MBPT vs (TD)DFT

a fight or a wedding ?

Francesco Sottile

Laboratoire des Solides Irradiés
Ecole Polytechnique, Palaiseau - France
European Theoretical Spectroscopy Facility (ETSF)

Lyon, 14 December 2007

ETSF
an initiative of the
Nanoquanta
Network of Excellence

Ecole POLYTECHNIQUE

Outline

Outline

A rough Summary

DFT - TDDFT

- √ fast (one-particle eqs)
- × lack of functionals

MBPT (GW-BSE)

- √ it works! (physical ingredients)
- × Cumbersome

Fast, efficient and reliable

A rough Summary

DFT - TDDFT

- √ fast (one-particle eqs)
- × lack of functionals

MBPT (GW-BSE)

- √ it works! (physical ingredients)
- × Cumbersome

Fast, efficient and reliable

A rough Summary

DFT - TDDFT

- √ fast (one-particle eqs)
- × lack of functionals

MBPT (GW-BSE)

- √ it works! (physical ingredients)
- × Cumbersome

Fast, efficient and reliable

A possible strategy

Combine the two approaches

A possible strategy

Dyson eq. for G

$$d\left[\quad G = G_0 + G_0 \left(\Sigma - V_{xc}\right) G \quad\right]$$

$$0 = G_0 \left(\Sigma - V_{xc}\right) G$$

$$\int d(23) G_0(12) \left[\; \Sigma(23) - V_{xc}(2)\delta(23) \;\right] G(31) = 0$$

A possible strategy

Dyson eq. for G

$$d\left[\quad G = G_0 + G_0\,(\Sigma - V_{xc})\,G \quad\right]$$

$$0 = G_0\,(\Sigma - V_{xc})\,G$$

$$\int d(23)G_0(12)\left[\,\Sigma(23) - V_{xc}(2)\delta(23)\,\right]G(31) = 0$$

A possible strategy

Dyson eq. for G

$$d\left[\quad G = G_0 + G_0 \left(\Sigma - V_{xc} \right) G \quad \right]$$

$$0 = G_0 \left(\Sigma - V_{xc} \right) G$$

$$\int d(23) G_0(12) \left[\Sigma(23) - V_{xc}(2)\delta(23) \right] G(31) = 0$$

A possible strategy

Dyson eq. for G

$$\int d(23) G_0(12) \left[\ \Sigma(23) - V_{xc}(2)\delta(23)\ \right] G(31) = 0$$

given a Σ (non-local and dynamic),
we obtain a V_{xc} (local and static) which provides the same density

Sham-Schlüter equation

L.J.Sham and M.Schlter, Phys. Rev. Lett. **51**, 1888 (1983)

A possible strategy

Dyson eq. for G

$$\int d(23)G_0(12)\left[\ \Sigma(23) - V_{xc}(2)\delta(23)\ \right]G(31) = 0$$

given a Σ (non-local and dynamic),

we obtain a V_{xc} (local and static) which provides the same density

Sham-Schlüter equation

L.J.Sham and M.Schlter, Phys. Rev. Lett. **51**, 1888 (1983)

A possible strategy

Dyson eq. for G

$$\int d(23) G_0(12) \left[\, \Sigma(23) - V_{xc}(2)\delta(23) \, \right] G(31) = 0$$

given a Σ (non-local and dynamic),
we obtain a V_{xc} (local and static) which provides the same density

Sham-Schlüter equation

L.J.Sham and M.Schlter, Phys. Rev. Lett. **51**, 1888 (1983)

A possible strategy

Dyson eq. for G

$$\int d(23) G_0(12) \left[\, \Sigma(23) - V_{xc}(2)\delta(23) \, \right] G(31) = 0$$

given a Σ (non-local and dynamic),
we obtain a V_{xc} (local and static) which provides the same density

Sham-Schlüter equation

L.J.Sham and M.Schlter, Phys. Rev. Lett. **51**, 1888 (1983)

