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U.S. DEPARTMENT OF ENERGY

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TEXAS ADVANCED COMPUTING CENTER

ODEN

Lecture Mon.1

Introduction to Electron-Phonon Interactions

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The University of Texas at Austin

Lecture Summary

- Manifestations of electron-phonon interactions
- Heuristic approach to the electron-phonon interaction
- Rayleigh-Schrödinger perturbation theory
- The electron-phonon matrix element
- Wannier interpolation

Manifestations of electron-phonon interactions

Electron mobility in monolayer MoS_2

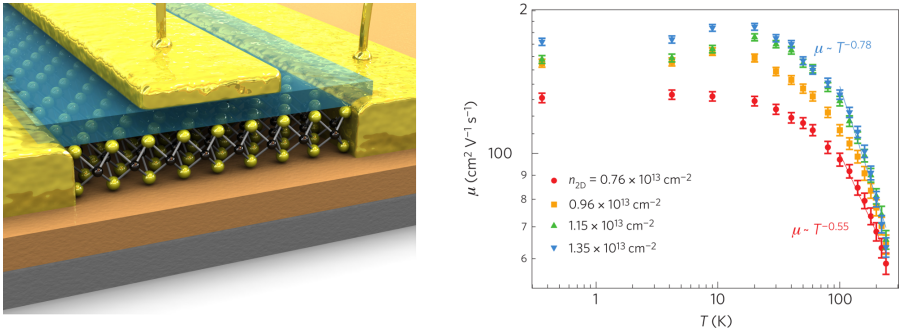
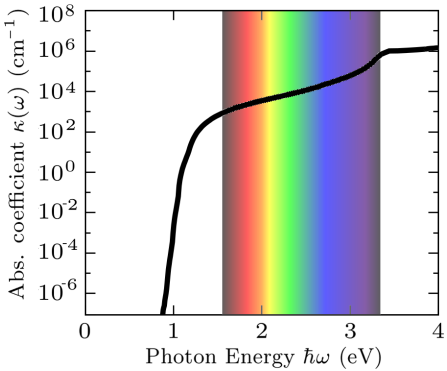


Figure from Radisavljevic and Kis, Nature Mater. 12, 815 (2013)

Manifestations of electron-phonon interactions

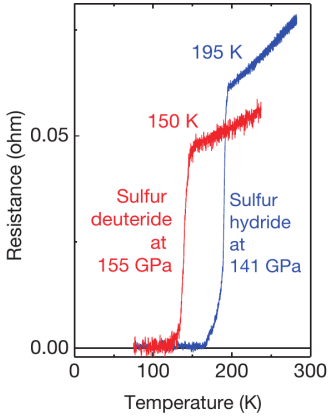
Phonon-assisted optical absorption in silicon



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

Manifestations of electron-phonon interactions

High-temperature superconductivity in compressed H_3S



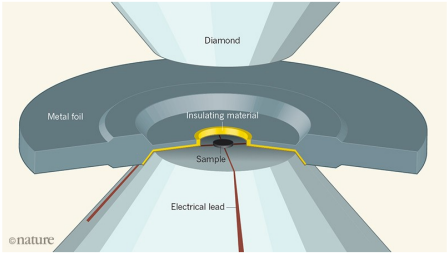


Figure from Drozdov et al, Nature 73, 525 (2015)

Manifestations of electron-phonon interactions

Temperature-dependent photoluminescence in hybrid perovskites

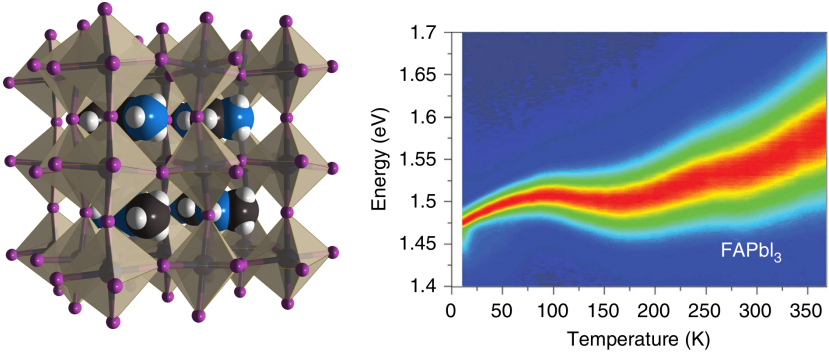


Figure from Wright et al, Nat. Commun. 7, 11755 (2016)

Where do electron-phonon interactions come from?

