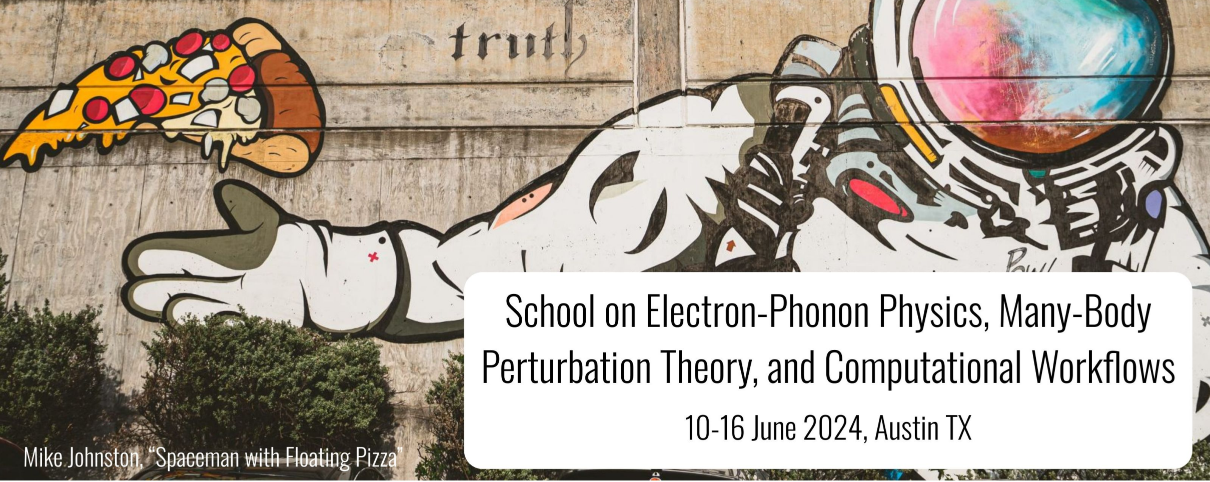


Mike Johnston, “Spaceman with Floating Pizza”

School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

10-16 June 2024, Austin TX

U.S. DEPARTMENT OF ENERGY

NSF

TACC
TEXAS ADVANCED COMPUTING CENTER

ODEN

Lecture Mon.1

Introduction to Electron-Phonon Physics and School Topics

Feliciano Giustino

Oden Institute & Department of Physics

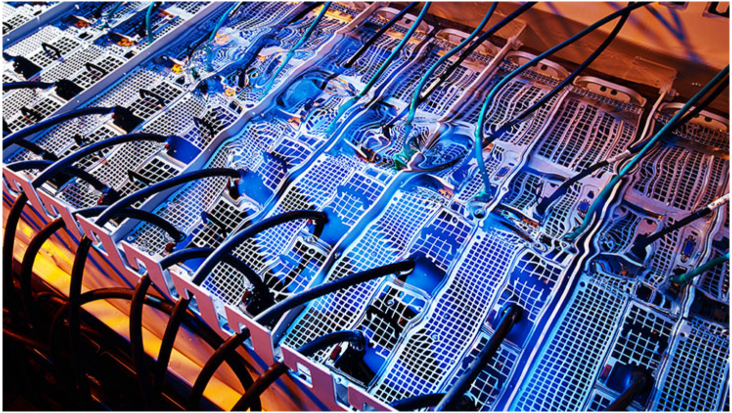
The University of Texas at Austin

Lecture summary

- Manifestations and impact of electron-phonon interactions
- Heuristic approach to the electron-phonon interaction
- Rayleigh-Schrödinger perturbation theory
- The electron-phonon matrix element
- Wannier interpolation
- Other topics in this school

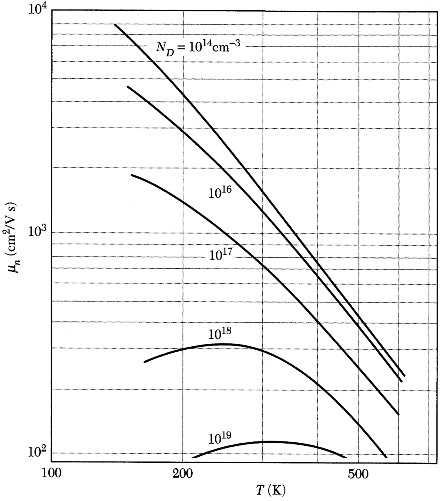
Manifestations of electron-phonon interactions

A **microscopic** phenomenon with **macroscopic** consequences



→ TACC visit Thu

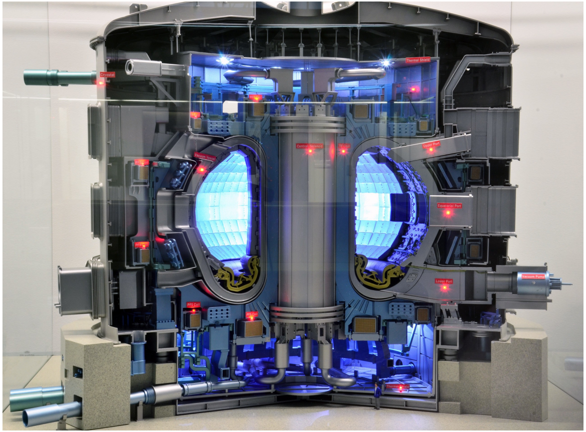
Frontera supercomputer with liquid-immersion cooling in GRC ICEraQ, TACC



→ Lec Wed.1 Poncé

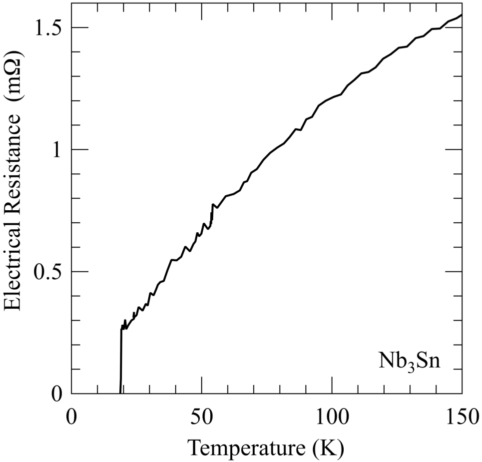
Electron mobility of silicon (Sze, "Semiconductor Devices")