A possible strategy

Sham-Schlüter equation

$$\int d(23) G_0(12) \left[\, \Sigma(23) - V_{xc}(2)\delta(23) \, \right] G(31) = 0$$

$$\int d(23) G_0(12) \left[\, \Sigma_x(23) - V_{xc}(2)\delta(23) \, \right] G_0(31) = 0$$

we obtain $V_{xc}^{\mathrm{EXX}} = G_0 G_0 v G_0 (\chi^0)^{-1}$

Exact-Exchange Approximation

A possible strategy

Sham-Schlüter equation

$$\int d(23) G_0(12) \left[\ \Sigma(23) - V_{xc}(2)\delta(23) \ \right] G(31) = 0$$

$$\int d(23) G_0(12) \left[\ \Sigma_x(23) - V_{xc}(2)\delta(23) \ \right] G_0(31) = 0$$

we obtain $V_{xc}^{\text{EXX}} = G_0 G_0 v G_0 (\chi^0)^{-1}$

Exact-Exchange Approximation

A possible strategy

Sham-Schlüter equation

$$\int d(23) G_0(12) \left[\, \Sigma(23) - V_{xc}(2)\delta(23) \, \right] G(31) = 0$$

$$\int d(23) G_0(12) \left[\, \Sigma_x(23) - V_{xc}(2)\delta(23) \, \right] G_0(31) = 0$$

we obtain $V_{xc}^{\text{EXX}} = G_0 G_0 v G_0 (\chi^0)^{-1}$

Exact-Exchange Approximation

A possible strategy

Sham-Schlüter equation

$$\int d(23)G_0(12)\left[\ \Sigma(23) - V_{xc}(2)\delta(23)\ \right]G(31) = 0$$

$$\int d(23)G_0(12)\left[\ \Sigma_x(23) - V_{xc}(2)\delta(23)\ \right]G_0(31) = 0$$

we obtain $V_{xc}^{\mathrm{EXX}} = G_0 G_0 v G_0 (\chi^0)^{-1}$

Exact-Exchange Approximation

A possible strategy

Generalized SSE

$$p\left[\quad G = G_0 + G_0\left(\Sigma - V_{xc}\right) G \quad\right]$$

M.Gatti *et al*, Phys. Rev. Lett. **99**, 057401 (2007)

A possible strategy

Generalized SSE

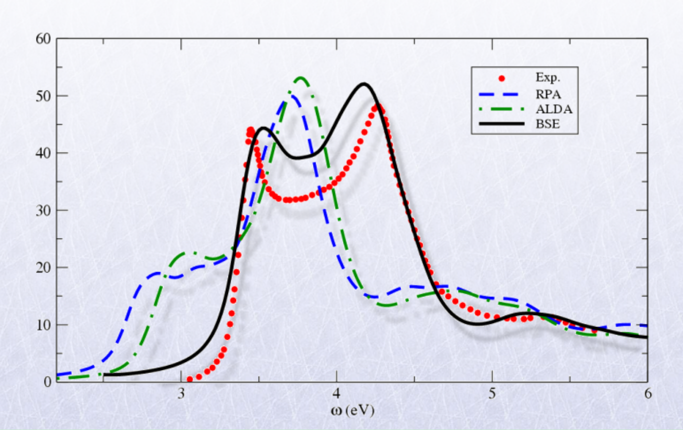
$$p\Big[\quad G = G_0 + G_0\left(\Sigma - V_{xc}\right)G \quad\Big]$$

M.Gatti *et al*, Phys. Rev. Lett. **99**, 057401 (2007)