Ionic degrees of freedom in the Kohn-Sham equations

cf. 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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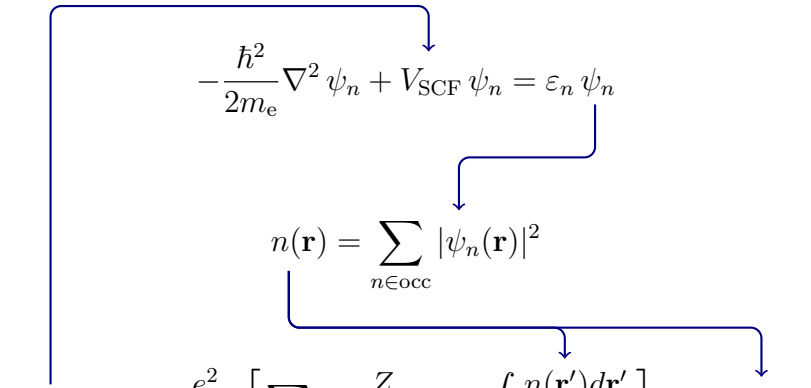

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Atom κ at position τ_κ

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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- Displace atom from equilibrium site, $\tau = \tau_0 + u$

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Perturbation Hamiltonian leading to EPIs

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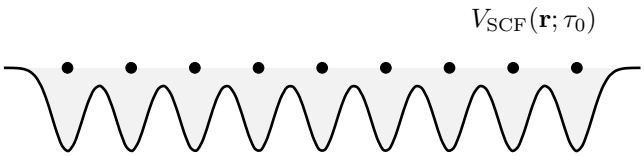

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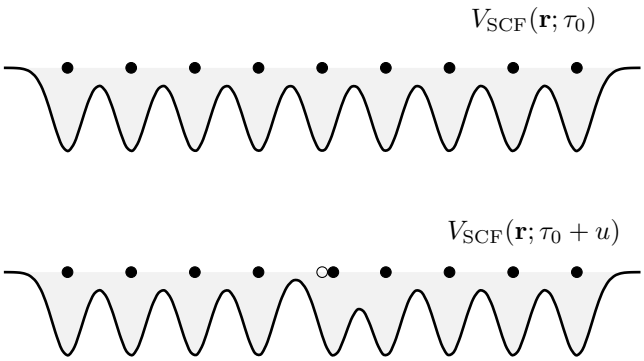

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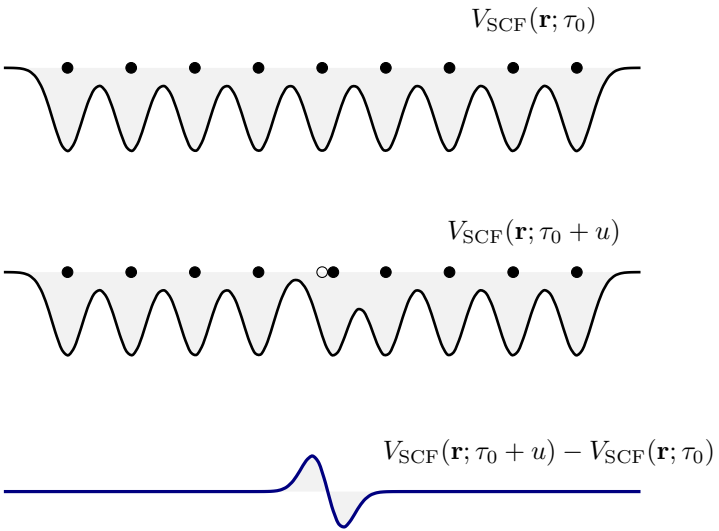

Rayleigh-Schrödinger perturbation theory

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Transition rate $$\Gamma_{n \to m} = \frac{2\pi}{\hbar} |\langle m| \frac{\partial V_{\rm SCF}}{\partial \tau} u \, |n\rangle|^2 \, \delta(E_m - E_n - \hbar\omega)$$

Rayleigh-Schrödinger perturbation theory

Energy

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

Temperature-dependent band structure

Wavefunction

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Phonon-assisted optical processes and polarons

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Phonon-limited transport phenomena

Displacement amplitudes

What is the atomic displacement u in the perturbation Hamiltonian?

