Ab initio Theoretical Optical Spectroscopy and the Bethe-Salpeter Equation (BSE)

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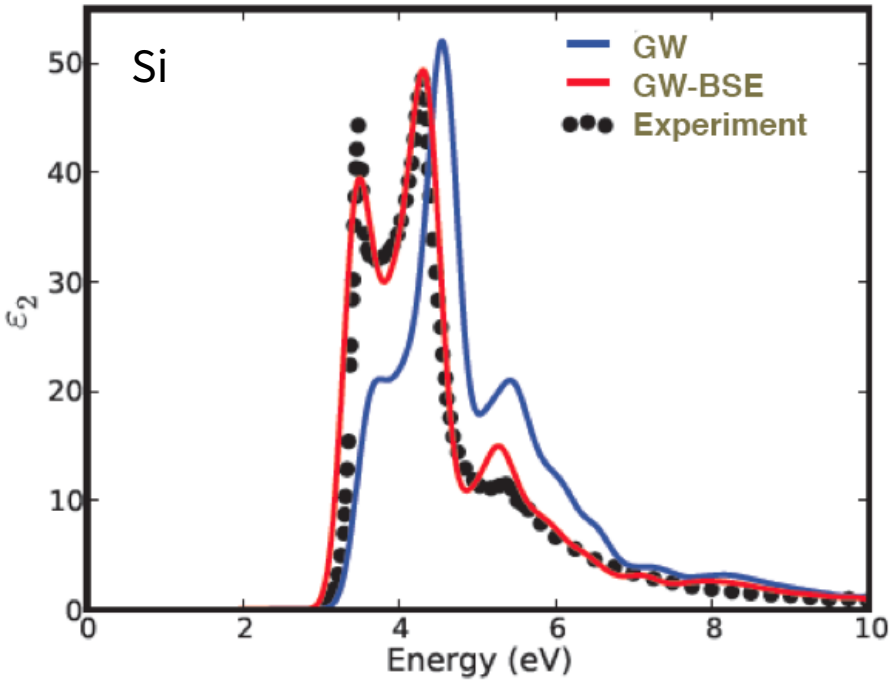
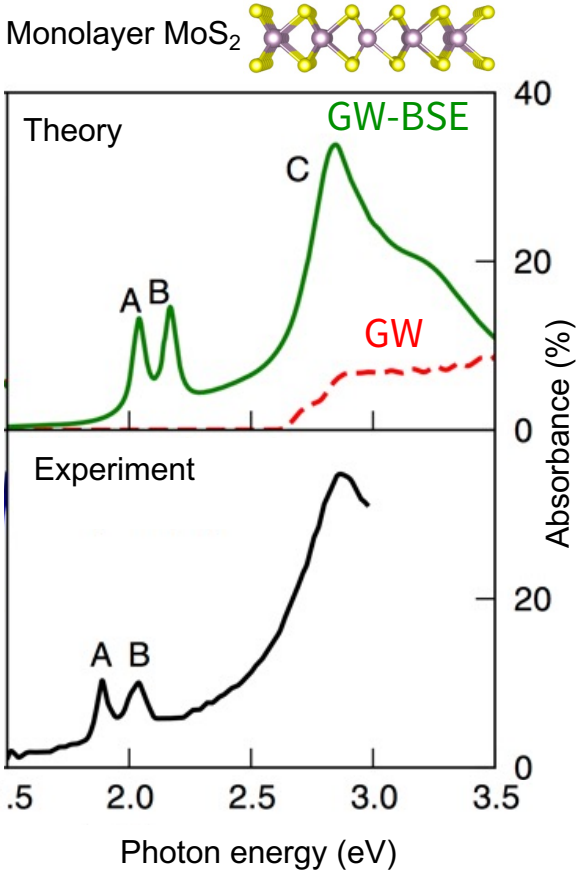
Why do we care about the BSE?



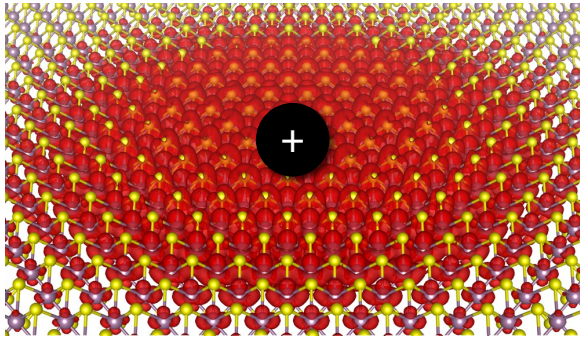
S. Albrecht, L. Reining, R. Del Sole, and G. Onida, PRL 80, 4510 (1998)
M. Rohlfing and S. G. Louie, PRL 81, 2312 (1998)
L. X. Benedict, E. L. Shirley, and R. B. Bohn, PRL 80, 4514 (1998)
J. R. Deslippe et al., CPC. 183, 1269 (2012)

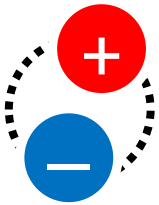


Qiu, Jornada, Louie, PRL 111, 216805 (2013).
Mak, Lee, Hone, Shan, Heinz, PRL 105, 136805 (2010).

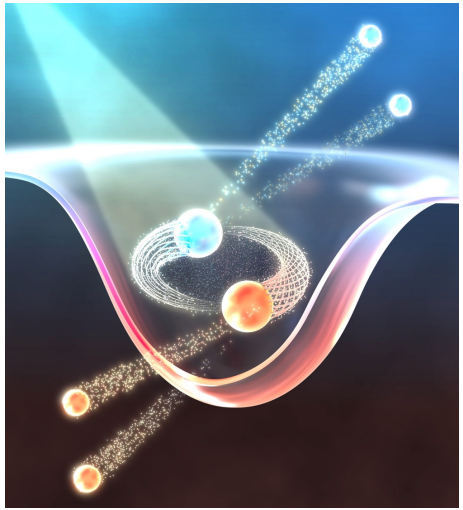
Some important phenomena cannot be *qualitatively* understood without the notion of excitons!

Exciton wavefunction in monolayer MoS_2





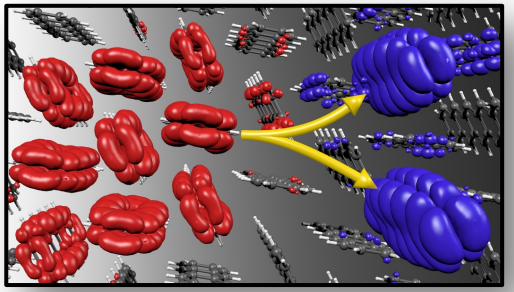
Exciton localization in moiré materials for QIS applications



Karni*, …, Jornada, Heinz, Dani, Nature 603, 247 (2022).

Barré, …, R.-Abramson, Jornada, Heinz, Science 376, 406 (2022).

Single fission in crystal pentacene

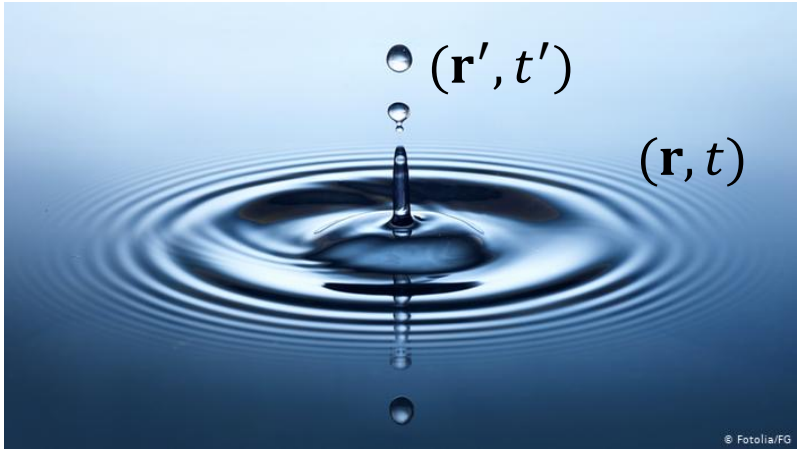


R.-Abramson, Jornada, Louie, Neaton, PRL 119, 267401 (2017).

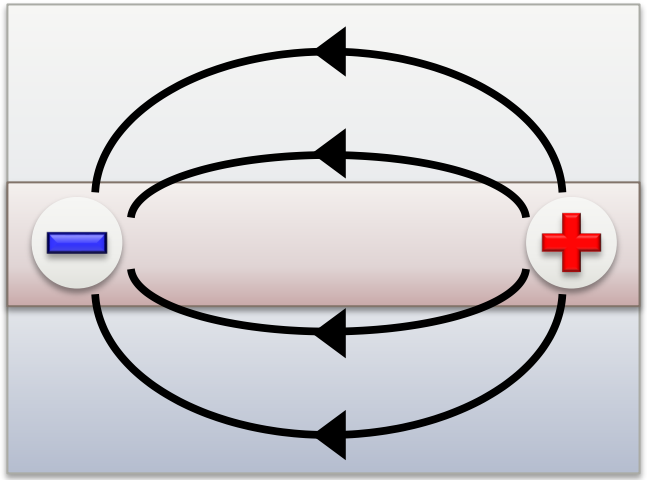
Altman, R.-Abramson, Jornada, JPCL 13, 747 (2022).

Outline

Theoretical spectroscopy and the Bethe-Salpeter equation (BSE)

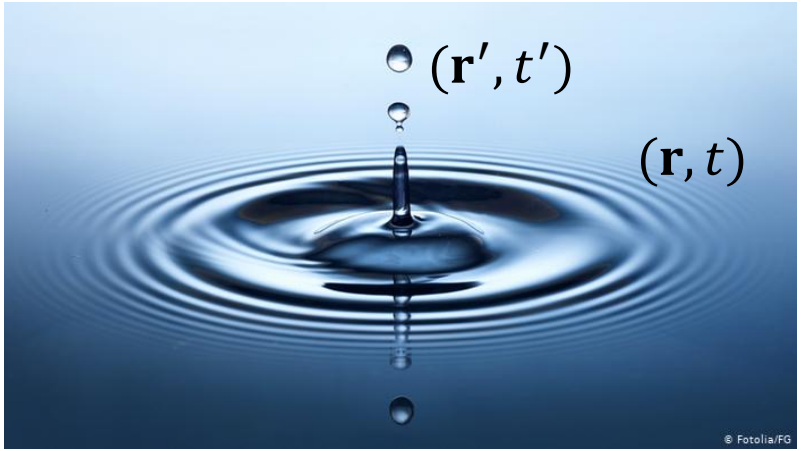


Example: Electronic and optical properties of 2D materials



Outline

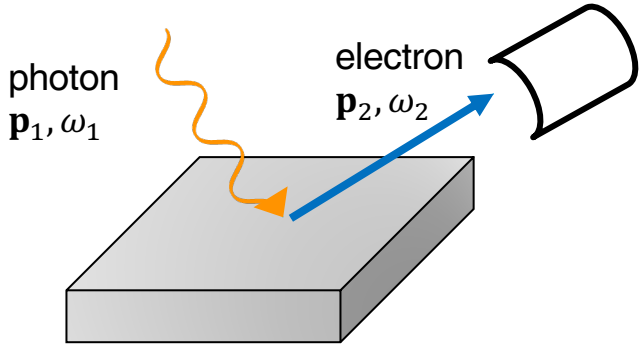
Theoretical spectroscopy and the Bethe-Salpeter equation (BSE)



- **Recap: Green's functions**
- BSE: intuition and derivation
- Kernel K of the BSE & connection w/ Wannier equations
- BSE & optical processes in practice

Recap: Green's functions formalism

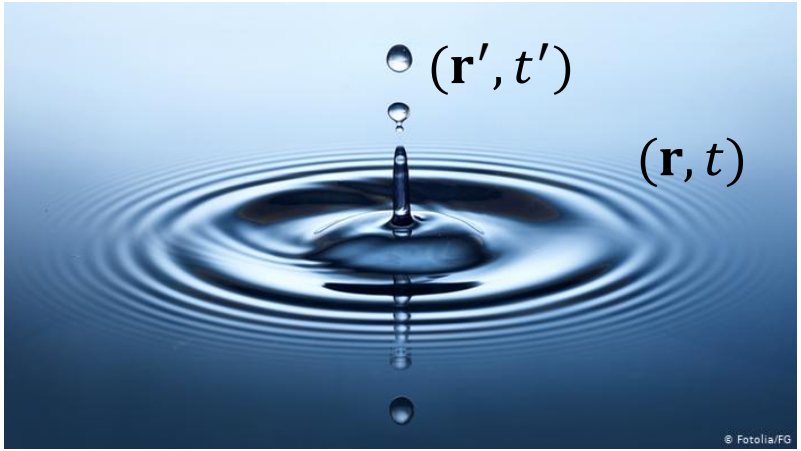
events detected:
spectral function $A(\omega)$