A **microscopic** phenomenon with **macroscopic** consequences



1:50 scale model of the ITER experiment (www.iter.org)

Manifestations of electron-phonon interactions



→ Lec Wed.2 Margine

Resistance of Nb_3Sn and superconducting transition

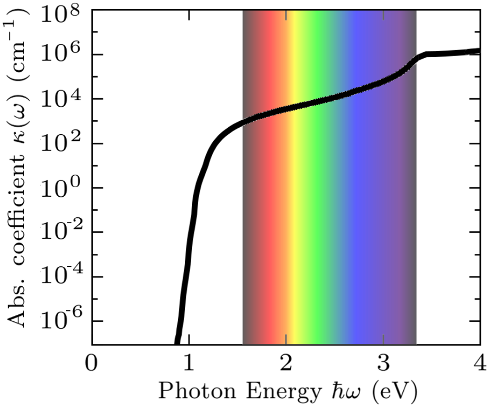
Akimitsu group, in "Superconductors: New Developments", 2015

Manifestations of electron-phonon interactions

A **microscopic** phenomenon with **macroscopic** consequences

Webberville Solar Farm, Austin TX (35 MW)

Optical absorption coefficient of silicon, 300 K



→ Lec Wed.3 Kioupakis

→ Lec Sat.3 Tiwari

Data from Green et al, Prog. Photovolt. Res. Appl. 3, 189 (1995)

Über die Quantenmechanik der Elektronen in Kristallgittern.

Von **Felix Bloch** in Leipzig.

Mit 2 Abbildungen. (Eingegangen am 10. August 1928.)

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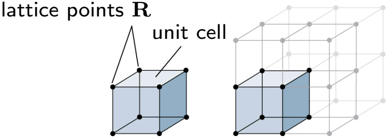

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Bloch theorem

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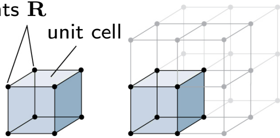

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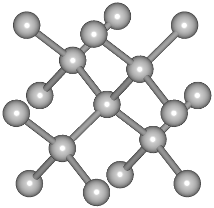
Bloch theorem

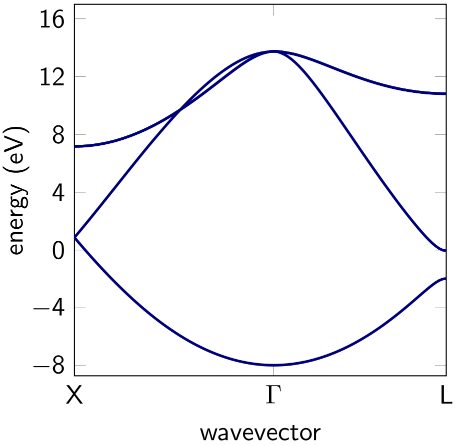
$$\rho = \frac{c_1}{T}\left(\frac{k_\mathrm{B}T}{\hbar C}\right)^6 \int_0^{\hbar C q_\mathrm{D}/k_\mathrm{B}T} \frac{x^5\,dx}{(e^x-1)\,(1-e^{-x})}$$

Bloch-Grüneisen formula for electrical resistivity

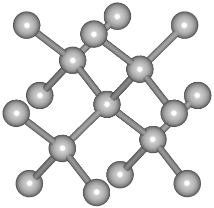
Where do electron-phonon interactions come from?



diamond



Heuristic notion of electron-phonon interactions



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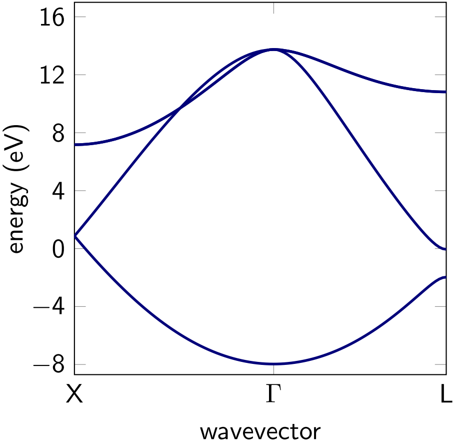
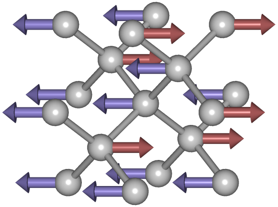
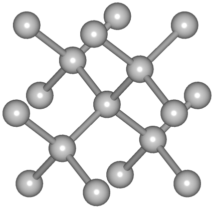




Γ-point optical mode

0.015 Å C-displacement

Heuristic notion of electron-phonon interactions



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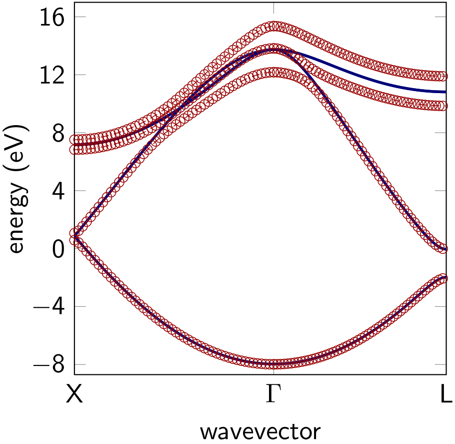

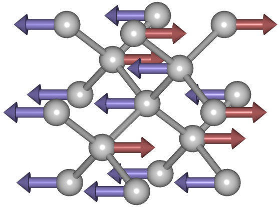

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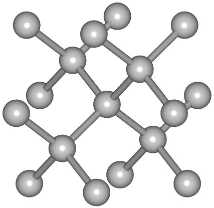

