TDDFT for extended systems II: Excitons

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Outline

- Introduction to excitons
- TDDFT for periodic systems
- Optical spectra and exciton binding energies
- \( xc \) functionals for excitons
- Real-time TDDFT for solids
- Summary
Absorption of light in a solid

Let us consider the absorption of light in a solid with a gap.
Absorption of light across the band gap

- Light comes in with photon energy at least as large as the band gap
- Photon gets absorbed, promotes electron across the gap, leaving a hole behind

GaAs

$\text{VB}$

$\text{CB}$

$h\nu$
Absorption spectra of insulators/semiconductors

will produce an absorption spectrum like this (in 3D):

\[ h\nu \]

\[ E_g \]

photons

gap

see John H. Davies
“The Physics of low-dimensional semiconductors”
Chapter 8
In the experiment, one finds sharp peaks at the absorption threshold…
In fact, there are peaks below the band gap energy: Excitons.
Excitons in nanoscale systems

Jang & Mennucci, Rev. Mod. Phys. 90, 035003 (2018)

Frenkel excitons in light-harvesting systems: purple bacteria
What is an exciton?

► After their creation, the electron and the hole are not completely free, but experience **Coulomb attraction**.

► This gain in (mostly electrostatic) energy can lower the onset of absorption and change the spectral strength.

**Excitons are bound electron-hole pairs.**

C. A. Ullrich and Zeng-hui Yang, Topics in Current Chemistry 368, 185 (2015)
Exciton wave functions in 3D solids

LiF


Erhart, Schleife, Sadigh and Aberg, PRB 89, 075132 (2014)
**Mott-Wannier exciton:** weakly bound, delocalized over many lattice constants

► In semiconductors with small band gap and large ε

**Frenkel exciton:** tightly bound, localized on a single (or a few) atoms

► In large-gap insulators, or in low-ε organic materials
Excitons: the Wannier equation

Derivation of Wannier eq. from many-body theory: Sham and Rice, Phys. Rev. 144, 708 (1966)

\[
\left[ -\frac{\hbar^2 \nabla^2}{2m_{eh}} - \frac{e^*^2}{4\pi\varepsilon_0 r} \right] \psi(r) = E \psi(r)
\]

\[
\frac{1}{m_{eh}} = \frac{1}{m_e^*} + \frac{1}{m_h^*} \quad E_n^* = -\frac{m_{eh}}{2\hbar^2 n^2} \left( \frac{e^*^2}{4\pi\varepsilon_0} \right)^2
\]

Exciton binding energy for GaAs:

\[ E_0^* = 4.75 \text{ meV} \]

Experiment:

\[ E_0^* = 3.3 \text{ meV} \]
Excitonic features in the absorption spectrum

- Sharp peaks below the onset of the single-particle gap
- Redistribution of oscillator strength: enhanced absorption close to the onset of the continuum

H. Haug & S.W. Koch
Quantum Theory of the
Optical and Electronic
Properties of Semiconductors

H-atom: Elliott formula
Wannier equation and excitonic Rydberg Series

Cu$_2$O


GaAs

Optical transitions in insulators are challenging for TDDFT:

- band gap opening
- excitons

Standard approach: Bethe-Salpeter equation (combined with GW)

▶ Gives good results, but computationally expensive
▶ Want to use TDDFT instead!
Insulators: three different gaps

Band gap: \[ E_g = E_{g,KS} + \Delta_{xc} \]

Optical gap: \[ E_g^{optical} = E_g - E_0^{exciton} \]

The Kohn-Sham gap approximates the optical gap (neutral excitation), not the band gap!
Hybrid functionals for the band gap

Matsushita, Nakamura & Oshiyama, PRB 84, 075205 (2011)
Marques, Vidal, Oliveira, Reining & Botti, PRB 83, 035119 (2011)

see also Skone, Govoni and Galli, PRB 93, 235106 (2016)
Excitons: comparison of first-principles methods

M. Rohlfing and S. Louie, PRB 62, 4927 (2000)

Many-body perturbation theory: Based on Green’s functions
- moves (quasi)particles around
- one-particle G: electron addition and removal – GW ground state
- two-particle L: electron-hole excitation – Bethe-Salpeter equation
- intuitive: contains the right physics (screened e-h interaction)
  by direct construction