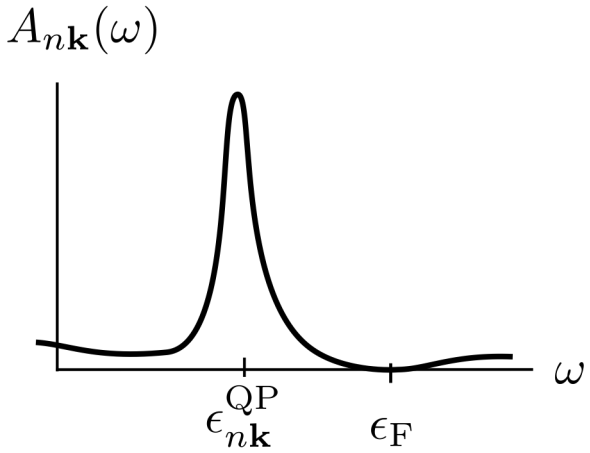


- Excitation properties from Green's function

$$G(\mathbf{r}, t; \mathbf{r}, t') = -i\langle \Psi_0 \left| \hat{T}\left[\hat{\psi}(\mathbf{r}, t)\hat{\psi}^{\dagger}(\mathbf{r}', t')\right] \right| \Psi_0 \rangle$$

- Add an electron, see the "ripple" it creates





Recap: Green's functions formalism

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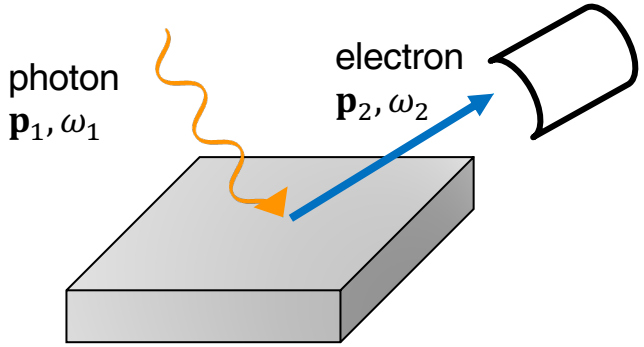


- Non-interacting Green's function (e.g. DFT)

$$G_0(\mathbf{r}, \mathbf{r}'; \omega) \sim [\omega - H^0(\mathbf{r}, \mathbf{r}')]^{-1}$$

- Interacting Green's function

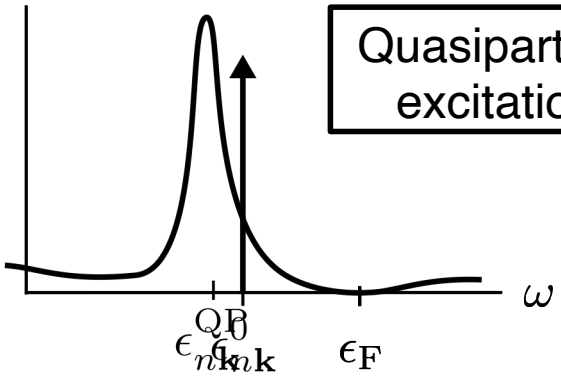
$$G(\omega) = [\omega - H^0 - \Sigma(\omega)]^{-1}$$

Self-energy

  - Exact, in principle.
  - No need to deal with many-body Hamiltonian.

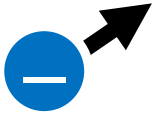
Peaks of Green's functions:
long-lived elementary excitations.

$A_{n\mathbf{k}}(\omega)$



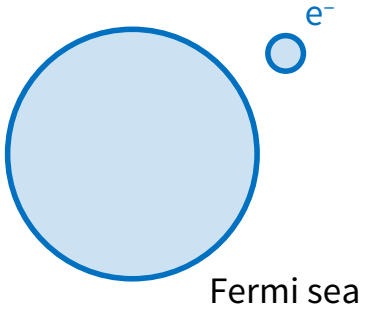
Quasiparticle excitation

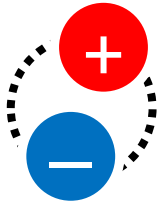
Spectroscopic properties = behavior of excited particles



Quasiparticle (QP) properties

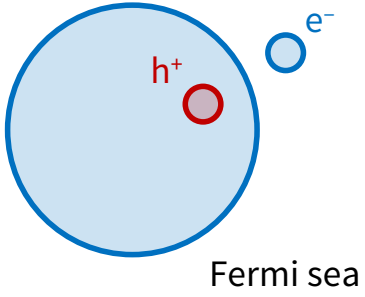
- “N+1” particle problem (add elec. or hole)
- Photoemission, tunneling, etc.
- Quasiparticle approach & GW approximation



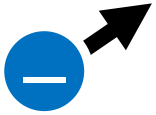


Optical properties

- “N” electron (or “+2” particle) problem
- Electron-hole interaction & excitonic effects
- Optical absorption, EELS, XAS, etc.



Spectroscopic properties = behavior of excited particles



Quasiparticle (QP) properties via single-particle Green's function:

$$G(1;1') = -i\langle\Psi_0|\hat{T}\left[\hat{\psi}(1)\hat{\psi}^\dagger(1')\right]|\Psi_0\rangle$$

Add electron at $(\mathbf{r}';t')$, measure amplitude at $(\mathbf{r};t)$

Dyson's equation:

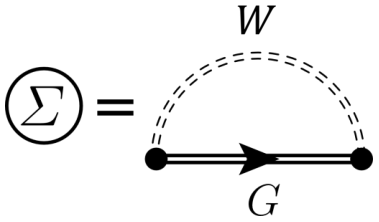
$$G^{-1}(\mathbf{r},\mathbf{r}';\omega) = G_0^{-1}(\mathbf{r},\mathbf{r}';\omega) - \Sigma(\mathbf{r},\mathbf{r}';\omega)$$

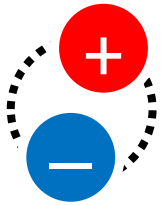
Inverse interacting Green's function

Inverse noninteracting Green's function

QP self-energy

GW approximation to Σ





Optical properties via eh correlation function L:

$$L(1,2;1',2') = -i\langle\Psi_0|\hat{T}\left[\hat{\psi}(1)\hat{\psi}^\dagger(2)\hat{\psi}(2')\hat{\psi}^\dagger(1')\right]|\Psi_0\rangle_{\text{joint}}$$

Bethe-Salpeter equation (BSE):

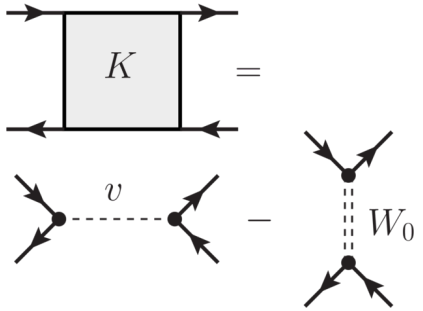
$$L^{-1} = L_0^{-1} - K$$

Inverse (non-)interacting eh propagator

Kernel of the BSE = e-h self-energy

Add eh pair $(\mathbf{r}_1',\mathbf{r}_2';t')$, measure amplitude at $(\mathbf{r}_1,\mathbf{r}_2;t)$

eh interaction kernel K



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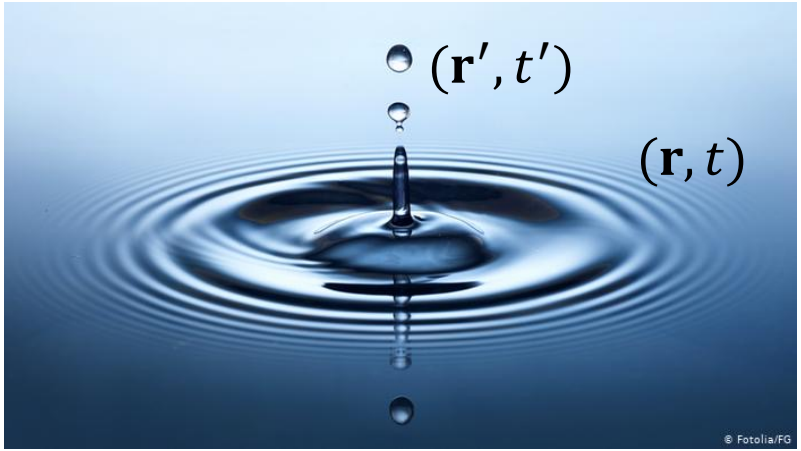
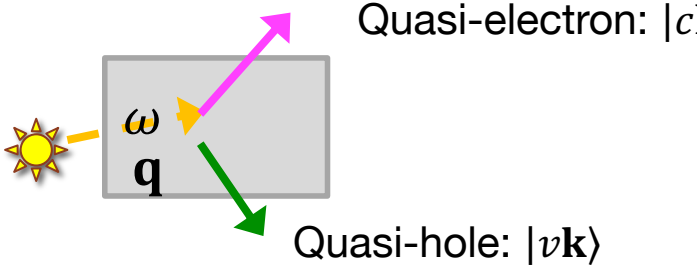


- Recap: Green's functions
- **BSE: intuition and derivation**
- Kernel K of the BSE & connection w/ Wannier equations
- BSE & optical processes in practice

Optical spectrum & excitonic effects

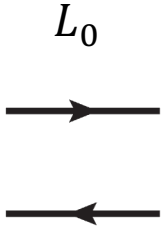
No electron-hole interactions



Quasi-electron: $|c\mathbf{k}+\mathbf{q}\rangle$

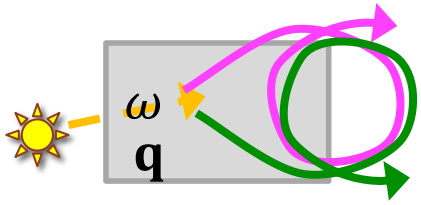
Quasi-hole: $|v\mathbf{k}\rangle$

Final state: uncorrelated electron & hole



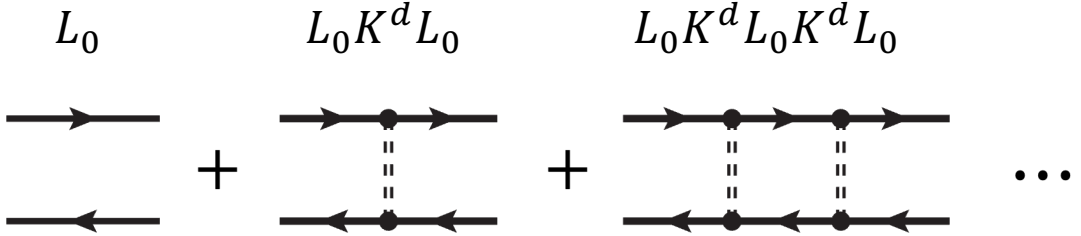
Two single-particle Green's functions!

With electron-hole interactions

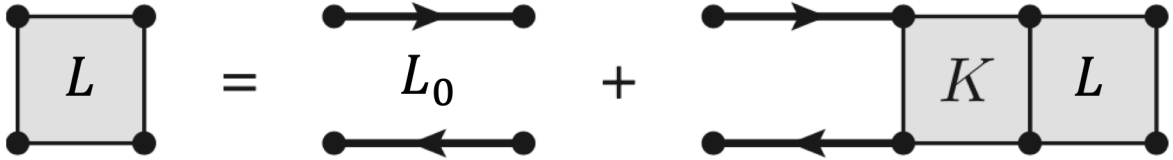


Excitonic state: $|S\rangle$

Final state: *correlated* electron-hole pair



The Bethe-Salpeter equation (BSE)



$$L = L_0 + L_0 K L$$

e-h correlation function

kernel of the BSE

$1 \equiv (\mathbf{x}, t)$

- Express quantities in quasiparticle basis
- Assume static kernel K

$$L(\omega) = L_{vc\mathbf{k},v'c'\mathbf{k}'}(\omega), \quad \cdots$$

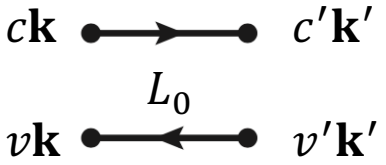
$$L^{-1}(\omega) = L_0^{-1}(\omega) - K$$

The BSE effective Hamiltonian

- L^0 is already diagonal in the QP basis

$$L^0_{vc\mathbf{k},v'c'\mathbf{k}'}(\omega) = \left[\omega - \left(E^{\mathrm{QP}}_{c\mathbf{k}} - E^{\mathrm{QP}}_{v\mathbf{k}}\right)\delta_{cc'}\delta_{vv'}\delta_{\mathbf{k}\mathbf{k}'}\right]^{-1}$$