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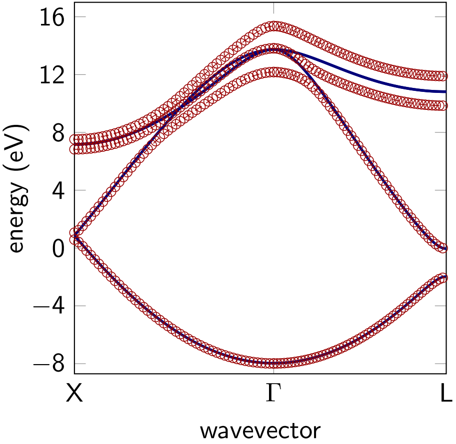

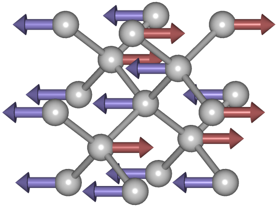

Γ-point optical mode

0.015 Å C-displacement

How far do atoms move? What is the oscillation frequency?

Can oscillations promote electronic transitions? What about finite-$\mathbf{q}$ modes?

Ionic degrees of freedom in the Kohn-Sham equations

→ Lec. Mon.2 Giannozzi

$$-\frac{\hbar^2}{2m_\mathrm{e}}\nabla^2\,\psi_n + V_\mathrm{SCF}\,\psi_n = \varepsilon_n\,\psi_n$$

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Atom κ at position τ_κ

Heuristic approach to electron-phonon interactions

The SCF potential depends parametrically on the atomic coordinates

$$V_{\mathrm{SCF}} = V_{\mathrm{SCF}}(\mathbf{r}; \boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3 \cdots)$$

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Perturbation Hamiltonian leading to EPIs

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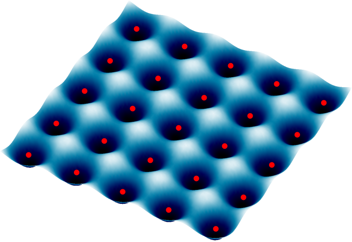
All atoms at equilibrium



$V_{\mathrm{SCF}}(\mathbf{r};\tau_0)$

Perturbation Hamiltonian leading to EPIs

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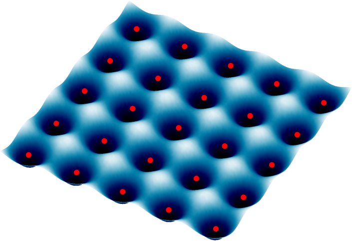
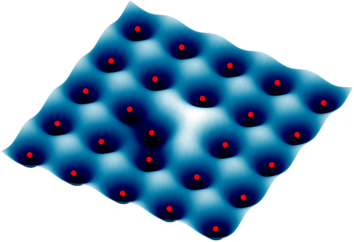


$V_{\mathrm{SCF}}(\mathbf{r}; \tau_0)$

One atom displaced



$V_{\mathrm{SCF}}(\mathbf{r}; \tau_0 + u)$

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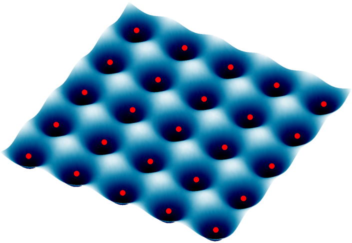
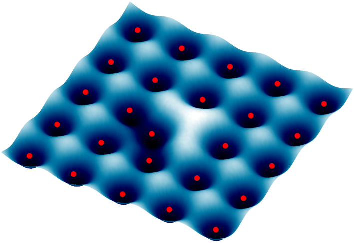


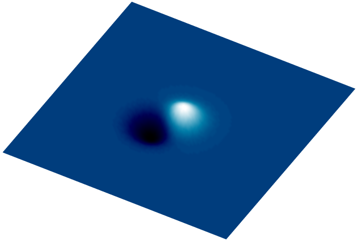
$V_{\mathrm{SCF}}(\mathbf{r};\tau_0)$

One atom displaced



$V_{\mathrm{SCF}}(\mathbf{r};\tau_0+u)$

Perturbation of the SCF potential



$V_{\mathrm{SCF}}(\mathbf{r};\tau_0+u) - V_{\mathrm{SCF}}(\mathbf{r};\tau_0)$

Rayleigh-Schrödinger perturbation theory

Rayleigh-Schrödinger perturbation theory

Energy $$\Delta E_n = \langle n | \frac{\partial V_{\rm SCF}}{\partial \tau} u | n \rangle$$

Rayleigh-Schrödinger perturbation theory

Energy

$$\Delta E_n = \langle n | \frac{\partial V_{\mathrm{SCF}}}{\partial \tau} u | n \rangle$$

Wavefunction

$$\Delta \psi_n = \sum_{m \neq n} \frac{\langle m | \frac{\partial V_{\mathrm{SCF}}}{\partial \tau} u | n \rangle}{E_n - E_m} \psi_m$$

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Wavefunction $$\Delta \psi_n = \sum_{m \neq n} \frac{\langle m | \frac{\partial V_{\rm SCF}}{\partial \tau} u | n \rangle}{E_n - E_m} \psi_m$$

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Energy
$$\Delta E_n = \langle n| \frac{\partial V_{\mathrm{SCF}}}{\partial \tau} u |n\rangle$$
Temperature-dependent band structures

Wavefunction
$$\Delta \psi_n = \sum_{m \neq n} \frac{\langle m| \frac{\partial V_{\mathrm{SCF}}}{\partial \tau} u |n\rangle}{E_n - E_m} \psi_m$$
Phonon-assisted optical processes and polarons

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Ultrafast relaxation and phonon-limited transport

Displacement amplitudes

What is the atomic displacement u in the perturbation Hamiltonian?

