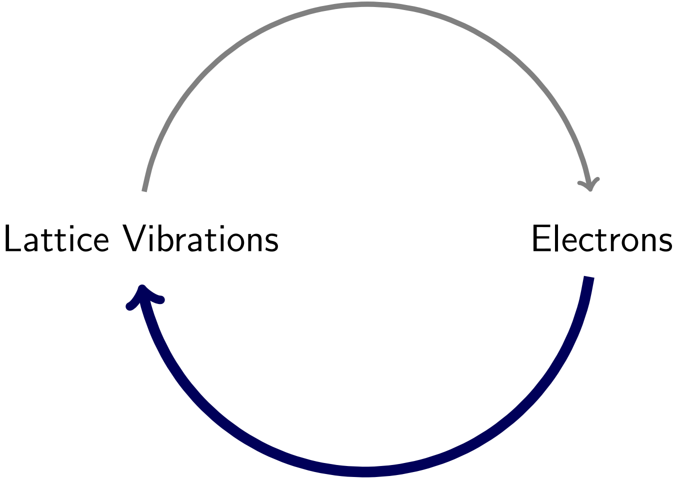


Figure adapted from Schlipf et al, Phys. Rev. Lett. 121, 086402 (2018)

Mutual interactions between electrons and vibrations




Lattice Vibrations
Electrons

Time-evolution of atomic displacements

Key quantity to study phonons in a many-body framework:

displacement-displacement correlation function

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

3×3 matrices in the Cartesian coordinates

Time-evolution of atomic displacements

Key quantity to study phonons in a many-body framework:

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

3×3 matrices in the Cartesian coordinates

Heisenberg time evolution of atomic displacements

$$i\hbar\frac{d}{dt}\Delta\hat{\boldsymbol{\tau}}_{\kappa}(t) = [\Delta\hat{\boldsymbol{\tau}}_{\kappa}(t), \hat{H}]$$

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$$M_{\kappa}\frac{d^2\Delta\hat{\boldsymbol{\tau}}_{\kappa}}{dt^2} = -\frac{M_{\kappa}}{\hbar^2}[[\Delta\hat{\boldsymbol{\tau}}_{\kappa}, \hat{H}], \hat{H}]$$

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Equation of motion for the displacement correlation function

$$M_\kappa \frac{\partial^2}{\partial t^2} \mathbf{D}_{\kappa\kappa'}(tt') =$$

Many-body phonon self-energy

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$$M_\kappa \frac{\partial^2}{\partial t^2} \mathbf{D}_{\kappa\kappa'}(tt') = -\mathbf{I}\,\delta_{\kappa\kappa'}\delta(tt') - \sum_{\kappa''}\int dt''\ \mathbf{\Pi}_{\kappa\kappa''}(tt'')\,\mathbf{D}_{\kappa''\kappa'}(t''t')$$

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Many-body phonon self-energy

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$\mathbf{\Pi}_{\kappa\kappa'}(\omega)$ contains the force constants resulting from the Coulomb interaction between nuclei, screened by the electronic dielectric matrix $\epsilon_{\mathrm{e}}(\mathbf{r},\mathbf{r}',\omega)$

$$\mathbf{D} = \begin{pmatrix} \mathbf{D}_{11} & \mathbf{D}_{12} & \dots & \mathbf{D}_{1N} \\ \mathbf{D}_{21} & \mathbf{D}_{22} & \dots & \mathbf{D}_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{D}_{N1} & \mathbf{D}_{N2} & \dots & \mathbf{D}_{NN} \end{pmatrix} \quad \mathbf{\Pi} = \begin{pmatrix} \mathbf{\Pi}_{11} & \mathbf{\Pi}_{12} & \dots & \mathbf{\Pi}_{1N} \\ \mathbf{\Pi}_{21} & \mathbf{\Pi}_{22} & \dots & \mathbf{\Pi}_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{\Pi}_{N1} & \mathbf{\Pi}_{N2} & \dots & \mathbf{\Pi}_{NN} \end{pmatrix} \quad \mathbf{M} = \begin{pmatrix} M_1\mathbf{I} & 0 & \dots & 0 \\ 0 & M_2\mathbf{I} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & M_N\mathbf{I} \end{pmatrix}$$

