The Bethe-Salpeter Equation

An Introduction

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Outline

Outline

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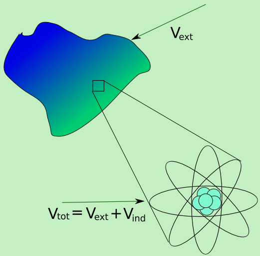
Linear Response Approach

System subject to an external perturbation



Linear Response Approach

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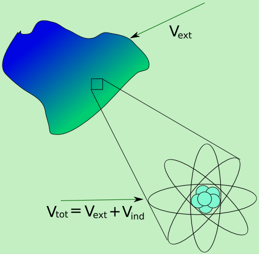
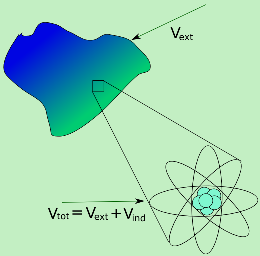


$$V_{tot} = \varepsilon^{-1} V_{ext}$$

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

Linear Response Approach

System subject to an external perturbation



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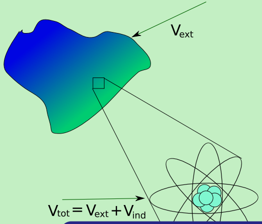
$$\mathbf{E} = \varepsilon^{-1} \mathbf{D}$$

Linear Response Approach

System subject to an external perturbation



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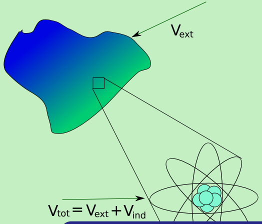
Dielectric function ε

$$\varepsilon$$

Linear Response Approach

System subject to an external perturbation



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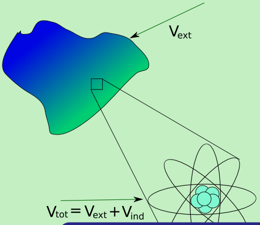
Dielectric function ε

ε

Abs

Linear Response Approach

System subject to an external perturbation



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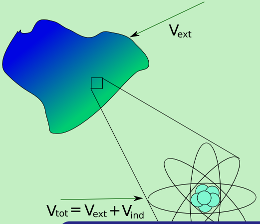
Dielectric function ε

EELS ↔ ε

Abs ↔ ε

Linear Response Approach

System subject to an external perturbation



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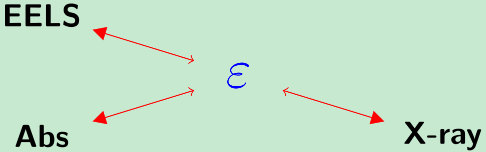

Linear Response Approach

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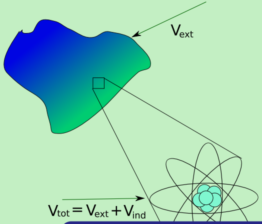

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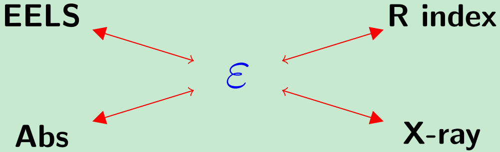

Linear Response Approach

Definition of polarizability

$$\varepsilon^{-1} = 1 + v\chi$$

χ is the polarizability of the system

Linear Response Approach

Polarizability

interacting system $\delta n = \chi \delta V_{ext}$

non-interacting system $\delta n_{n-i} = \chi^0 \delta V_{tot}$

Linear Response Approach

Polarizability

interacting system $\delta n = \chi \delta V_{ext}$

non-interacting system $\delta n_{n-i} = \chi^0 \delta V_{tot}$

Single-particle polarizability

$$\chi^0 = \sum_{ij} \frac{\phi_i(\mathbf{r})\phi_j^*(\mathbf{r})\phi_i^*(\mathbf{r}')\phi_j(\mathbf{r}')}{\omega - (\epsilon_i - \epsilon_j) + i\eta}$$

hartree, hartree-fock, dft, etc.

G.D. Mahan *Many Particle Physics* (Plenum, New York, 1990)

Linear Response Approach

Polarizability

interacting system $\delta n = \chi \delta V_{ext}$

non-interacting system $\delta n_{n-i} = \chi^0 \delta V_{tot}$

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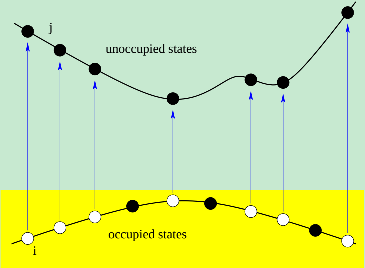

Linear Response Approach

First approximation: IP-RPA

$$\chi^0 = \sum_{ij} \frac{\phi_i(\mathbf{r})\phi_j^*(\mathbf{r})\phi_i^*(\mathbf{r}')\phi_j(\mathbf{r}')}{\omega - (\epsilon_i - \epsilon_j) + i\eta}$$

$$\text{Abs} = \text{Im}\left\langle \chi^0 \right\rangle = \sum_{ij} \left|\langle j|D|i\rangle\right|^2 \delta(\omega - (\epsilon_j - \epsilon_i))$$

