# Introduction to the Bethe-Salpeter equation for excitons

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ISTPC 2024

# Acknowledgements


Palaiseau theoretical spectroscopy group

Pierluigi Cudazzo Jaakko Koskelo

# References

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G. Onida, L. Reining, and A. Rubio
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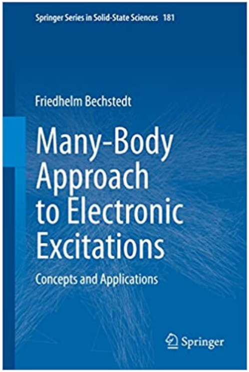
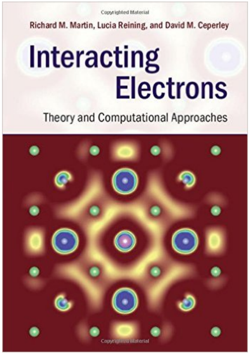
# Books


Springer Series in Solid-State Sciences 181
Friedhelm Bechstedt
Many-Body Approach to Electronic Excitations
Concepts and Applications
Springer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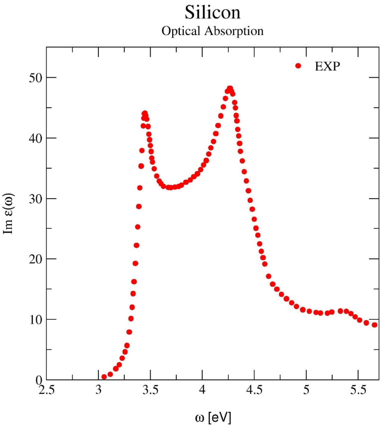
Interacting Electrons
Theory and Computational Approaches

# Outline

# Outline

# Motivation




Exp. at 30 K from: P. Lautenschlager *et al.*, Phys. Rev. B **36**, 4821 (1987).

## Theoretical spectroscopy

- Calculate and reproduce
- Understand and explain
- Predict

$\alpha(\omega) \propto \mathrm{Im}\epsilon(\mathbf{q} \to 0, \omega)$ (extended systems) absorption coefficient

$\sigma(\omega) \propto \mathrm{Im}\epsilon(\mathbf{q} \to 0, \omega)$ (finite systems) photoabsorption cross section

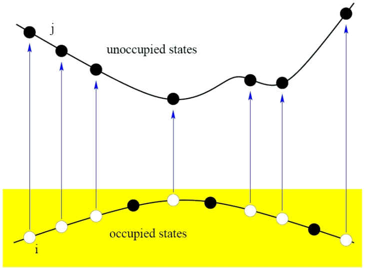
## Theoretical Spectroscopy

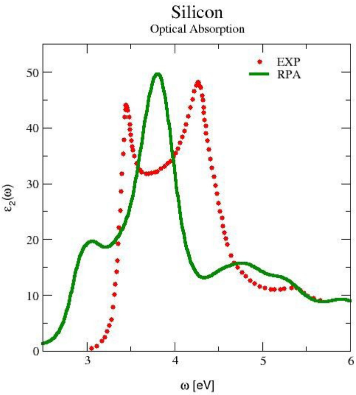
- Which kind of spectra?
- Which kind of tools?

# Independent particles: Kohn-Sham

Independent transitions:

$$\epsilon_2(\omega) = \frac{8\pi^2}{\Omega\omega^2} \sum_{ij} |\langle\varphi_j|\mathbf{e}\cdot\mathbf{v}|\varphi_i\rangle|^2 \delta(\varepsilon_j - \varepsilon_i - \omega)$$



What is wrong?

What is missing?

# GW corrections

## Standard perturbative $G_0W_0$

$$H_0(\mathbf{r})\varphi_i(\mathbf{r}) + V_{xc}(\mathbf{r})\varphi_i(r) = \epsilon_i\varphi_i(\mathbf{r})$$

$$H_0(\mathbf{r})\phi_i(\mathbf{r}) + \int d\mathbf{r}' \; \Sigma(\mathbf{r},\mathbf{r}',\omega = E_i) \; \phi_i(\mathbf{r}') = E_i \, \phi_i(\mathbf{r})$$

First-order perturbative corrections with $\Sigma = iGW$:

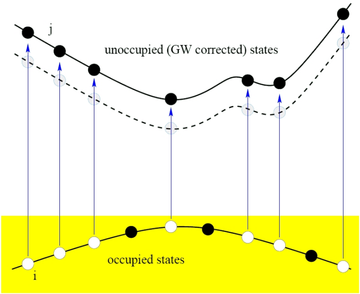
$$E_i - \epsilon_i = \langle\varphi_i|\Sigma - V_{xc}|\varphi_i\rangle$$

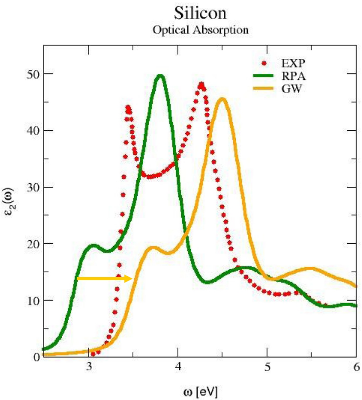
Hybersten and Louie, PRB **34** (1986);
Godby, Schlüter and Sham, PRB **37** (1988)

# Independent (quasi)particles: GW

Independent transitions:

$$\epsilon_2(\omega) = \frac{8\pi^2}{\Omega\omega^2} \sum_{ij} |\langle\varphi_j|\mathbf{e}\cdot\mathbf{v}|\varphi_i\rangle|^2 \delta(E_j - E_i - \omega)$$

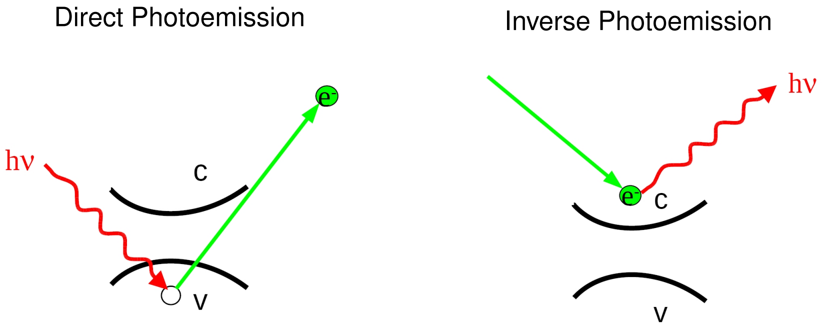


What is wrong?

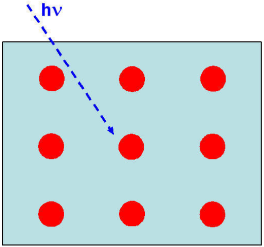
What is missing?

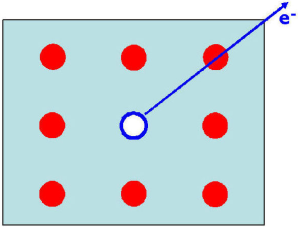
# GW bandstructure: photoemission




One-particle excitations → poles of one-particle Green's function $G$

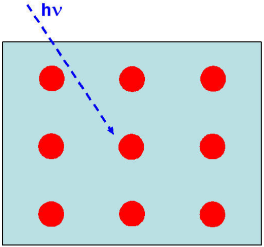
# GW bandstructure: photoemission

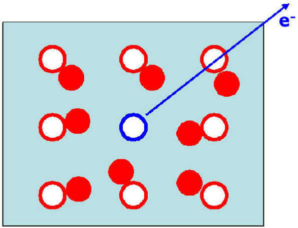



additional charge →

# GW bandstructure: photoemission



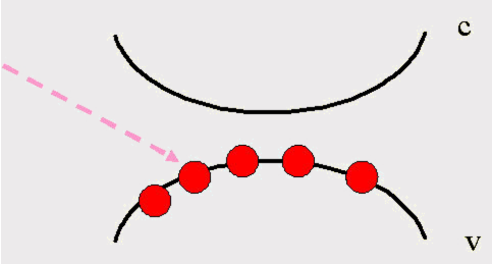




additional charge → reaction: polarization, screening

## GW approximation

1. polarization made of noninteracting electron-hole pairs (RPA)
2. classical (Hartree) interaction between additional charge and polarization charge

