Introduction to many-body Green's functions

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ELK school - CECAM 2011

Outline

References

Francesco Sottile
PhD thesis, Ecole Polytechnique (2003)
http://etsf.polytechnique.fr/system/files/users/francesco/Tesi_dot.pdf

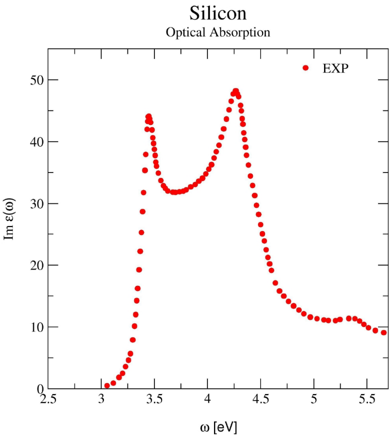
Fabien Bruneval
PhD thesis, Ecole Polytechnique (2005)
http://theory.polytechnique.fr/people/bruneval/bruneval_these.pdf

Giovanni Onida, Lucia Reining, and Angel Rubio
Rev. Mod. Phys. **74**, 601 (2002).

G. Strinati
Rivista del Nuovo Cimento **11**, (12)1 (1988).

Outline

Motivation



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

Theoretical spectroscopy

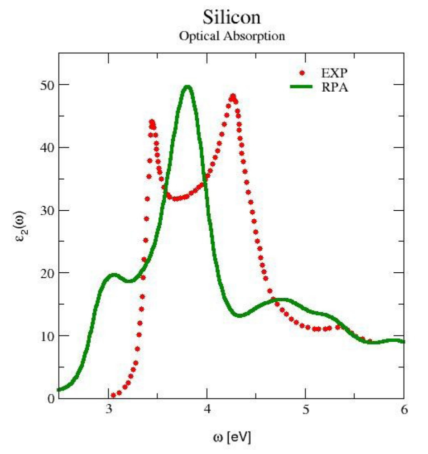
- Calculate and reproduce
- Understand and explain
- Predict

Theoretical Spectroscopy

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

Why do we have to study more than DFT?

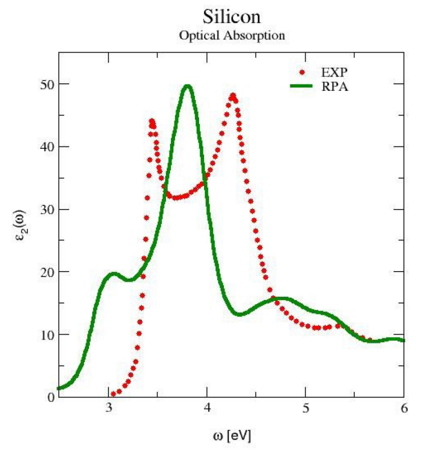
Absorption spectrum of bulk silicon in DFT



How can we understand this?

Why do we have to study more than DFT?

Absorption spectrum of bulk silicon in DFT



Spectroscopy is exciting!

MBPT vs. TDDFT: different worlds, same physics

MBPT

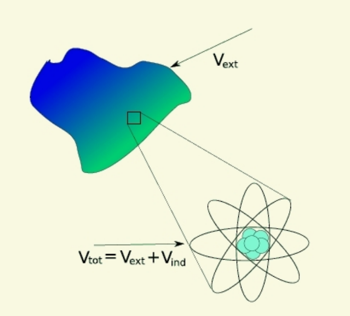
- based on Green's functions
- one-particle G: electron addition and removal - GW
  two-particle L: electron-hole excitation - BSE
- moves (quasi)particles around
- is intuitive (easy)

TDDFT

- based on the density
- response function χ: neutral excitations
- moves density around
- is efficient (simple)

Response functions

External perturbation V_{ext} applied on the sample
$\rightarrow V_{tot}$ acting on the electronic system



Potentials

$$\delta V_{tot} = \delta V_{ext} + \delta V_{ind}$$

$$\delta V_{ind} = v \delta \rho$$

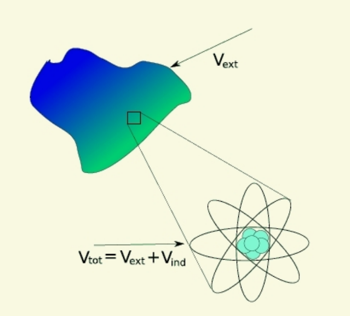
Dielectric function

$$\epsilon = \frac{\delta V_{ext}}{\delta V_{tot}} = 1 - v \frac{\delta \rho}{\delta V_{tot}}$$

$$\epsilon^{-1} = \frac{\delta V_{tot}}{\delta V_{ext}} = 1 + v \frac{\delta \rho}{\delta V_{ext}}$$

Response functions

External perturbation V_{ext} applied on the sample
$\rightarrow$ V_{tot} acting on the electronic system



Dielectric function

$$\epsilon = \frac{\delta V_{ext}}{\delta V_{tot}} = 1 - vP$$

$$\epsilon^{-1} = \frac{\delta V_{tot}}{\delta V_{ext}} = 1 + v\chi$$

$$P = \frac{\delta \rho}{\delta V_{tot}} \qquad \chi = \frac{\delta \rho}{\delta V_{ext}}$$

$$\chi = P + Pv\chi$$

$$P = \chi_0 + \chi_0 f_{xc} P$$

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).