Time-dependent DFT: Based on the electron density
- moves the density around
- Ground state: Kohn-Sham DFT
- response function $\chi$: neutral excitations of the KS system
- efficient (all interactions are local), but less intuitive how
  the right physics is built in

* thanks to Matteo Gatti
1. **Calculate the dielectric function via Dyson equation**  
   (computationally more efficient, gives optical spectrum)

2. **Solve Casida equation**  
   (more expensive, can give precise exciton binding energies)

3. **Via real-time propagation**  
   (can consider ultrafast or nonlinear regime)

---

\[ \chi(\mathbf{r}, \mathbf{r}', \omega) = \chi_s(\mathbf{r}, \mathbf{r}', \omega) + \int d\mathbf{x} \int d\mathbf{x}' \chi_s(\mathbf{r}, \mathbf{x}, \omega) \left\{ \frac{1}{|\mathbf{x} - \mathbf{x}'|} + f_{xc}(\mathbf{x}, \mathbf{x}', \omega) \right\} \chi(\mathbf{x}', \mathbf{r}', \omega) \]

Periodic systems: \[ \chi(\mathbf{r}, \mathbf{r}', \omega) = \chi(\mathbf{r} + \mathbf{R}, \mathbf{r}' + \mathbf{R}, \omega) \]

Fourier transform:

\[ \chi(\mathbf{r}, \mathbf{r}', \omega) = \sum_{\mathbf{q} \in BZ} \sum_{\mathbf{G}, \mathbf{G}'} e^{-i(\mathbf{q}+\mathbf{G}) \cdot \mathbf{r}} e^{i(\mathbf{q}+\mathbf{G}') \cdot \mathbf{r}'} \chi(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}', \omega) \]

\[ \chi_{\mathbf{G}G'}(\mathbf{q}, \omega) = \chi_{s\mathbf{G}G'}(\mathbf{q}, \omega) + \sum_{\mathbf{G}_1 \mathbf{G}_2} \chi_{s\mathbf{GG}_1}(\mathbf{q}, \omega) \times \left\{ V_{\mathbf{G}_1}(\mathbf{q}) \delta_{\mathbf{G}_1 \mathbf{G}_2} + f_{xc\mathbf{G}_1 \mathbf{G}_2}(\mathbf{q}, \omega) \right\} \chi_{\mathbf{G}_2 G'}(\mathbf{q}, \omega) \]
The dielectric tensor

\[
\begin{align*}
\nabla \cdot \mathbf{D} &= n_{\text{free}} \\
\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \times \mathbf{H} &= j_{\text{free}} + \frac{\partial \mathbf{D}}{\partial t}
\end{align*}
\]

Maxwell equations

Def. of dielectric tensor:

\[
D(\mathbf{r}, \omega) = \int d^3 r' \varepsilon(\mathbf{r}, \mathbf{r}', \omega) \mathbf{E}(\mathbf{r}', \omega)
\]

In periodic solids:

\[
D_G(\mathbf{q}, \omega) = \sum_{G'} \varepsilon_{GG'}(\mathbf{q}, \omega) \mathbf{E}_{G'}(\mathbf{q}, \omega)
\]

This is the \textbf{microscopic} dielectric tensor. But for comparison with spectroscopy, we would like the \textbf{macroscopic} dielectric function:

\[
D_{\text{mac}}(\omega) = \varepsilon_{\text{mac}}(\omega) \mathbf{E}_{\text{mac}}(\omega)
\]

Problem: we cannot calculate the macroscopic dielectric function directly! This would ignore the \textbf{local-field effects} (microscopic fluctuations).
In a homogeneous, isotropic system, things would be easy:

\[
\varepsilon_{\text{mac}}^\text{hom}(\omega) = \lim_{q \to 0} \varepsilon_{\text{hom}}^\text{hom}(q, \omega)
\]

and

\[
\varepsilon_{\text{hom}}^\text{hom}(q, \omega) = \varepsilon_{L}^\text{hom}(q, \omega) \hat{q} \hat{q}^T + \varepsilon_{T}^\text{hom}(1 - \hat{q} \hat{q}^T)
\]

and

\[
\varepsilon_{L}^\text{hom}(0, \omega) = \varepsilon_{T}^\text{hom}(0, \omega)
\]