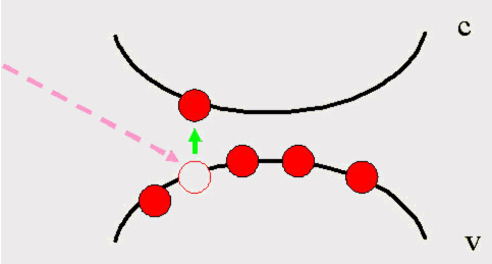
# Absorption




Two-particle excitations → poles of two-particle Green's function

Excitonic effects = electron - hole interaction

# Absorption




Two-particle excitations → poles of two-particle Green's function

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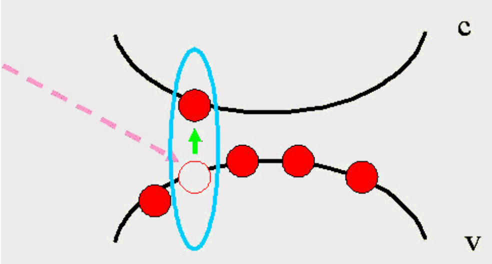
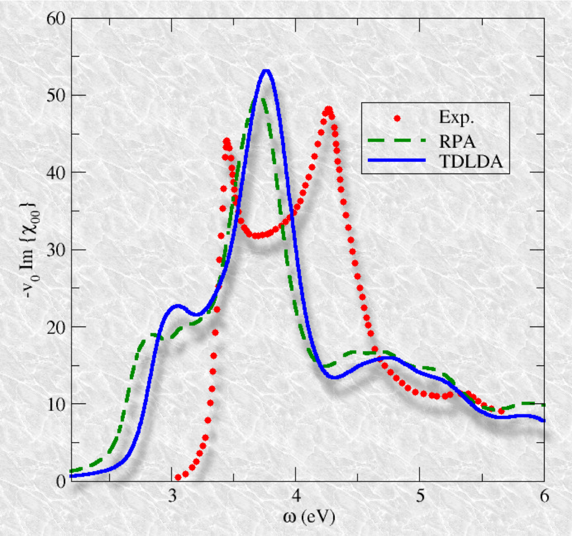
# Absorption




Two-particle excitations → poles of two-particle Green's function

Excitonic effects = electron - hole interaction

# Why do we have to study more than TDDFT?




Bulk silicon: absorption

# TDDFT vs. MBPT: different worlds, same physics

## TDDFT

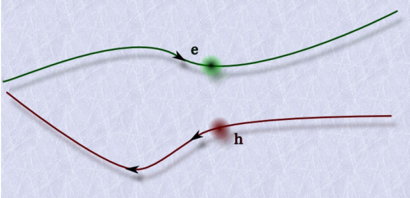
- based on the density: a many-body theory of a collective variable
- moves density around
- response function $\chi$: neutral excitations
- is efficient (simple)

## MBPT

- based on Green's functions
- moves (quasi)particles around
- one-particle $G$: electron addition and removal - GW
  two-particle $L$: electron-hole excitation - BSE
- is intuitive (easy)

# Two-particle correlation function $L$

$$L_0(1234) = -iG(13)G(42)$$

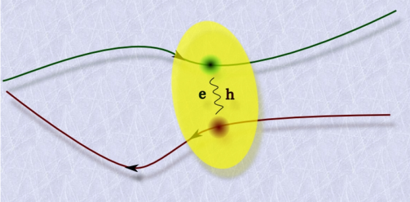



Independent particles

Notation: index 1 stands for space,time (and spin)

# Two-particle correlation function $L$

$$L(1234)$$




Interacting particles (excitonic effects)

Notation: index 1 stands for space,time (and spin)

# Outline

# TDDFT vs. MBPT

## TDDFT

- Key variable: density $\rho(1)$

## MBPT

- Key variable: Green's function $G(12)$

# TDDFT vs. MBPT

## TDDFT

- Key variable: density $\rho(1)$
- Linear response:

$$\chi(12) = \frac{\delta\rho(1)}{\delta V_{ext}(2)}$$

## MBPT

- Key variable: Green's function $G(12)$
- Linear response:

$$L(1234) = -i\frac{\delta G(12)}{\delta V_{ext}(34)}$$

# TDDFT vs. MBPT

## TDDFT

- Key variable: density $\rho(1)$
- Linear response:

$$\chi(12) = \frac{\delta\rho(1)}{\delta V_{ext}(2)}$$

- Dyson equation:

$$\chi(12) = \chi^0(12) + \int d34\chi^0(13)[v(34) + f_{xc}(34)]\chi(42)$$

with $f_{xc}(34) = \delta V_{xc}(3)/\delta\rho(4)$

## MBPT

- Key variable: Green's function $G(12)$
- Linear response:

$$L(1234) = -i\frac{\delta G(12)}{\delta V_{ext}(34)}$$

- Dyson equation = Bethe-Salpeter equation:

$$L(1234) = L_0(1234) + \int d5678L_0(1256)\left[v(57)\delta(56)\delta(78) + i\frac{\delta\Sigma(56)}{\delta G(78)}\right]L(7834)$$

# TDDFT - MBPT connection

## The connection

$$-iG(11^+) = \rho(1) \quad \Rightarrow \quad L(11^+22^+) = \chi(12)$$

Notation: $1^+$ means $r_1 t_1 + \eta$ with $\eta \to 0$

# Reminder: Dyson equation

## Dyson equation

$$G(12) = G_H(12) + \int d34\, G_H(13)[\Sigma(34) + V_{ext}(34)]G(42)$$

where $G_H$ is the Hartree Green's function:

$$G_H(\omega) = (\omega - H_0)^{-1} \Rightarrow G_H^{-1}(\omega) = (\omega - H_0)$$

where $H_0$ is the Hartree Hamiltonian = $T + V_H$

From now on: integration over repeated variables is understood

# Reminder: Dyson equation

## Dyson equation

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where $H_0$ is the Hartree Hamiltonian = $T + V_H$

From now on: integration over repeated variables is understood

## Exercise

$$G^{-1}(12) = G_H^{-1}(12) - \Sigma(12) - V_{ext}(12)$$

# The Bethe-Salpeter equation

## Exercise

Formal derivation

$$L(1234) = -i \frac{\delta G(12)}{\delta V_{ext}(34)}$$

# The Bethe-Salpeter equation

## Exercise

Formal derivation

$$L(1234) = -i\frac{\delta G(12)}{\delta V_{ext}(34)} = +iG(15)\frac{\delta G^{-1}(56)}{\delta V_{ext}(34)}G(62)$$

# The Bethe-Salpeter equation

## Exercise

Formal derivation

$$L(1234) = -i\frac{\delta G(12)}{\delta V_{ext}(34)} = +iG(15)\frac{\delta G^{-1}(56)}{\delta V_{ext}(34)}G(62)$$
$$= +iG(15)\frac{\delta[G_H^{-1}(56) - V_{ext}(56) - \Sigma(56)]}{\delta V_{ext}(34)}G(62)$$

# The Bethe-Salpeter equation

## Exercise

Formal derivation

$$L(1234) = -i\frac{\delta G(12)}{\delta V_{ext}(34)} = +iG(15)\frac{\delta G^{-1}(56)}{\delta V_{ext}(34)}G(62)$$

$$= +iG(15)\frac{\delta[G_H^{-1}(56) - V_{ext}(56) - \Sigma(56)]}{\delta V_{ext}(34)}G(62)$$

$$= -iG(13)G(42) + iG(15)G(62)\left[\frac{\delta V_H(5)\delta(56)}{\delta V_{ext}(34)} - \frac{\delta\Sigma(56)}{\delta V_{ext}(34)}\right]$$

# The Bethe-Salpeter equation

## Exercise

Formal derivation

$$\begin{aligned}
L(1234) &= -i\frac{\delta G(12)}{\delta V_{ext}(34)} = +iG(15)\frac{\delta G^{-1}(56)}{\delta V_{ext}(34)}G(62) \\
&= +iG(15)\frac{\delta[G_H^{-1}(56) - V_{ext}(56) - \Sigma(56)]}{\delta V_{ext}(34)}G(62) \\
&= -iG(13)G(42) + iG(15)G(62)\left[\frac{\delta V_H(5)\delta(56)}{\delta V_{ext}(34)} - \frac{\delta\Sigma(56)}{\delta V_{ext}(34)}\right] \\
&= -iG(13)G(42) + iG(15)G(62)\left[\frac{\delta V_H(5)\delta(56)}{\delta G(78)} - \frac{\delta\Sigma(56)}{\delta G(78)}\right]\frac{\delta G(78)}{\delta V_{ext}(34)}
\end{aligned}$$