Micro-macro connection

Microscopic-Macroscopic connection: local fields

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

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

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

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

Absorption spectra

Absorption spectra

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

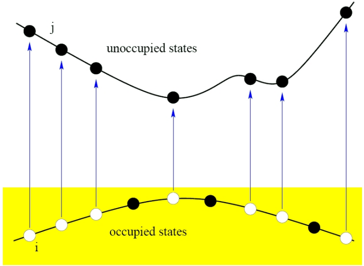
$$\mathrm{Abs}(\omega) = -\lim_{\mathbf{q}\to 0} \mathrm{Im}\left[v_{\mathbf{G}=0}(\mathbf{q})\bar{\chi}_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega)\right]$$

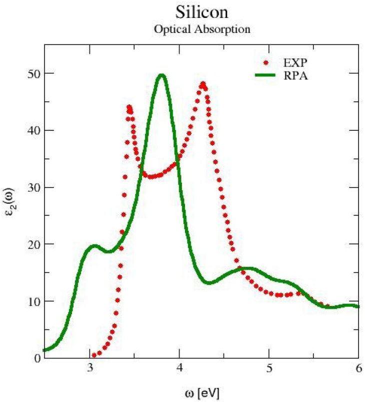
Absorption $\rightarrow$ response to $V_{ext} + V_{ind}^{macro}$

Independent particles: Kohn-Sham

Independent transitions:

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

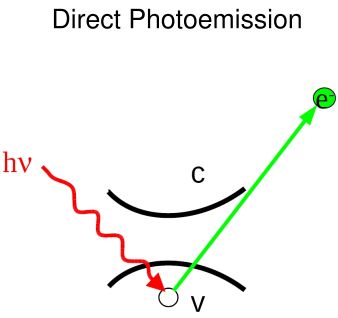


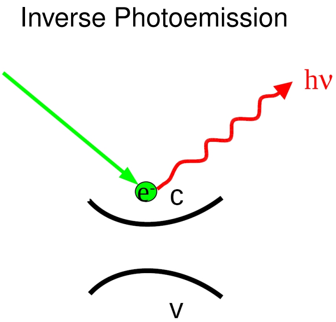


What is an electron?

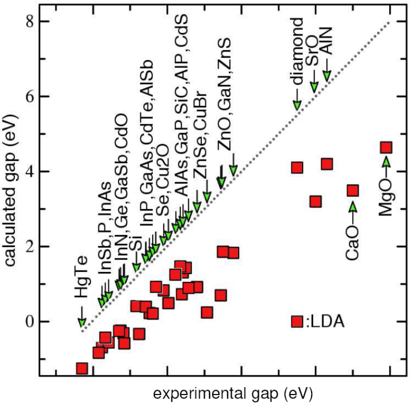
Outline

Photoemission





Why do we have to study more than DFT?



adapted from M. van Schilfgaarde *et al.*, PRL **96** (2006).

One-particle Green's function

The one-particle Green's function G

Definition and meaning of G:

$$iG(\mathbf{x_1}, t_1; \mathbf{x_2}, t_2) = \langle N| T\left[\psi(\mathbf{x_1}, t_1)\psi^\dagger(\mathbf{x_2}, t_2)\right]|N\rangle$$

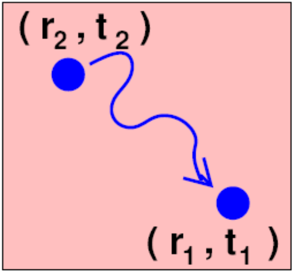
for $t_1 > t_2 \Rightarrow iG(\mathbf{x_1}, t_1; \mathbf{x_2}, t_2) = \langle N|\psi(\mathbf{x_1}, t_1)\psi^\dagger(\mathbf{x_2}, t_2)|N\rangle$

for $t_1 < t_2 \Rightarrow iG(\mathbf{x_1}, t_1; \mathbf{x_2}, t_2) = -\langle N|\psi^\dagger(\mathbf{x_2}, t_2)\psi(\mathbf{x_1}, t_1)|N\rangle$

One-particle Green's function

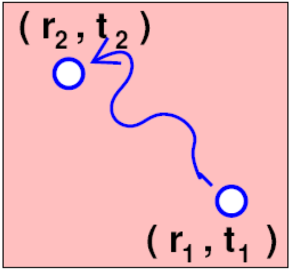
$t_1 > t_2$

$\langle N|\psi(\mathbf{x_1}, t_1)\psi^\dagger(\mathbf{x_2}, t_2)|N\rangle$



$t_1 < t_2$

$-\langle N|\psi^\dagger(\mathbf{x_2}, t_2)\psi(\mathbf{x_1}, t_1)|N\rangle$



One-particle Green's function

What is G ?

Definition and meaning of G:

$$G(\mathbf{x_1},t_1;\mathbf{x_2},t_2) = -i < N|T\left[\psi(\mathbf{x_1},t_1)\psi^\dagger(\mathbf{x_2},t_2)\right]|N>$$

Insert a complete set of $N+1$ or $N-1$-particle states. This yields

$$\begin{aligned} G(\mathbf{x_1},t_1;\mathbf{x_2},t_2) &= -i\sum_j f_j(\mathbf{x_1})f_j^*(\mathbf{x_2})e^{-i\varepsilon_j(t_1-t_2)}\times \\ &\times [\theta(t_1-t_2)\theta(\varepsilon_j-\mu)-\theta(t_2-t_1)\Theta(\mu-\varepsilon_j)]; \end{aligned}$$

where:

$$\varepsilon_j = \begin{array}{ll} E(N+1,j)-E(N), & \varepsilon_j>\mu \\ E(N)-E(N-1,j), & \varepsilon_j<\mu \end{array}$$

$$f_j(\mathbf{x_1}) = \begin{array}{ll} \langle N|\psi(\mathbf{x_1})|N+1,j\rangle, & \varepsilon_j>\mu \\ \langle N-1,j|\psi(\mathbf{x_1})|N\rangle, & \varepsilon_j<\mu \end{array}$$

One-particle Green's function

What is G? - Fourier transform

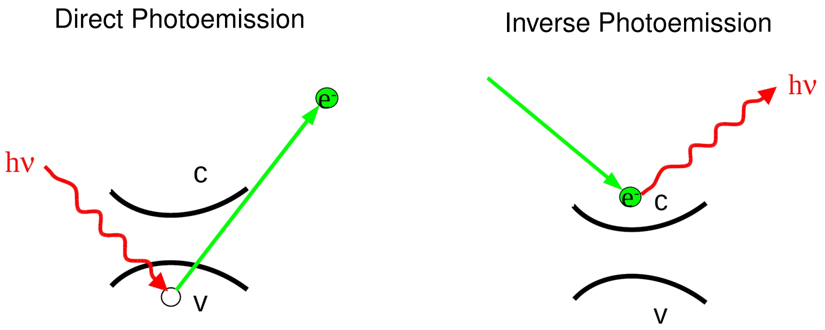
Fourier Transform:

$$G(\mathbf{x},\mathbf{x}',\omega) = \sum_j \frac{f_j(\mathbf{x})f_j^*(\mathbf{x}')}{\omega - \varepsilon_j + i\eta sgn(\varepsilon_j - \mu)}.$$