Displacement amplitudes

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equilibrium

e.g.: fixed temperature

out of equilibrium

e.g.: driven systems

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Mean square displacements at given temperature

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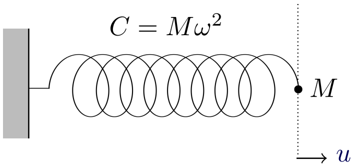
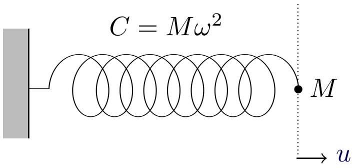
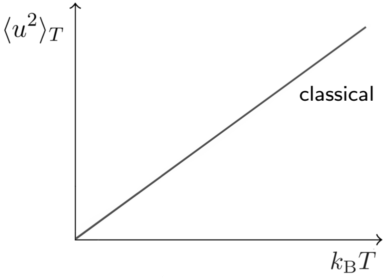


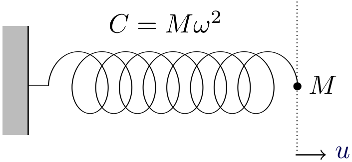
Mean square displacements at given temperature

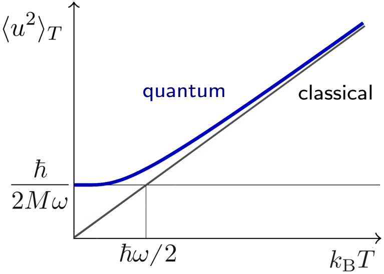




$$\langle u^2 \rangle_T = \frac{k_{\rm B}T}{M\omega^2}$$

Mean square displacements at given temperature





$$\langle u^2 \rangle_T = \frac{k_{\mathrm{B}}T}{M\omega^2}$$

$$\langle u^2 \rangle_T = \frac{\hbar}{2M\omega}\left[2\, n\left(\frac{\hbar\omega}{k_{\mathrm{B}}T}\right) + 1\right]$$

Bose-Einstein

Allen-Heine theory

$$\Delta E_n = \langle n| \frac{\partial V_{\mathrm{SCF}}}{\partial \tau} |n\rangle \, u$$

Allen-Heine theory

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Allen-Heine theory

$$\Delta E_n = \cancel{\langle n|\frac{\partial V_{\mathrm{SCF}}}{\partial \tau}|n\rangle}\, u + \sum_{m\neq n} \frac{\left|\langle m|\frac{\partial V_{\mathrm{SCF}}}{\partial \tau}|n\rangle\right|^2}{E_n - E_m}\, u^2$$

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$$\Delta E_n = \cancel{\langle n|\frac{\partial V_{\mathrm{SCF}}}{\partial \tau}|n\rangle}\, u + \sum_{m\neq n} \frac{\left|\langle m|\frac{\partial V_{\mathrm{SCF}}}{\partial \tau}|n\rangle\right|^2}{E_n - E_m}\, u^2 + \frac{1}{2}\langle n|\frac{\partial^2 V_{\mathrm{SCF}}}{\partial \tau^2}|n\rangle\, u^2$$

Temperature-dependent band structures

Allen-Heine theory

$$\Delta E_n = \cancel{\langle n| \frac{\partial V_{\text{SCF}}}{\partial \tau} |n\rangle} \, u + \sum_{m \neq n} \frac{\left| \langle m| \frac{\partial V_{\text{SCF}}}{\partial \tau} |n\rangle \right|^2}{E_n - E_m} \, u^2 + \frac{1}{2} \langle n| \frac{\partial^2 V_{\text{SCF}}}{\partial \tau^2} |n\rangle \, u^2$$

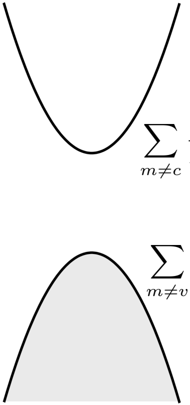
$$\Delta E_n = \left[\sum_{m \neq n} \frac{\left| \langle m| \frac{\partial V_{\text{SCF}}}{\partial \tau} |n\rangle \right|^2}{E_n - E_m} + \frac{1}{2} \langle n| \frac{\partial^2 V_{\text{SCF}}}{\partial \tau^2} |n\rangle \right] u^2$$

Allen-Heine theory

$$\Delta E_n = \cancel{\langle n | \frac{\partial V_{\rm SCF}}{\partial \tau} | n \rangle} \, u + \sum_{m \neq n} \frac{\left| \langle m | \frac{\partial V_{\rm SCF}}{\partial \tau} | n \rangle \right|^2}{E_n - E_m} \, u^2 + \frac{1}{2} \langle n | \frac{\partial^2 V_{\rm SCF}}{\partial \tau^2} | n \rangle \, u^2$$

$$\langle \Delta E_n \rangle_T = \left[\sum_{m \neq n} \frac{\left| \langle m | \frac{\partial V_{\rm SCF}}{\partial \tau} | n \rangle \right|^2}{E_n - E_m} + \frac{1}{2} \langle n | \frac{\partial^2 V_{\rm SCF}}{\partial \tau^2} | n \rangle \right] \frac{\hbar}{2 M \omega} \left(2 \, n_T + 1 \right)$$

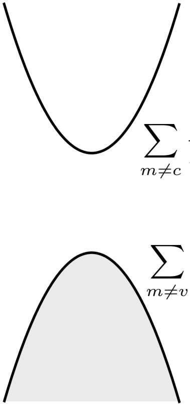
Temperature-dependent band structures: Basic trends