The connection to optics is via the refractive index:

\[
\varepsilon_{\text{mac}}(\omega) = \tilde{n}^2
\]

\[
\text{Re} \varepsilon_{\text{mac}} = n^2 + \kappa^2
\]

\[
\text{Im} \varepsilon_{\text{mac}} = 2n\kappa
\]

see Yu and Cardona

*The Physics of Semiconductors*
For cubic symmetry, one can prove that

\[ \varepsilon_{\text{mac}}(\omega) = \lim_{q \to 0} \left[ \varepsilon^{-1}_{G G'}(q, \omega) \right]^{-1} \]

Adler 1962

Wiser 1963

\( \varepsilon_{G G'}(q, \omega) \): longitudinal component of dielectric tensor
(a.k.a. dielectric matrix)

To make progress, we need a connection with response theory:

\[ V_1(r, \omega) = \int d^3r' \varepsilon(r, r', \omega) \left[ V_1(r, \omega) + \int d^3r'' \frac{n_1(r'', \omega)}{|r' - r''|} \right] \]

so that

\[ \varepsilon^{-1}(r, r', \omega) = \delta(r - r') + \int d^3r'' \frac{\chi(r'', r', \omega)}{|r - r''|} \]

and for a periodic system,

\[ \varepsilon_{G G'}^{-1}(q, \omega) = \delta_{G G'} + V_G(q) \chi_{G G'}(q, \omega) \]
The macroscopic dielectric function

From this, one obtains

\[ \varepsilon_{\text{mac}}(\omega) = 1 - \lim_{q \to 0} V_0(q) \chi_{00}(q, \omega) \]

Notice a subtle, but very important point: we use a modified response function \( \chi_{GG'}(q, \omega) \):

\[ \chi_{GG'}(q, \omega) = \chi_{GG'}(q, \omega) + \sum_{G_1G_2} \chi_{GG_1}(q, \omega) \left\{ V_{G_1}(q) \delta_{G_1G_2} + f_{xcG_1G_2}(q, \omega) \right\} \chi_{G_2G'}(q, \omega) \]

where the long-range part of the Coulomb interaction has been removed:

\[ V_G(q) = \begin{cases} 0 & \text{for } G = 0 \\ \frac{4\pi}{|q + G|^2} & \text{for } G \neq 0 \end{cases} \]

Density response of periodic systems

\[ \delta n_G(q, \omega) = \sum_{G'} \chi_{sGG'}(q, \omega) \left\{ \delta V_{G'}^{\text{ext}}(q, \omega) + \sum_{G''} f_{G'G''}^{Hxc}(q, \omega) \delta n_{G''}(q, \omega) \right\} \]

**Loss function:**
response to a microscopic external scalar potential.
**Loss spectrum** includes **plasmons**.

**Density eigenmode:**
set \( \delta V_{G'}^{\text{ext}}(q, \omega) = 0 \)

**Optical absorption:**
response to total macroscopic classical perturbation.
**Optical spectrum** includes **excitons**.

**Density eigenmode:**
set \( \delta V_{G'}^{\text{ext}}(q, \omega) + f_{00}^{H} \delta n_{0}(q, \omega) = 0 \)
Excitation energies follow from eigenvalue problem (Casida 1995):

\[
\begin{pmatrix}
A & B \\
B^* & A^*
\end{pmatrix}
\begin{pmatrix}
X \\
Y
\end{pmatrix}
= \Omega_n
\begin{pmatrix}
-1 & 0 \\
0 & 1
\end{pmatrix}
\begin{pmatrix}
X \\
Y
\end{pmatrix}
\]

\[
A_{vck,v'c'k'} = (E_{ck} - E_{vk}) \delta_{vv'} \delta_{cc'} \delta_{kk'} + F_{vck,v'c'k'}^{Hxc}
\]

\[
B_{vck,v'c'k'} = F_{vck,v'c'k'}^{Hxc}
\]

\[
F_{vck,v'c'k'}^{H} = \frac{2}{V} \sum_{G \neq 0} \frac{4\pi}{G^2} \left< c_{k} | e^{iG \cdot r} | v_{k} \right> \left< v'_{k'} | e^{-iG \cdot r} | c'_{k'} \right>
\]

\[
F_{vck,v'c'k'}^{xc} = \frac{2}{V} \lim_{q \to 0} \sum_{G,G'} f_{xc,GG'}(q) \left< c_{k} | e^{i(q+G) \cdot r} | v_{k} \right> \left< v'_{k'} | e^{-i(q+G) \cdot r} | c'_{k'} \right>
\]
Using time-reversal symmetry, Full Casida eq. can be transformed into