Spectral function:

$$A(\mathbf{x},\mathbf{x}';\omega) = \frac{1}{\pi} \mid \mathrm{Im} G(\mathbf{x},\mathbf{x}';\omega) \mid = \sum_j f_j(\mathbf{x})f_j^*(\mathbf{x}')\delta(\omega - \varepsilon_j).$$

Photoemission



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

One-particle Green's function

One-particle Green's function

From one-particle G we can obtain:

- one-particle excitation spectra
- ground-state expectation value of any one-particle operator: e.g. density ρ or density matrix γ:
  $\rho(\mathbf{r}, t) = -iG(\mathbf{r}, \mathbf{r}, t, t^+) \qquad \gamma(\mathbf{r}, \mathbf{r}', t) = -iG(\mathbf{r}, \mathbf{r}', t, t^+)$
- ground-state total energy

One-particle Green's function

Straightforward?

$$G(\mathbf{x},t;\mathbf{x}',t') = -i < N|T\left[\psi(\mathbf{x},t)\psi^{\dagger}(\mathbf{x}',t')\right]|N>$$

$|N> = ???$ Interacting ground state!

Perturbation Theory?

Time-independent perturbation theories: messy.
Textbooks: adiabatically switched on interaction, Gell-Mann-Low theorem, Wick's theorem, expansion (diagrams). Lots of diagrams.....

One-particle Green's function

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Functional approach to the MB problem

Equation of motion

To determine the 1-particle Green's function:

$$\left[i\frac{\partial}{\partial t_1} - h_0(1)\right]G(1,2) = \delta(1,2) - i\int d3v(1,3)G_2(1,3,2,3^+)$$

Do the Fourier transform in frequency space:

$$[\omega - h_0]G(\omega) + i\int vG_2(\omega) = 1$$

where $h_0 = -\frac{1}{2}\nabla^2 + v_{ext}$ is the independent particle Hamiltonian.
The 2-particle Green's function describes the motion of 2 particles.

Unfortunately, hierarchy of equations

$$
\begin{array}{ccc}
G_1(1,2) & \leftarrow & G_2(1,2;3,4) \\
G_2(1,2;3,4) & \leftarrow & G_3(1,2,3;4,5,6) \\
\vdots & \vdots & \vdots
\end{array}
$$

Self-energy

Perturbation theory starts from what is known to evaluate what is not known, hoping that the difference is small...
Let's say we know $G_0(\omega)$ that corresponds to the Hamiltonian h_0
Everything that is unknown is put in

$$\Sigma(\omega) = G_0^{-1}(\omega) - G^{-1}(\omega)$$

This is the definition of the self-energy

Thus,

$$[\omega - h_0]G(\omega) - \int \Sigma(\omega)G(\omega) = 1$$

to be compared with

$$[\omega - h_0]G(\omega) + i \int vG_2(\omega) = 1$$

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One-particle Green's function

Trick due to Schwinger (1951):
introduce a small external potential $U(3)$, that will be made equal to zero at the end, and calculate the variations of G with respect to U

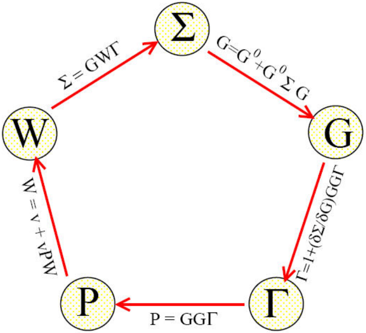
$$\frac{\delta G(1,2)}{\delta U(3)} = -G_2(1,3;2,3) + G(1,2)G(3,3).$$

Hedin's equation

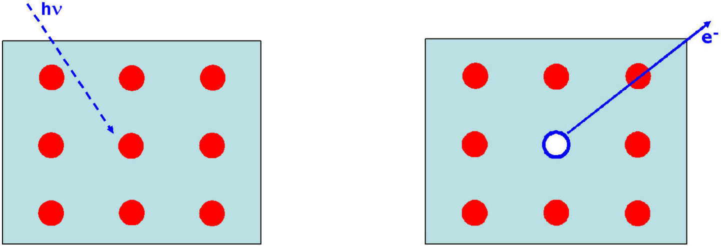
Hedin's equations

$$\Sigma = iGW\Gamma$$
$$G = G_0 + G_0 \Sigma G$$
$$\Gamma = 1 + \frac{\delta\Sigma}{\delta G} GG\Gamma$$
$$P = -iGG\Gamma$$
$$W = v + vPW$$

L. Hedin, Phys. Rev. **139** (1965)

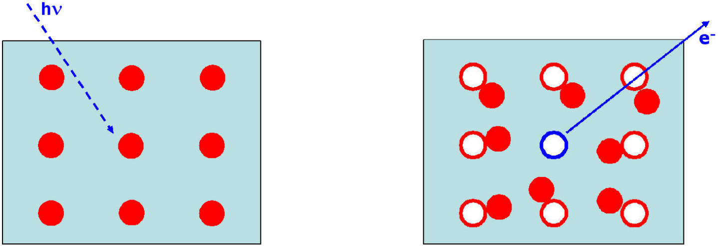


GW bandstructure: photoemission



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

Hedin's equation and GW

GW approximation

$$\Sigma = iGW\Gamma$$
$$G = G_0 + G_0\Sigma G$$
$$\Gamma = 1$$
$$P = -iGG\Gamma$$
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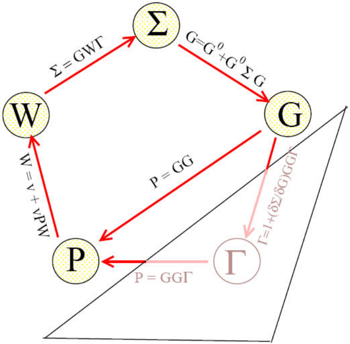