D: diagonal term = kinetic energy of free e-h pairs



- Define the BSE effective Hamiltonian H_{BSE}

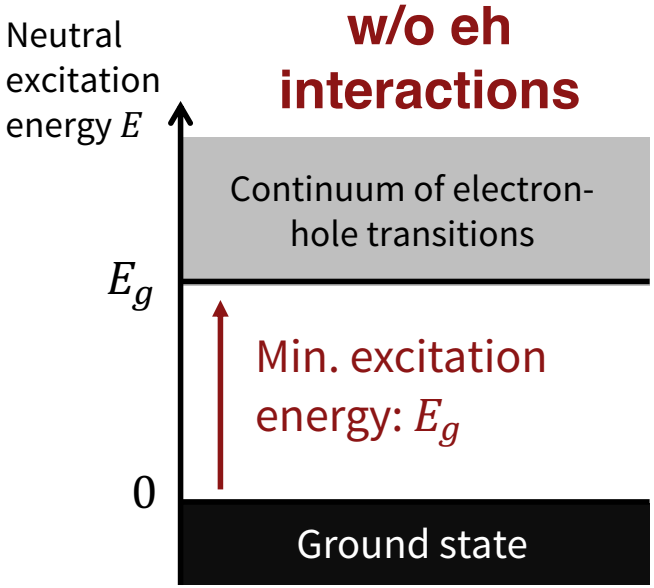
$$L^{-1}(\omega) = L_0^{-1}(\omega) - K = \omega - D - K := \omega - H_{\mathrm{BSE}}$$

$$H_{\mathrm{BSE}} := D + K$$

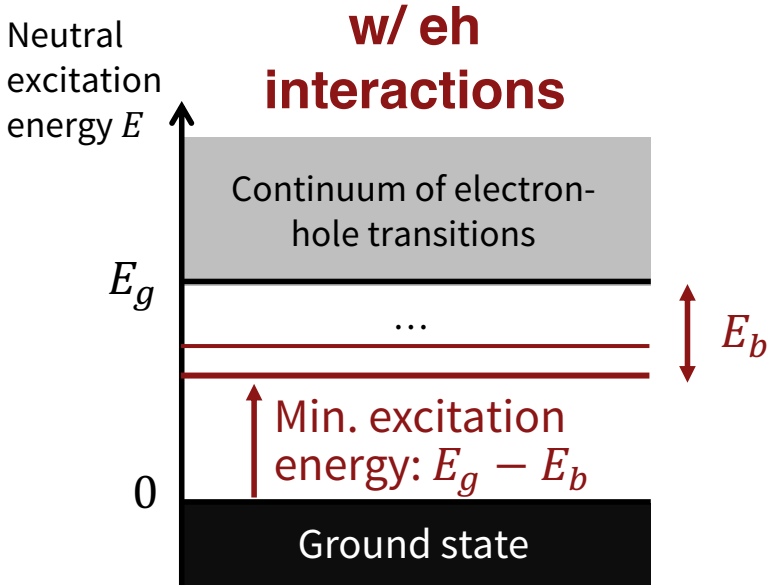
Poles of $L(\omega)$ = collective, neutral excitations
= eigenstates of H_{BSE}

$$H_{\mathrm{BSE}}|S\rangle = \Omega_S|S\rangle$$

Representing excited states & excitonic effects



- Lowest-energy excitation: electron at CBM, hole at VBM
- Excitation energy: E_g
- Only continuum of states in bulk materials



- There's a finite e-h binding (E_b)
- Lowering of the excitation energy: $E_g - E_b$
- Presence of discrete sub-bandgap excitations → **excitons**!

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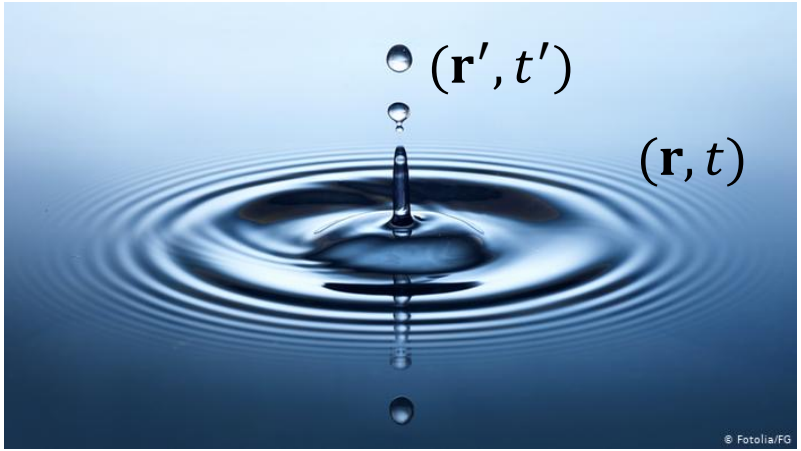

- Recap: Green's functions
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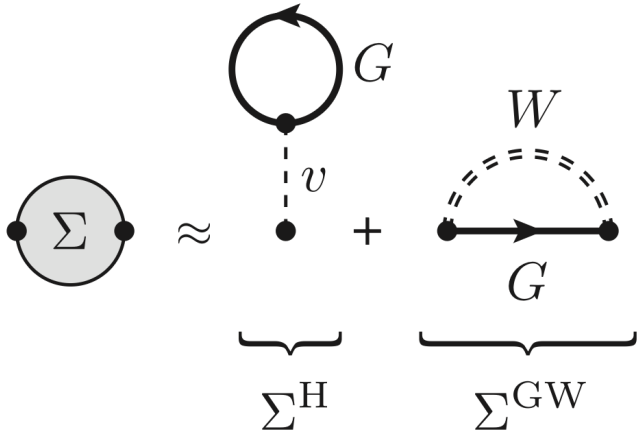
- **Kernel K of the BSE & connection w/ Wannier equations**
- BSE & optical processes in practice

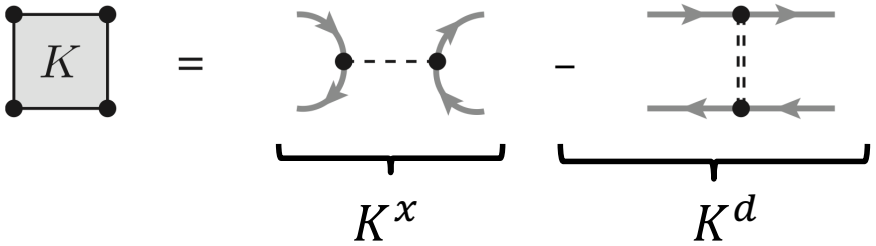
The electron-hole interaction kernel K

- K is related to the single-particle self-energy Σ $K = \frac{\delta \Sigma}{\delta G}$

GW approximation

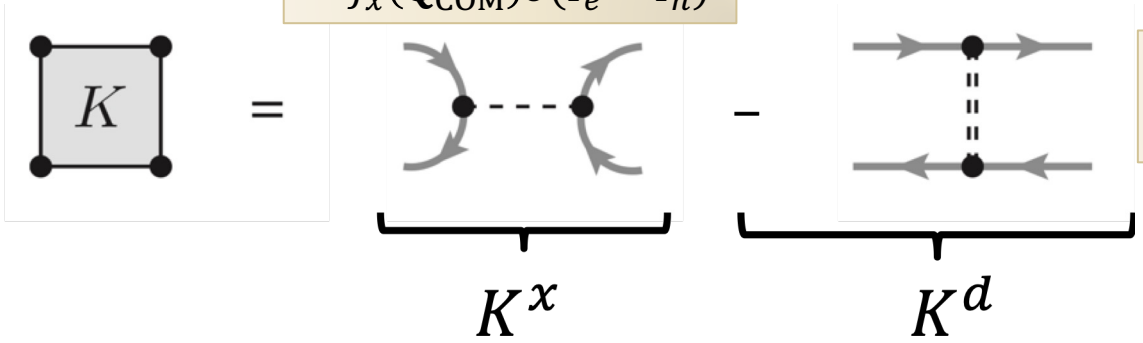


Corresponding K
(neglect $\delta W / \delta G$)



The electron-hole interaction kernel K

$\sim J_x(\mathbf{Q}_{\mathrm{COM}})\delta(\mathbf{r}_e - \mathbf{r}_h)$



$\sim -\varepsilon^{-1}\dfrac{e^2}{|\mathbf{r}_e - \mathbf{r}_h|}$

Exchange interaction K^x

- **Repulsive**, density-density interaction
- Involves **bare** Coulomb interaction (v)
- Requires overlap. e-h pairs in space & spin
- Can couple two e-h pairs far apart
- Responsible for splitting of spin-singlet & triplet excitons, plasmons, Föster-like coupling, etc.

Direct interaction K^d

- **Attractive**, orbital-dependent interaction
- Involves **screened** Coulomb interaction (W)
- Requires overlap. initial+final electrons & initial+final holes
- Does not require e-h to overlap
- Responsible **binding of excitons**, Rydberg-like solutions, etc.

Physical picture & Wannier equations

- Assuming 2-band model, smooth WFNs, constant screening, effective mass dispersion

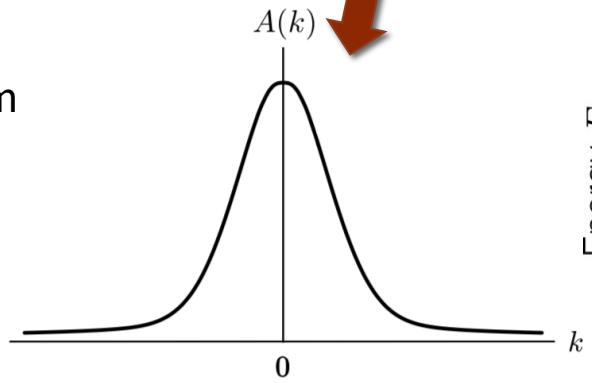
$$H_{\mathrm{BSE}} = D - K^d + K^x$$

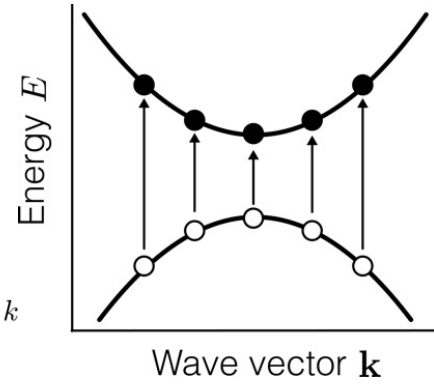
$$\left[\left(E_g - \frac{\nabla^2}{2\mu}\right) - \frac{e^2}{\varepsilon|\mathbf{r}_e - \mathbf{r}_h|} + \delta_{M_S,0}\, J_x\, \delta(\mathbf{r}_e - \mathbf{r}_h)\right] F_S(\mathbf{r}_e - \mathbf{r}_h) = \Omega_S\, F_S(\mathbf{r}_e - \mathbf{r}_h)$$

- Hydrogenic equation!
  - Bound excitonic states ⟷ bound electronic states in a hydrogenic atom

- K^x often small in solids (~meV), but important in localized excitons (e.g., Frankel excitons)

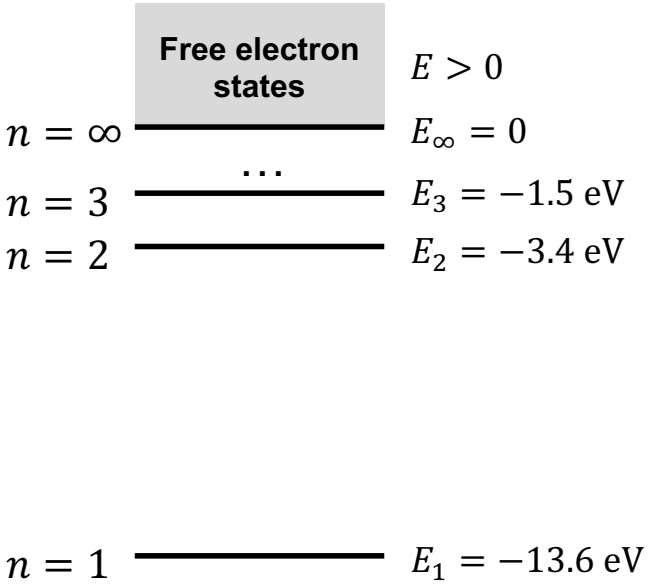
Fourier pairs!