$$\sum_{m \neq c} \frac{|\cdots|^2}{E_c - E_m} < 0$$

$$\sum_{m \neq v} \frac{|\cdots|^2}{E_v - E_m} > 0$$

Temperature-dependent band structures: Basic trends



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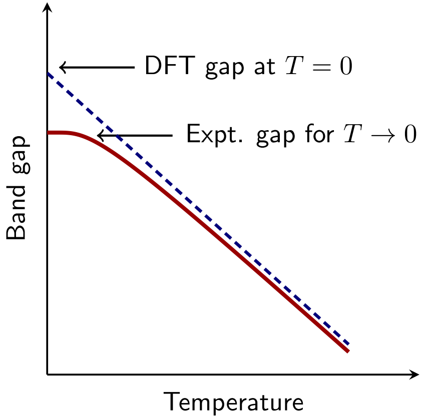
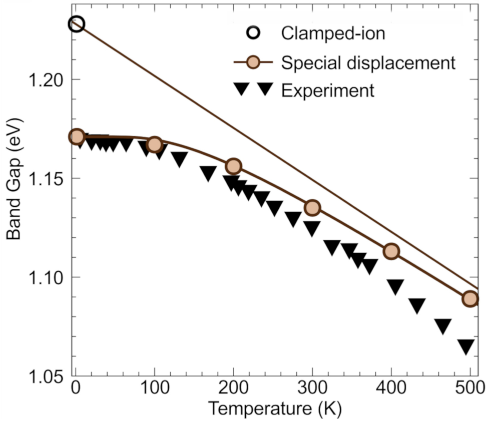
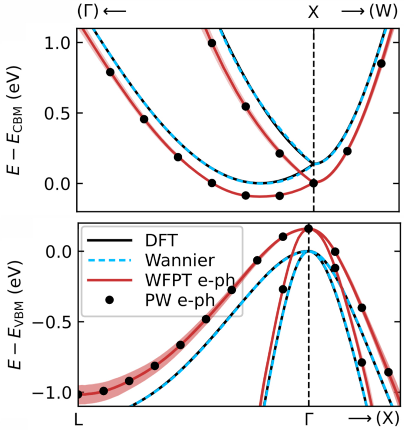


Example: Temperature-dependent bands of silicon

→ Lec Fri.1 Zacharias



→ Lec Sat.2 Lihm



Left figure: Zacharias et al, PRR 2, 013357 (2020); Right figure: Lihm et al, PRX 11, 041053 (2021)

Phonon-assisted optical absorption

$$\Delta\psi_n(\mathbf{r}) = \sum_{m\neq n} \frac{\langle m|\, \dfrac{\partial V_{\rm SCF}}{\partial \tau}\, u\,|n\rangle}{E_n - E_m}\psi_m(\mathbf{r})$$

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$$\epsilon_2(\omega) = \frac{\mathrm{const}}{\omega^2}\sum_{cv} |\langle c|\,\hat{p}\,|v\rangle|^2\,\delta(E_c - E_v - \hbar\omega)$$

$$\Delta\psi_n(\mathbf{r}) = \sum_{m\neq n} \frac{\langle m|\, \frac{\partial V_{\rm SCF}}{\partial \tau}\, u\, |n\rangle}{E_n - E_m} \psi_m(\mathbf{r})$$

$\langle c + \Delta c\,|$ $\qquad$ $|\, v + \Delta v\rangle$

$$\epsilon_2(\omega) = \frac{\rm const}{\omega^2} \sum_{cv} |\langle c|\, \hat{p}\, |v\rangle|^2\, \delta(E_c - E_v - \hbar\omega)$$

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$$\left|\,\sum_{m\neq c} \frac{\langle c|\, \dfrac{\partial V_{\mathrm{SCF}}}{\partial\tau}\,|m\rangle\langle m|\,\hat{p}\,|v\rangle}{E_c - E_m} + \cdots\right|^2 u^2$$

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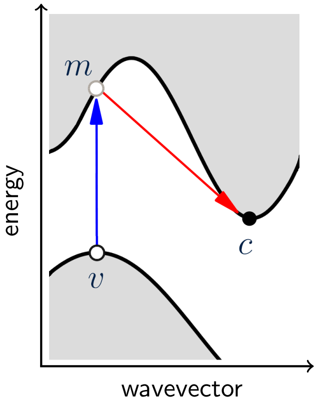

Example: Absorption spectrum of silicon

→ Lec Wed.3 Kioupakis & Lec Sat.3 Tiwari

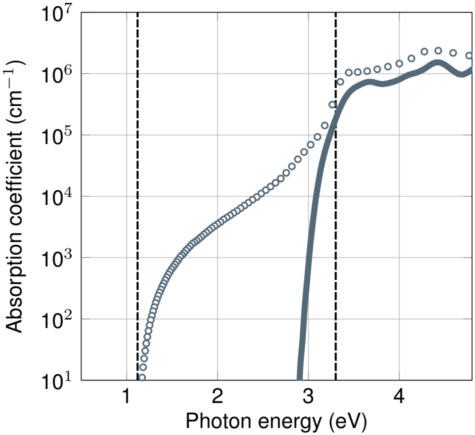

Figure from Tiwari et al, PRB 109, 195127 (2024)

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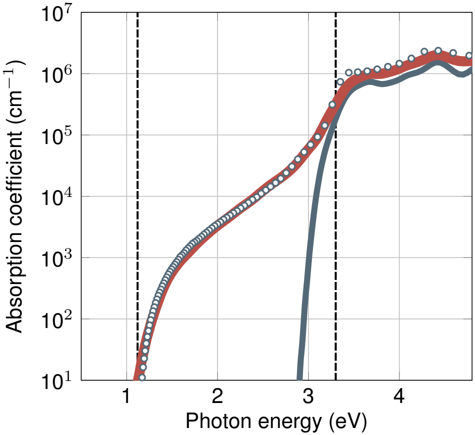

Figure from Tiwari et al, PRB 109, 195127 (2024)