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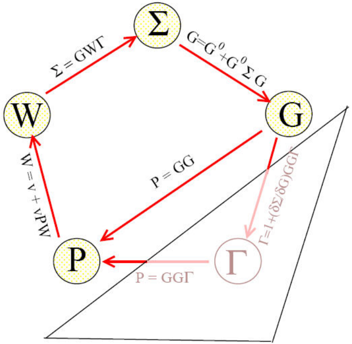


GW corrections

Standard perturbative G_0W_0

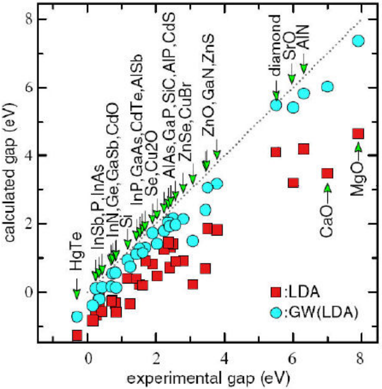
$$
\begin{aligned}
H_0(\mathbf{r})\varphi_i(\mathbf{r}) + V_{xc}(\mathbf{r})\varphi_i(r) &= \epsilon_i\varphi_i(\mathbf{r}) \\
H_0(\mathbf{r})\phi_i(\mathbf{r}) + \int d\mathbf{r}'\ \Sigma(\mathbf{r},\mathbf{r}',\omega = E_i)\ \phi_i(\mathbf{r}') &= E_i\,\phi_i(\mathbf{r})
\end{aligned}
$$

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)

GW results

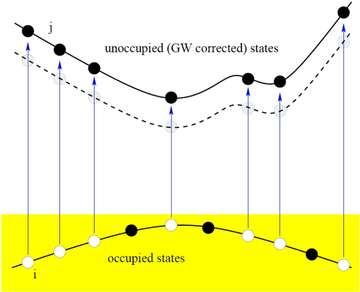


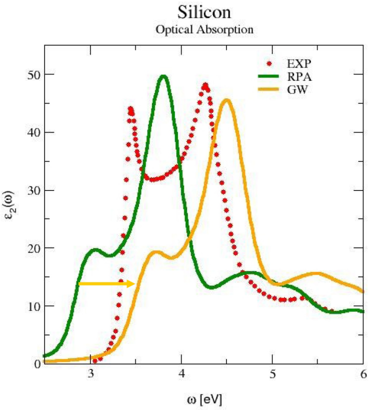
M. van Schilfgaarde *et al.*, PRL **96** (2006).

Independent (quasi)particles: GW

Independent transitions:

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

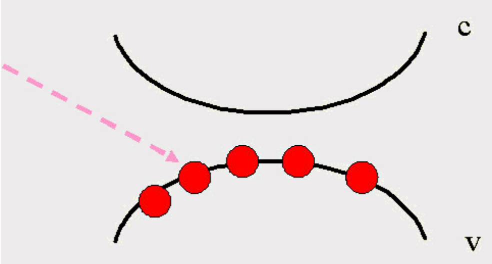




What is wrong?

What is missing?

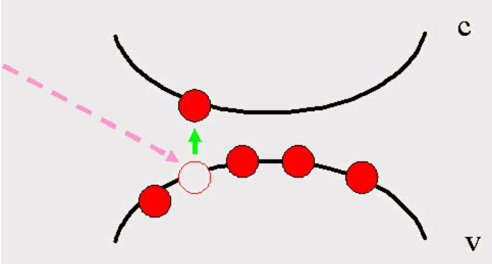
Absorption



Two-particle excitations $\rightarrow$ poles of two-particle Green's function L

Excitonic effects = electron - hole interaction

Absorption



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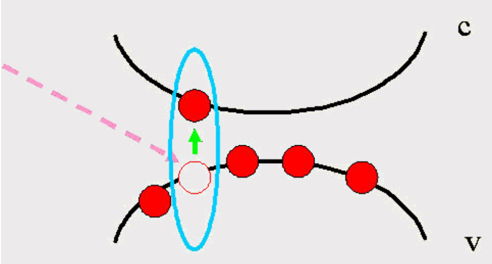


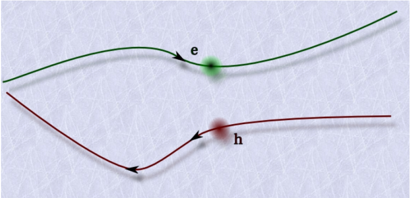
Two-particle excitations $\rightarrow$ poles of two-particle Green's function L

Excitonic effects = electron - hole interaction

Outline

Beyond RPA

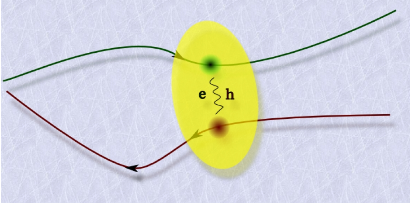
$$P(12) = -iG(12)G(21) = P_0(12)$$



Independent particles (RPA)

Beyond RPA

$$P(12) = -iG(13)G(42)\Gamma(342)$$



Interacting particles (excitonic effects)

From Hedin's equations to BSE

From Hedin...

$$P = -iGG\Gamma$$

$$\Gamma = 1 + \frac{\delta\Sigma}{\delta G}GG\Gamma$$

From Hedin's equations to BSE

From Hedin...

$$P = -iGG\Gamma$$

$$\Gamma = 1 + \frac{\delta\Sigma}{\delta G} GG\Gamma$$

...to Bethe-Salpeter

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

The Bethe-Salpeter equation

Exercise

Formal derivation

$$
\begin{aligned}
L(1234) =& -i\frac{\delta G(12)}{\delta V_{ext}(34)} = +iG(15)\frac{\delta G^{-1}(56)}{\delta V_{ext}(34)}G(62) \\
=& +iG(15)\frac{\delta[G_0^{-1}(56) - V_{ext}(56) - \Sigma(56)]}{\delta V_{ext}(34)}G(62) \\
=& -iG(13)G(42) + iG(15)G(62)\left[\frac{\delta V_H(5)\delta(56)}{\delta V_{ext}(34)} - \frac{\delta\Sigma(56)}{\delta V_{ext}(34)}\right] \\
=& -iG(13)G(42) + iG(15)G(62)\left[\frac{\delta V_H(5)\delta(56)}{\delta G(78)} - \frac{\delta\Sigma(56)}{\delta G(78)}\right]\frac{\delta G(78)}{\delta V_{ext}(34)}
\end{aligned}
$$