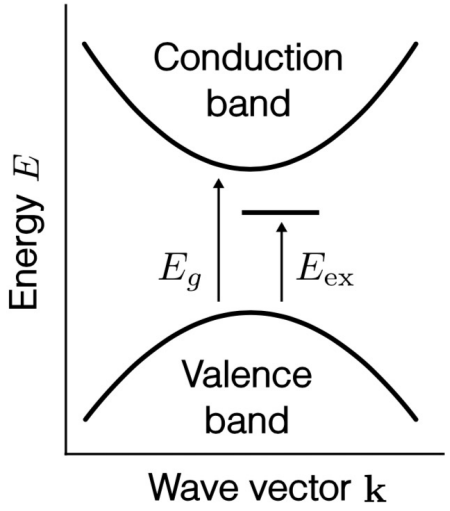


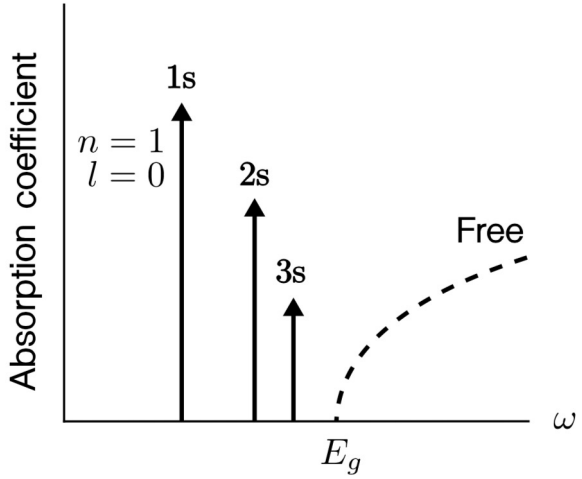
Physical picture & Wannier equations

Hydrogen atom



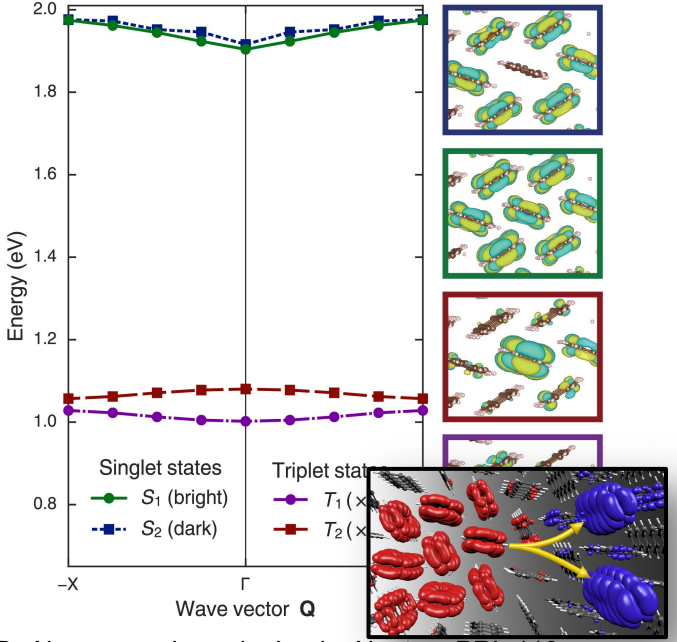
(Wannier-Mott) excitons





Excitons beyond a Wannier model

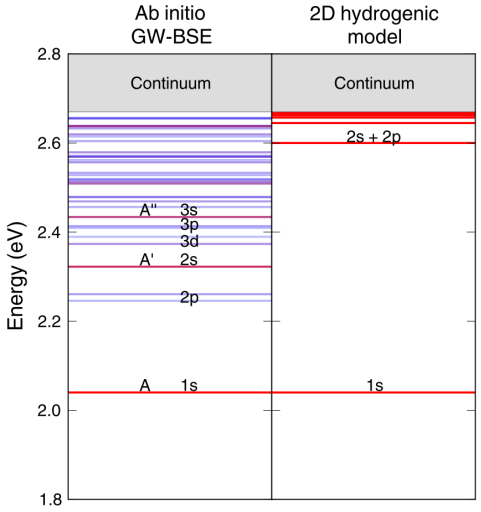
Wannier & Frankel excitons in bulk pentacene, singlet fission, etc.



R.-Abramson, Jornada, Louie, Neaton, PRL 119, 267401 (2017).

Altman, R.-Abramson, Jornada, JPCL 13, 747 (2022).

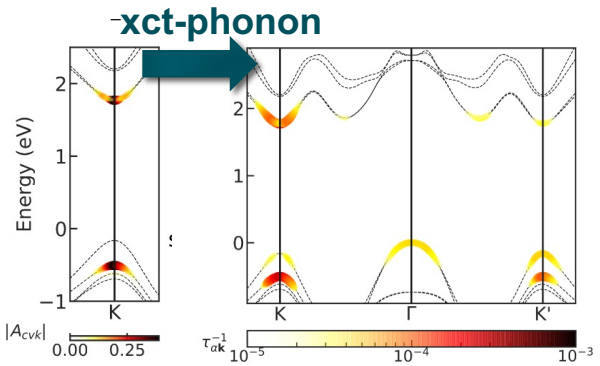
Non-hydrogenic excitons in monolayer materials



Qiu, Jornada, Louie, PRL 111, 216805 (2013).

Qiu, Jornada, Louie, PRB 93, 235435 (2016).

Exciton linewidth, dynamics, and thermalization

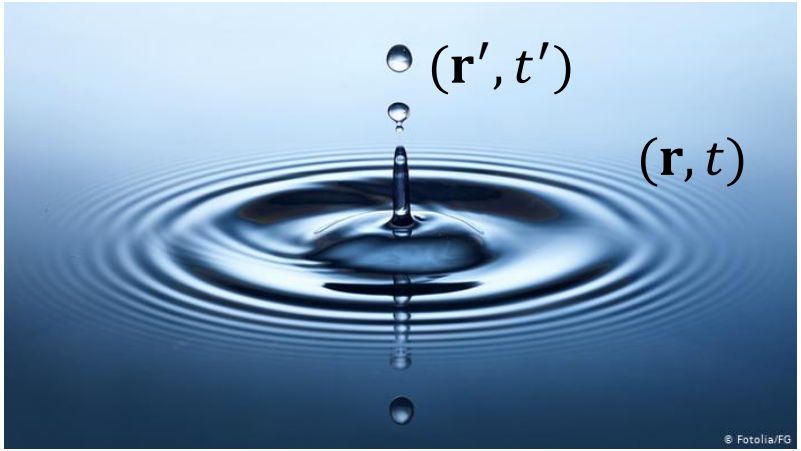


Chan*, Haber, Naik, Neaton, Qiu*, Jornada*, Louie*, Nano Lett. 23, 3971 (2023).

Chan*, Naik, Haber, Neaton, Louie, Qiu*, Jornada*, Nano Lett. 24, 7972 (2024).

Outline

Theoretical spectroscopy and the Bethe-Salpeter equation (BSE)



- Recap: Green's functions
- BSE: intuition and derivation
- Kernel K of the BSE & connection w/ Wannier equations
- **BSE & optical processes in practice**

The BSE in practice

- Our previous expression for the BSE:

$$H_{\mathrm{BSE}}|S\rangle = (D+K)|S\rangle = \Omega_S|S\rangle$$

- Express exciton → linear combination of several electron-hole transitions

$$|S\rangle = \sum_{vc\mathbf{k}} A^S_{vc\mathbf{k}}\, c^\dagger_{c\mathbf{k}} c_{v\mathbf{k}}\, |0\rangle$$

$A^S_{vc\mathbf{k}}$: exciton electron-hole expansion coefficients

- BSE → eigenvalue problem

$$\sum_{v'c'\mathbf{k}'} \left[\left(E^{\mathrm{QP}}_{c\mathbf{k}} - E^{\mathrm{QP}}_{v\mathbf{k}}\right)\delta_{cc'}\delta_{vv'}\delta_{kk'} + \langle vc\mathbf{k}|K|v'c'\mathbf{k}'\rangle\right] A^S_{v'c'\mathbf{k}'} = \Omega^S A^{\mathrm{S}}_{vc\mathbf{k}}$$

Notes:

- H_{BSE}: matrix of size $n_v n_c n_k$, diagonalize it is $(n_v n_c n_k)^3$!
- Need fine k-point sampling to resolve fine spatial features of excitons features
- Size of BSE can be very large $> 10^6$!

The BSE & optical absorption spectrum

- Optical properties : ~ $H_{\mathrm{el-ph}} \sim \mathbf{A} \cdot \mathbf{v}$

$$\varepsilon_2(\omega) \propto \sum_S |\langle 0|\mathbf{v}\cdot\hat{e}|S\rangle|^2 \delta(\omega - \Omega_S)$$

Oscillator strength

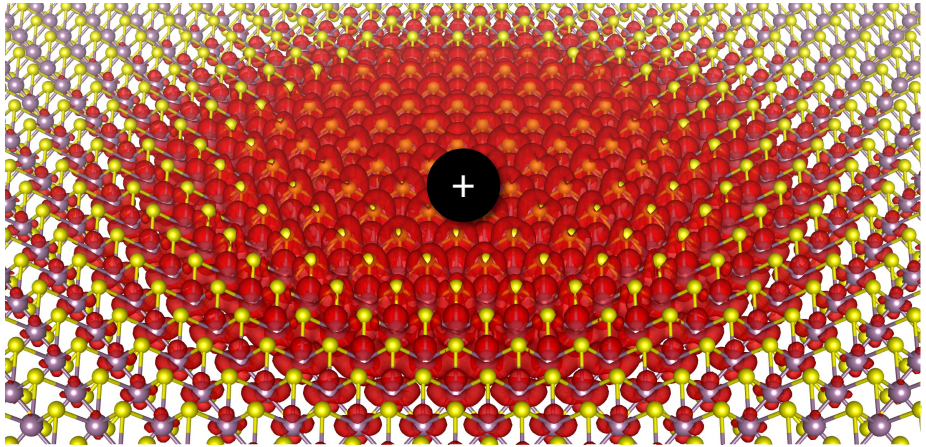
Opt. excitation energy

$\mathbf{v}$: velocity matrix elements

- Optical properties follow directly from eigenvalues and eigenvectors of the BSE
- There are approaches that directly yield ε_2 without diagonalizing H_{BSE} (Haydock/Lanczos), but they typically can't access the exciton wavefunctions

The exciton wavefunction

Exciton wavefunction: $\Psi_S(\mathbf{r}_e, \mathbf{r}_h) = \sum_{vck} A_{vc\mathbf{k}} \psi_{c\mathbf{k}}(\mathbf{r}_e) \psi^*_{v\mathbf{k}}(\mathbf{r}_h)$



$|\Psi_S(\mathbf{r}_e, \mathbf{r}_h = (+))|^2$

- Note that the exciton wavefunction depends on two coordinates.
- Typically, one fixes one of them (e.g., hole)
- Q: What if you integrate, e.g., the hole coordinate?

The Bethe-Salpeter equation calculation in practice

Desired expressions

$$\sum_{v'c'\mathbf{k}'} \left[\left(E^{\mathrm{QP}}_{c\mathbf{k}} - E^{\mathrm{QP}}_{v\mathbf{k}} \right) \delta_{cc'} \delta_{vv'} \delta_{kk'} + \langle vc\mathbf{k}|K|v'c'\mathbf{k}'\rangle \right] A^{S}_{v'c'\mathbf{k}'} = \Omega^{S} A^{S}_{vc\mathbf{k}}$$

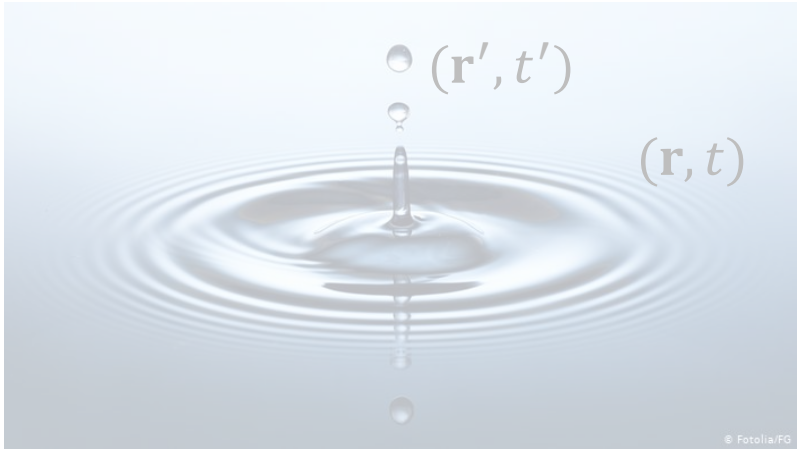
$$\varepsilon(\omega) \propto \sum_{S} |\langle 0|\mathbf{v}\cdot\hat{e}|S\rangle|^2 \delta(\omega - \Omega_S)$$

Main ingredients/ steps

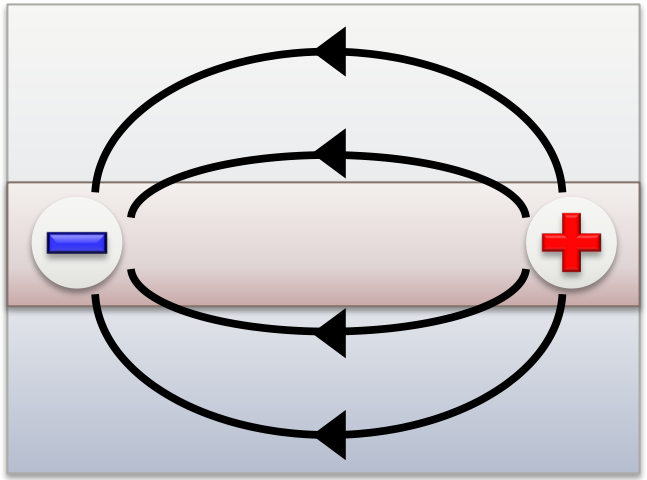
- **Quasiparticle** states on a dense set of k-points [**`sigma`** code]
  - In practice, use WFNs from DFT
  - Only correct QP energies with a GW calculation
- Evaluation of **K** [**`kernel`** code]
  - Requires screened Coulomb interaction W → dielectric screening ε^{-1} [**`epsilon`** code]
- Diag. of H_{BSE} [**`absorption`** code]