# The Bethe-Salpeter equation

## Exercise

Formal derivation

$$L(1234) = -i\frac{\delta G(12)}{\delta V_{ext}(34)} = +iG(15)\frac{\delta G^{-1}(56)}{\delta V_{ext}(34)}G(62)$$

$$= +iG(15)\frac{\delta[G_H^{-1}(56) - V_{ext}(56) - \Sigma(56)]}{\delta V_{ext}(34)}G(62)$$

$$= -iG(13)G(42) + iG(15)G(62)\left[\frac{\delta V_H(5)\delta(56)}{\delta V_{ext}(34)} - \frac{\delta\Sigma(56)}{\delta V_{ext}(34)}\right]$$

$$= -iG(13)G(42) + iG(15)G(62)\left[\frac{\delta V_H(5)\delta(56)}{\delta G(78)} - \frac{\delta\Sigma(56)}{\delta G(78)}\right]\frac{\delta G(78)}{\delta V_{ext}(34)}$$

$$L(1234) = L_0(1234) + L_0(1256)\left[v(57)\delta(56)\delta(78) + i\frac{\delta\Sigma(56)}{\delta G(78)}\right]L(7834)$$

# The Bethe-Salpeter equation in the GW approximation

## Approximations

$$L = L_0 + L_0\left(v + i\frac{\delta\Sigma}{\delta G}\right)L$$

# The Bethe-Salpeter equation in the GW approximation

## Approximations

$$L = L_0 + L_0\left(v + i\frac{\delta\Sigma}{\delta G}\right)L$$

Approximation:

$\Sigma \approx iGW$

# The Bethe-Salpeter equation in the GW approximation

## Approximations

$$L = L_0 + L_0 \left( v - \frac{\delta(GW)}{\delta G} \right) L$$

Approximation:

$$\Sigma \approx iGW \qquad \frac{\delta(GW)}{\delta G} = W + G\frac{\delta W}{\delta G} \approx W$$

# The Bethe-Salpeter equation in the GW approximation

## Approximations

We finally obtain:

$$L = L_0 + L_0(v - W)L$$

# Static BSE

## Further approximation: Cancellations between

1. Quasiparticle approximation to $G$ in $L_0(1234) = -iG(13)G(42)$
   $\Rightarrow$ Only GW quasiparticle energies $E_i$ at the place of Kohn-Sham eigenvalues $\epsilon_i$
2. Static approximation to $W$

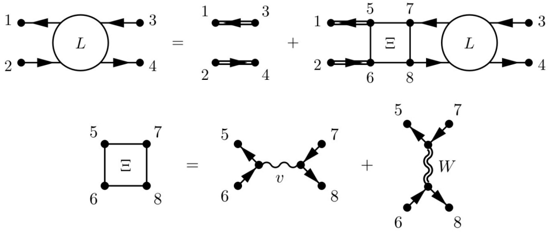
$$W(\mathbf{r}_1, \mathbf{r}_2, t_1 - t_2) \Rightarrow W(\mathbf{r}_1, \mathbf{r}_2, \omega = 0)\delta(t_1 - t_2)$$

F. Bechstedt *et al.* Phys. Rev. Lett. **78** (1997).
P. Cudazzo and L. Reining, Phys. Rev. Research **2** (2020)

# The Bethe-Salpeter equation in the GW approximation

## The Bethe-Salpeter equation in the GW approximation

$$L(1234) = L_0(1234) + L_0(1256)[v(57)\delta(56)\delta(78) - W(56)\delta(57)\delta(68)]L(7834)$$




- $v$ = repulsive e-h exchange interaction (dipole-dipole type)
- $W$ = attractive e-h direct interaction (monopole-monopole type)

# Outline

## Absorption

$$\mathrm{Abs}(\omega) = \lim_{\mathbf{q}\to 0} \mathrm{Im}\epsilon_M(\mathbf{q},\omega)$$

$$\mathrm{Abs}(\omega) = -\lim_{\mathbf{q}\to 0} \mathrm{Im}\left[v_{\mathbf{G}=0}(\mathbf{q})\bar{\chi}_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega)\right]$$

$$\bar{\chi} = P + P\bar{v}\bar{\chi}$$

Absorption $\rightarrow$ response to $V_{ext} + V_{ind}^{macro}$

## EELS

$$\mathrm{EELS}(\omega) = -\lim_{\mathbf{q}\to 0} \mathrm{Im}[1/\epsilon_M(\mathbf{q},\omega)]$$

$$\mathrm{EELS}(\omega) = -\lim_{\mathbf{q}\to 0} \mathrm{Im}\left[v_{\mathbf{G}=0}(\mathbf{q})\chi_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega)\right]$$

$$\chi = P + P(v_0 + \bar{v})\chi$$

EELS $\rightarrow$ response to $V_{ext}$

# Micro-macro connection

## Microscopic-Macroscopic connection: local fields

$$\epsilon_M(\mathbf{q},\omega) = 1 - v_{\mathbf{G}=0}(\mathbf{q})\bar{\chi}_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega)$$

$$\bar{\chi}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = P_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) + P_{\mathbf{G},\mathbf{G}_1}(\mathbf{q},\omega)\bar{v}_{\mathbf{G}_1}(\mathbf{q})\bar{\chi}_{\mathbf{G}_1,\mathbf{G}'}(\mathbf{q},\omega)$$

$$\bar{v}_{\mathbf{G}}(\mathbf{q}) = \begin{cases} 0 & \text{for } \mathbf{G} = 0 \\ v_{\mathbf{G}}(\mathbf{q}) & \text{for } \mathbf{G} \neq 0 \end{cases}$$

Hanke, Adv. Phys. **27** (1978).

# Micro-macro connection

## Microscopic-Macroscopic connection: local fields

$$\chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = P_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) + P_{\mathbf{G},\mathbf{G}_1}(\mathbf{q},\omega) v_{\mathbf{G}_1}(\mathbf{q}) \chi_{\mathbf{G}_1,\mathbf{G}'}(\mathbf{q},\omega)$$

$$\epsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \delta_{\mathbf{G},\mathbf{G}'} + v_{\mathbf{G}}(\mathbf{q}) \chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$$

$$\epsilon_M(\mathbf{q},\omega) = \frac{1}{\epsilon^{-1}_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega)}$$

Adler, Phys. Rev. **126** (1962); Wiser, Phys. Rev. **129** (1963).

# Solving BSE

$$L(1234) = L_0(1234) + L_0(1256)[v(57)\delta(56)\delta(78) - W(56)\delta(57)\delta(68)]L(7834)$$

# Solving BSE

$$\bar{L}(1234) = L_0(1234) + L_0(1256)[\bar{v}(57)\delta(56)\delta(78) - W(56)\delta(57)\delta(68)]\bar{L}(7834)$$

# Solving BSE

$$\bar{L}(1234) = L_0(1234) + L_0(1256)[\bar{v}(57)\delta(56)\delta(78) - W(56)\delta(57)\delta(68)]\bar{L}(7834)$$

## Static $W$

Simplification:

$$W(\mathbf{r}_1, \mathbf{r}_2, t_1 - t_2) \Rightarrow W(\mathbf{r}_1, \mathbf{r}_2)\delta(t_1 - t_2)$$

$$\bar{L}(1234) \Rightarrow \bar{L}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4, t - t') \Rightarrow \bar{L}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4, \omega)$$

# Solving BSE

## Dielectric function

$$\bar{L}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4\omega) = L_0(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4\omega) + \int d\mathbf{r}_5 d\mathbf{r}_6 d\mathbf{r}_7 d\mathbf{r}_8\, L_0(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_5\mathbf{r}_6\omega)\times$$
$$\times\,[\bar{v}(\mathbf{r}_5\mathbf{r}_7)\delta(\mathbf{r}_5\mathbf{r}_6)\delta(\mathbf{r}_7\mathbf{r}_8) - W(\mathbf{r}_5\mathbf{r}_6)\delta(\mathbf{r}_5\mathbf{r}_7)\delta(\mathbf{r}_6\mathbf{r}_8)]\bar{L}(\mathbf{r}_7\mathbf{r}_8\mathbf{r}_3\mathbf{r}_4\omega)$$

$$\epsilon_M(\omega) = 1 - \lim_{\mathbf{q}\to 0}\left[v_{\mathbf{G}=0}(\mathbf{q})\int d\mathbf{r}d\mathbf{r}'\, e^{-i\mathbf{q}(\mathbf{r}-\mathbf{r}')}\bar{L}(\mathbf{r},\mathbf{r},\mathbf{r}',\mathbf{r}',\omega)\right]$$

# Solving BSE

$$\bar{L}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4\omega) = L_0(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4\omega) + \int d\mathbf{r}_5 d\mathbf{r}_6 d\mathbf{r}_7 d\mathbf{r}_8 \, L_0(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_5\mathbf{r}_6\omega) \times$$
$$\times \left[\bar{v}(\mathbf{r}_5\mathbf{r}_7)\delta(\mathbf{r}_5\mathbf{r}_6)\delta(\mathbf{r}_7\mathbf{r}_8) - W(\mathbf{r}_5\mathbf{r}_6)\delta(\mathbf{r}_5\mathbf{r}_7)\delta(\mathbf{r}_6\mathbf{r}_8)\right]\bar{L}(\mathbf{r}_7\mathbf{r}_8\mathbf{r}_3\mathbf{r}_4\omega)$$

How to solve it?