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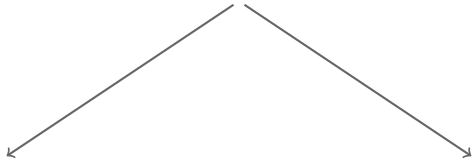

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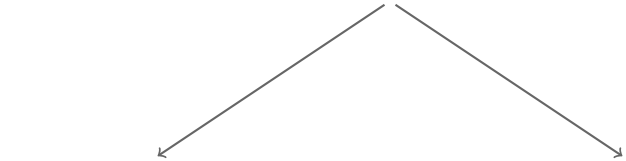

Mean square displacements at given temperature

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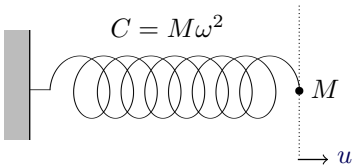

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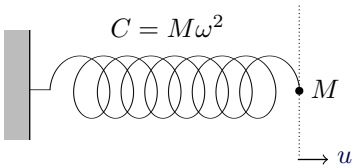

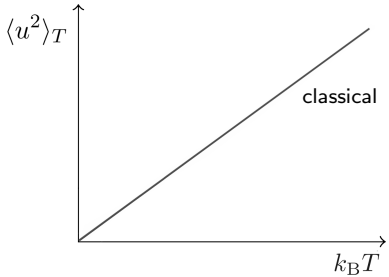

$$\langle u^2 \rangle_T = \frac{k_\mathrm{B}T}{M\omega^2}$$

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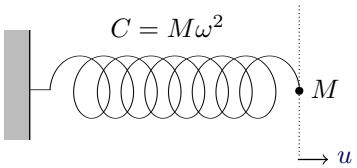

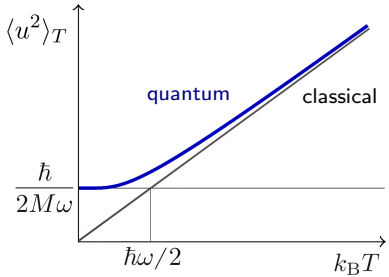

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$$\langle u^2 \rangle_T = \frac{\hbar}{2M\omega}\left[2\,n\left(\frac{\hbar\omega}{k_\mathrm{B}T}\right)+1\right]$$

Bose-Einstein

Temperature-dependent band structures

Allen-Heine theory

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Temperature-dependent band structures

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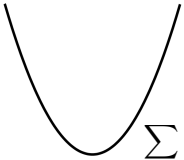
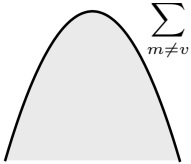
Temperature-dependent band structures: Basic trends



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



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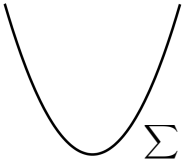

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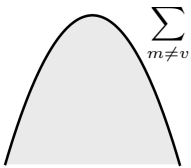

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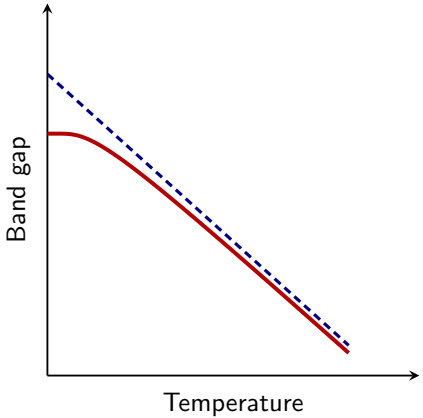

Example: Temperature-dependent bands of silicon

cf. Lec. Fri.1 Zacharias

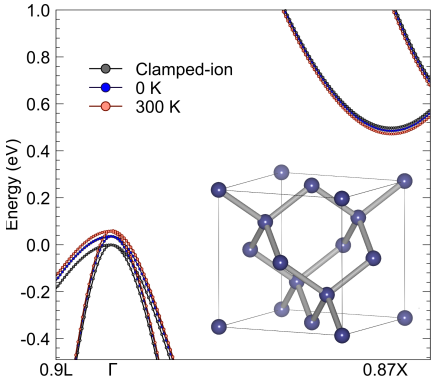

Figure from Zacharias et al, Phys. Rev. Research 2, 013357 (2020)