$$\sum_{v'c'k'} \left[ \delta_{vk,v'k'} \delta_{ck,c'k'} \omega_{cvk} + F_{vcv,k,v'c'k'}^{Hxc} \right] X_{v'c'k'} + \sum_{v'c'k'} F_{vcv,k,v'c'k'}^{Hxc} Y_{v'c'k'} = -\Omega_n X_{vcv}$$

$$\sum_{v'c'k'} F_{vcv,k,v'c'k'}^{Hxc} X_{v'c'k'} + \sum_{v'c'k'} \left[ \delta_{vk,v'k'} \delta_{ck,c'k'} \omega_{cvk} + F_{vcv,k,v'c'k'}^{Hxc} \right] Y_{v'c'k'} = \Omega_n Y_{vcv}$$

**Tamm-Dancoff Approximation (TDA)**

More expensive than calculating $\text{Im } \epsilon(\omega)$ via Dyson eqn, but can resolve very small exciton binding energies

Sander, Maggio & Kresse, PRB 92, 045209 (2015)
Optical absorption in Insulators: TDDFT

RPA and ALDA both bad!

- absorption edge red shifted (electron self-interaction)
- first excitonic peak missing (electron-hole interaction)

Why does the LDA fail??
- lacks long spatial range
- need new classes of xc functionals

The xc kernel for periodic systems

\[ f_{xc}(\mathbf{r}, \mathbf{r}', \omega) = \sum_{\mathbf{q} \in \text{FBZ}} \sum_{G,G'} e^{i(\mathbf{q}+G)\mathbf{r}} f_{xc,GG'}(\mathbf{q}, \omega) e^{-i(\mathbf{q}+G')\mathbf{r}} \]

TDDFT requires the following matrix elements as input:

\[ F_{\nu c\mathbf{k}, \nu' c'\mathbf{k}'}^{xc} = \lim_{q \to 0} \sum_{GG'} f_{xc,GG'}(\mathbf{q}, \omega) \left< c\mathbf{k} \left| e^{i(q+G)\mathbf{r}} \right| \nu\mathbf{k} \right> \left< \nu'\mathbf{k}' \left| e^{-i(q+G)\mathbf{r}} \right| c'\mathbf{k}' \right> \]

**Most important: long-range** (\(q \to 0\)) **limit of “head”** (\(G = G' = 0\)):

\[ \left< c\mathbf{k} \left| e^{iqr} \right| \nu\mathbf{k} \right> \xrightarrow{q \to 0} q \quad f_{xc,00}^{\text{exact}}(\mathbf{q}, \omega) \xrightarrow{q \to 0} \frac{1}{q^2} \]

**but** \(f_{xc,00}^{\text{ALDA}}(\mathbf{q}) \xrightarrow{q \to 0} \text{const.} \)

Therefore, no excitons in ALDA!
The exact xc kernel can be written as

\[ f_{xc} = f_{xc}^{qp} + f_{xc}^{ex} \]

“quasiparticle”, opens the gap
\[ c_{KS} \rightarrow c_{qp} \]

“excitonic”, accounts for electron-hole interaction

- Usually, \( f_{xc}^{qp} \) is neglected. Instead, one uses hybrids, GW, or DFT+ scissors, which directly approximates \( c_{qp} \)

- Only \( f_{xc}^{ex} \) is then approximated

See also: Cavo, Berger & Romaniello, PRB 101, 115109 (2020)
Di Sabatino, Berger & Romaiello, Faraday Discuss. 224, 467 (2020)
Long-range xc kernels for solids

- **LRC** (long-range corrected) kernel (with fitting parameter $\alpha$):
  
  $f_{xc,GG'}^{LRC}(q) = -\frac{\alpha}{|q + G|^2} \delta_{GG'}$

- **“bootstrap”** kernel (S. Sharma et al., PRL 107, 186401 (2011))

  $f_{xc,GG'}^{\text{boot}}(q, \omega) = \frac{\mathcal{E}^{-1}_{GG'}(q,0)}{\chi_{s00}(q,0)}$

  (depends on unoccupied bands, may need large number of bands)

- **Functionals from many-body theory:** (requires matrix inversion)

  - exact exchange
  - “nanoquanta” kernel, reverse-engineered from BSE (L. Reining et al., 2002)
Excitons: which xc kernels to use?