# Solving BSE

$$\bar{L}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4\omega) = L_0(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4\omega) + \int d\mathbf{r}_5 d\mathbf{r}_6 d\mathbf{r}_7 d\mathbf{r}_8\, L_0(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_5\mathbf{r}_6\omega)\times$$
$$\times\, [\bar{v}(\mathbf{r}_5\mathbf{r}_7)\delta(\mathbf{r}_5\mathbf{r}_6)\delta(\mathbf{r}_7\mathbf{r}_8) - W(\mathbf{r}_5\mathbf{r}_6)\delta(\mathbf{r}_5\mathbf{r}_7)\delta(\mathbf{r}_6\mathbf{r}_8)]\bar{L}(\mathbf{r}_7\mathbf{r}_8\mathbf{r}_3\mathbf{r}_4\omega)$$

How to solve it?

## Transition space

$$\bar{L}_{(n_1 n_2)(n_3 n_4)}(\omega) = \langle \phi^*_{n_1}(\mathbf{r}_1)\phi_{n_2}(\mathbf{r}_2)|\bar{L}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4\omega)|\phi^*_{n_3}(\mathbf{r}_3)\phi_{n_4}(\mathbf{r}_4)\rangle = \langle\langle \bar{L}\rangle\rangle$$

## Exercise

$$L_0(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4, \omega) = \sum_{ij} (f_j - f_i) \frac{\phi_i^*(\mathbf{r}_1)\phi_j(\mathbf{r}_2)\phi_i(\mathbf{r}_3)\phi_j^*(\mathbf{r}_4)}{\omega - (E_i - E_j)}$$

Calculate:

$$\langle\langle L_0 \rangle\rangle = \frac{f_{n_1} - f_{n_2}}{\omega - (E_{n_2} - E_{n_1})} \delta_{n_1 n_3} \delta_{n_2 n_4}$$

# Solving BSE

## BSE in transition space

We consider only resonant optical transitions
for a nonmetallic system: $(n_1 n_2) = (v\mathbf{k}c\mathbf{k}) \Rightarrow (vc)$

$$\bar{L} = L_0 + L_0(\bar{v} - W)\bar{L}$$

$$\bar{L} = [1 - L_0(\bar{v} - W)]^{-1} L_0$$

$$\bar{L} = [L_0^{-1} - (\bar{v} - W)]^{-1}$$

$$\bar{L}_{(vc)(v'c')}(\omega) = [(E_c - E_v - \omega)\delta_{vv'}\delta_{cc'} + (f_v - f_c)\langle\langle\bar{v} - W\rangle\rangle]^{-1}(f_{c'} - f_{v'})$$

# Solving BSE

$$\bar{L}_{(vc)(v'c')}(\omega) = [(E_c - E_v - \omega)\delta_{vv'}\delta_{cc'} + (f_v - f_c)\langle\langle \bar{v} - W \rangle\rangle]^{-1}(f_{c'} - f_{v'})$$

# Solving BSE

$$\bar{L}_{(vc)(v'c')}(\omega) = [(E_c - E_v - \omega)\delta_{vv'}\delta_{cc'} + (f_v - f_c)\langle\langle \bar{v} - W\rangle\rangle]^{-1}(f_{c'} - f_{v'})$$

$$\bar{L} \rightarrow [H_{exc} - \omega I]^{-1}$$

$$H_{exc}^{(vc)(v'c')} = (E_c - E_v)\delta_{vv'}\delta_{cc'} + (f_v - f_c)\langle vc|\bar{v} - W|v'c'\rangle$$

# Solving BSE

## Excitonic hamiltonian

$$H_{exc}^{(vc)(v'c')} = (E_c - E_v)\delta_{vv'}\delta_{cc'} + (f_v - f_c)\langle vc|\bar{v} - W|v'c'\rangle$$

## Spectral representation of a hermitian operator

$$[H_{exc} - \omega I]^{-1} = \sum_\lambda \frac{|A_\lambda\rangle\langle A_\lambda|}{E_\lambda - \omega}$$

$$H_{exc}A_\lambda = E_\lambda A_\lambda$$

$$\bar{L}_{(vc)(v'c')}(\omega) = \sum_\lambda \frac{A_\lambda^{(vc)} A_\lambda^{*(v'c')}}{E_\lambda - \omega}(f_{c'} - f_{v'})$$

# Absorption spectra in BSE

## Excitonic hamiltonian

$$H_{exc} A_\lambda = E_\lambda A_\lambda$$

$$H_{exc}^{(vc)(v'c')} = (E_c - E_v)\delta_{vv'}\delta_{cc'} + (f_v - f_c)\langle vc|\bar{v} - W|v'c'\rangle$$

## Matrix elements

$$\langle vc|\bar{v}|v'c'\rangle = 2\int dr_1 \int dr_2 \phi_v(r_1)\phi_c^*(r_1)\bar{v}(r_1, r_2)\phi_{v'}^*(r_2)\phi_{c'}(r_2)$$

$$\langle vc| - W|v'c'\rangle = -\int dr_1 \int dr_2 \phi_v(r_1)\phi_{v'}^*(r_1)W(r_1, r_2)\phi_c^*(r_2)\phi_{c'}(r_2)$$

## Absorption spectrum

$$Abs(\omega) \propto \sum_\lambda \Big| \sum_{vc} A_\lambda^{(vc)} \langle v|D|c\rangle \Big|^2 \delta(E_\lambda - \omega)$$

# Absorption spectra in BSE

## Independent (quasi)particles

$$Abs(\omega) \propto \sum_{vc} |\langle v|D|c\rangle|^2 \delta(E_c - E_v - \omega)$$

## Excitonic effects

$$[H_{el} + H_{hole} + H_{el-hole}]A_\lambda = E_\lambda A_\lambda$$

$$Abs(\omega) \propto \sum_{\lambda} |\sum_{vc} A_\lambda^{(vc)} \langle v|D|c\rangle|^2 \delta(E_\lambda - \omega)$$

- mixing of transitions: $|\langle v|D|c\rangle|^2 \rightarrow |\sum_{vc} A_\lambda^{(vc)} \langle v|D|c\rangle|^2$
- modification of excitation energies: $E_c - E_v \rightarrow E_\lambda$

# BSE calculations

## A three-step method

1. LDA calculation
   $\Rightarrow$ Kohn-Sham wavefunctions $\varphi_i$
2. GW calculation
   $\Rightarrow$ GW energies $E_i$ and screened Coulomb interaction $W$
3. BSE calculation

   solution of $H_{exc} A_\lambda = E_\lambda A_\lambda$ with:

   $$H_{exc}^{(vc)(v'c')} = (E_c - E_v)\delta_{vv'}\delta_{cc'} + (f_v - f_c)\langle vc|\bar{v} - W|v'c'\rangle$$

   $\Rightarrow$ excitonic eigenstates $A_\lambda, E_\lambda$
   $\Rightarrow$ spectra $\epsilon_M(\omega)$

# Screening the Coulomb interaction

## Bethe-Salpeter equation: GW approximation

$$L(1234) = L_0(1234) + L_0(1256)[v(57)\delta(56)\delta(78) - W(56)\delta(57)\delta(68)]L(7834)$$

# Screening the Coulomb interaction

**Bethe-Salpeter equation: Hartree-Fock approximation**

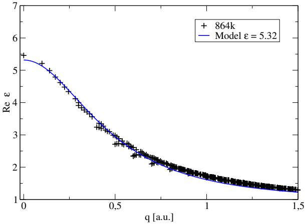
$$L(1234) = L_0(1234) + L_0(1256)[v(57)\delta(56)\delta(78) - v(56)\delta(57)\delta(68)]L(7834)$$

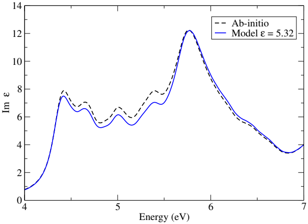
$$W = \epsilon^{-1} v$$

GW with no screening is Hartree-Fock

BSE with no screening is time-dependent Hartree-Fock

# Screening the Coulomb interaction




Silver chloride, A. Lorin *et al.*, PRB 104 (2021)