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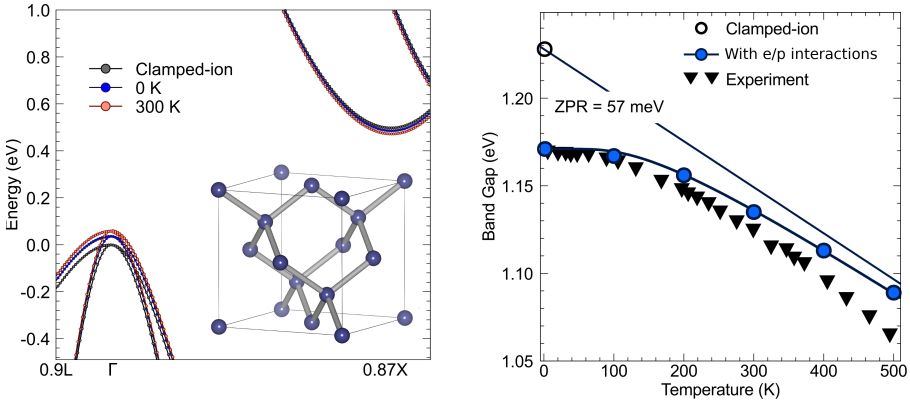

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Phonon-assisted optical absorption

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

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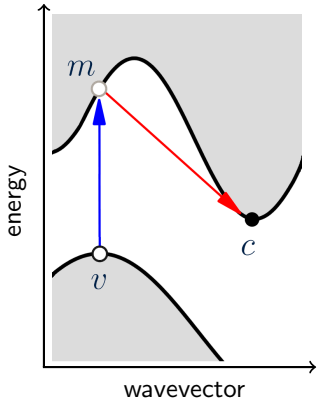

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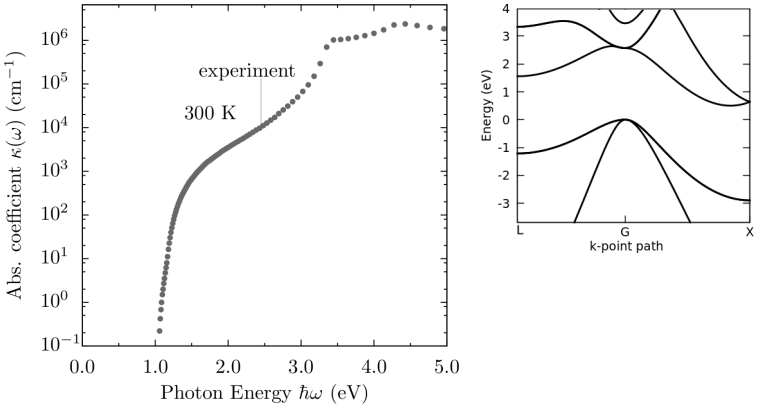

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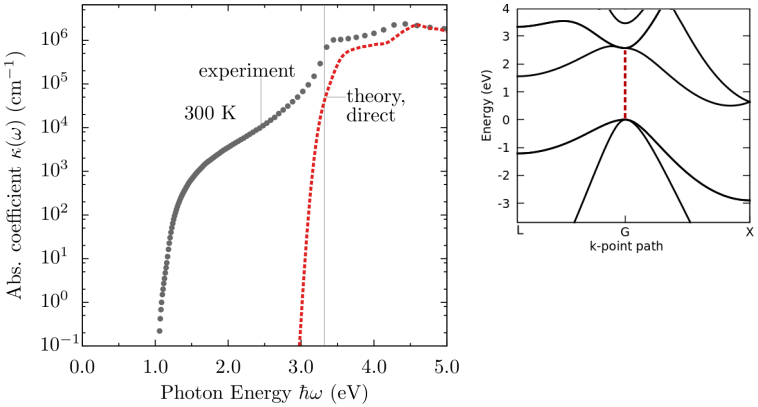