Outline

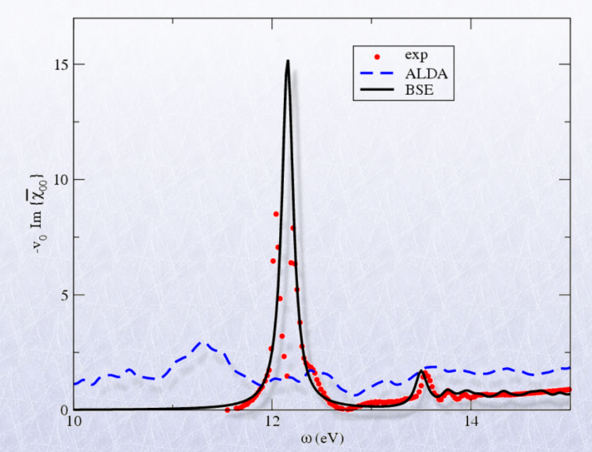
Optical Absorption Spectra of Solids

Semiconductors: Silicon



Optical Absorption Spectra of Solids

Insulators: Argon



Optical Absorption Spectra of Solids

- ALDA bad for any solids!! though quick
- BSE good but cumbersome

Optical Absorption Spectra of Solids

The problem of Abs in solids. Towards a better understanding

- Reining *et al.* Phys.Rev.Lett. **88**, 66404 (2002)
  Long-range kernel
- de Boeij *et al.* J.Chem.Phys. **115**, 1995 (2002)
  Polarization density functional. Long-range.
- Kim and Görling Phys.Rev.Lett. **89**, 96402 (2002)
  Exact-exchange
- Sottile *et al.* Phys.Rev.B **68**, 205112 (2003)
  Long-range and contact exciton.
- Botti *et al.* Phys. Rev. B **72**, 125203 (2005)
  Dynamic long-range component

Parameters to fit to experiments.

Optical Absorption Spectra of Solids

The problem of Abs in solids. Towards a better understanding

- Reining *et al.* Phys.Rev.Lett. **88**, 66404 (2002)
  Long-range kernel
- de Boeij *et al.* J.Chem.Phys. **115**, 1995 (2002)
  Polarization density functional. Long-range.
- Kim and Görling Phys.Rev.Lett. **89**, 96402 (2002)
  Exact-exchange
- Sottile *et al.* Phys.Rev.B **68**, 205112 (2003)
  Long-range and contact exciton.
- Botti *et al.* Phys. Rev. B **72**, 125203 (2005)
  Dynamic long-range component

Parameters to fit to experiments.

Beyond ALDA approximation

Abs in solids. Insights from MBPT

Parameter-free Ab initio kernels

- Sottile *et al.* Phys.Rev.Lett. **91**, 56402 (2003)
  Full many-body kernel. Mapping Theory.
- Marini *et al.* Phys.Rev.Lett. **91**, 256402 (2003)
  Full many-body kernel. Perturbation Theory.

$$f_{xc} = \chi_0^{-1} GGWGG \chi_0^{-1}$$

Outline

Outline

1. Introduction
2. BSE and TDDFT up to 2002
3. The Mapping Theory Kernel
   - Theory
   - Results
4. Conclusions and Perspectives

The Mapping Theory

The idea

BSE works ⇒ { we get the ingredients of the BSE
and we put them in TDDFT

The Mapping Theory

BSE: Excitonic Hamiltonian 4-point

$$H^{\text{BSE}}_{(vc)(v'c')} = \Big[(E_c - E_v)\, \delta_{vv'}\delta_{cc'} + v^{v'c'}_{vc} - W^{v'c'}_{vc} \Big]$$

The Mapping Theory

BSE: Excitonic Hamiltonian 4-point

$$H^{\text{BSE}} = \Big[(E_c - E_v) + \ll v \gg - \ll W \gg \Big]$$

The Mapping Theory

BSE: Excitonic Hamiltonian — 4-point

$$H^{\text{BSE}} = \left[\left(\epsilon_c + \Delta_c^{\text{GW}} - \epsilon_v - \Delta_v^{\text{GW}} \right) + \ll v \gg - \ll W \gg \right]$$

The Mapping Theory

BSE: Excitonic Hamiltonian — 4-point

$$H^{\text{BSE}} = \left[\left(\epsilon_c + \Delta_c^{\text{GW}} - \epsilon_v - \Delta_v^{\text{GW}} \right) + \ll v \gg - \ll W \gg \right]$$

TDDFT: Polarizability equation — 2-point

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

The Mapping Theory

BSE: Excitonic Hamiltonian 4-point

$$H^{\mathrm{BSE}} = \left[\left(\epsilon_c + \Delta_c^{\mathrm{GW}} - \epsilon_v - \Delta_v^{\mathrm{GW}} \right) + \ll v \gg - \ll W \gg \right]$$

TDDFT: written in transition space 4-point

$$H^{\mathrm{TDDFT}} = \left[(\epsilon_c - \epsilon_v) + \ll v \gg + \ll f_{xc} \gg \right]$$

The Mapping Theory

BSE: Excitonic Hamiltonian 4-point

$$H^{\text{BSE}} = \left[\left(\epsilon_c + \Delta_c^{\text{GW}} - \epsilon_v - \Delta_v^{\text{GW}} \right) + \ll v \gg - \ll W \gg \right]$$

TDDFT: written in transition space 4-point

$$H^{\text{TDDFT}} = \left[(\epsilon_c - \epsilon_v) + \ll v \gg + \ll f_{xc} \gg \right]$$

The exchange-correlation kernel f_{xc} has to take into account both GW corrections and excitonic effects !!