Example: Luminescence spectrum of germanium

→ Lec Sat.3 Tiwari

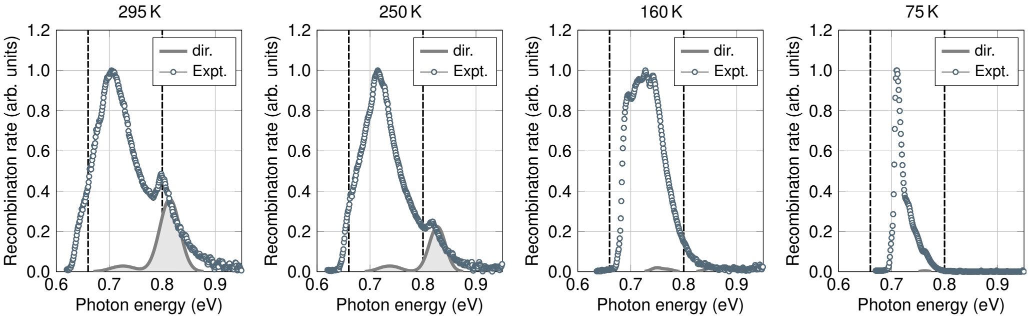

Figure from Tiwari et al, PRB 109, 195127 (2024)

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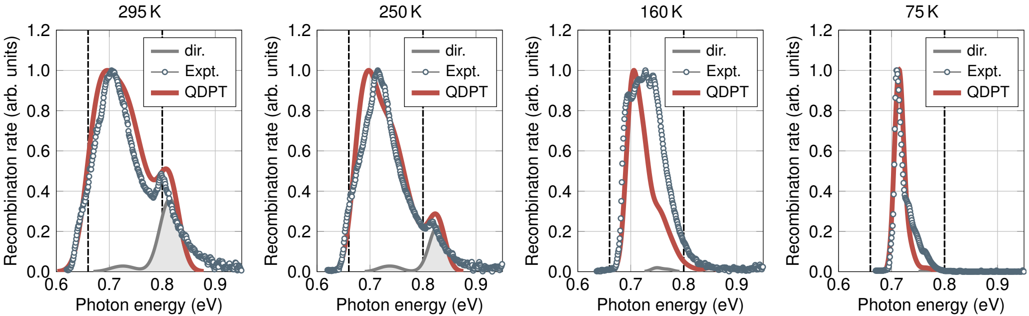

Figure from Tiwari et al, PRB 109, 195127 (2024)

Phonon-limited carrier mobilities

→ Lec. Wed.1 Poncé

Carrier relaxation time

$$\frac{1}{\tau_n} = \sum\nolimits_m \Gamma_{n\to m}$$

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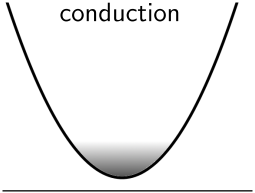

Weighted average of relaxation times near Fermi level

$$\langle \tau \rangle = \frac{1}{N_c} \sum_{n \in c} \left[\frac{m |\mathbf{v}_n|^2 / 2}{3 k_\mathrm{B} T / 2} \exp\left(-\frac{\varepsilon_n - \varepsilon_\mathrm{F}}{k_\mathrm{B} T} \right) \right] \tau_n$$

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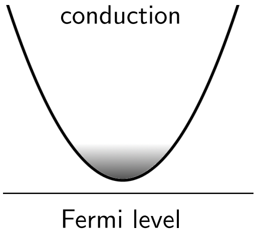

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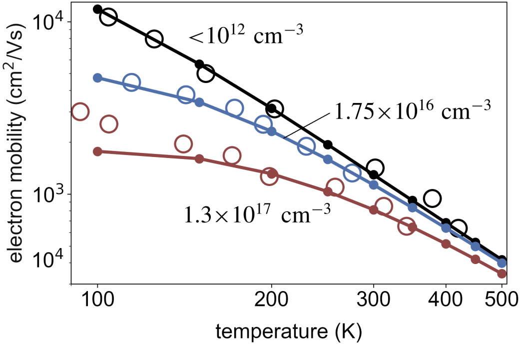
Electron mobility (simplified)

$$\mu = \frac{e\langle\tau\rangle}{m}$$

Example: Mobility of silicon

→ Tut. Wed.1 Poncé
→ Tut. Wed.2 Ha



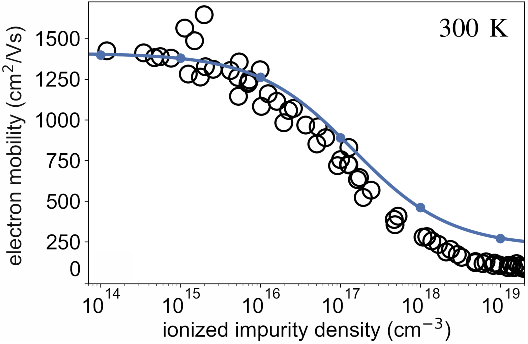


Figure from Leveillee et al, PRB 107, 125207 (2023)

How difficult is to perform these calculations?

The electron-phonon matrix element

→ Lec. Mon.2 Giannozzi

$$\langle \psi_m | \frac{\partial V_{\mathrm{SCF}}}{\partial \tau} | \psi_n \rangle$$

The electron-phonon matrix element

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$$\langle \psi_m | \frac{\partial V_{\rm SCF}}{\partial \tau} | \psi_n \rangle \quad \longrightarrow \quad g_{mn\nu}(\mathbf{k},\mathbf{q}) = \langle u_{m\mathbf{k}+\mathbf{q}} | \Delta_{\mathbf{q}\nu} v_{\rm SCF} | u_{n\mathbf{k}} \rangle_{\rm uc}$$

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Lattice-periodic part of the wavefunction

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Lattice-periodic part of the wavefunction

Lattice-periodic variation of the self-consistent potential

Zero-point amplitude

Potential change from ionic displacement

$$\Delta_{\mathbf{q}\nu} v_{\rm SCF} = \sum_{\kappa\alpha p} e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_p)} \sqrt{\frac{\hbar}{2M_\kappa \omega_{\mathbf{q}\nu}}}\, e_{\kappa\alpha,\nu}(\mathbf{q}) \frac{\partial V_{\rm SCF}(\mathbf{r})}{\partial \tau_{\kappa\alpha p}}$$

Incommensurate modulation

Phonon polarization

Example: Electron lifetimes & relaxation rates

$$\frac{1}{\tau_{n\mathbf{k}}} = \sum_{m\nu} \int_{\mathrm{BZ}} d\mathbf{q}\, [\cdots]\, |g_{nm\nu}(\mathbf{k},\mathbf{q})|^2 \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} \pm \hbar\omega_{\mathbf{q}\nu})$$