Outline

Many-body perturbation theory

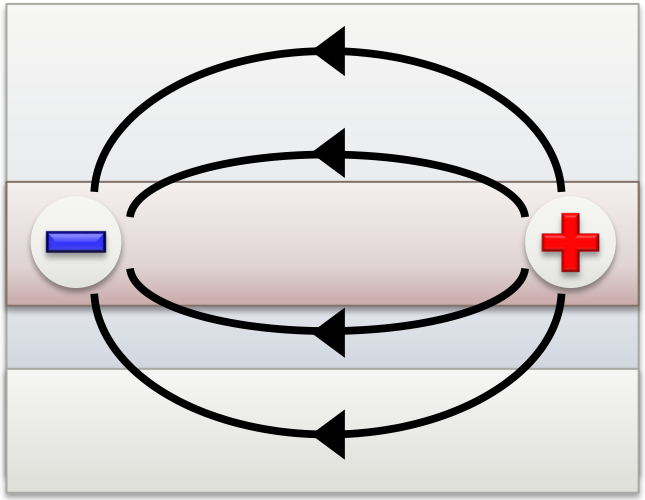


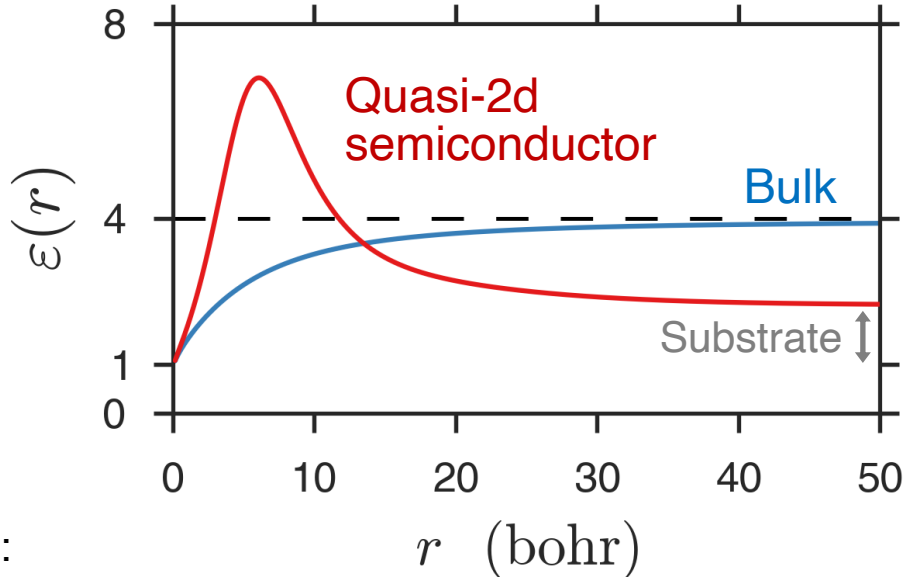
Electronic and optical properties of 2D materials



Low-dimensional materials and reduced screening

Screening is highly **spatially dependent** in semicond. with reduced dimensionality.



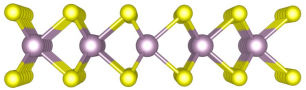


Spatial dependence of screening leads to:

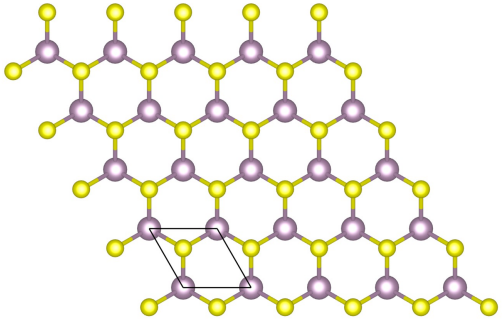
- Enhancement of **many-electron effects**.
- **Breakdown of simpler continuum models** (non-hydrogenic excitonic series, etc.)
- **Environment-dependent** results (substrate, etc.).

Monolayer TMDCs

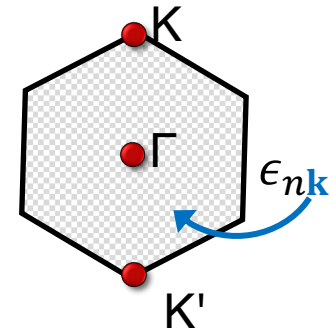
Monolayer TMD/MX_2 – side view:



Monolayer TMD/MX_2 – top view:



Brillouin zone



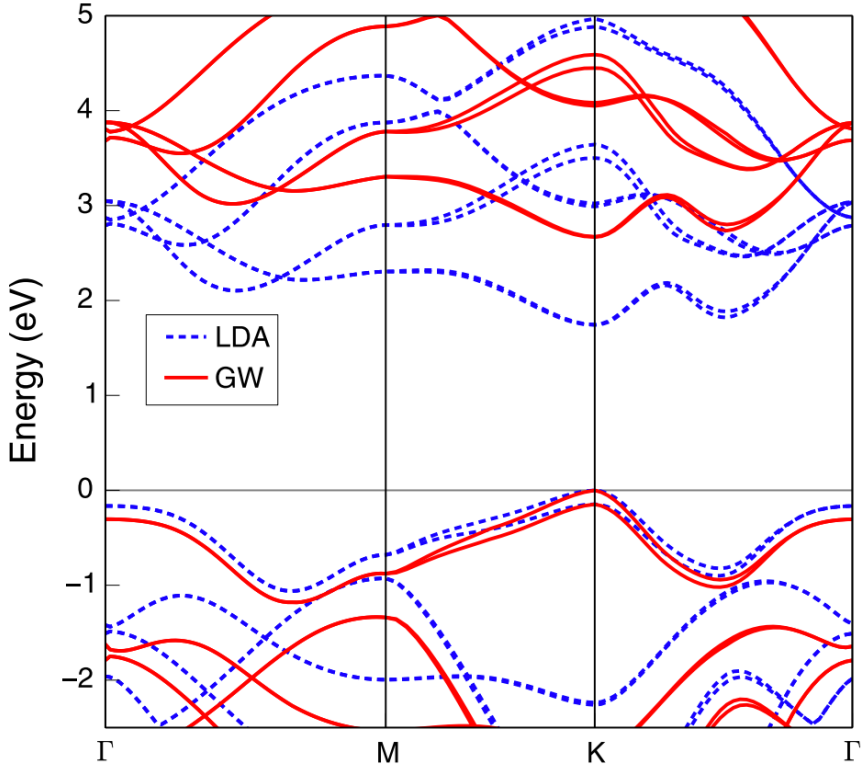
M = Mo, W, etc. (transition metal)

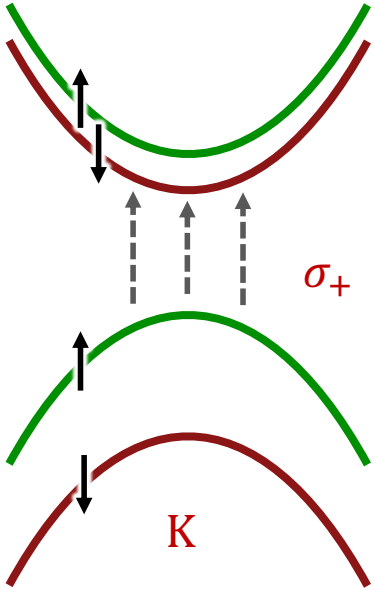
X = S, Se, etc. (chalcogen)

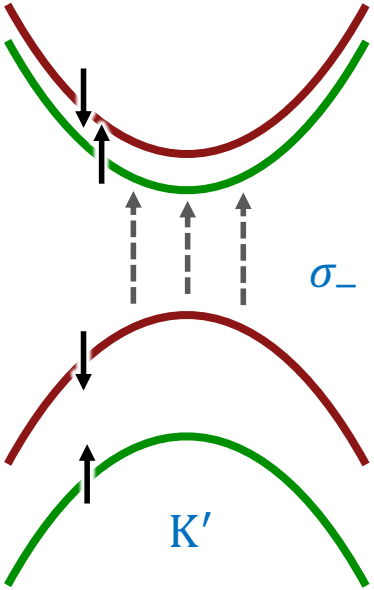
- Unusual/exciting properties:
  - Large optical absorption; [1-3]
  - **Locked spin/valley degrees of freedom / valley Hall effect; [4]**
  - Tunable electronic screening, non-hydrogenic excitonic physics;
  - Large catalytic activity (H_2 evolution reaction) [5]; etc.

[1] Mak, Lee, Hone, Shan, Hein, PRL 105, 136805 (2010); [2] Qiu, **da Jornada**, Louie, PRL 111, 216805 (2013).
[3] Bernardi, Palummo, Grossman, Nano Lett 13, 3664 (2013);
[4] D. Xiao, et al. PRL (2012); T. Cao,et al. Nat. Comm. (2012); K. F. Mak, et al. Science (2014).
[5] Jaramillo, et al., Science 317, 100 (2007).

MoS_2 quasiparticle band structure

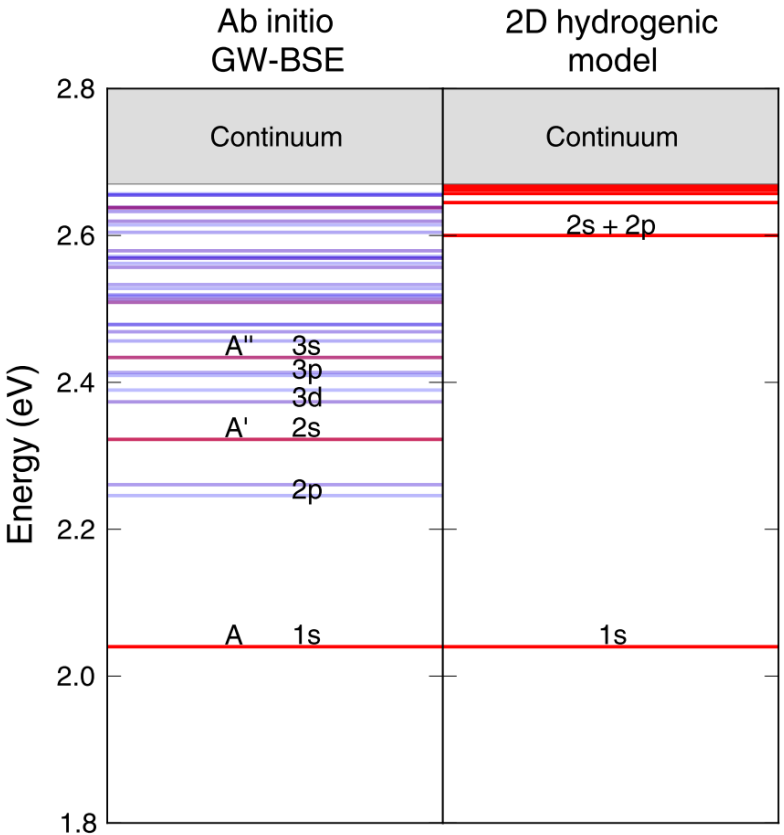




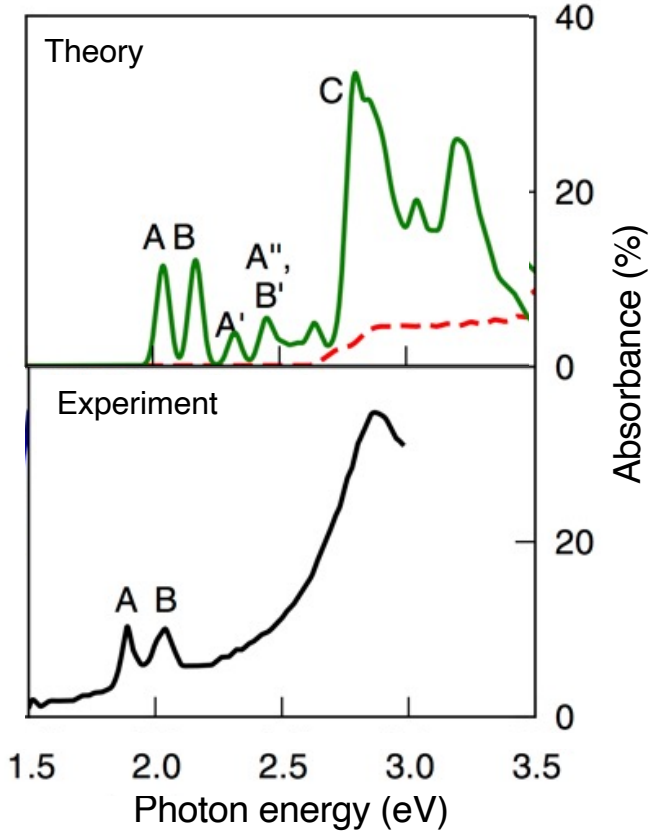


Qiu, Jornada, Louie, PRL 111, 216805 (2013); Qiu, Jornada, Louie, PRB 93, 235435 (2016).