The Mapping Theory

BSE: Excitonic Hamiltonian — 4-point

$$H^{\text{BSE}} = \left[(E_c - E_v) + \ll v \gg - \ll W \gg \right]$$

TDDFT: written in transition space — 4-point

$$H^{\text{TDDFT}} = \left[(E_c - E_v) + \ll v \gg + \ll f_{xc} \gg \right]$$

Same starting point for both BSE and TDDFT: the GW band-structure.

The Mapping Theory

BSE: Excitonic Hamiltonian 4-point

$$H^{\mathrm{BSE}} = \Big[(E_c - E_v) + \ll v \gg - \ll W \gg \Big]$$

TDDFT: written in transition space 4-point

$$H^{\mathrm{TDDFT}} = \Big[(E_c - E_v) + \ll v \gg + \ll f_{xc} \gg \Big]$$

We concentrate, then, only on the excitonic effects.

The Mapping Theory

BSE: Excitonic Hamiltonian 4-point

$$H^{\mathrm{BSE}} = \left[(E_c - E_v) + \ll v \gg - \ll W \gg \right]$$

TDDFT: written in transition space 4-point

$$H^{\mathrm{TDDFT}} = \left[(E_c - E_v) + \ll v \gg - \ll W \gg \right]$$

We substitute the 'unknown' $\ll f_{xc} \gg$ with $\ll W \gg$.

The Mapping Theory

The idea

We want to use $\ll W \gg$, but in a 2-point equation.

$$\chi(12,\omega) = \chi_0(12,\omega) + \chi_0(13,\omega)\left(v(34) + f_{xc}(34,\omega)\right)\chi(42,\omega)$$

The Mapping Theory

The idea

We want to use $\ll W \gg$, but in a 2-point equation.

$$\chi(12,\omega) = \chi_0(12,\omega) + \chi_0(13,\omega)\left(v(34) + f_{xc}(34,\omega)\right)\chi(42,\omega)$$

The Mapping Theory

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

$$\chi = \left(1 - \chi_0 v - \chi_0 f_{xc}\right)^{-1} \chi_0$$

Let's define an invertible matrix $X(12,\omega) = \sum_{vc} \phi_v(1)\phi_c(1) g_{vc}(2,\omega)$

$$\chi = X X^{-1} \left(1 - \chi_0 v - \chi_0 X^{-1} X f_{xc}\right)^{-1} \chi_0$$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} X f_{xc} X\right)^{-1} \chi_0$$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} T\right)^{-1} \chi_0$$

The Mapping Theory

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

$$\chi = \left(1 - \chi_0 v - \chi_0 f_{xc} \right)^{-1} \chi_0$$

Let's define an invertible matrix $X(12,\omega) = \sum_{vc} \phi_v(1)\phi_c(1) g_{vc}(2,\omega)$

$$\chi = XX^{-1} \left(1 - \chi_0 v - \chi_0 X^{-1} X f_{xc} \right)^{-1} \chi_0$$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} X f_{xc} X \right)^{-1} \chi_0$$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} T \right)^{-1} \chi_0$$

The Mapping Theory

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

$$\chi = \left(1 - \chi_0 v - \chi_0 f_{xc} \right)^{-1} \chi_0$$

Let's define an invertible matrix $X(12,\omega) = \sum_{vc} \phi_v(1)\phi_c(1) g_{vc}(2,\omega)$

$$\chi = X X^{-1} \left(1 - \chi_0 v - \chi_0 X^{-1} X f_{xc} \right)^{-1} \chi_0$$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} X f_{xc} X \right)^{-1} \chi_0$$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} T \right)^{-1} \chi_0$$

The Mapping Theory

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

$$\chi = \left(1 - \chi_0 v - \chi_0 f_{xc} \right)^{-1} \chi_0$$

Let's define an invertible matrix $X(12,\omega) = \sum_{vc} \phi_v(1)\phi_c(1) g_{vc}(2,\omega)$

$$\chi = XX^{-1} \left(1 - \chi_0 v - \chi_0 X^{-1} X f_{xc} \right)^{-1} \chi_0$$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} X f_{xc} X \right)^{-1} \chi_0$$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} T \right)^{-1} \chi_0$$