Many-body vibrational eigenfrequencies

$$\mathbf{D} = \begin{pmatrix} \mathbf{D}_{11} & \mathbf{D}_{12} & \dots & \mathbf{D}_{1N} \\ \mathbf{D}_{21} & \mathbf{D}_{22} & \dots & \mathbf{D}_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{D}_{N1} & \mathbf{D}_{N2} & \dots & \mathbf{D}_{NN} \end{pmatrix} \quad \mathbf{\Pi} = \begin{pmatrix} \mathbf{\Pi}_{11} & \mathbf{\Pi}_{12} & \dots & \mathbf{\Pi}_{1N} \\ \mathbf{\Pi}_{21} & \mathbf{\Pi}_{22} & \dots & \mathbf{\Pi}_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{\Pi}_{N1} & \mathbf{\Pi}_{N2} & \dots & \mathbf{\Pi}_{NN} \end{pmatrix} \quad \mathbf{M} = \begin{pmatrix} M_1\mathbf{I} & 0 & \dots & 0 \\ 0 & M_2\mathbf{I} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & M_N\mathbf{I} \end{pmatrix}$$

Equation of motion for the displacement-displacement correlation function in matrix form and in frequency domain

$$\mathbf{M}\,\omega^2\,\mathbf{D}(\omega) = \mathbf{I} + \mathbf{\Pi}(\omega)\,\mathbf{D}(\omega)$$

Formal solution: phonon Green's function in Cartesian coordinates

$$\mathbf{D}(\omega) = \frac{1}{\mathbf{M}\,\omega^2 - \mathbf{\Pi}(\omega)}$$

Many-body vibrational eigenfrequencies

Formal solution: phonon Green's function in Cartesian coordinates

$$\mathbf{D}(\omega) = \frac{1}{\mathbf{M}\,\omega^2 - \mathbf{\Pi}(\omega)} = \mathbf{M}^{-1/2}\frac{1}{\mathbf{I}\,\omega^2 - \mathbf{M}^{-1/2}\mathbf{\Pi}(\omega)\mathbf{M}^{-1/2}}\mathbf{M}^{-1/2}$$

Many-body vibrational eigenfrequencies

Formal solution: phonon Green's function in Cartesian coordinates

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the quantity

$$\mathbf{M}^{-1/2}\,\mathbf{\Pi}(\omega)\,\mathbf{M}^{-1/2} \longrightarrow \frac{\Pi_{\kappa\alpha,\kappa'\alpha'}(\omega)}{\sqrt{M_\kappa M_{\kappa'}}}$$

is the many-body dynamical matrix

The resonant frequencies are the solutions of the nonlinear equations

$$\Omega(\omega) = \omega$$

where $\Omega^2(\omega)$ is an eigenvalue of $\mathbf{M}^{-1/2}\,\mathbf{\Pi}(\omega)\,\mathbf{M}^{-1/2}$

Connection with density-functional perturbation theory

$$\Pi_{\kappa\alpha,\kappa'\alpha'}(\omega) = \frac{\partial^2}{\partial\tau_{\kappa\alpha}\,\partial\tau_{\kappa'\alpha'}} \int\! d\mathbf{r}\; \epsilon_{\mathrm{e}}^{-1}(\boldsymbol{\tau}_\kappa, \mathbf{r}, \omega)\, \frac{e^2 Z_\kappa Z_{\kappa'}}{4\pi\epsilon_0|\mathbf{r} - \boldsymbol{\tau}_{\kappa'}|} - \text{(static force)}$$

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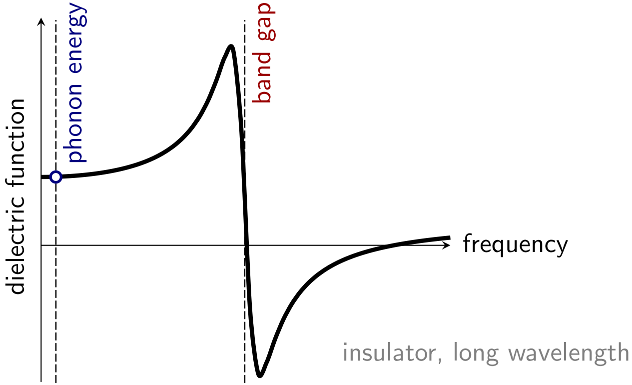