Excitons in monolayer TMDCs

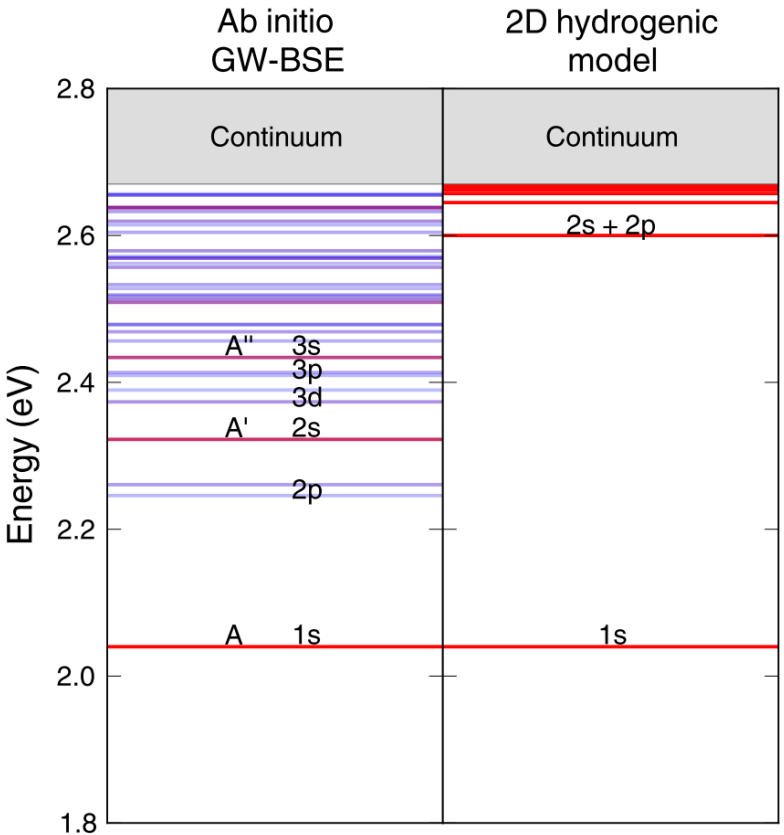


Optical absorption spectrum
(monolayer MoS_2)

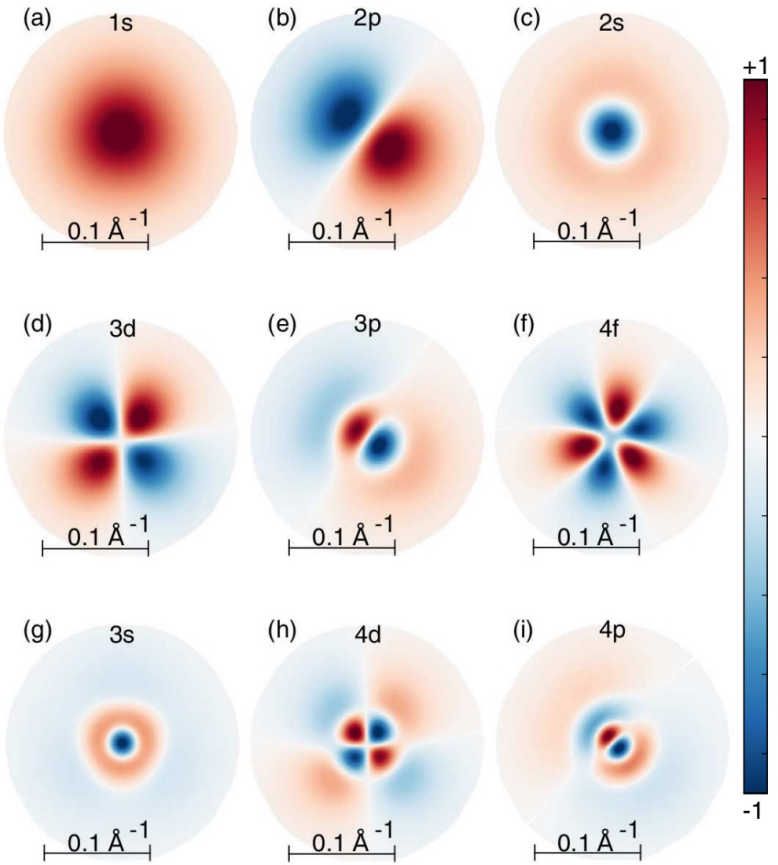


Qiu, Jornada, Louie, PRL 111, 216805 (2013); Qiu, Jornada, Louie, PRB 93, 235435 (2016).

Excitons in monolayer TMDCs

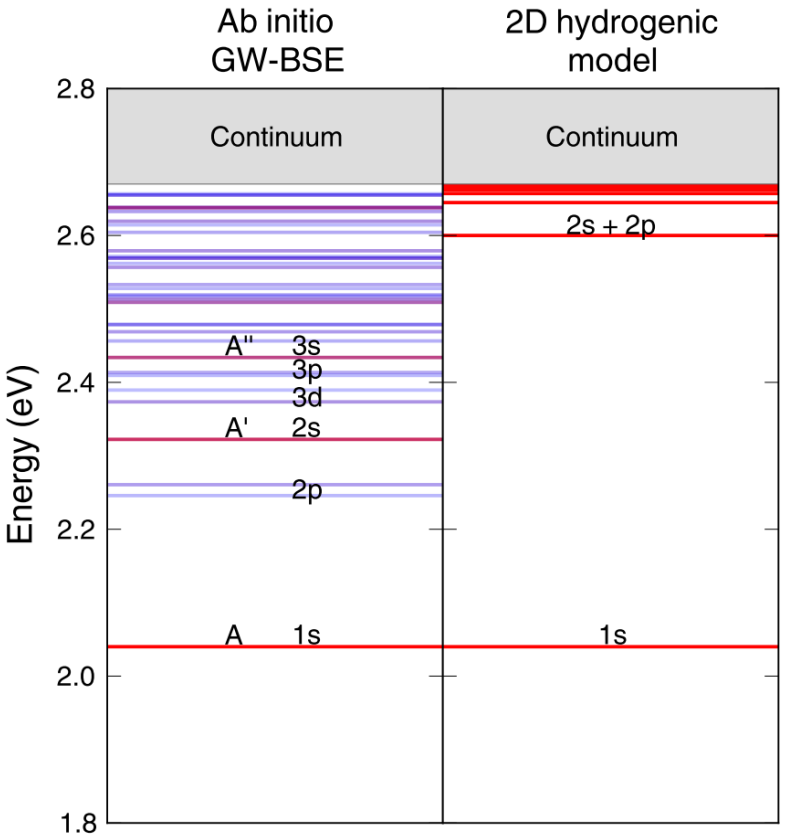


$A^S_{vc\mathbf{k}}$

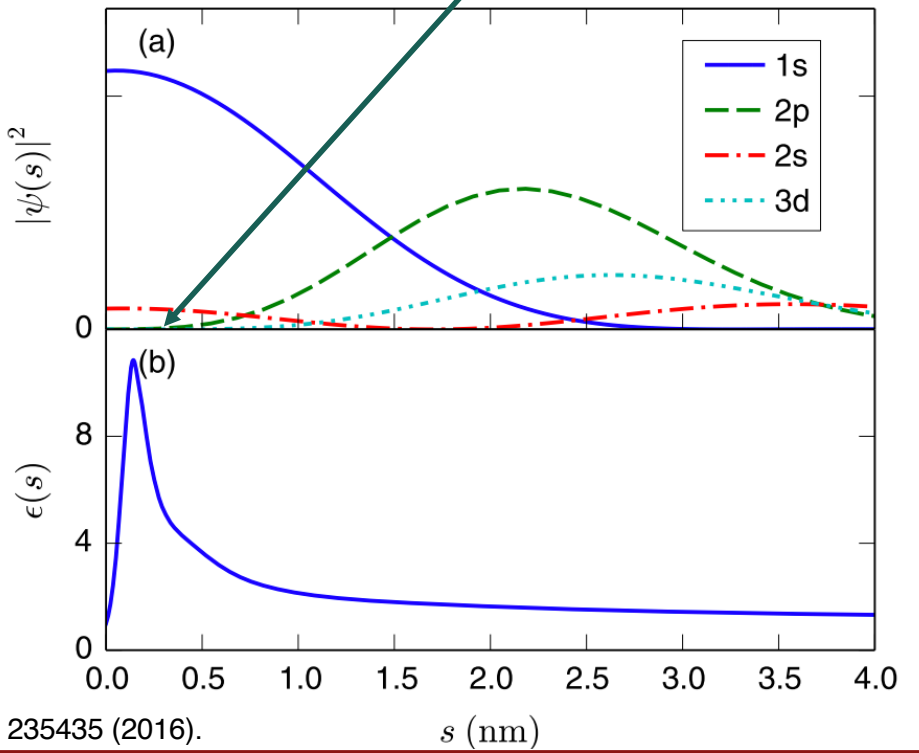


Qiu, Jornada, Louie, PRL 111, 216805 (2013); Qiu, Jornada, Louie, PRB 93, 235435 (2016).

Excitons in monolayer TMDCs

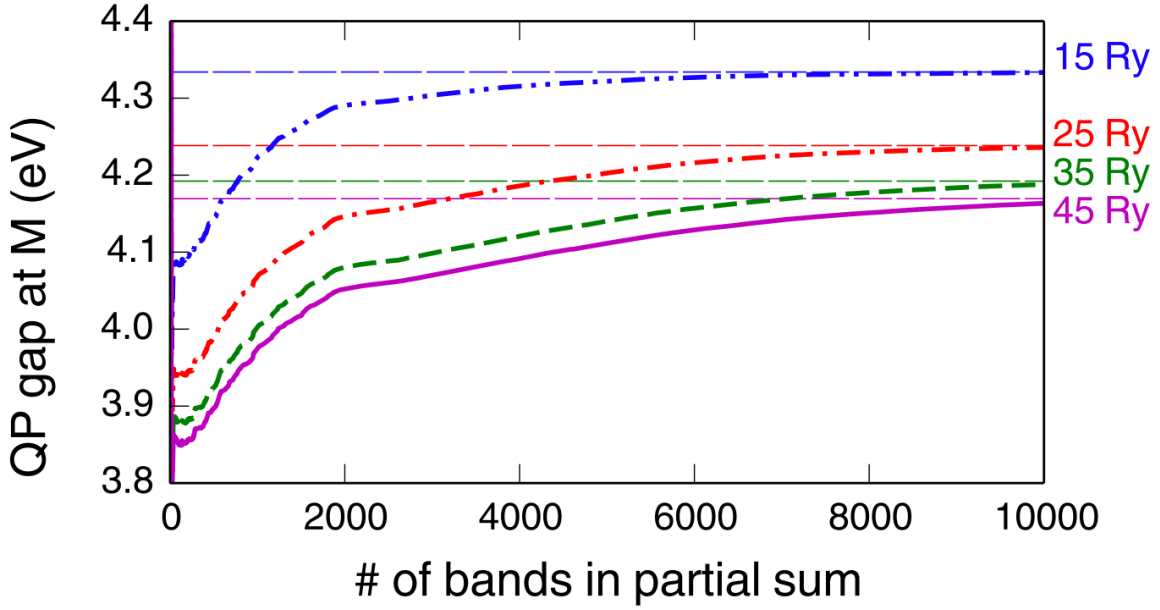


Wavefunction is small where screening is strongest!
2p has stronger binding energy than 2s



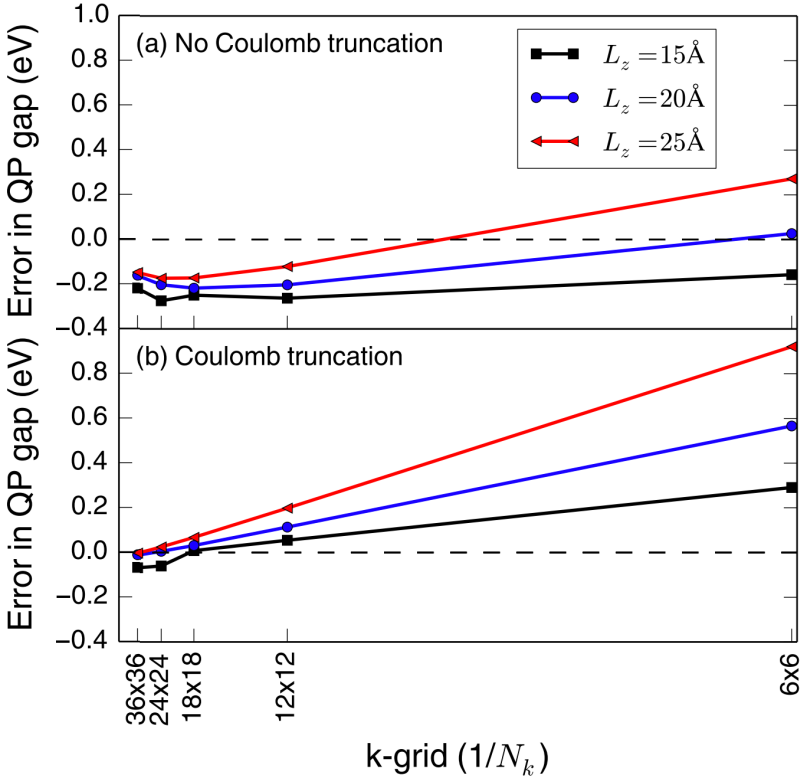
Qiu, Jornada, Louie, PRL 111, 216805 (2013); Qiu, Jornada, Louie, PRB 93, 235435 (2016).