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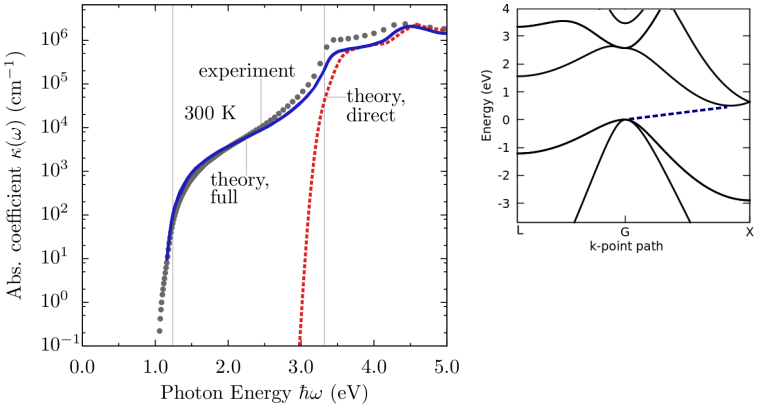

Figure from Zacharias et al, Phys. Rev. Lett. 115, 177401 (2015)
see also: Noffinger et al, Phys. Rev. Lett. 108, 167402 (2012)

Phonon-limited carrier mobilities

cf. Lec. Wed.1 Poncé

Carrier relaxation time

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

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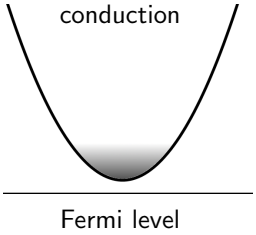
Electron mobility from Boltzmann equation (SERTA, simplified)



$$\mu_{\mathrm{e}} = \frac{e}{m}\frac{1}{N_c}\sum_{n\in c}\frac{m|\mathbf{v}_n|^2}{3}\left(-\frac{\partial f}{\partial \varepsilon_n}\right)\tau_n$$

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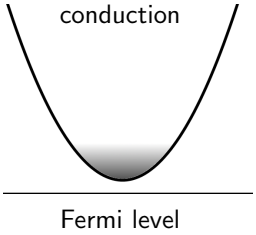

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$$\mu = \frac{e\langle\tau\rangle}{m}$$ Drude formula

Example: Mobility of lead-halide perovskite $MAPbI_3$

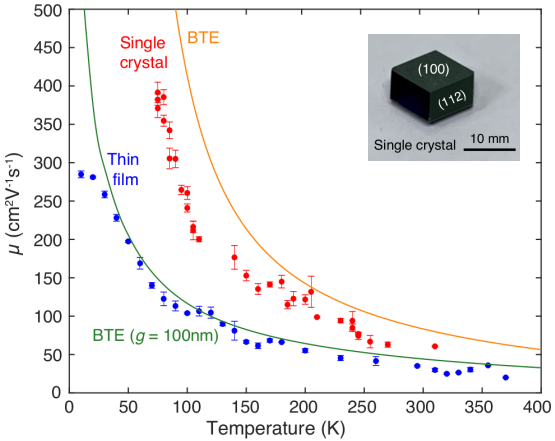

Figure from Xia et al, J. Phys. Chem. Lett. 12, 3607 (2021)

The electron-phonon matrix element

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

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

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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

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

Incommensurate modulation

Phonon polarization

The challenge of Brillouin Zone sampling

Example: Electron lifetimes

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

The challenge of Brillouin Zone sampling

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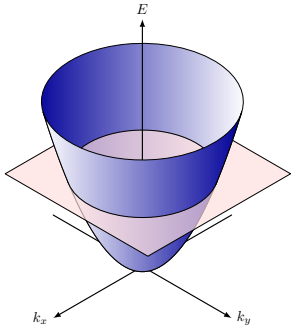

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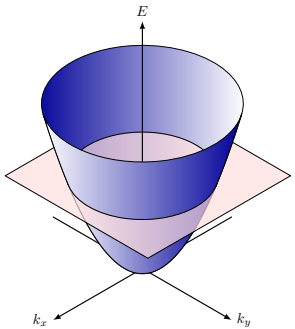
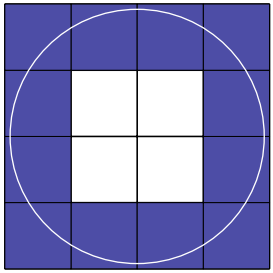