- **Nanoquanta kernel**: accurate but expensive

- **Long-range corrected (LRC) kernel**: simple but ad-hoc

- **Bootstrap kernel**: several versions
  Sharma, Dewhurst, Sanna and Gross, PRL **107**, 186401 (2011)

- **Jellium with a gap**:  
  Trevisanutto *et al.*, PRB **87**, 205143 (2013)

- **Current-TDDFT**:  
  Cavo, Berger & Romaniello, PRB **101**, 115109 (2020)

- **Hybrid functionals**:  
  Wing *et al.*, PRMat **3**, 064603 (2019)
  Tal, Liu, Kresse & Pasquarello, PRREs **2**, 032019 (2020)
  Zivkovic, de Leeuw, Searle & Bernasconi, JPC C **124**, 24995 (2020)
  Sun, Li & Liang, PCCP **21**, 16296 (2021)
The family of LRC/Bootstrap xc kernels

With some tricks, LRC kernel can produce quite accurate optical spectra!

Cannot get good exciton binding energies and good spectral shapes at the same time! No exciton Rydberg series.

Byun and Ullrich, PRB 95, 205136 (2017)
TDDFT vs MBPT

TDDFT coupling matrix:

$$
\sum_{v'c'k'} \left[ \delta_{v_k,v'_k} \delta_{c_k,c'_k} \omega_{vck}^2 + 2\sqrt{\omega_{cvk} \omega_{c'v'k'}} F_{vck,v'c'k'}^{Hxc} \right] Z_{v'c'k'} = \Omega_n^2 Z_{vck}
$$

Bethe-Salpeter equation (BSE) coupling matrix:

$$
F_{vck,v'c'k'}^{xc} = \sum_{GG'} f_{xc,GG'}(q \rightarrow 0) \langle ck | e^{iG \cdot r} | vk \rangle \langle v'k' | e^{-iG \cdot r} | c'k' \rangle
$$

$$
F_{vck,v'c'k'}^{xc} = \sum_{GG'} g_{GG'}(q) \langle ck | e^{i(q+G) \cdot r} | c'k' \rangle \langle v'k' | e^{-i(q+G) \cdot r} | v'k' \rangle \delta_{q,k-k'}
$$

screened Coulomb interaction
Screened exact exchange (SXX)

**BSE:**
\[ g_{GG'}(q) = -4\pi \frac{\epsilon_{GG'}^{-1}(q, \omega = 0)}{|q + G'|^2} \]

**TDHF:**
\[ g_{GG'}(q) = -4\pi \frac{1}{|q + G'|^2} \delta_{GG'} \]

**SXX:**
\[ g_{GG'}(q) = -4\pi \frac{\gamma}{|q + G'|^2} \delta_{GG'} \]

\[ \gamma = \epsilon_{00}^{-1}(0,0) \]

Calculated with RPA

Dielectrically screened hybrid functionals

\[
K_{xc}^{\text{hybrid}} = \gamma K_{xc}^{XX} + (1 - \gamma) K_{xc}^{ALDA}
\]

\[
\gamma = \varepsilon_{00}^{-1}(0,0)
\]

Very close to BSE, but 1-2 orders of magnitude faster.

Sun, Yang, and Ullrich, Phys. Rev. Research 2, 013091 (2020)
Optical spectra with screened range-separated hybrid

pentacene

Refaely-Abramson, Jain, Sharifzadeh, Neaton & Kronik, PRB 92, 081204 (2015)

Wing, Haber, Noff, Barker, Egger, Ramasubramaniam, Louie, Neaton & Kronik, PRMat 3, 064603 (2019)

\[ A_{laser}(t) = -c \int_{0}^{t} E(t') dt' \]
Equivalence of LR- and RT-TDDFT for optical spectra

- 4 electrons per unit cell
- two lowest valence bands are occupied
- use simple plane-wave basis
Equivalence of LR- and RT-TDDFT for optical spectra

\[ i \frac{\partial}{\partial t} \varphi_j (r, t) = \left[ \frac{1}{2} \left( \frac{\nabla}{i} + A(t) \right)^2 + V_{\text{eff}} (r, t) \right] \varphi_j (r, t) \]

"delta-kick": \[ V(r, t) = E_0 r \delta(t - t_0) \quad \overset{\leftrightarrow}{=} \quad A(t) = E_0 \theta(t - t_0) \]