The Mapping Theory

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

$$\chi = \left(1 - \chi_0 v - \chi_0 f_{xc} \right)^{-1} \chi_0$$

Let's define an invertible matrix $X(12,\omega) = \sum_{vc} \phi_v(1)\phi_c(1)g_{vc}(2,\omega)$

$$\chi = XX^{-1} \left(1 - \chi_0 v - \chi_0 X^{-1} X f_{xc} \right)^{-1} \chi_0$$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} X f_{xc} X \right)^{-1} \chi_0$$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} T \right)^{-1} \chi_0$$

The Mapping Theory

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

$$\chi = \left(1 - \chi_0 v - \chi_0 f_{xc}\right)^{-1} \chi_0$$

Let's define an invertible matrix $X(12,\omega) = \sum_{vc} \phi_v(1)\phi_c(1)g_{vc}(2,\omega)$

$$\chi = XX^{-1} \left(1 - \chi_0 v - \chi_0 X^{-1} X f_{xc}\right)^{-1} \chi_0$$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} X f_{xc} X\right)^{-1} \chi_0$$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} T\right)^{-1} \chi_0$$

The Mapping Theory

$$\chi = X\left(X - \chi_0 v X - \chi_0 X^{-1} T\right)^{-1} \chi_0$$

$$T(12,\omega) = X(13,\omega) f_{xc}(34,\omega) X(42,\omega) = \sum_{vc} \int d(34) g_{vc}(1,\omega)\phi_v(3)\phi_c(3) f_{xc}(34,\omega)\phi_{v'}(4)\phi_{c'}(4) g_{v'c'}(2,\omega)$$

$$T(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll f_{xc} \gg g_{v'c'}(2,\omega)$$

$$T_{\text{BSE}}(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll W \gg g_{v'c'}(2,\omega)$$

The Mapping Theory

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} T \right)^{-1} \chi_0$$

$$T(12,\omega) = X(13,\omega) f_{xc}(34,\omega) X(42,\omega) =$$

$$\sum_{vc} \int d(34) g_{vc}(1,\omega) \phi_v(3) \phi_c(3) f_{xc}(34,\omega) \phi_{v'}(4) \phi_{c'}(4) g_{v'c'}(2,\omega)$$

$$T(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll f_{xc} \gg g_{v'c'}(2,\omega)$$

$$T_{\text{BSE}}(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll W \gg g_{v'c'}(2,\omega)$$

The Mapping Theory

$$\chi = X\left(X - \chi_0 v X - \chi_0 X^{-1} T\right)^{-1} \chi_0$$

$$T(12,\omega) = X(13,\omega) f_{xc}(34,\omega) X(42,\omega) =$$

$$\sum_{vc} \int d(34) g_{vc}(1,\omega)\phi_v(3)\phi_c(3) f_{xc}(34,\omega)\phi_{v'}(4)\phi_{c'}(4) g_{v'c'}(2,\omega)$$

$$T(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll f_{xc} \gg g_{v'c'}(2,\omega)$$

$$T_{\text{BSE}}(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll W \gg g_{v'c'}(2,\omega)$$

The Mapping Theory

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} T \right)^{-1} \chi_0$$

$$T(12,\omega) = X(13,\omega) f_{xc}(34,\omega) X(42,\omega) =$$

$$\sum_{vc} \int d(34) g_{vc}(1,\omega)\phi_v(3)\phi_c(3) f_{xc}(34,\omega)\phi_{v'}(4)\phi_{c'}(4) g_{v'c'}(2,\omega)$$

$$T(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll f_{xc} \gg g_{v'c'}(2,\omega)$$

$$T_{\mathrm{BSE}}(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll W \gg g_{v'c'}(2,\omega)$$

The Mapping Theory

$$\chi = X\left(X - \chi_0 v X - \chi_0 X^{-1} T\right)^{-1} \chi_0$$

$$T(12,\omega) = X(13,\omega) f_{xc}(34,\omega) X(42,\omega) =$$

$$\sum_{\substack{vc \\ v'c'}} \int d(34) g_{vc}(1,\omega)\phi_v(3)\phi_c(3) f_{xc}(34,\omega)\phi_{v'}(4)\phi_{c'}(4) g_{v'c'}(2,\omega)$$

$$T(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll f_{xc} \gg g_{v'c'}(2,\omega)$$

$$T_{\mathrm{BSE}}(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll W \gg g_{v'c'}(2,\omega)$$