Connection with density-functional perturbation theory

We call **adiabatic** self-energy the $\mathbf{\Pi}$ evaluated using the **static** screening (electrons adjust instantaneously to atomic displacements)

$$\mathbf{\Pi}^{\mathrm{A}} \stackrel{\mathsf{def}}{=} \mathbf{\Pi}\,(\omega\!=\!0)$$

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After rearranging:

$$\Pi^{\mathrm{A}}_{\kappa\alpha,\kappa'\alpha'} = \frac{\partial^2 U_{\mathrm{nn}}}{\partial\tau_{\kappa\alpha}\,\partial\tau_{\kappa'\alpha'}} + \int d\mathbf{r}\,\frac{\partial^2 V^{\mathrm{en}}(\mathbf{r})}{\partial\tau_{\kappa\alpha}\,\partial\tau_{\kappa'\alpha'}}\langle\hat{n}_{\mathrm{e}}(\mathbf{r})\rangle + \int d\mathbf{r}\,\frac{\partial V^{\mathrm{en}}(\mathbf{r})}{\partial\tau_{\kappa\alpha}}\frac{\partial\langle\hat{n}_{\mathrm{e}}(\mathbf{r})\rangle}{\partial\tau_{\kappa'\alpha'}}$$

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replace with DFT electron density

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replace with DFT electron density

$$\Pi^{\mathrm{A}}_{\kappa\alpha,\kappa'\alpha'} = \frac{\partial^2 E^{\mathrm{DFT}}_{\mathrm{tot}}}{\partial\tau_{\kappa\alpha}\,\partial\tau_{\kappa'\alpha'}}$$

DFPT matrix of force constants

Phonons beyond DFPT: Dyson's equation

Relation between **adiabatic** and **non-adiabatic** Green's functions

$$\mathbf{D}^{-1}(\omega) \quad = \quad \mathbf{M}\,\omega^2 - \mathbf{\Pi}(\omega)$$

Relation between **adiabatic** and **non-adiabatic** Green's functions

$$\begin{aligned}\mathbf{D}^{-1}(\omega) &= \mathbf{M}\,\omega^2 - \mathbf{\Pi}(\omega)\\ \mathbf{D}^{\mathrm{A},-1}(\omega) &= \mathbf{M}\,\omega^2 - \mathbf{\Pi}^{\mathrm{A}}\end{aligned}$$

Phonons beyond DFPT: Dyson's equation

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$$\mathbf{D}^{-1}(\omega) = \mathbf{M}\,\omega^2 - \mathbf{\Pi}(\omega)$$

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$$-\mathbf{D}^{-1}(\omega) + \mathbf{D}^{\mathrm{A},-1}(\omega) = \mathbf{\Pi}(\omega) - \mathbf{\Pi}^{\mathrm{A}}$$

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$$-\,\mathbf{D}^{-1}(\omega) + \mathbf{D}^{\mathrm{A},-1}(\omega) = \underbrace{\mathbf{\Pi}(\omega) - \mathbf{\Pi}^{\mathrm{A}}}$$

non-adiabatic self-energy $\mathbf{\Pi}^{\mathrm{NA}}$

Relation between **adiabatic** and **non-adiabatic** Green's functions

$$\begin{aligned}
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\mathbf{D}^{\mathrm{A},-1}(\omega) &= \mathbf{M}\,\omega^2 - \mathbf{\Pi}^{\mathrm{A}} \\
\hline
-\,\mathbf{D}^{-1}(\omega) + \mathbf{D}^{\mathrm{A},-1}(\omega) &= \underbrace{\mathbf{\Pi}(\omega) - \mathbf{\Pi}^{\mathrm{A}}}_{\text{non-adiabatic self-energy } \mathbf{\Pi}^{\mathrm{NA}}}
\end{aligned}$$

Dyson's equation for the phonon Green's function

$$\mathbf{D} = \mathbf{D}^{\mathrm{A}} + \mathbf{D}^{\mathrm{A}}\,\mathbf{\Pi}^{\mathrm{NA}}\,\mathbf{D}$$