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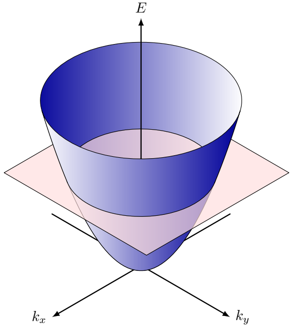

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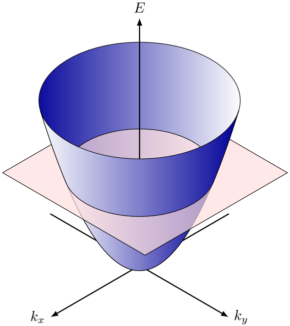
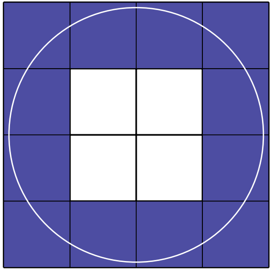


4 x 4 grid



Coarse BZ sampling

The challenge of Brillouin Zone sampling

Example: Electron lifetimes & relaxation rates

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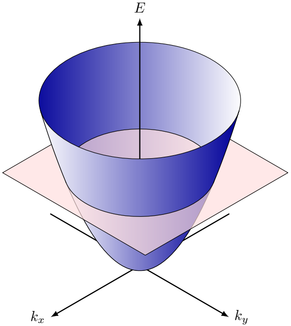

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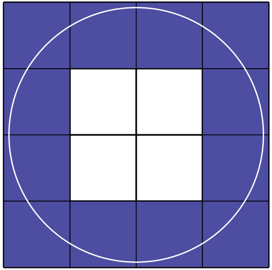
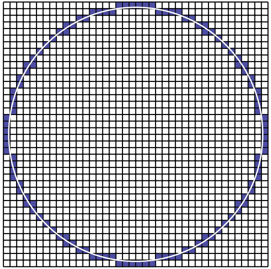


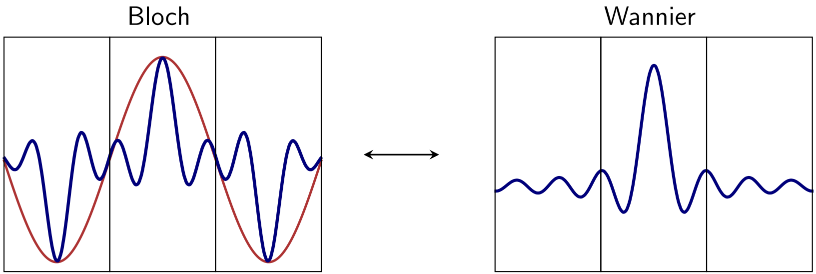
Coarse BZ sampling

40 x 40 grid



Fine BZ sampling

→ Lec. Mon.3 Marzari → Lec. Tue.1 Marrazzo → Lec. Sat.1 Qiao

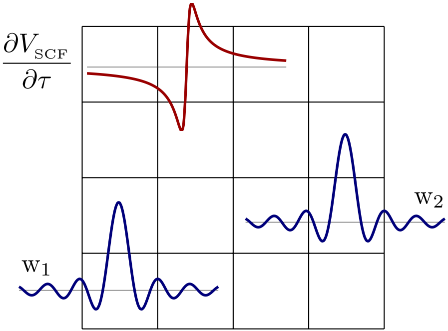


$$\mathrm{w}_{m\mathbf{R}}(\mathbf{r}) = \frac{1}{N_p} \sum_{n\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}}\, U_{nm\mathbf{k}}\, \psi_{n\mathbf{k}}(\mathbf{r})$$

Review article: Marzari et al, Rev. Mod. Phys. 84, 1419 (2012)

Wannier interpolation of electron-phonon matrix elements

$$\langle w_1 | \frac{\partial V_{\mathrm{SCF}}}{\partial \tau} | w_2 \rangle$$



Scheme from FG, Cohen, Louie, PRB 76, 165108 (2007)

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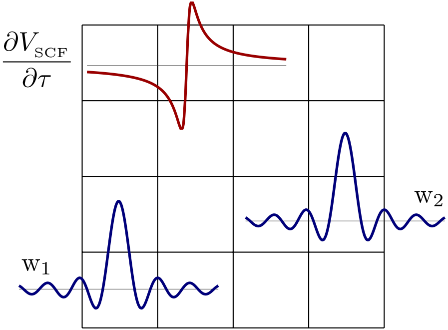

$$\mathbf{g}_\nu(\mathbf{k},\mathbf{q}) = \sqrt{\frac{\hbar}{2M_\kappa \omega_{\mathbf{q}\nu}}} \sum_{\mathbf{R}\mathbf{R}'} e^{i(\mathbf{k}\cdot\mathbf{R}+\mathbf{q}\cdot\mathbf{R}')} U_{\mathbf{k}+\mathbf{q}}\, \mathbf{g}(\mathbf{R},\mathbf{R}') \cdot \mathbf{e}_{\mathbf{q}\nu}\, U^\dagger_{\mathbf{k}}$$

Scheme from FG, Cohen, Louie, PRB 76, 165108 (2007)

Example: Electron-phonon matrix elements of diamond

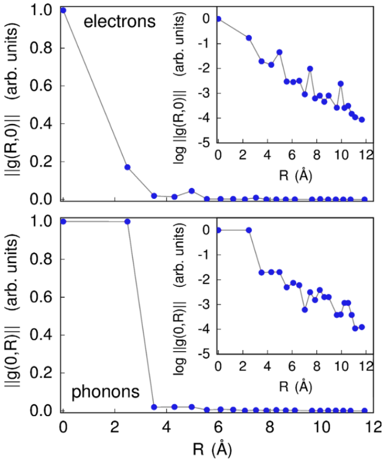

Figure from FG et al, Phys. Rev. B 76, 165108 (2007)