Calculate the time-dependent dipole moment:
\[ d(t) = \int_{\text{cell}} r n(r, t) dr \]
\[ = \int dr \sum_{\text{cell}} \sum_k \sum_i u_{ik}^* (r, t) ru_{ik} (r, t) \]

expand time-dependent Bloch fcts:
\[ u(r, t) = \sum_n \xi(t) u_{nk}^{(0)} (r) \]
ill defined for periodic solids!
Dipole matrix elements:

$$
\mu_{nn'k} = \int_{cell} d\mathbf{r} u_{nk}^{(0)*}(\mathbf{r}) u_{nk}^{(0)}(\mathbf{r}) = \int d\mathbf{r} \frac{u_{nk}^{(0)*}(\mathbf{r})(i\nabla - \mathbf{k})u_{nk}^{(0)}(\mathbf{r})}{E_{nk} - E_{n'k}} \quad \text{well behaved!}
$$

Fourier transform:

$$
\mathbf{d}(\omega) = \int dt \mathbf{d}(t)e^{-i\omega t}e^{i\omega t}
$$

Dynamic polarizability:

$$
\alpha(\omega) = \frac{d(\omega)}{E_0}
$$

T. Sander and G. Kresse, JCP 146, 064110 (2017)
LR TDDFT:
\[
\epsilon_{mac}^{RPA}(\omega) = 1 - \lim_{q \to 0} \nu_q \chi_{00}(q, \omega)
\]

RT TDDFT:
\[
\epsilon_{mac}^{RPA}(\omega) = 1 - 4\pi\alpha(\omega)
\]

How to get excitons with this?
See my talk on Wednesday morning!
Real-time electron dynamics in solids: codes

- **Ultrafast magnetization dynamics, femtomagnetism**
  ELK (Full-potential LAPW)

- **High-harmonic generation, magnons**
  Octopus (real-space grid)

- **Core-level spectroscopy.**
  SIESTA (LCAO)

- **Ultrafast nonlinear spectroscopy, coherent phonons.**
  Salmon (real-space grid, norm-conserving PP)

- **Stopping power of materials under ion impact.**
  Qb@ll, INQ (plane waves)
  Andrade et al. JCTC 17, 7447 (2021)

...and there are more.....
Dielectric breakdown
Yabana et al., PRB 85, 045134 (2012)

High harmonic generation (HHG) in Si
Tancogne-Dejean et al. (2017)
RT-TDDFT for periodic solids: magnetic materials

N. Tancogne-Dejean, F.G. Eich & A. Rubio,
JCTC 16, 1007 (2020)

RT-TDDFT to calculate magnon dispersions

see also: Singh, Elliott, Dewhurst, Gross & Sharma,
pss-b 257, 1900654 (2020)

Krieger, Dewhurst, Elliott, Sharma & Gross
JCTC 11, 4870 (2015)

Nonlinear regime: ultrafast demagnetization
TDDFT methods can describe excitons, but difficult to get good exciton BE and good oscillator strengths. No exciton Rydberg series with LRC-type adiabatic xc kernels.

Challenges: xc kernel that works for small-gap semiconductors and for large-gap insulators; numerically very sensitive.

Alternative to BSE: hybrid functionals – similar accuracy but cheaper. Very promising! But more expensive than pure TDDFT.

Real-time TDDFT for solids now more and more common. Allows description of ultrafast/nonlinear effects.

Suggested exercises

- Test the **Wannier model** for different materials, and compare with experimental data. For what materials does it give reasonable exciton binding energies, when does it fail?

- Go over the derivation of the **Elliott formula** in the textbook of **Haug and Koch**, Chapter 10. This is a highly instructive exercise, and a beautiful analytic derivation. Then write a short Python code to implement the formula to produce optical absorption spectra like the one on slide 7. You can do it for 3D, 2D and 1D.

- An excellent introduction to light-matter interaction, dielectric properties, and excitons is given in the textbook of **Yu and Cardona, “Fundamental of Semiconductors.”** It is highly recommended to read Chapter 6.

- To learn more about the many-body formalism in solids, consult:
  - **Martin, Reining & Ceperley, “Interacting Electrons”**
  - **Bechstedt, “Many-Body Approach to Electronic Excitations”**
Thanks to all collaborators, students and postdocs over the years.