4 x 4 grid

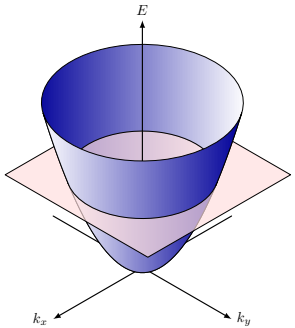


Coarse BZ sampling

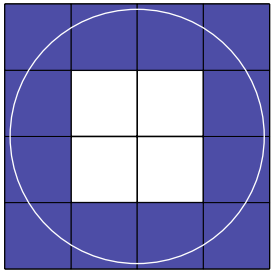
The challenge of Brillouin Zone sampling

Example: Electron lifetimes

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

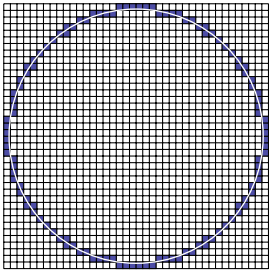


4 x 4 grid



Coarse BZ sampling

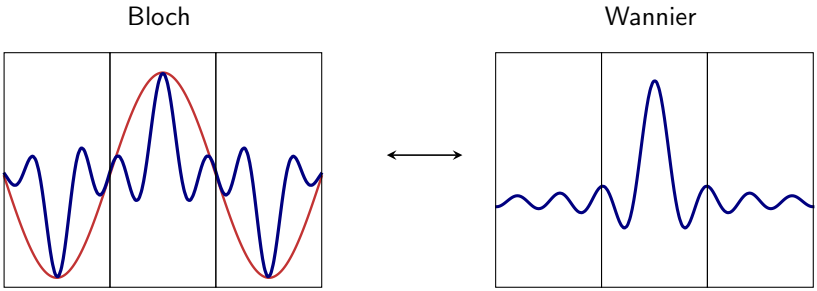
40 x 40 grid



Fine BZ sampling

Wannier functions

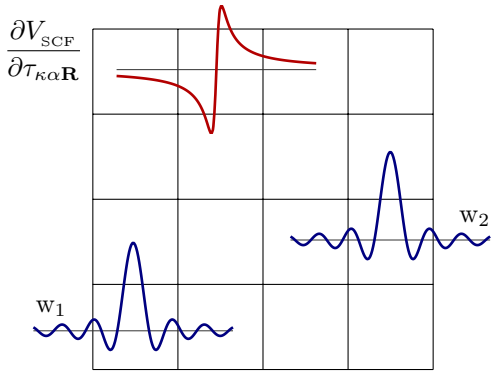
cf. Lecs. Mon.3 Marzari, Tue.1 Marrazzo



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

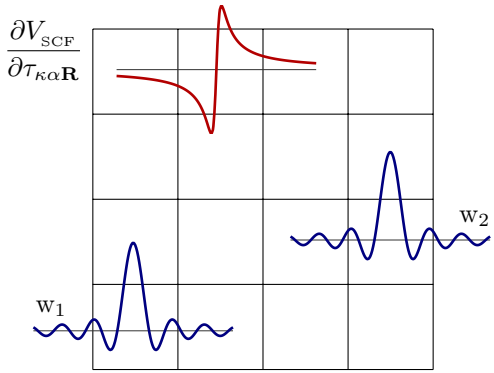
Review article: Marzari, Mostofi, Yates, Souza, Vanderbilt, Rev. Mod. Phys. 84, 1419 (2012)

Wannier interpolation of electron-phonon matrix elements



FG, Cohen, Louie, Phys. Rev. B 76, 165108 (2007)

Wannier interpolation of electron-phonon matrix elements



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

FG, Cohen, Louie, Phys. Rev. B 76, 165108 (2007)

Example: Electron-phonon matrix elements of diamond

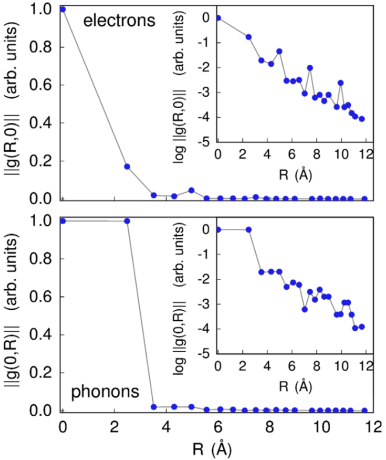
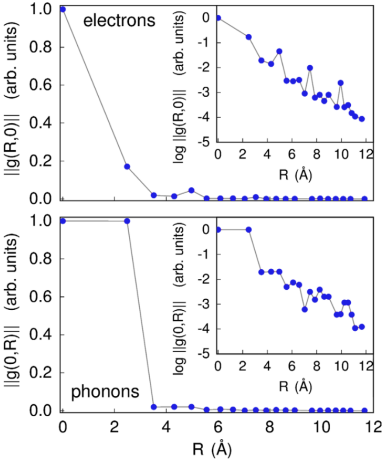