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

The Bethe-Salpeter equation

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

Polarizabilities

$$L(1234) = -i\frac{\delta G(12)}{\delta V_{ext}(34)} \qquad \chi(12) = \frac{\delta\rho(1)}{\delta V_{ext}(2)}$$

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

The Bethe-Salpeter equation

Approximations

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

The Bethe-Salpeter equation

Approximations

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

Approximation:

$\Sigma \approx iGW$

The Bethe-Salpeter equation

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

Approximations

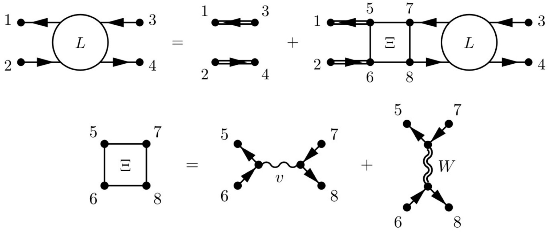
Final result:

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

The Bethe-Salpeter equation

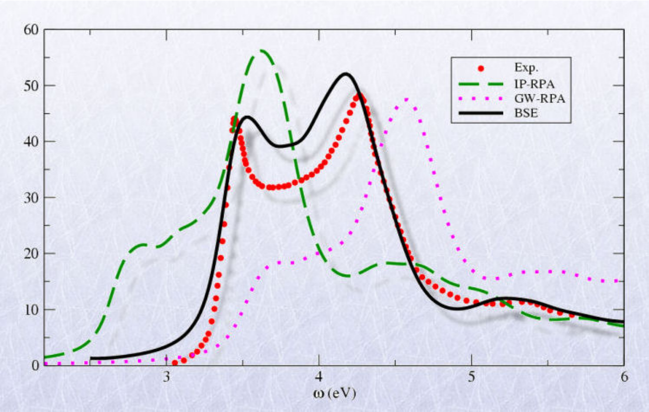
Bethe-Salpeter equation

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



Absorption spectra in BSE

Bulk silicon



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

Solving BSE

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

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

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

Static W

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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?

Transition space

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

Solving BSE

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

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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

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

Spectral representation of a hermitian operator

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

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

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

Solving BSE

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

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

Spectral representation of a hermitian operator

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

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

Absorption spectra in BSE

Independent (quasi)particles

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

Excitonic effects

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

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

- 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 φ_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:

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

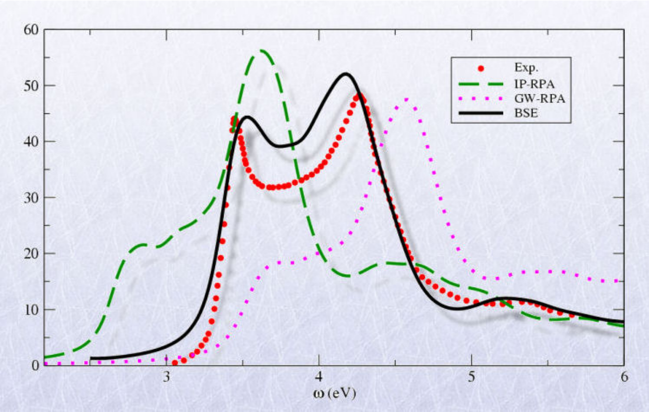
   $\Rightarrow$ excitonic eigenstates A_λ, E_λ
   $\Rightarrow$ spectra $\epsilon_M(\omega)$

A bit of history

- derivation of the equation (bound state of deuteron)
  - E. E. Salpeter and H. A. Bethe, PR **84**, 1232 (1951).
- BSE for exciton calculations
  - L.J. Sham and T.M. Rice, PR **144**, 708 (1966).
  - W. Hanke and L. J. Sham, PRL **43**, 387 (1979).
- first *ab initio* calculation
  - G. Onida, L. Reining, R. W. Godby, R. Del Sole, and W. Andreoni, PRL **75**, 818 (1995).
- first *ab initio* calculations in extended systems
  - S. Albrecht, L. Reining, R. Del Sole, and G. Onida, PRL **80**, 4510 (1998).
  - L. X. Benedict, E. L. Shirley, and R. B. Bohn, PRL **80**, 4514 (1998).
  - M. Rohlfing and S. G. Louie, PRL **81**, 2312 (1998).

Continuum excitons

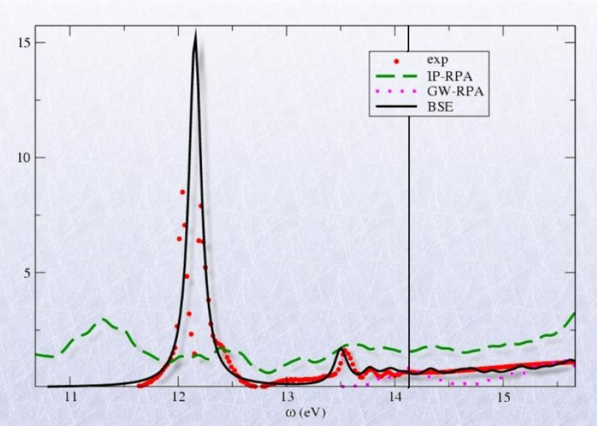
Bulk silicon



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

Bound excitons

Solid argon



F. Sottile, M. Marsili, V. Olevano, and L. Reining, PRB **76** (2007).

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

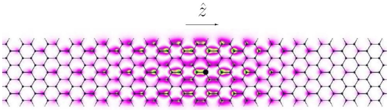
$$W(\mathbf{r}, \mathbf{r}') = \frac{1}{\epsilon_0 |\mathbf{r} - \mathbf{r}'|}$$