Phonons beyond DFPT: Dyson's equation

Adiabatic phonon Green's function from DFPT

(diagonal part in eigenmode representation)

$$D^{\mathrm{A}}_{\mathbf{q}\nu}(\omega) = \frac{1}{\omega - \omega_{\mathbf{q}\nu}} - \frac{1}{\omega + \omega_{\mathbf{q}\nu}} = \frac{2\omega_{\mathbf{q}\nu}}{\omega^2 - \omega^2_{\mathbf{q}\nu}}$$

Phonons beyond DFPT: Dyson's equation

Adiabatic phonon Green's function from DFPT

(diagonal part in eigenmode representation)

$$D^{\mathrm{A}}_{\mathbf{q}\nu}(\omega) = \frac{1}{\omega - \omega_{\mathbf{q}\nu}} - \frac{1}{\omega + \omega_{\mathbf{q}\nu}} = \frac{2\omega_{\mathbf{q}\nu}}{\omega^2 - \omega^2_{\mathbf{q}\nu}}$$

Combine D^{A} with Dyson's equation to find the complete Green's function

$$D_{\mathbf{q}\nu}(\omega) = \frac{2\omega_{\mathbf{q}\nu}}{\omega^2 - \omega^2_{\mathbf{q}\nu} - 2\omega_{\mathbf{q}\nu}\Pi^{\mathrm{NA}}_{\mathbf{q}\nu}(\omega)}$$

Phonons beyond DFPT: Quasiparticle approximation

$$\frac{2\,\omega_{\mathbf{q}\nu}}{\omega^2 - \omega_{\mathbf{q}\nu}^2 - 2\omega_{\mathbf{q}\nu}\Pi_{\mathbf{q}\nu}^{\mathrm{NA}}(\omega)} \longrightarrow \frac{2\,\tilde{\Omega}_{\mathbf{q}\nu}}{\omega^2 - \tilde{\Omega}_{\mathbf{q}\nu}^2} \quad \text{with} \quad \tilde{\Omega}_{\mathbf{q}\nu} = \Omega_{\mathbf{q}\nu} + i\gamma_{\mathbf{q}\nu}$$

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Frequency shift $\quad \Omega_{\mathbf{q}\nu} \simeq \omega_{\mathbf{q}\nu} + \mathrm{Re}\,\Pi_{\mathbf{q}\nu}^{\mathrm{NA}}(\omega_{\mathbf{q}\nu})$

Line broadening $\quad \gamma_{\mathbf{q}\nu} \simeq \mathrm{Im}\,\Pi_{\mathbf{q}\nu}^{\mathrm{NA}}(\omega_{\mathbf{q}\nu})$

valid for $|\Pi_{\mathbf{q}\nu}^{\mathrm{NA}}(\omega_{\mathbf{q}\nu})| \ll \omega_{\mathbf{q}\nu}$

$$\frac{2\,\omega_{\mathbf{q}\nu}}{\omega^2-\omega_{\mathbf{q}\nu}^2-2\omega_{\mathbf{q}\nu}\Pi^{\rm NA}_{\mathbf{q}\nu}(\omega)} \longrightarrow \frac{2\,\tilde\Omega_{\mathbf{q}\nu}}{\omega^2-\tilde\Omega_{\mathbf{q}\nu}^2} \quad \text{with} \quad \tilde\Omega_{\mathbf{q}\nu}=\Omega_{\mathbf{q}\nu}+i\gamma_{\mathbf{q}\nu}$$

Frequency shift $\quad \Omega_{\mathbf{q}\nu}\simeq\omega_{\mathbf{q}\nu}+{\rm Re}\,\Pi^{\rm NA}_{\mathbf{q}\nu}(\omega_{\mathbf{q}\nu})$