Figure from Giustino et al, Phys. Rev. B 76, 165108 (2007)

Example: Electron-phonon matrix elements of diamond



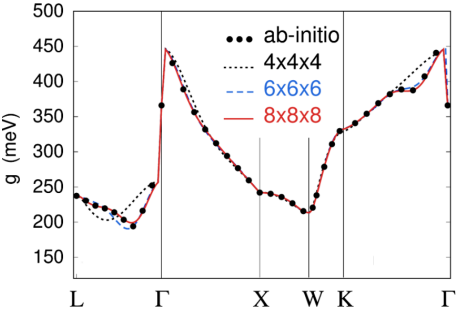


Figure from Giustino et al, Phys. Rev. B 76, 165108 (2007)

Example: EP matrix elements of various semiconductors

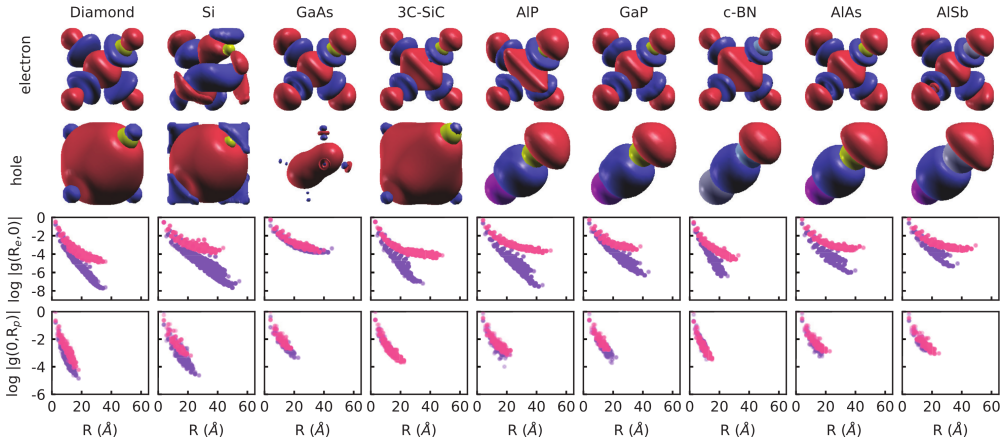
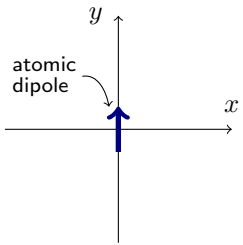


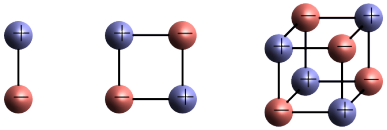
Figure from Poncé et al, Phys. Rev. Res. 3, 043022 (2021)

Spatial decay of induced potential



dipole quadrupole octupole

$$\frac{\partial V_{\mathrm{SCF}}}{\partial \tau}(\mathbf{r}) \sim \epsilon^{-1}\left[D_\alpha \frac{\hat{r}_\alpha}{r^2} + Q_{\alpha\beta}\frac{\hat{r}_\alpha \hat{r}_\beta}{r^3} + O_{\alpha\beta\gamma}\frac{\hat{r}_\alpha \hat{r}_\beta \hat{r}_\gamma}{r^4} + \cdots\right]$$



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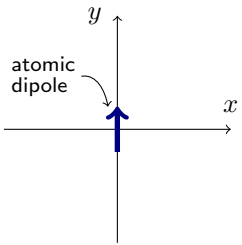

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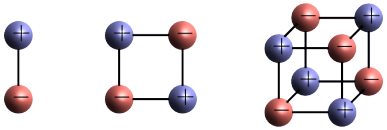
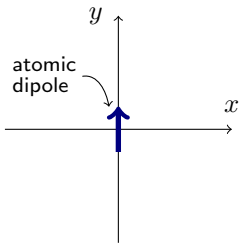