## Model dielectric function

$$\epsilon(q) = 1 + \frac{1}{\frac{1}{\epsilon(q{=}0)-1} + \alpha\left(\frac{q}{q_{TF}}\right)^2 + \frac{q^4}{4\omega_p}}.$$

G. Cappellini *et al.*, PRB 47 (1993).

Note the similarities with TDDFT hybrids (with local range separation)

# Adiabatic TDDFT vs. BSE

## Bethe-Salpeter equation

- Non-local self-energy: $V_{ext}(1) + V_H(1) + \Sigma(1,2)$
- Four-point Dyson equation:
  $L(1234) = L_0(1234) + L_0(1256)\left[v(57)\delta(56)\delta(78) + i\frac{\delta\Sigma(56)}{\delta G(78)}\right]L(7834)$
- Matrix elements (excitonic hamiltonian):

$$\langle vc|v|v'c'\rangle = 2\int dr_1 dr_2 \phi_v(r_1)\phi_c^*(r_1)v(r_1,r_2)\phi_{v'}^*(r_2)\phi_{c'}(r_2)$$

$$\langle vc| - W|v'c'\rangle = -\int dr_1 dr_2 \phi_v(r_1)\phi_{v'}^*(r_1)W(r_1,r_2)\phi_c^*(r_2)\phi_{c'}(r_2)$$

## Adiabatic TDDFT

- Local Kohn-Sham potential: $V_{ext}(1) + V_H(1) + V_{xc}(1)$
- Two-point Dyson equation: $\chi(12) = \chi^0(12) + \chi^0(13)[v(34) + f_{xc}(34)]\chi(42)$
- Matrix elements (Casida equation):

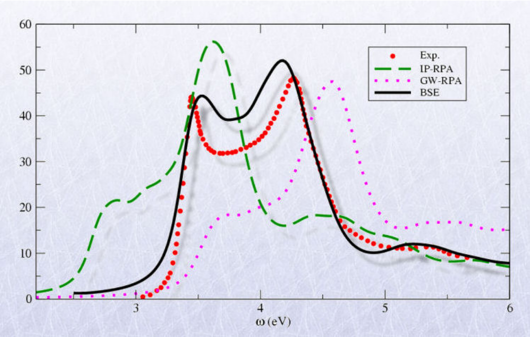
$$\langle vc|v|v'c'\rangle = 2\int dr_1 dr_2 \phi_v(r_1)\phi_c^*(r_1)v(r_1,r_2)\phi_{v'}^*(r_2)\phi_{c'}(r_2)$$

$$\langle vc|f_{xc}|v'c'\rangle = 2\int dr_1 dr_2 \phi_v(r_1)\phi_c^*(r_1)f_{xc}(r_1,r_2)\phi_{v'}^*(r_2)\phi_{c'}(r_2)$$

# Outline

# Continuum excitons

Bulk silicon

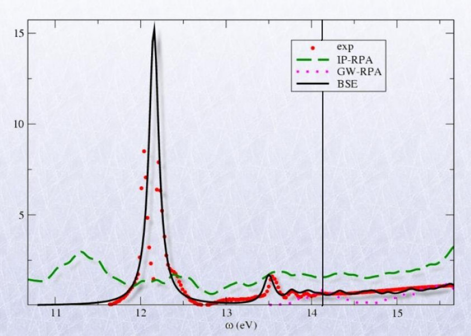



G. Onida, L. Reining, and A. Rubio, RMP **74** (2002).

# Bound excitons

$$\text{Binding energy} = E_{GW}^{gap} - E_\lambda$$

Solid argon

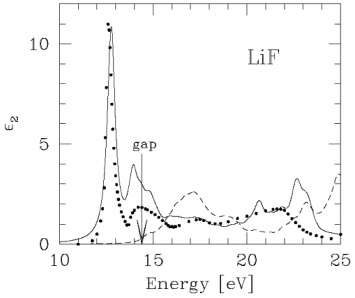


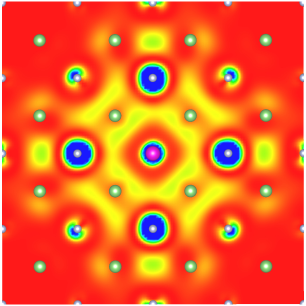

F. Sottile *et al.* PRB **76** (2007).

# Exciton analysis

Exciton amplitude: $\Psi_\lambda(\mathbf{r}_h, \mathbf{r}_e) = \sum_{vc} A_\lambda^{(vc)} \phi_v^*(\mathbf{r}_h)\phi_c(\mathbf{r}_e)$

Lithium Fluoride: fix $\bar{\mathbf{r}}_h$ and plot $|\Psi_\lambda(\bar{\mathbf{r}}_h, \mathbf{r}_e)|^2$

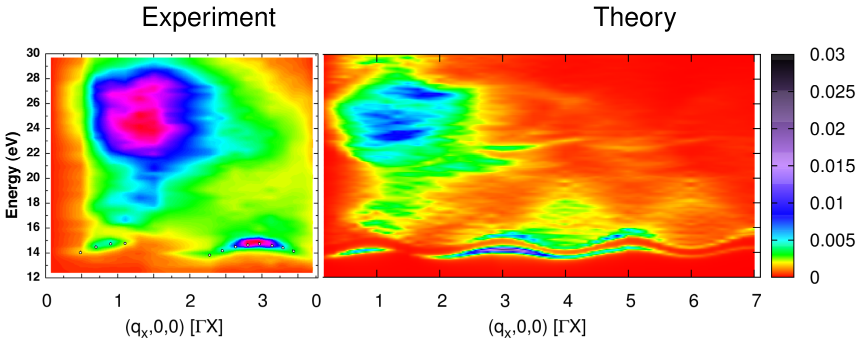


M. Rohlfing and S. G. Louie, PRL **81** (1998); M. Gatti and F. Sottile, PRB **88** (2013).

# Exciton dispersion: IXS

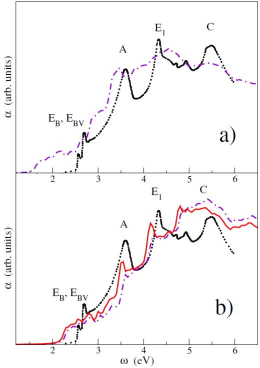
Lithium Fluoride




P. Abbamonte *et al.*, PNAS **105** (2008); M. Gatti and F. Sottile, PRB **88** (2013).

# Self-consistency in the BSE

Difference between $G_0W_0$ and QSGW ingredients in the BSE: $Cu_2O$




F. Bruneval *et al.*, PRL **97** (2006)

# Finite systems: atoms and molecules

## Molecular systems

Calculations of vertical excitation energies $E_\lambda$ from full BSE matrix

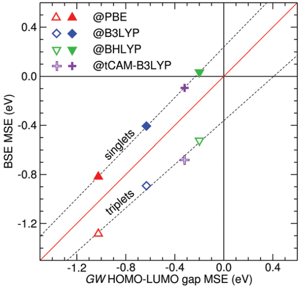
$$\begin{pmatrix} R & C \\ -C^* & -R^* \end{pmatrix} \begin{pmatrix} X_\lambda \\ Y_\lambda \end{pmatrix} = E_\lambda \begin{pmatrix} X_\lambda \\ Y_\lambda \end{pmatrix}$$

- Benchmarks of singlet/triplet energies with respect to accurate quantum chemical methods
- Assessment of quality of ingredients (different levels of self-consistency)
- Charge-transfer excitations $E_{CT}(R) = EA - IP - 1/R$

Reviewed in: X. Blase, I. Duchemin, D. Jacquemin, Chem. Soc. Rev. **47** (2018)

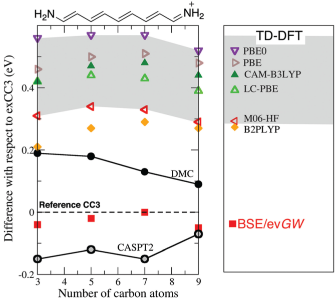
# Finite systems: atoms and molecules

Mean-signed errors for Thiel's set




F. Bruneval *et al.*
J. Chem. Phys. **142** (2015).

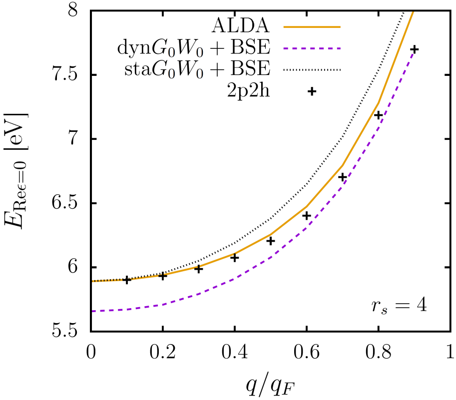
Errors for streptocyanine chains




P. Boulanger *et al.*
J. Chem. Theory Comput. **10** (2014)

# Problem of consistency

Plasmon dispersion in HEG




Jaakko Koskelo *et al.*, arXiv:2301.00474.