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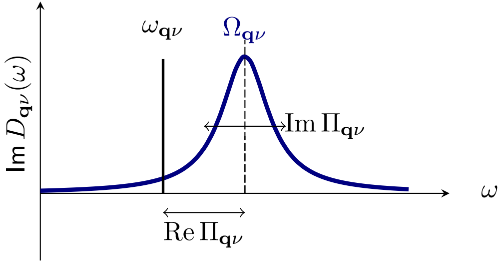
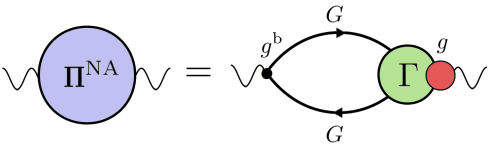
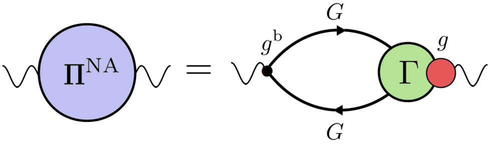




$$\Pi^{\rm NA}_{\mathbf{q}\nu} = \frac{2}{\hbar}\sum_{mn}\int\frac{d\mathbf{k}}{\Omega_{\rm BZ}}\, g^{\rm b}_{mn\nu}(\mathbf{k},\mathbf{q})\, g^{*}_{mn\nu}(\mathbf{k},\mathbf{q})\left[\frac{f_{m\mathbf{k}+\mathbf{q}}-f_{n\mathbf{k}}}{\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{n\mathbf{k}}-\hbar\omega_{\mathbf{q}\nu}-i\eta} - \frac{f_{m\mathbf{k}+\mathbf{q}}-f_{n\mathbf{k}}}{\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{n\mathbf{k}}}\right]$$

This is Eq. (145) of FG, RMP2017

Phonon self-energy in practice

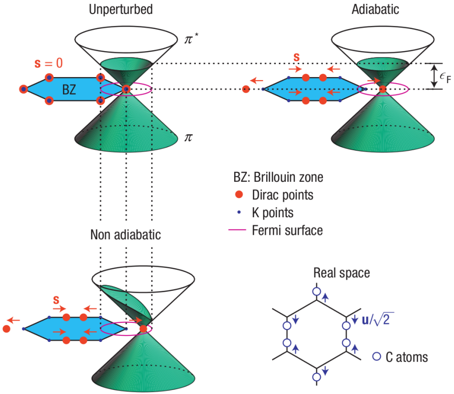


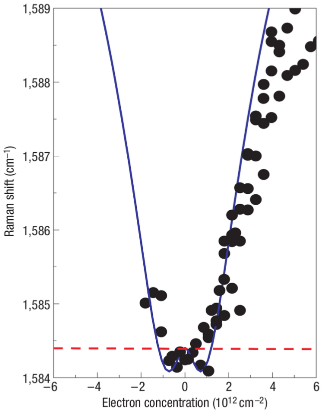
$$\Pi^{\rm NA}_{\mathbf{q}\nu} = \frac{2}{\hbar}\sum_{mn}\int\frac{d\mathbf{k}}{\Omega_{\rm BZ}}\, g^{\rm b}_{mn\nu}(\mathbf{k},\mathbf{q})\, g^{*}_{mn\nu}(\mathbf{k},\mathbf{q})\left[\frac{f_{m\mathbf{k}+\mathbf{q}}-f_{n\mathbf{k}}}{\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{n\mathbf{k}}-\hbar\omega_{\mathbf{q}\nu}-i\eta} - \frac{f_{m\mathbf{k}+\mathbf{q}}-f_{n\mathbf{k}}}{\varepsilon_{m\mathbf{k}+\mathbf{q}}-\varepsilon_{n\mathbf{k}}}\right]$$

- For $(f_{m\mathbf{k}+\mathbf{q}}-f_{n\mathbf{k}})$ to be nonvanishing, n and m should be occupied/empty
- Can be large only for metals, semimetals, degenerate semiconductors
- Very small effect in wide-gap insulators