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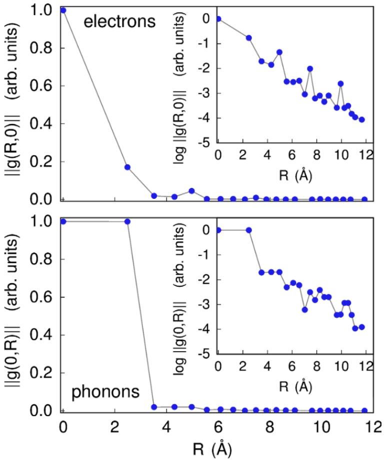

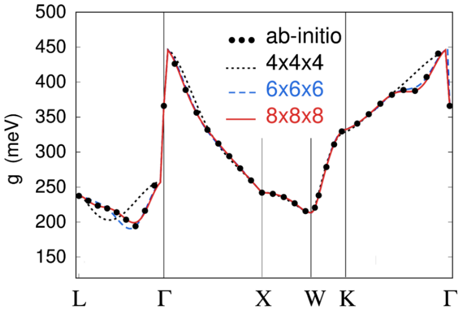

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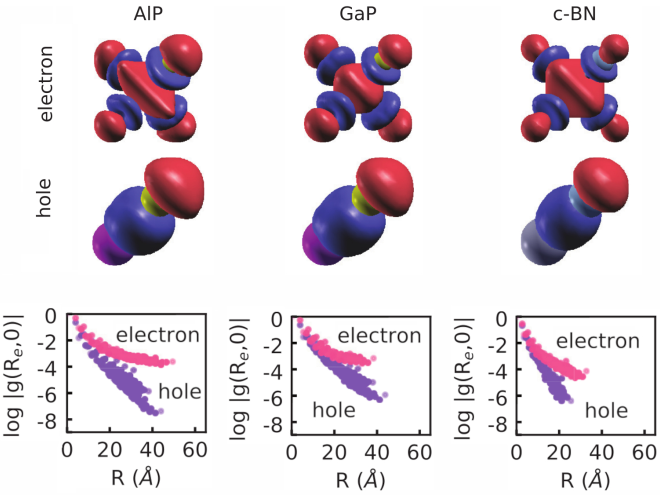

Figure from Poncé et al, Phys. Rev. Res. 3, 043022 (2021)

Example: Electron lifetimes & relaxation rates

$$\frac{1}{\tau_{n\mathbf{k}}} = \sum_{m\nu} \int_{\mathrm{BZ}} d\mathbf{q}\, [\cdots]\, |g_{nm\nu}(\mathbf{k},\mathbf{q})|^2 \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} \pm \hbar\omega_{\mathbf{q}\nu})$$

Other school topics not covered in this intro

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↑

DFT band structures often
not good enough

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DFT band structures often not good enough

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many-body GW calculations

→ Lec. Thu.1 Louie

Other school topics not covered in this intro

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GW perturbation theory

→ Lec. Thu.3 Li

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KS eigenvalues depend on temperature

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DFT matrix elements sometimes not good enough → GW perturbation theory → Lec. Thu.3 Li

DFT band structures often not good enough → many-body GW calculations → Lec. Thu.1 Louie

KS eigenvalues depend on temperature → Special displacement method → Lec. Fri.1 Zacharias

Wannier function perturbation theory → Lec. Sat.2 Lihm

Other school topics not covered in this intro

Example: Electron lifetimes & relaxation rates

$$\frac{1}{\tau_{n\mathbf{k}}} = \sum_{m\nu} \int_{\rm BZ} d\mathbf{q} \, [\cdots] \, |g_{nm\nu}(\mathbf{k},\mathbf{q})|^2 \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} \pm \hbar\omega_{\mathbf{q}\nu})$$

DFT matrix elements sometimes not good enough → GW perturbation theory → Lec. Thu.3 Li

DFT band structures often not good enough → many-body GW calculations → Lec. Thu.1 Louie

KS eigenvalues depend on temperature → Special displacement method → Lec. Fri.1 Zacharias

Wannier function perturbation theory → Lec. Sat.2 Lihm

Why should we use this formula?

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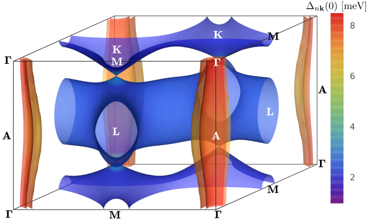
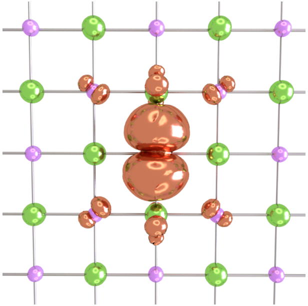
Why should we use this formula? → Many-body theory of EP couplings → Lec. Tue.2 Giustino

Superconductivity



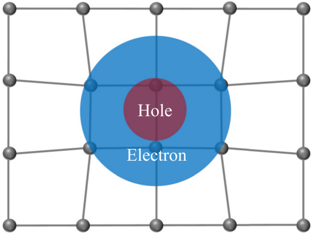
→ Lec. Wed.2 Margine

Polarons



→ Lec. Thu.2 Giustino

Excitons



→ Lec. Thu.1 Louie
→ Lec. Thu.4 Dai

Take-home messages

- We can understand the basics of electron-phonon physics using elementary perturbation theory
- Calculations for electron-phonon physics usually require a fine sampling of matrix elements across the Brillouin zone
- Wannier functions are very useful to address the Brillouin zone sampling challenge

Further reading

- Baroni et al, Rev. Mod. Phys. 73, 515 (2001) [link]
- Marzari et al, Rev. Mod. Phys. 84, 1419 (2012) [link]
- Giustino, Rev. Mod. Phys. 89, 015003 (2017) [link]
- Grimvall, The electron-phonon interaction in metals, 1981 (North-Holland)