# Missing dynamical effects

## Beyond static BSE

- Correction to excitation energies and spectra
  G. Strinati, PRL **49** (1982) and PRB **29** (1984); M. Rohlfing and S. G. Louie, PRB **62** (2000); A. Marini and R. Del Sole, PRL **91** (2003); Y. Ma, M. Rohlfing, and C. Molteni, PRB **80** (2009); S. Gao *et al.*, Nanolett. **16** (2016); P. F. Loos and X. Blase, J. Chem. Phys. **153** (2020)

# Missing dynamical effects

## Beyond static BSE

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- Multiple excitations in molecules (and also solids: *dd* excitations and double plasmons)
  P. Romaniello *et al.*, J. Chem. Phys. **130** (2009); D. Sangalli *et al.*, J. Chem. Phys 134 (2011); E. Rebolini and J. Toulouse, J. Chem. Phys. **144** (2016); V. Olevano, J. Toulouse, and P. Schuck, J. Chem. Phys. **150** (2019).

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## Beyond static BSE

- Correction to excitation energies and spectra
  G. Strinati, PRL **49** (1982) and PRB **29** (1984); M. Rohlfing and S. G. Louie, PRB **62** (2000); A. Marini and R. Del Sole, PRL **91** (2003); Y. Ma, M. Rohlfing, and C. Molteni, PRB **80** (2009); S. Gao *et al.*, Nanolett. **16** (2016); P. F. Loos and X. Blase, J. Chem. Phys. **153** (2020)
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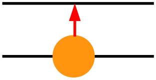
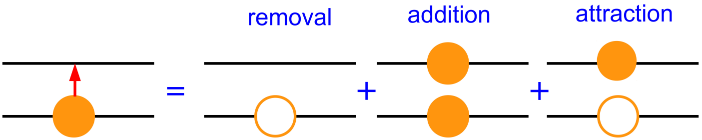
- Exciton self-energy and cumulant expansion (coupling with bosons)
  P. Cudazzo and L. Reining, Phys. Rev. Research **2** (2020)

# One electron limit: A detour?



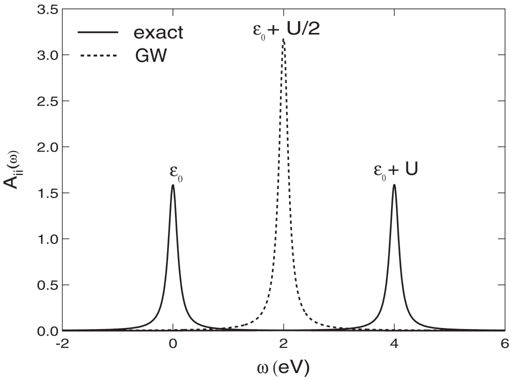
# One electron limit: A detour?




Perfect cancellation

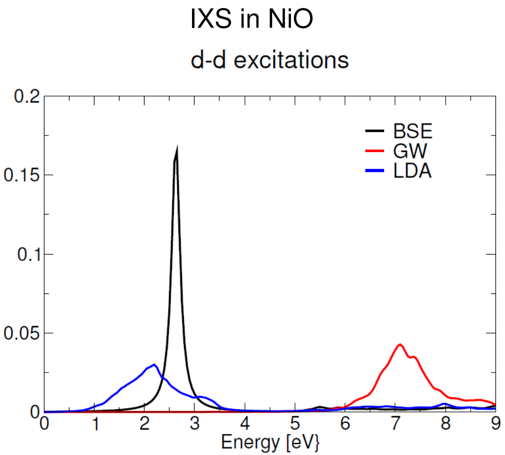
# One electron limit: A detour?

Atomic limit of Hubbard dimer with one spin-up electron: addition of one spin-down electron




P. Romaniello, S. Guyot, and L. Reining JCP **131** (2009).

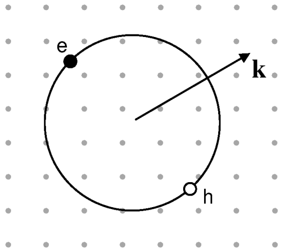
# Problem of consistency



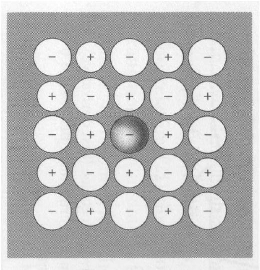
# Outline

# Wannier and Frenkel excitons

Wannier exciton




Frenkel exciton



weakly bound: delocalised over many lattice sites

*semiconductors*

tightly bound: localised on few sites

*wide gap insulators*

R. S. Knox, *Theory of Excitons* (1963); C. Kittel, *Introduction to Solid State Physics*

# The Wannier model

## Bethe-Salpeter equation

$$H_{exc} A_\lambda = E_\lambda A_\lambda$$

$$H_{exc}^{(vc)(v'c')} = (E_c - E_v)\delta_{vv'}\delta_{cc'} + \langle\langle \bar{v} - W \rangle\rangle$$

## Wannier model

- two parabolic bands

$$E_c - E_v = E_g + \frac{k^2}{2\mu} \quad \rightarrow \quad -\frac{\nabla^2}{2\mu}$$

- no local fields ($\bar{v} = 0$) and effective screened $W$

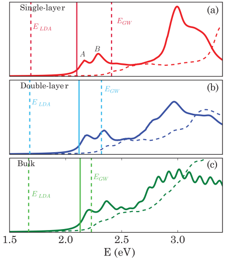
$$W(\mathbf{r}, \mathbf{r}') = \frac{1}{\epsilon|\mathbf{r} - \mathbf{r}'|}$$

- solution = Rydberg series for effective H atom

$$E_\lambda = E_g - \frac{R_{eff}}{\lambda^2} \quad \text{with} \quad R_{eff} = \frac{\mu}{2\epsilon^2}$$

# Two dimensions

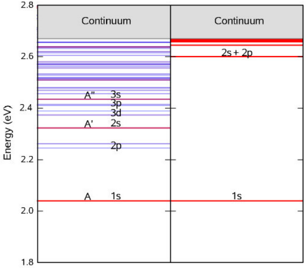
## Larger binding energy




MoS$_2$ absorption spectrum

A. Molina Sanchez *et al.*, PRB **88** (2013).

## Non-hydrogenic series




Exciton energies

E.g. A. Chernikov *et al.*, PRL **113** (2014).

## Macroscopic interaction in 2D

$$W(r) = \frac{1}{4\alpha_{2D}} \left[ H_0\left(\frac{r}{r_0}\right) - Y_0\left(\frac{r}{r_0}\right) \right]$$

$r_0 = 2\pi\alpha_{2D}$ and $H_0, Y_0$ Struve and Bessel functions 2nd kind

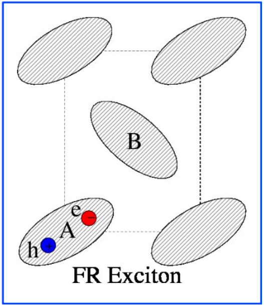
L.V. Keldysh, JETP Lett. **29** (1979); P. Cudazzo, I.V. Tokatly, A. Rubio, PRB **84** (2011).