This is Eq. (145) of FG, RMP2017

Non-adiabatic Kohn-anomaly in graphene

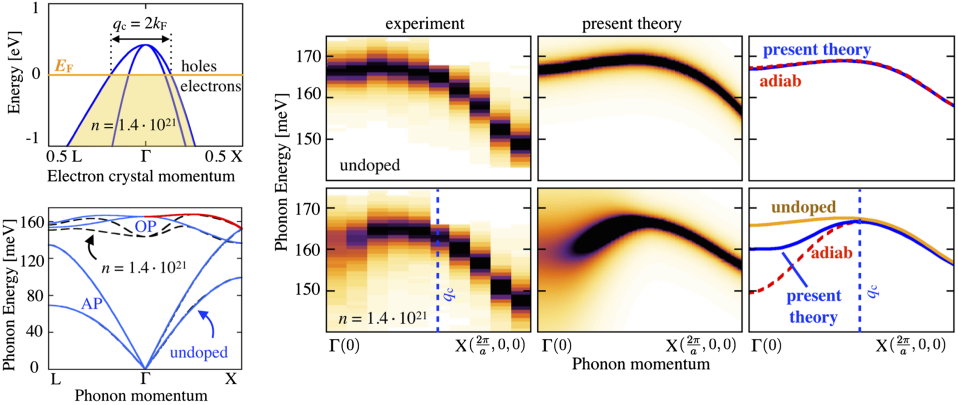




Figures from Pisana et al, Nat. Mater. 6, 198 (2007)

Examples of non-adiabatic phonons

Non-adiabatic phonons in B-doped diamond



Figures from Caruso et al, Phys. Rev. Lett. 119, 017001 (2017)

Phonon lifetimes from electron-phonon interactions

$$\tau_{\mathbf{q}\nu}^{-1} = \frac{2\pi}{\hbar} 2 \sum_{mn} \int \frac{d\mathbf{k}}{\Omega_{\mathrm{BZ}}} g^{\mathrm{b}}_{mn\nu}(\mathbf{k},\mathbf{q}) g^{*}_{mn\nu}(\mathbf{k},\mathbf{q}) (f_{m\mathbf{k}+\mathbf{q}} - f_{n\mathbf{k}})\, \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu})$$

Top equation is Eq. (146) of FG, RMP2017

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$$\downarrow$$

$$|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$$ overscreening approximation

Top equation is Eq. (146) of FG, RMP2017

$$\tau_{\mathbf{q}\nu}^{-1} = \frac{2\pi}{\hbar} 2 \sum_{mn} \int \frac{d\mathbf{k}}{\Omega_{\rm BZ}} \underline{g_{mn\nu}^{\rm b}(\mathbf{k},\mathbf{q}) g_{mn\nu}^{*}(\mathbf{k},\mathbf{q})} (f_{m\mathbf{k}+\mathbf{q}} - f_{n\mathbf{k}})\, \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu})$$

↓

$|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$ overscreening approximation

$$g^{\rm b}(\mathbf{q}) g^{*}(\mathbf{q}) \simeq \epsilon(\mathbf{q}) |g(\mathbf{q})|^2$$

Top equation is Eq. (146) of FG, RMP2017

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↓

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$$g^{\rm b}(\mathbf{q}) g^{*}(\mathbf{q}) \simeq \epsilon(\mathbf{q}) |g(\mathbf{q})|^2$$

The phonon self-energy in EPW is still overscreened and needs correction: use with caution

Top equation is Eq. (146) of FG, RMP2017

Overscreening of the phonon linewidths in MgB_2

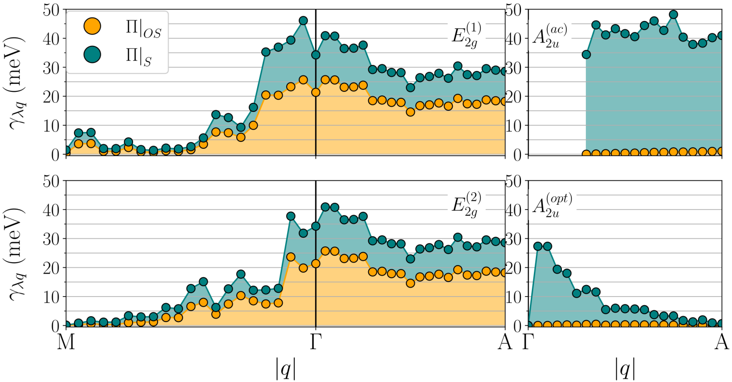

Figure from Marini, Phys. Rev. B 107, 024305 (2023)

see also discussion in Berges et al, arXiv:2212.11806 (2023)

Take-home messages

- Field theory provides a rigorous and systematic framework to study electron-phonon physics
- The Fan-Migdal self-energy yields the electron mass enhancement and lifetimes
- The non-adiabatic phonon self-energy yields frequency shift and phonon lifetimes

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