- solution = Rydberg series for effective H atom

$$E_n = E_g - \frac{R_{eff}}{n^2} \quad \text{with} \quad R_{eff} = \frac{R_\infty \mu}{\epsilon_0^2}$$

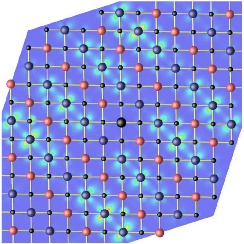
Exciton analysis

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



Graphene nanoribbon

D. Prezzi, *et al.*, PRB **77** (2008).



Manganese Oxide

C. Rödl, *et al.*, PRB **77** (2008).

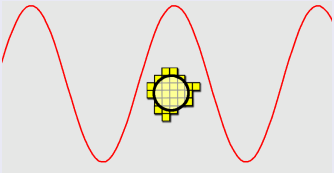
Outline

Micro-macro connection

Observation

At long wavelength, external fields are slowly varying over the unit cell:

- dimension of the unit cell for silicon: 0.5 nm
- visible radiation 400 nm $< \lambda <$ 800 nm



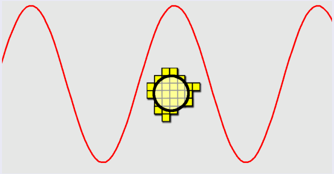
Total and induced fields are rapidly varying: they include the contribution from electrons in all regions of the cell.
Large and irregular fluctuations over the atomic scale.

Micro-macro connection

Observation

One usually measures quantities that vary on a macroscopic scale. When we calculate microscopic quantities we need to average over distances that are

- large compared to the cell parameter
- small compared to the wavelength of the external perturbation.



The differences between the microscopic fields and the averaged (macroscopic) fields are called the crystal local fields.

Suppose that we are able
to calculate the microscopic dielectric function ϵ,
how do we obtain the macroscopic dielectric function ϵ_M
that we measure in experiments ?

Micro-macro connection

Fourier transform

In a periodic medium, every function $V(\mathbf{r},\omega)$ can be represented by the Fourier series

$$V(\mathbf{r},\omega)=\sum_{\mathbf{qG}} V(\mathbf{q}+\mathbf{G},\omega)e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}}$$

or:

$$V(\mathbf{r},\omega)=\sum_{\mathbf{q}} e^{i\mathbf{qr}}\sum_{\mathbf{G}} V(\mathbf{q}+\mathbf{G},\omega)e^{i\mathbf{Gr}}=\sum_{\mathbf{q}} e^{i\mathbf{qr}}V(\mathbf{q},\mathbf{r},\omega)$$

where:

$$V(\mathbf{q},\mathbf{r},\omega)=\sum_{\mathbf{G}} V(\mathbf{q}+\mathbf{G},\omega)e^{i\mathbf{Gr}}$$

$V(\mathbf{q},\mathbf{r},\omega)$ is periodic with respect to the Bravais lattice and hence is the quantity that one has to average to get the corresponding macroscopic potential $V_M(\mathbf{q},\omega)$.

Micro-macro connection

Averages

$$V_M(\mathbf{q},\omega) = \frac{1}{\Omega_c}\int d\mathbf{r}\, V(\mathbf{q},\mathbf{r},\omega)$$

$$V(\mathbf{q},\mathbf{r},\omega) = \sum_{\mathbf{G}} V(\mathbf{q}+\mathbf{G},\omega) e^{i\mathbf{G}\mathbf{r}}$$

Therefore:

$$V_M(\mathbf{q},\omega) = \sum_{\mathbf{G}} V(\mathbf{q}+\mathbf{G},\omega)\frac{1}{\Omega_c}\int d\mathbf{r} e^{i\mathbf{G}\mathbf{r}} = V(\mathbf{q}+\mathbf{0},\omega)$$

The macroscopic average V_M corresponds to the $\mathbf{G}=0$ component of the microscopic V.

Example

$$V_{ext}(\mathbf{q},\omega) = \epsilon_M(\mathbf{q},\omega) V_{tot,M}(\mathbf{q},\omega)$$

Micro-macro connection

Averages

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Example

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Micro-macro connection

Fourier transforms

Fourier transform of a function $f(\mathbf{r},\mathbf{r}',\omega)$:

$$f(\mathbf{q}+\mathbf{G},\mathbf{q}+\mathbf{G}',\omega)=\int d\mathbf{r}d\mathbf{r}' e^{-i(\mathbf{q}+\mathbf{G})\mathbf{r}} f(\mathbf{r},\mathbf{r}',\omega) e^{+i(\mathbf{q}+\mathbf{G}')\mathbf{r}'} \equiv f_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$$

Therefore the relation

$$V_{tot}(\mathbf{r}_1,\omega)=\int d\mathbf{r}_2 \epsilon^{-1}(\mathbf{r}_1,\mathbf{r}_2,\omega) V_{ext}(\mathbf{r}_2,\omega)$$

in the Fourier space becomes:

$$V_{tot}(\mathbf{q}+\mathbf{G},\omega)=\sum_{\mathbf{G}'} \epsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) V_{ext}(\mathbf{q}+\mathbf{G}',\omega)$$

Micro-macro connection

Fourier transforms

Fourier transform of a function $f(\mathbf{r}, \mathbf{r}', \omega)$:

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Micro-macro connection

Example

$$V_{tot,M}(\mathbf{q},\omega) = \epsilon_M^{-1}(\mathbf{q},\omega) V_{ext}(\mathbf{q},\omega)$$

Macroscopic dielectric function

$$V_{tot}(\mathbf{q}+\mathbf{G},\omega) = \sum_{\mathbf{G}'} \epsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) V_{ext}(\mathbf{q}+\mathbf{G}',\omega)$$

$$V_{M,tot}(\mathbf{q},\omega) = V_{tot}(\mathbf{q}+\mathbf{0},\omega)$$

V_{ext} is a macroscopic quantity:

$$V_{tot,M}(\mathbf{q},\omega) = \epsilon^{-1}_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega) V_{ext}(\mathbf{q},\omega)$$

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

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

Micro-macro connection

Example

$$V_{tot,M}(\mathbf{q},\omega) = \epsilon_M^{-1}(\mathbf{q},\omega)\,V_{ext}(\mathbf{q},\omega)$$