The Mapping Theory

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} T \right)^{-1} \chi_0$$

$$T(12,\omega) = X(13,\omega) f_{xc}(34,\omega) X(42,\omega) = \sum_{\substack{vc \\ v'c'}} \int d(34) g_{vc}(1,\omega)\phi_v(3)\phi_c(3) f_{xc}(34,\omega)\phi_{v'}(4)\phi_{c'}(4) g_{v'c'}(2,\omega)$$

$$T(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll f_{xc} \gg g_{v'c'}(2,\omega)$$

$$T_{\mathrm{BSE}}(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll W \gg g_{v'c'}(2,\omega)$$

The Mapping Theory

$$\chi = X\left(X - \chi_0 vX - \chi_0 X^{-1} T\right)^{-1}\chi_0$$

$$T(12,\omega) = X(13,\omega)f_{xc}(34,\omega)X(42,\omega) =$$

$$\sum_{\substack{vc\\v'c'}} \int d(34) g_{vc}(1,\omega)\phi_v(3)\phi_c(3)f_{xc}(34,\omega)\phi_{v'}(4)\phi_{c'}(4)g_{v'c'}(2,\omega)$$

$$T(12,\omega) = \sum_{\substack{vc\\v'c'}} g_{vc}(1,\omega) \ll f_{xc} \gg g_{v'c'}(2,\omega)$$

$$T_{\mathrm{BSE}}(12,\omega) = \sum_{\substack{vc\\v'c'}} g_{vc}(1,\omega) \ll W \gg g_{v'c'}(2,\omega)$$

The Mapping Theory

$$\chi = X\left(X - \chi_0 v X - \chi_0 X^{-1} T\right)^{-1} \chi_0$$

$$T(12,\omega) = X(13,\omega) f_{xc}(34,\omega) X(42,\omega) =$$

$$\sum_{\substack{vc \\ v'c'}} \int d(34) g_{vc}(1,\omega)\phi_v(3)\phi_c(3) f_{xc}(34,\omega)\phi_{v'}(4)\phi_{c'}(4) g_{v'c'}(2,\omega)$$

$$T(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll f_{xc} \gg g_{v'c'}(2,\omega)$$

$$T_{\text{BSE}}(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll W \gg g_{v'c'}(2,\omega)$$

The Mapping Theory

TDDFT 2-point equation containing $\ll W \gg$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} T \right)^{-1} \chi_0$$

$$T_{\text{BSE}}(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll W \gg g_{v'c'}(2,\omega)$$

$$X(12,\omega) = \sum_{vc} \phi_v(1)\phi_c(1) g_{vc}(2,\omega)$$

What about the application ??

The Mapping Theory

TDDFT 2-point equation containing $\ll W \gg$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} T \right)^{-1} \chi_0$$

$$T_{\mathrm{BSE}}(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll W \gg g_{v'c'}(2,\omega)$$

$$X(12,\omega) = \sum_{vc} \phi_v(1)\phi_c(1) g_{vc}(2,\omega)$$

What about the application ??

The Mapping Theory

TDDFT 2-point equation containing $\ll W \gg$

$$\chi = X \left(X - \chi_0 v X - \chi_0 X^{-1} T \right)^{-1} \chi_0$$

$$T_{\mathrm{BSE}}(12,\omega) = \sum_{\substack{vc \\ v'c'}} g_{vc}(1,\omega) \ll W \gg g_{v'c'}(2,\omega)$$

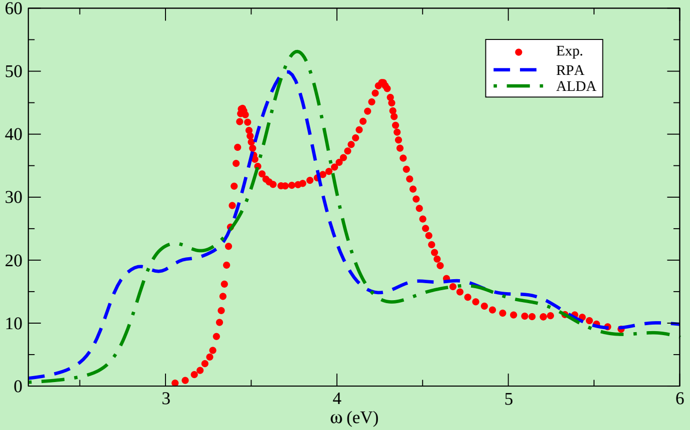
$$X(12,\omega) = \sum_{vc} \phi_v(1)\phi_c(1) g_{vc}(2,\omega)$$

What about the application ??