# Frenkel and charge transfer excitons

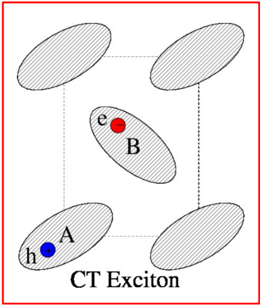
When electrons are localised
(wavefunctions with small overlap)

$$\hat{H}_{ex} = \begin{pmatrix} \hat{H}^{FR} & \hat{H}^{hopping} \\ \hat{H}^{hopping} & \hat{H}^{CT} \end{pmatrix}$$

Frenkel exciton




Charge transfer exciton



# Frenkel and charge transfer excitons

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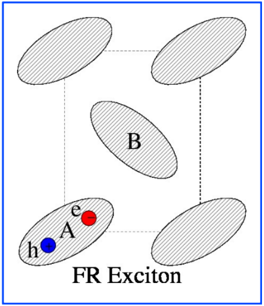
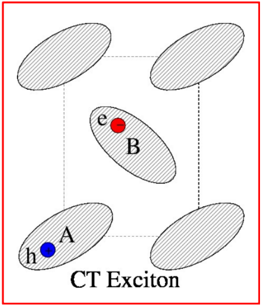
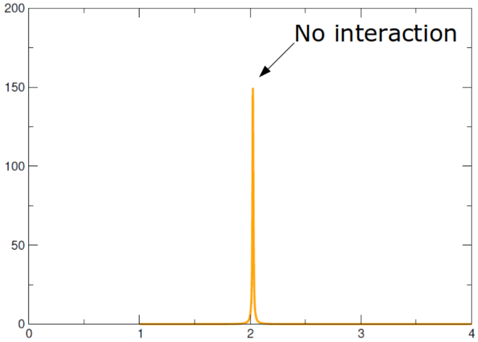
Frenkel exciton | Charge transfer exciton



# Frenkel and charge transfer excitons

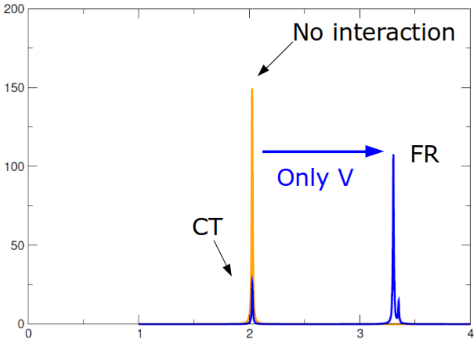
$$E^{\pm}_{FR} = \Delta\epsilon$$
$$E^{\pm}_{CT} = \Delta\epsilon$$




Reviewed in P. Cudazzo *et al.* J. Phys.: Condens. Matter **27** (2015).

# Frenkel and charge transfer excitons

$$
\begin{aligned}
E^{\pm}_{FR} &= \Delta\epsilon + I \pm J \\
E^{\pm}_{CT} &= \Delta\epsilon
\end{aligned}
$$




Reviewed in P. Cudazzo *et al.* J. Phys.: Condens. Matter **27** (2015).

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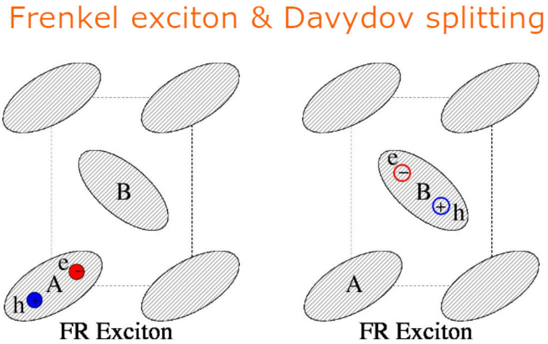
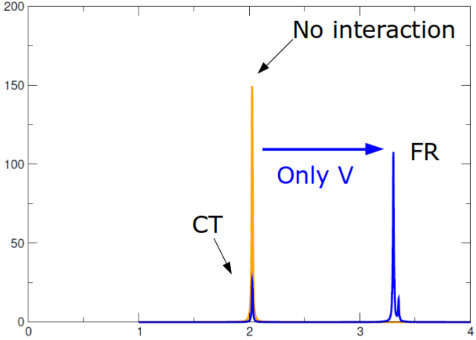
E^{\pm}_{CT} &= \Delta\epsilon
\end{aligned}
$$




Reviewed in P. Cudazzo *et al.* J. Phys.: Condens. Matter **27** (2015).

# Frenkel and charge transfer excitons

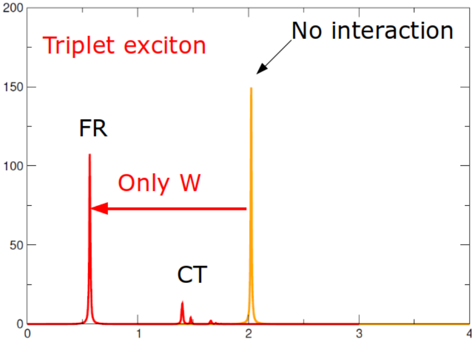
$$E_{FR}^{\pm} = \Delta\epsilon + I \pm J$$
$$E_{CT}^{\pm} = \Delta\epsilon$$




Reviewed in P. Cudazzo *et al.* J. Phys.: Condens. Matter **27** (2015).

# Frenkel and charge transfer excitons

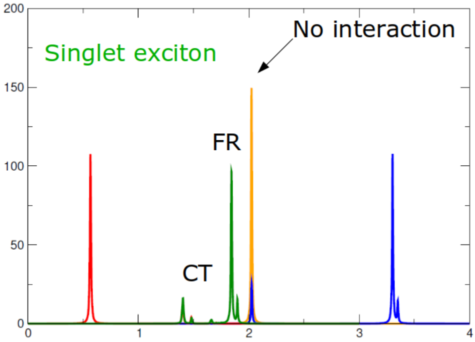
$$E_{FR}^{\pm} = \Delta\epsilon - W$$
$$E_{CT}^{\pm} = \Delta\epsilon - \tilde{W}$$




Reviewed in P. Cudazzo *et al.* J. Phys.: Condens. Matter **27** (2015).

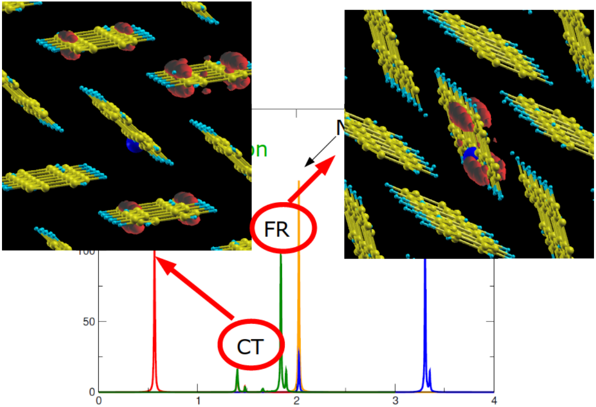
# Frenkel and charge transfer excitons

$$E^{\pm}_{FR} = \Delta\epsilon + I \pm J - W$$
$$E^{\pm}_{CT} = \Delta\epsilon - \tilde{W}$$




Reviewed in P. Cudazzo *et al.* J. Phys.: Condens. Matter **27** (2015).

# Frenkel and charge transfer excitons




Reviewed in P. Cudazzo *et al.* J. Phys.: Condens. Matter **27** (2015).

# Wannier and Frenkel excitons: dispersion

## Exciton dispersion

$E_\lambda(\mathbf{q})$ = Exciton dispersion: exciton energy as a function of the momentum carried by the electron-hole pair

## Wannier and Frenkel models

- Wannier exciton

$$E_\lambda(\mathbf{q}) = E_\lambda(\mathbf{q}=0) + \frac{q^2}{2(m_e^* + m_h^*)}$$

Free propagation: band structure effect (singlet=triplet)

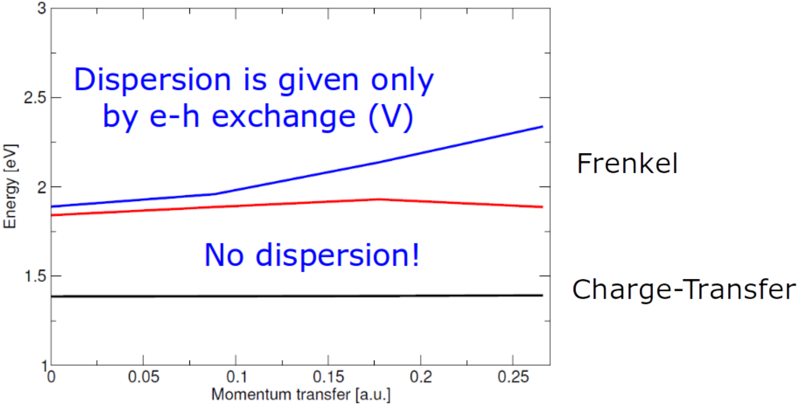
- Frenkel exciton

$$E_\lambda(\mathbf{q}) = E_\lambda^{ii} + \sum_j e^{i\mathbf{q}(\mathbf{R}_j - \mathbf{R}_i)} E_\lambda^{ij}$$

Dipole-dipole interaction: Destroy electron-hole pair at site $i$ and create at site $j$

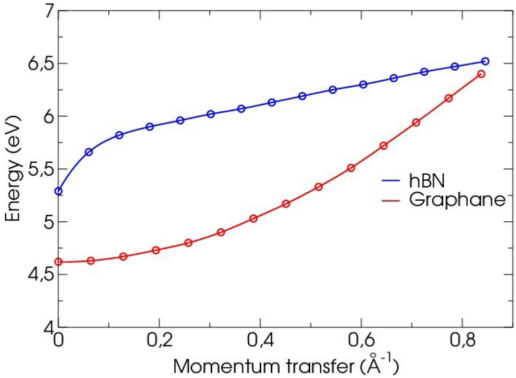
# Exciton dispersion: Frenkel and charge transfer

$$E^{\pm}_{FR}(\mathbf{q}) = \Delta\epsilon + I(\mathbf{q}) \pm J(\mathbf{q}) - W$$
$$E^{\pm}_{CT}(\mathbf{q}) = \Delta\epsilon - \tilde{W}$$