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Micro-macro connection

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Micro-macro connection

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Micro-macro connection

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Macroscopic dielectric function

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Micro-macro connection

Macroscopic dielectric function

$$V_{ext}(\mathbf{q}+\mathbf{G},\omega) = \sum_{\mathbf{G}'} \epsilon_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) V_{tot}(\mathbf{q}+\mathbf{G}',\omega)$$

Remember: V_{ext} is a macroscopic quantity:

$$V_{ext}(\mathbf{q},\omega) = \sum_{\mathbf{G}'} \epsilon_{\mathbf{G}=0,\mathbf{G}'}(\mathbf{q},\omega) V_{tot}(\mathbf{q}+\mathbf{G}',\omega)$$

$$V_{ext}(\mathbf{q},\omega) = \epsilon_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega) V_{tot,M}(\mathbf{q},\omega) + \sum_{\mathbf{G}'\neq 0} \epsilon_{\mathbf{G}=0,\mathbf{G}'}(\mathbf{q},\omega) V_{tot}(\mathbf{q}+\mathbf{G}',\omega)$$

$$V_{ext}(\mathbf{q},\omega) = \epsilon_M(\mathbf{q},\omega) V_{tot,M}(\mathbf{q},\omega)$$

$$\epsilon_M(\mathbf{q},\omega) \neq \epsilon_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega)$$

Micro-macro connection

Macroscopic dielectric function

$$V_{ext}(\mathbf{q}+\mathbf{G},\omega) = \sum_{\mathbf{G}'} \epsilon_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) V_{tot}(\mathbf{q}+\mathbf{G}',\omega)$$

Remember: V_{ext} is a macroscopic quantity:

$$V_{ext}(\mathbf{q},\omega) = \sum_{\mathbf{G}'} \epsilon_{\mathbf{G}=0,\mathbf{G}'}(\mathbf{q},\omega) V_{tot}(\mathbf{q}+\mathbf{G}',\omega)$$

$$V_{ext}(\mathbf{q},\omega) = \epsilon_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega) V_{tot,M}(\mathbf{q},\omega) + \sum_{\mathbf{G}'\neq 0} \epsilon_{\mathbf{G}=0,\mathbf{G}'}(\mathbf{q},\omega) V_{tot}(\mathbf{q}+\mathbf{G}',\omega)$$

$$V_{ext}(\mathbf{q},\omega) = \epsilon_{M}(\mathbf{q},\omega) V_{tot,M}(\mathbf{q},\omega)$$

$$\epsilon_{M}(\mathbf{q},\omega) \neq \epsilon_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega)$$

Micro-macro connection

Macroscopic dielectric function

$$V_{ext}(\mathbf{q}+\mathbf{G},\omega) = \sum_{\mathbf{G}'} \epsilon_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) V_{tot}(\mathbf{q}+\mathbf{G}',\omega)$$

Remember: V_{ext} is a macroscopic quantity:

$$V_{ext}(\mathbf{q},\omega) = \sum_{\mathbf{G}'} \epsilon_{\mathbf{G}=0,\mathbf{G}'}(\mathbf{q},\omega) V_{tot}(\mathbf{q}+\mathbf{G}',\omega)$$

$$V_{ext}(\mathbf{q},\omega) = \epsilon_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega) V_{tot,M}(\mathbf{q},\omega) + \sum_{\mathbf{G}'\neq 0} \epsilon_{\mathbf{G}=0,\mathbf{G}'}(\mathbf{q},\omega) V_{tot}(\mathbf{q}+\mathbf{G}',\omega)$$

$$V_{ext}(\mathbf{q},\omega) = \epsilon_M(\mathbf{q},\omega) V_{tot,M}(\mathbf{q},\omega)$$

$$\epsilon_M(\mathbf{q},\omega) \neq \epsilon_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega)$$

Micro-macro connection

Spectra

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

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

$$\mathrm{EELS}(\omega) = -\lim_{\mathbf{q}\to 0} \mathrm{Im}\,\epsilon^{-1}_M(\omega) = -\lim_{\mathbf{q}\to 0} \mathrm{Im}\,\epsilon^{-1}_{\mathbf{G}=0,\mathbf{G}'=0}(\mathbf{q},\omega)$$

Micro-macro connection

Spectra

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

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BSE vs. TDDFT: what in common ?

BSE

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

TDDFT

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

The Coulomb term v

The Coulomb term

$$v = v_0 + \bar{v}$$

Local fields reloaded

Microscopic-Macroscopic connection: local fields

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

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

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

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

Local fields reloaded

Microscopic-Macroscopic connection: local fields

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

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

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

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

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}

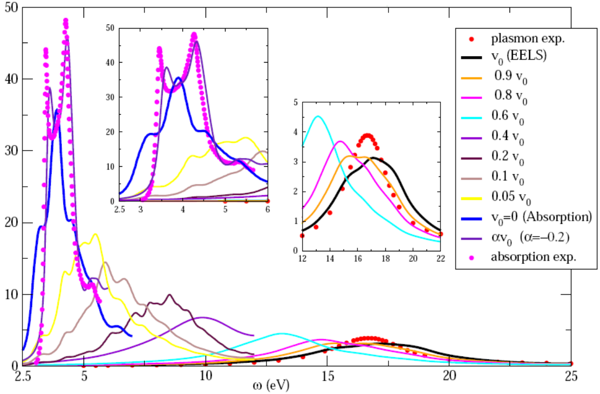
The Coulomb term v

The Coulomb term

$$v = v_0 + \bar{v}$$

long-range $v_0 \Rightarrow$ difference between Abs and Eels

Coulomb term v_0: Abs vs. Eels



F. Sottile, PhD thesis (2003) - Bulk silicon: absorption vs. EELS.

The Coulomb term v

The Coulomb term

$$v = v_0 + \bar{v}$$

long-range $v_0 \Rightarrow$ difference between Abs and Eels

what about $\bar{v}$?

The Coulomb term v

The Coulomb term

$$v = v_0 + \bar{v}$$

long-range $v_0 \Rightarrow$ difference between Abs and Eels

what about $\bar{v}$?