Outline

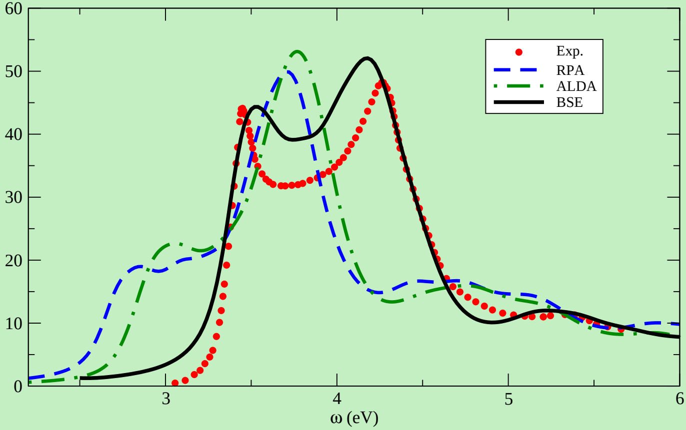
The Mapping Theory: Results

Absorption of Silicon



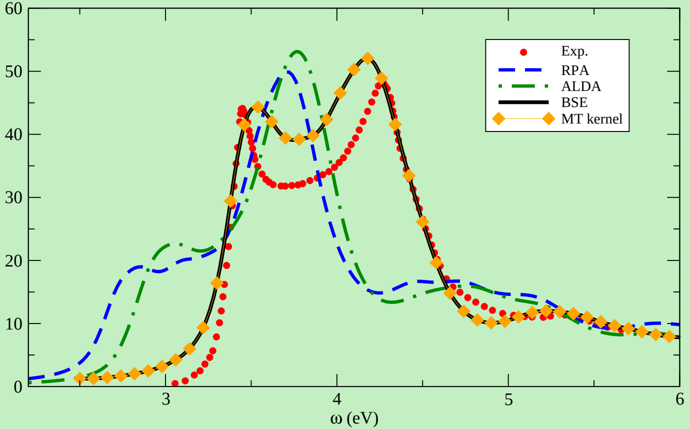
The Mapping Theory: Results

Absorption of Silicon



The Mapping Theory: Results

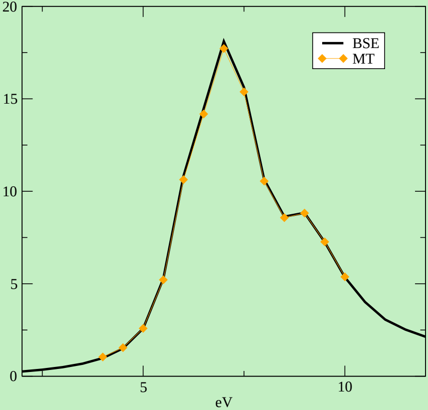
Absorption of Silicon

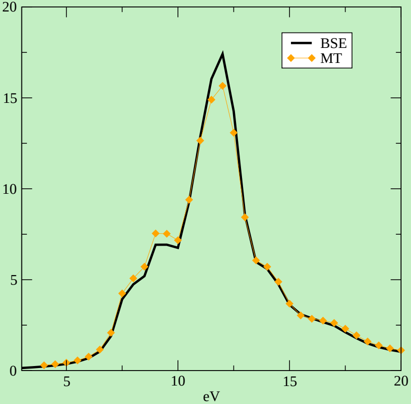


F.Sottile *et al.* Phys.Rev.Lett **91**, 56402 (2003)