P. Cudazzo *et al.* J. Phys.: Condens. Matter **27** (2015).

# Exciton dispersion: two dimensions




P. Cudazzo *et al.* PRL **116** (2016)

# Outline

# MBPT vs. TDDFT: different electrons

**MBPT**

$$L = L_0 + L_0(v + \Xi)L$$

**TDDFT**

$$\chi = \chi_0 + \chi_0(v + f_{xc})\chi$$

# MBPT vs. TDDFT: different electrons

**MBPT**

$L = L_0$ $\Rightarrow$ GW energies

**TDDFT**

$\chi = \chi_0$ $\Rightarrow$ Kohn-Sham energies

**Observation**

$f_{xc}$ has 2 tasks:

- bandgap opening ($\rightarrow$ GW)
- excitonic effects ($\rightarrow$ BSE)

# $f_{xc}$ kernel

## Definitions

$P = \chi_0 + \chi_0 f_{xc} P$ : irreducible polarizability $P$

$\chi = P + Pv\chi$ : reducible polarizability $\chi$

# $f_{xc}$ kernel

## Definitions

$P = \chi_0 + \chi_0 f_{xc} P$ : irreducible polarizability $P$

$\chi = P + Pv\chi$ : reducible polarizability $\chi$

$$f_{xc} = f_{xc}^{(1)} + f_{xc}^{(2)}$$

$f_{xc}^{(1)} \Rightarrow$ bandgap opening    $f_{xc}^{(2)} \Rightarrow$ excitonic effects

$$P_0 = \chi_0 + \chi_0 f_{xc}^{(1)} P_0 \qquad P = P_0 + P_0 f_{xc}^{(2)} P$$

$\chi_0 \Rightarrow$ Kohn-Sham energies    $P_0 \Rightarrow$ GW energies

# MBPT vs. TDDFT: different maths

**MBPT**

$$L = L_0 + L_0(v + \Xi)L$$

**TDDFT**

$$\chi = P_0 + P_0(v + f_{xc}^{(2)})\chi$$

**Observation**

- BSE is a 4-point equation
- TDDFT is a 2-point equation

# MBPT vs. TDDFT: different maths

**MBPT**

$$L = L_0 + L_0(v + \Xi)L$$

**TDDFT**

$$\chi = P_0 + P_0(v + f_{xc}^{(2)})\chi$$

**Observation**

- BSE is a 4-point equation $\Rightarrow$ unavoidable
- TDDFT is a 2-point equation $\Rightarrow$ can be rewritten as 4-point eq.

# TDDFT: 4-point formulation

**Definition**

$$\chi = P_0 + P_0(v + f_{xc}^{(2)})\chi$$

$$\Downarrow$$

$$^4\chi = L_0 + L_0(v + F_{xc})\,^4\chi$$

$$^4\chi(1122) = \chi(12) \qquad L_0(1122) = P_0(12)$$

Hamiltonian (Casida) formulation:

$$H_{TDDFT}^{(vc)(v'c')} = (E_c - E_v)\delta_{vv'}\delta_{cc'} + (f_v - f_c)[\langle\langle v\rangle\rangle + \langle\langle f_{xc}\rangle\rangle]$$

# MBPT & TDDFT

## MBPT

$$L = L_0 + L_0(v + \Xi)L$$

## TDDFT

$$^4\chi = L_0 + L_0(v + F_{xc})\,^4\chi$$

## Combination

$$L = {}^4\chi + {}^4\chi(\Xi - F_{xc})L$$

# $f_{xc}$ kernel

**What is the $f_{xc}$ kernel of TDDFT?**

It is the 2-point kernel $f_{xc}^{(2)}$:

$$F_{xc}(1234) = f_{xc}^{(2)}(13)\delta(12)\delta(34)$$

that yields equal 2-point polarizabilities:

$$^4\chi(1122) = \chi(12) = L(1122)$$

# $f_{xc}$ kernel

## Exact $f_{xc}$

$$L(1234) = {}^4\chi(1234) + {}^4\chi(1256)[\Xi(5678) - f_{xc}^{(2)}(57)\delta(56)\delta(78)]L(7834)$$

# $f_{xc}$ kernel

## Exact $f_{xc}$

$$L(1234) = {}^4\chi(1234) + {}^4\chi(1256)[\Xi(5678) - f_{xc}^{(2)}(57)\delta(56)\delta(78)]L(7834)$$

$$L(1122) = {}^4\chi(1122) + {}^4\chi(1156)[\Xi(5678) - f_{xc}^{(2)}(57)\delta(56)\delta(78)]L(7822)$$

# $f_{xc}$ kernel

## Exact $f_{xc}$

$$L(1234) = {}^4\chi(1234) + {}^4\chi(1256)[\Xi(5678) - f_{xc}^{(2)}(57)\delta(56)\delta(78)]L(7834)$$

$$L(1122) = {}^4\chi(1122) + {}^4\chi(1156)[\Xi(5678) - f_{xc}^{(2)}(57)\delta(56)\delta(78)]L(7822)$$

Since $L(1122) = {}^4\chi(1122) = \chi(12)$:

$$0 = {}^4\chi(1156)[\Xi(5678) - f_{xc}^{(2)}(57)\delta(56)\delta(78)]L(7822)$$

... solve for $f_{xc}^{(2)}$

# $f_{xc}$ kernel

## Exact $f_{xc}$

$$f_{xc}^{(2)}(34) = \chi^{-1}(31)\,{}^{4}\chi(1156)\Xi(5678)L(7822)\chi^{-1}(24)$$

# The Nanoquanta kernel

## Approximations

1. usual BSE implementation: $\Xi(1234) = -W(12)\delta(13)\delta(24)$
2. first-order linearizations:
   $\chi(12) = P_0(12)$ and $L(1233) = \chi(1233) = -iG(13)G(32)$

## Nanoquanta $f_{xc}$

$$f_{xc}^{(2)}(34) = P_0^{-1}(31)G(15)G(61)W(56)G(52)G(26)P_0^{-1}(24)$$

# The Nanoquanta kernel

## Approximations

1. usual BSE implementation: $\Xi(1234) = -W(12)\delta(13)\delta(24)$
2. first-order linearizations: $\chi(12) = P_0(12)$ and $L(1233) = \chi(1233) = -iG(13)G(32)$

## Nanoquanta $f_{xc}$

$$f_{xc}^{(2)}(34) = P_0^{-1}(31)G(15)G(61)W(56)G(52)G(26)P_0^{-1}(24)$$

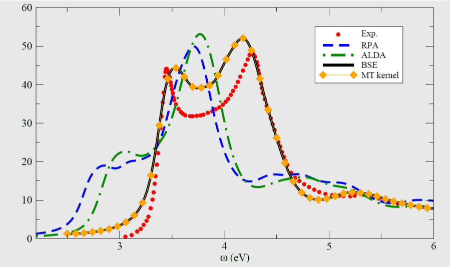
## Observations

- $f_{xc}$ is "ultranonlocal"
- $f_{xc}$ is frequency dependent ("memory") – but $W$ is static...

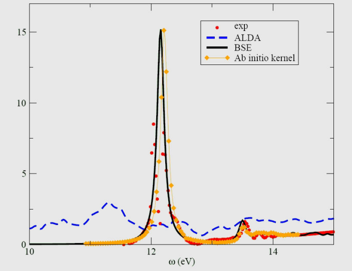
Reviewed in S. Botti *et al.* Rep. Prog. Phys. **70** (2007).

# The Nanoquanta kernel

Bulk Silicon



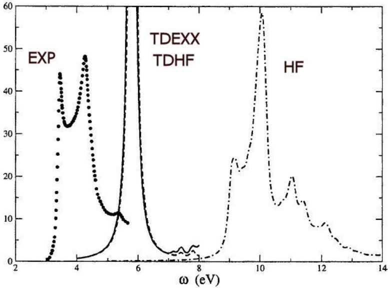

Solid Argon




Reviewed in S. Botti *et al.* Rep. Prog. Phys. **70** (2007).

# TDEXX

Bulk Silicon




TDEXX misses long-range screening

F. Bruneval, F. Sottile, V. Olevano, and L. Reining, JCP **124** (2006).

Many thanks!