$\bar{v}$ is responsible for crystal local-field effects

Coulomb term $\bar{v}$: local fields

$\bar{v}$: local fields

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

Set $\bar{v} = 0$ in:

$$\bar{\chi}_{\mathbf{G},\mathbf{G}'} = \chi^0_{\mathbf{G},\mathbf{G}'} + \sum_{\mathbf{G}_1} \chi^0_{\mathbf{G},\mathbf{G}_1} \bar{v}_{\mathbf{G}_1} \bar{\chi}_{\mathbf{G}_1,\mathbf{G}'}$$

$$\Rightarrow \bar{\chi}_{\mathbf{G},\mathbf{G}'} = \chi^0_{\mathbf{G},\mathbf{G}'}$$

Result:

$$\epsilon_M = 1 - v_{\mathbf{G}=0}\chi^0_{\mathbf{G}=\mathbf{0},\mathbf{G}'=\mathbf{0}}$$

that is: no local-field effects!
(equivalent to Fermi's golden rule)

Coulomb term $\bar{v}$: local fields

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

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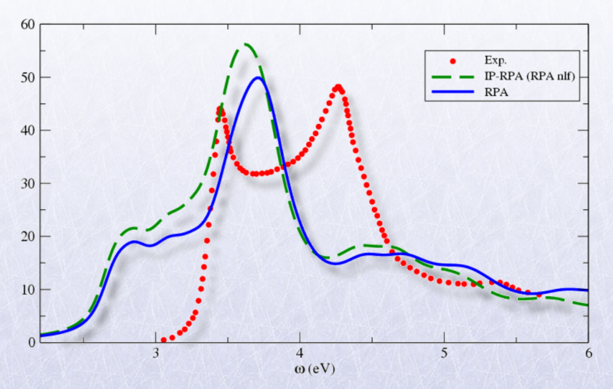
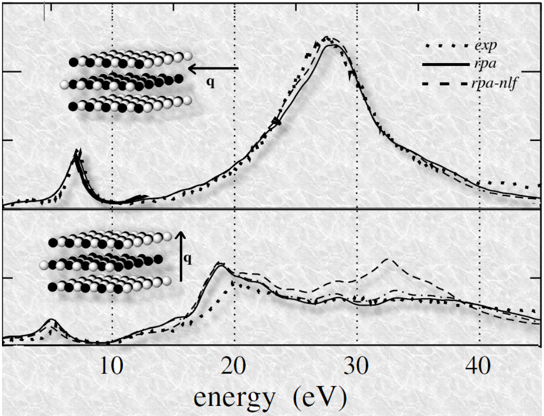
Coulomb term $\bar{v}$: local fields



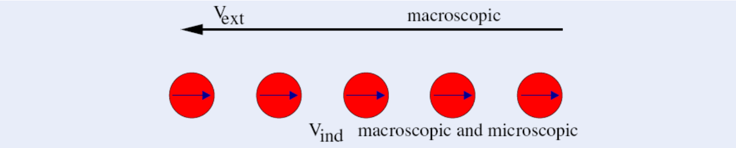
Bulk silicon: absorption

Coulomb term $\bar{v}$: local fields



A. G. Marinopoulos *et al.*, PRL **89** (2002) - Graphite EELS

What are local fields?



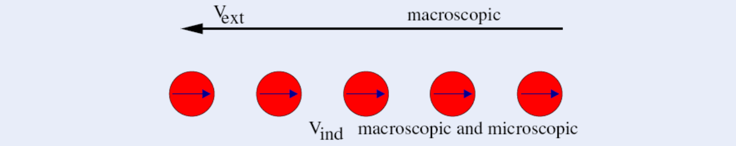
Effective medium theory

Uniform field E_0 applied to a dielectric sphere with dielectric constant ϵ in vacuum. From continuity conditions at the interface:

$$P = \frac{3}{4\pi} \frac{\epsilon - 1}{\epsilon + 2} E_0$$

Jackson, Classical electrodynamics, Sec. 4.4.

What are local fields?



Effective medium theory

Regular lattice of objects dimensionality d of material ϵ_1 in vacuum
Maxwell-Garnett formulas

- dot (O D system)

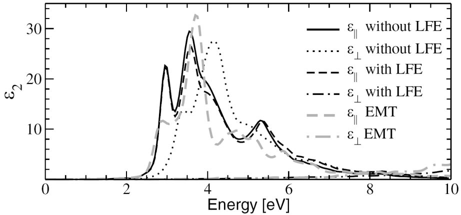
$$\mathrm{Im}\epsilon_M(\omega) \propto 9\frac{\mathrm{Im}\epsilon_1(\omega)}{[\mathrm{Re}\epsilon_1(\omega)+2]^2+[\mathrm{Im}\epsilon_1(\omega)]^2}$$

- wire (1D system)

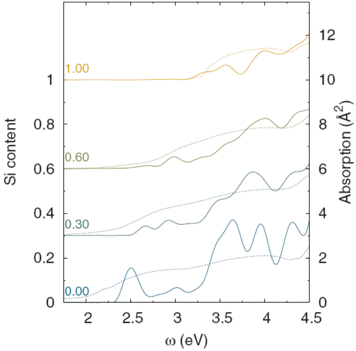
$$\mathrm{Im}\epsilon_M^{\parallel}(\omega) \propto \mathrm{Im}\epsilon_1(\omega)$$

$$\mathrm{Im}\epsilon_M^{\perp}(\omega) \propto 4\frac{\mathrm{Im}\epsilon_1(\omega)}{[\mathrm{Re}\epsilon_1(\omega)+1]^2+[\mathrm{Im}\epsilon_1(\omega)]^2}$$

What are local fields?



F. Bruneval *et al.*, PRL **94** (2005) -
Si nanowires



S. Botti *et al.*, PRB **79** (2009) -
SiGe nanodots

MBPT & TDDFT

MBPT helps improving DFT & TDDFT

DFT & TDDFT help improving MBPT

Conclusion

(TD)DFT & MBPT...

try to learn both!

Many thanks!

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- Francesco Sottile
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