TECHNICAL DETAIL #1: Convergence wrt energy cutoff for QP energies



Qiu, Jornada, Louie, PRL 111, 216805 (2013); Qiu, Jornada, Louie, PRB 93, 235435 (2016).

TECHNICAL DETAIL #2: convergence wrt k-point sampling & cell size



Calculations are hard to converge wrt **k-point sampling** (at least 36x36 at GW vs. 6x6 @ DFT)

In GW calculations on a supercell arrangement (out-of-plane sep. L_z):

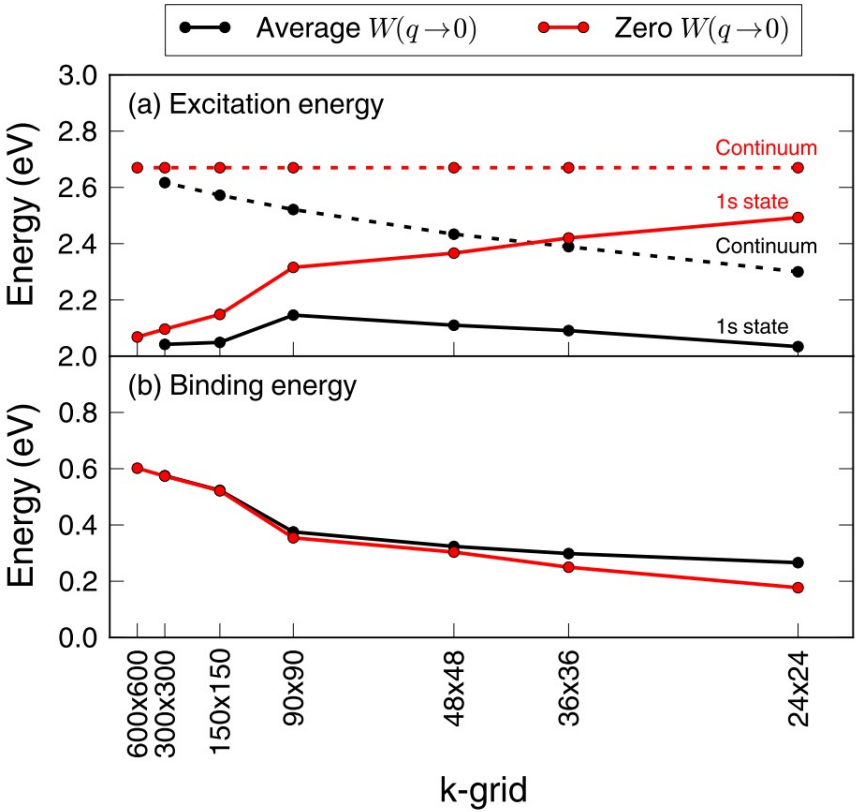
- Polarizability from repeated cells leads to an **overscreening**!
- This effect is hard to converge: decays as $1/L_z$, and couples to k-point sampling.
- Proper solution: truncate the Coulomb interaction:

$$\frac{1}{r} \rightarrow \frac{1}{r}\theta(z_c - |z|)$$

Qiu, Jornada, Louie, PRL 111, 216805 (2013); Qiu, Jornada, Louie, PRB 93, 235435 (2016).

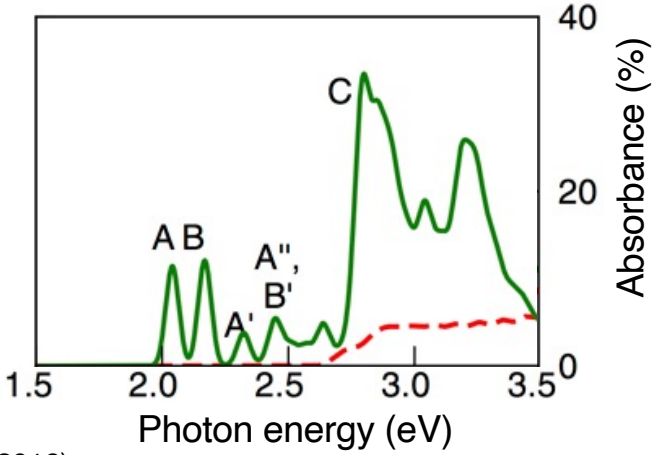
S. Ismail-Beigi, Physical Review B **73**, (2006).

TECHNICAL DETAIL #3: k-point sampling



Even harder to converge exitonic properties!

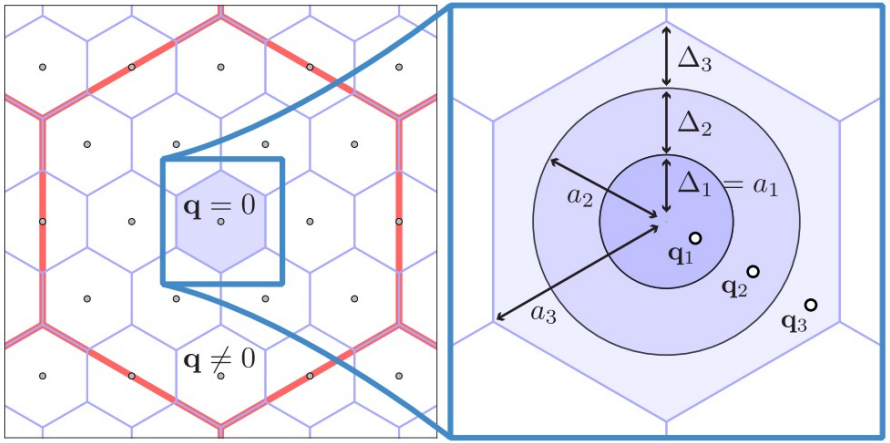
- At least **300x300 k-point sampling** to converge energy difference from 1s to continuum!
- Cancellation of errors if only interested in the binding energy.

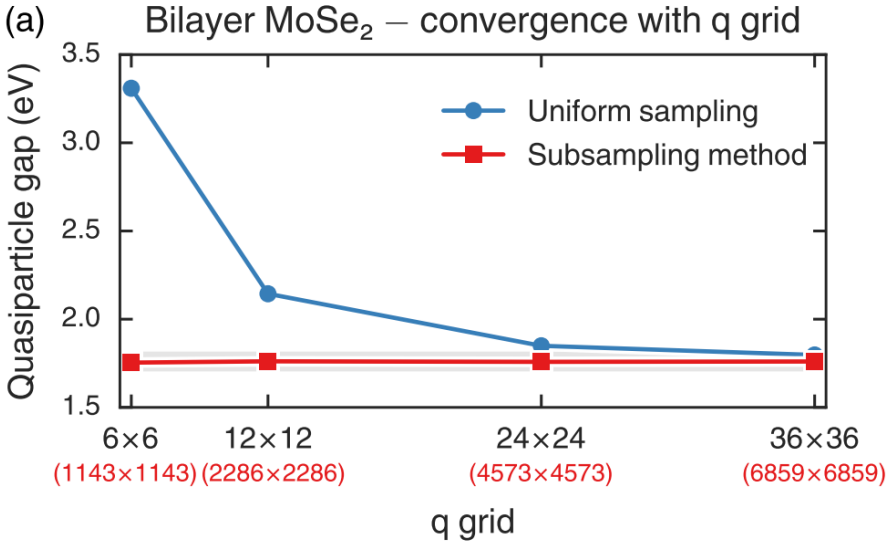


Qiu, Jornada, Louie, PRL 111, 216805 (2013); Qiu, Jornada, Louie, PRB 93, 235435 (2016).

Solution: non-uniform k-point sampling of the BZ

Simple idea: sample more finely (and only radially) $\varepsilon(\mathbf{q})$ for $\mathbf{q}$ close to Γ.
Order of magnitude savings in CPU resources!



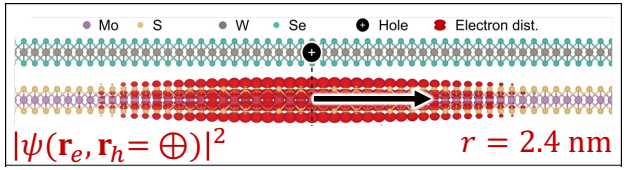


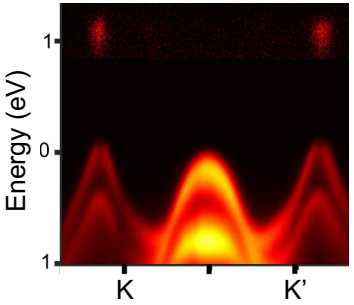
Jornada*, Qiu*, Louie, PRB 95, 035109 (2017).

Final examples:
Optical properties in reduced dimensional materials: dynamics, dephasing, and many-body interactions

Novel excitonic properties in 2D materials

Resolving the exciton localization and wavefunction

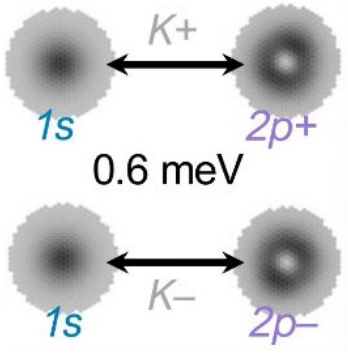




	r (nm)	R_{COM} (nm)
Expt.	2.7	0.8
Theory	2.4	1.3

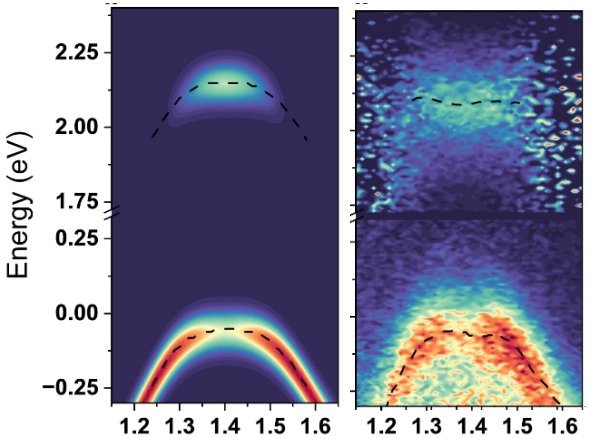
Karni*, …, Jornada, Heinz, Dani, Nature 603, 247 (2022).
Barré, …, Jornada, Heinz, Science 376, 406 (2022).

Angular momentum redistribution in TMDC bilayers



Yao, Wang, Chen, … Jornada, Heinz, Nano Lett. 26, 6820 (2026).

Floquet physics induced by the *excitonic field*

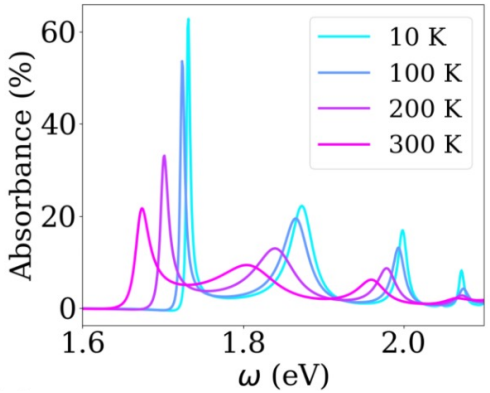


Pareek, …, Jornada*, Dani*, Nat. Phys. 22, 209 (2026).

First-principles methods for exciton dynamics

Exciton linewidth: need for coherent, 2nd-order formalism

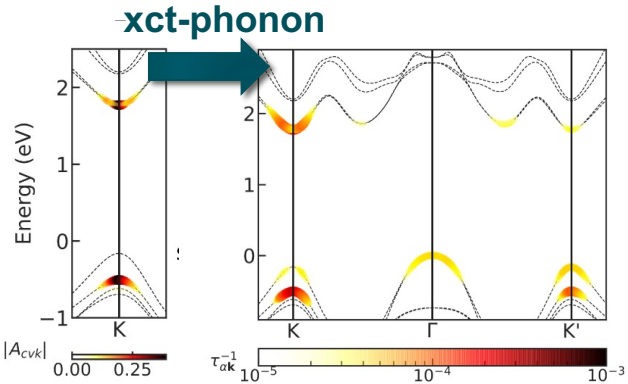
See also: Toyozawa(1958), Toyozawa(1964), Knorr(2016)



Chan*, Haber, Naik, Neaton, Qiu*, Jornada*, Louie*, Nano Lett. 23, 3971 (2023).