Fourier: $\frac{1}{q}$ 1 q

Spatial decay of induced potential



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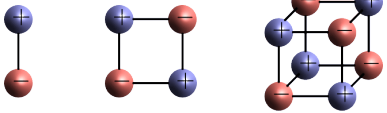
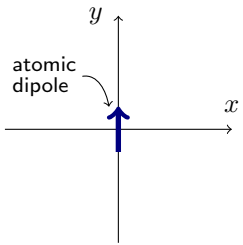


Fourier: $\frac{1}{q}$ 1 q

Metals: $\epsilon(q) = 1 + \dfrac{q_{\mathrm{TF}}^2}{q^2}$

Insulator: $\epsilon(q) = 1 + \dfrac{\epsilon_0 - 1}{1 + q^2/q_0^2}$

Spatial decay of induced potential



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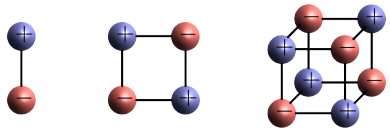

Fourier: $\frac{1}{q}$ 1 q

Metals: $\epsilon(q) = 1 + \frac{q_{\mathrm{TF}}^2}{q^2}$ smooth smooth smooth

Insulator: $\epsilon(q) = 1 + \frac{\epsilon_0 - 1}{1 + q^2/q_0^2}$ singular discontinuous smooth

Example: Fröhlich interaction matrix element in TiO_2

cf. Lec. Tue.5 Lee

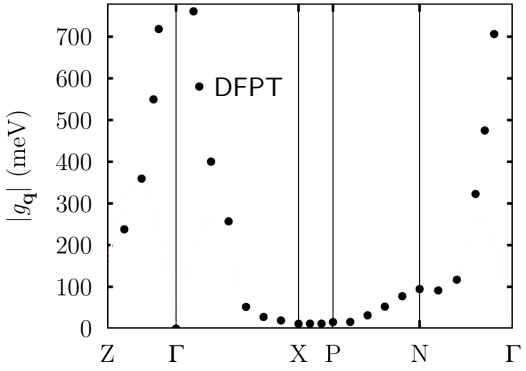

Figure from Verdi et al, Phys. Rev. Lett. 115, 176401 (2015)

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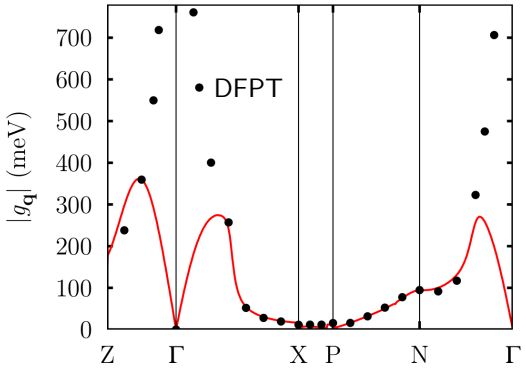

standard Wannier

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

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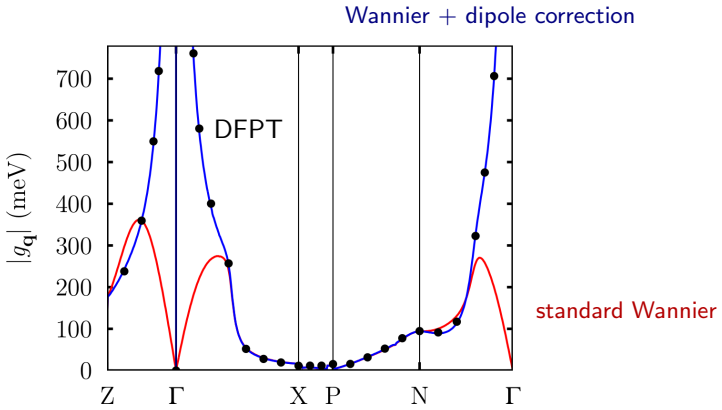

Figure from Verdi et al, Phys. Rev. Lett. 115, 176401 (2015)

Take-home messages

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

References

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- Jhalani et al, Phys. Rev. Lett. 125, 136602 (2020) [link]