The Mapping Theory: Results

Absorption of Silicon Carbide and Diamond

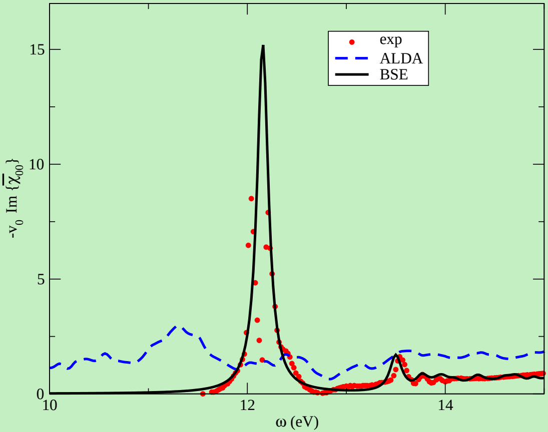




last week preliminary results :-)

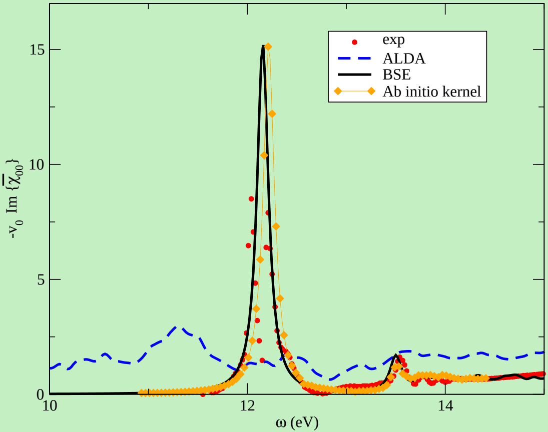
The Mapping Theory: Results

Absorption of Argon



The Mapping Theory: Results

Absorption of Argon



F.Sottile, M.Marsili *et al.*, PRB(R) **76**, 161103 (2007)

The Mapping Theory: Results

Tested also on absorption of SiO_2, DNA bases, Ge-nanowires, RAS of diamond surface, and EELS of LiF.

- Marini *et al.* Phys.Rev.Lett. **91**, 256402 (2003).
- Bruno *et al.* Phys.Rev.B **72** 153310, (2005).
- Palummo *et al.* Phys.Rev.Lett. **94** 087404 (2005).
- Varsano *et al.* J.Phys.Chem.B **110** 7129 (2006).

Outline

Conclusions

TDDFT is the method of choice

- √ Absorption spectra of simple molecules
- √ Electron energy loss spectra
- √ Inelastic X-ray scattering spectroscopy
- √ Absorption of Solids (BSE-like scaling)

Conclusions

DFT-MBPT

- ⇒ Mapping Theory
- ⇒ OEP (EXX, etc.)

Functionals [ρ]

- ⇒ Meta-GGA
- ⇒ Orbital dependency

Extensions of TDDFT

- ⇒ TD-CDFT
- ⇒ Deformation Theory

Today challenges

- ⇒ Open shells systems
- ⇒ Charge transfer excitations
- ⇒ Efficient calculations of Solids

Conclusions

DFT-MBPT

- ⇒ Mapping Theory
- ⇒ OEP (EXX, etc.)

Functionals [ρ]

- ⇒ Meta-GGA
- ⇒ Orbital dependency

Extensions of TDDFT

- ⇒ TD-CDFT
- ⇒ Deformation Theory

Today challenges

- ⇒ Open shells systems
- ⇒ Charge transfer excitations
- ⇒ Efficient calculations of Solids

Conclusions

DFT-MBPT

- ⇒ Mapping Theory
- ⇒ OEP (EXX, etc.)

Functionals $[\rho]$

- ⇒ Meta-GGA
- ⇒ Orbital dependency

Extensions of TDDFT

- ⇒ TD-CDFT
- ⇒ Deformation Theory

Today challenges

- ⇒ Open shells systems
- ⇒ Charge transfer excitations
- ⇒ Efficient calculations of Solids

Conclusions

DFT-MBPT

- ⇒ Mapping Theory
- ⇒ OEP (EXX, etc.)

Functionals [ρ]

- ⇒ Meta-GGA
- ⇒ Orbital dependency

Extensions of TDDFT

- ⇒ TD-CDFT
- ⇒ Deformation Theory

Today challenges

- ⇒ Open shells systems
- ⇒ Charge transfer excitations
- ⇒ Efficient calculations of Solids