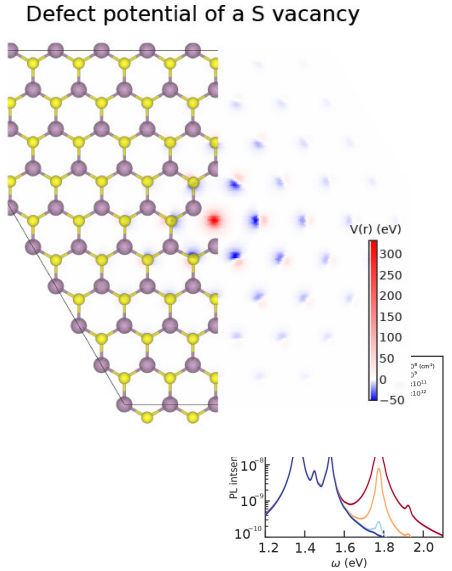
Exciton dynamics in complex TMDC heterostructures

Intralayer exciton: Fano resonance! Need:
~200 excitonic bands
~100 TB for matrix elements!



Chan*, Naik, Haber, Neaton, Louie, Qiu*, Jornada*, Nano Lett. 24, 7972 (2024).

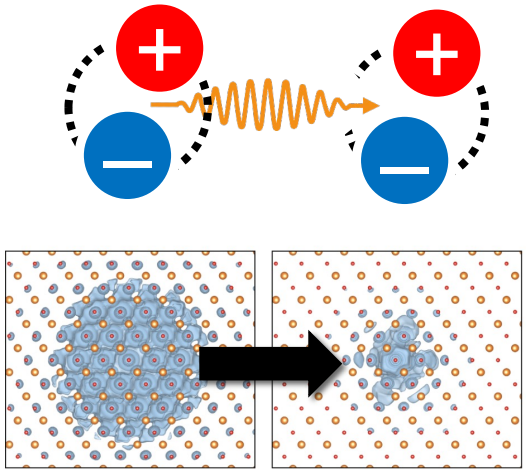
Exciton-defect interactions



Chan, Haber, Naik, Qiu, Jornada, Nano Lett. 26, 961 (2026).

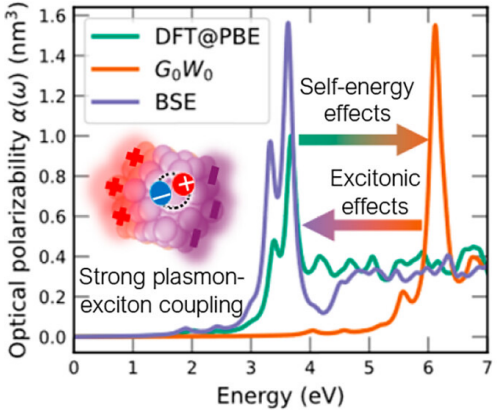
Other frontier problems in first-principles optical spectroscopy

Exciton-polaritons from MBPT & exciton Bohr radius collapse



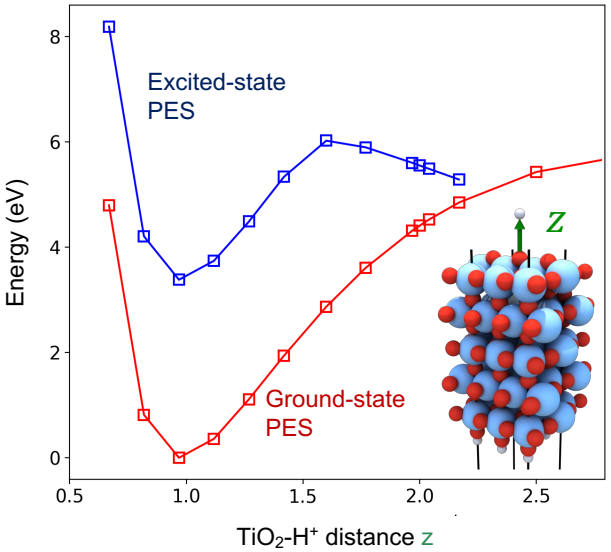
Mauri, Ciccarino, Haber, Qiu, Jornada, PRL 136, 206904 (2026)

Plexcitons in metallic nanoparticles



Simmerman, Altman, Jornada. Nano Lett. 26, 1697 (2026).

Excited-state energy surfaces & chemical reactions



Altman, Jornada, Npj Comput Mater 11, 122 (2025).

Quiz

1. Bound excitons can originate from transitions involving bands other than the VBM to the CBM.

2. For a semiconductor described within a 2-band model, the exciton binding energy cannot exceed the quasiparticle bandgap.

3. Excitonic effects are typically negligible in bulk metals.

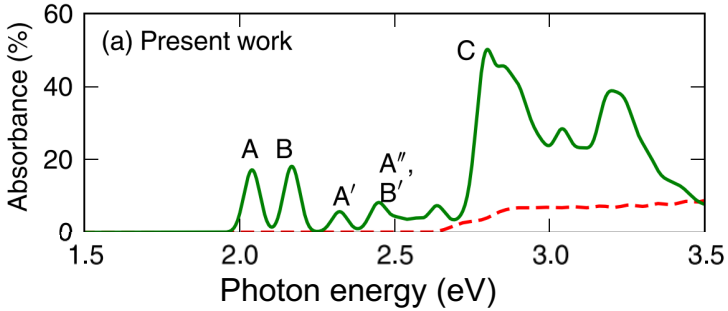
4. There is a continuous of bound exciton states

5. Excitons are detrimental for the performance of PV devices (need to "waste" binding energy to break-up excitons into free carriers).

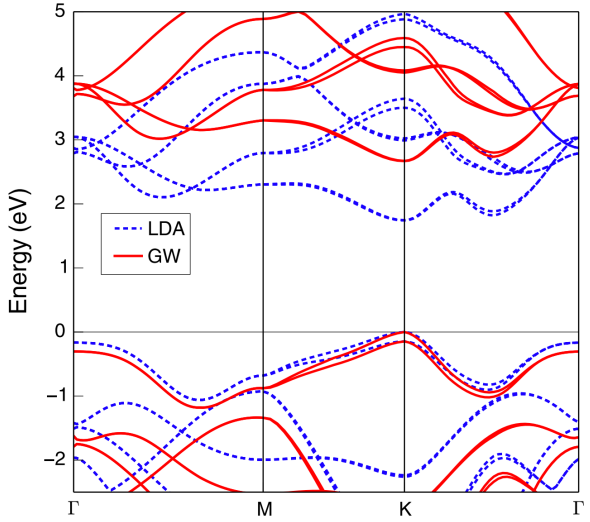
Quiz

1. Bound excitons can originate from transitions involving bands other than the VBM to the CBM.

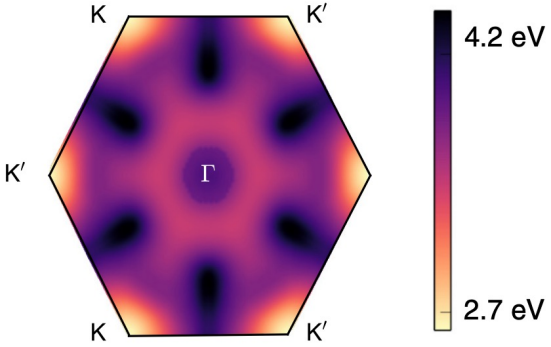
Example: monolayer MoS_2



Qiu, Jornada, Louie, PRL (2013)
Qiu, Jornada, Louie, PRB (2016)



(d) Interband transition energies:



Quiz

1. Bound excitons can originate from transitions involving bands other than the VBM to the CBM.

2. For a semiconductor described within a 2-band model, the exciton binding energy cannot exceed the quasiparticle bandgap.

3. Excitonic effects are typically negligible in bulk metals.

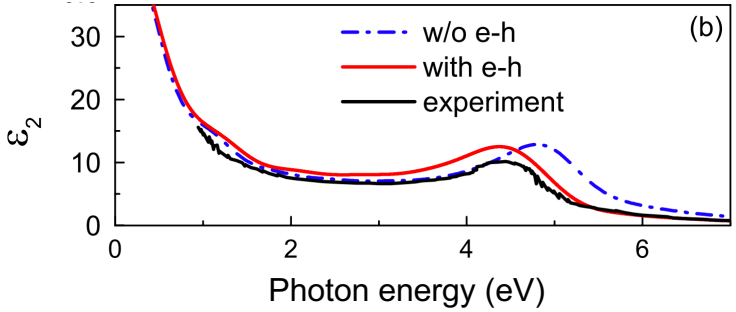
4. There is a continuous of bound exciton states

5. Excitons are detrimental for the performance of PV devices (need to "waste" binding energy to break-up excitons into free carriers).

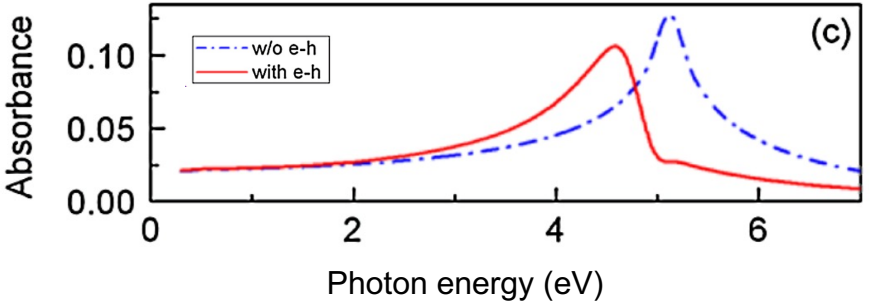
Quiz

3. Excitonic effects are typically negligible in bulk metals.

Graphite



Graphene



Yang, Deslipe, Park, Cohen, Louie (2009)

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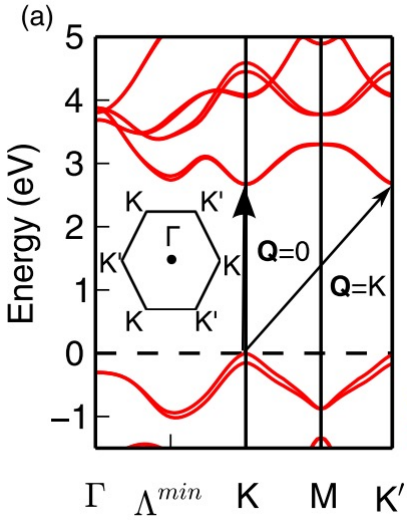
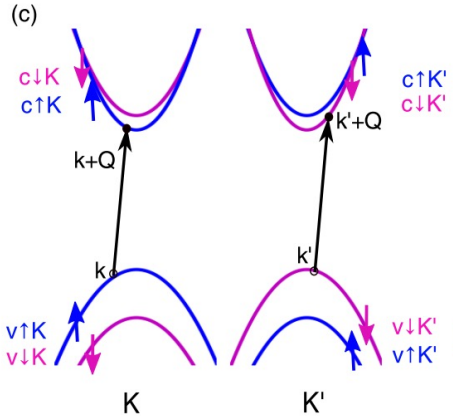
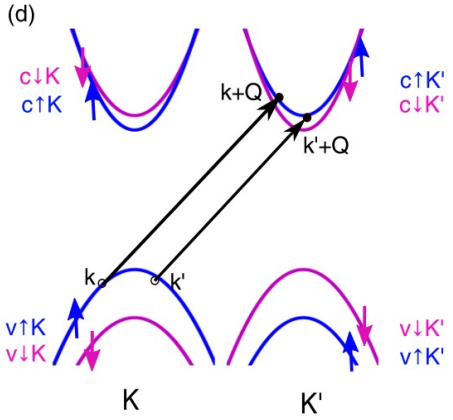
Quiz

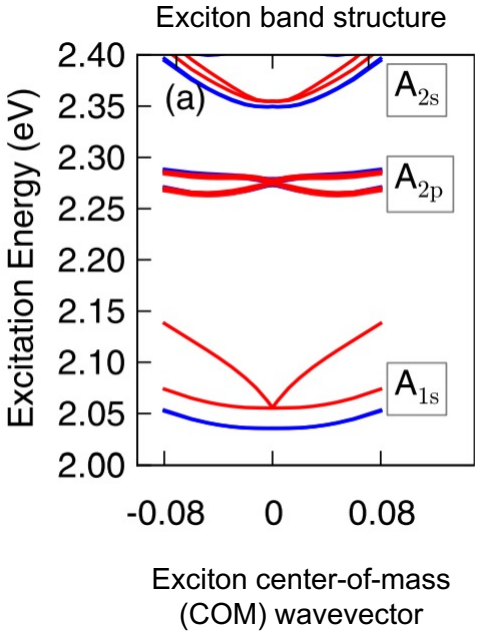
Excitons form bands!
But only $\mathbf{Q} \approx \mathbf{0}$ states are optically accessible.

4. There is a continuous of bound exciton states









Qiu, Cao, Louie, PRL 115, 176801 (2015); Cudazzo et al, PRL 116, 066803 (2016), …

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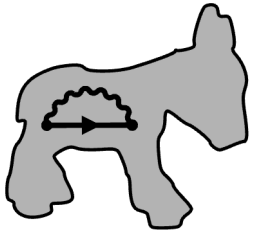

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