Linear Response Approach

First approximation: IP-RPA

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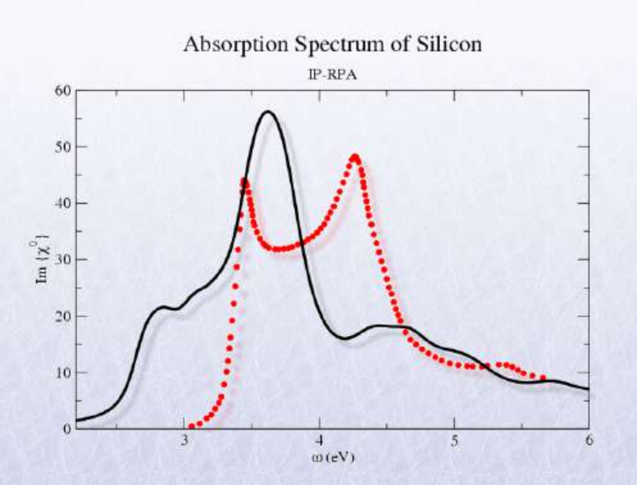

Linear Response Approach

How to go beyond χ^0 ?

Outline

TDDFT - Linear Response Approach

Polarizability

interacting system $\delta n = \chi \delta V_{ext}$

non-interacting system $\delta n_{n-i} = \chi^0 \delta V_{tot}$

$\Updownarrow$

Density Functional Formalism

$$\delta n = \delta n_{n-i}$$

$$\delta V_{tot} = \delta V_{ext} + \delta V_H + \delta V_{xc}$$

TDDFT - Linear Response Approach

Polarizability

interacting system $\delta n = \chi \delta V_{ext}$

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$$\Updownarrow$$

Density Functional Formalism

$$\delta n = \delta n_{n-i}$$

$$\delta V_{tot} = \delta V_{ext} + \delta V_H + \delta V_{xc}$$

TDDFT - Linear Response Approach

Polarizability

$$\chi \delta V_{ext} = \chi^0 \left(\delta V_{ext} + \delta V_H + \delta V_{xc}\right)$$

$$\chi = \chi^0 \left(1 + \frac{\delta V_H}{\delta V_{ext}} + \frac{\delta V_{xc}}{\delta V_{ext}}\right)$$

$$\frac{\delta V_H}{\delta V_{ext}} = \frac{\delta V_H}{\delta n}\frac{\delta n}{\delta V_{ext}} = v\chi$$

$$\frac{\delta V_{xc}}{\delta V_{ext}} = \frac{\delta V_{xc}}{\delta n}\frac{\delta n}{\delta V_{ext}} = f_{xc}\chi$$

with $f_{xc} = \frac{\delta V_{xc}}{\delta n}$ **exchange-correlation kernel**

with $v = \frac{\delta V_H}{\delta n}$ **coulomb interaction**

TDDFT - Linear Response Approach

Polarizability

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$$\frac{\delta V_H}{\delta V_{ext}} = \frac{\delta V_H}{\delta n} \frac{\delta n}{\delta V_{ext}} = v\chi$$

$$\frac{\delta V_{xc}}{\delta V_{ext}} = \frac{\delta V_{xc}}{\delta n} \frac{\delta n}{\delta V_{ext}} = f_{xc}\chi$$

$$\chi = \chi^0 + \chi^0 \left(v + f_{xc} \right) \chi$$

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TDDFT - Linear Response Approach

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$$\chi = \left[1 - \chi^0 \left(v + f_{xc} \right) \right]^{-1} \chi^0$$

with $f_{xc} = \frac{\delta V_{xc}}{\delta n}$ **exchange-correlation kernel**

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Linear Response Approach - Polarizability in TDDFT

Approximation for the x-c kernel

- $f_{xc}^{\text{RPA}} = 0$
- $f_{xc}^{\text{ALDA}} = \frac{\delta V_{xc}^{\text{LDA}}}{\delta n} \delta_{12}(\omega = 0)$
- f_{xc} GGA, Meta-GGA, EXX, etc.

Linear Response Approach - Polarizability in TDDFT

ALDA & GGA

Good results in simple molecules. Promising results for new frontier applications.

Serious shortcomings

Optical Response of Solids

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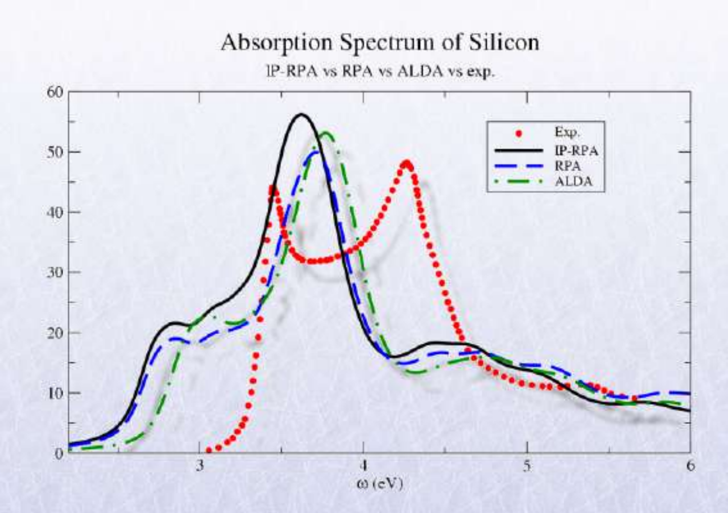
First approximation: IP-RPA



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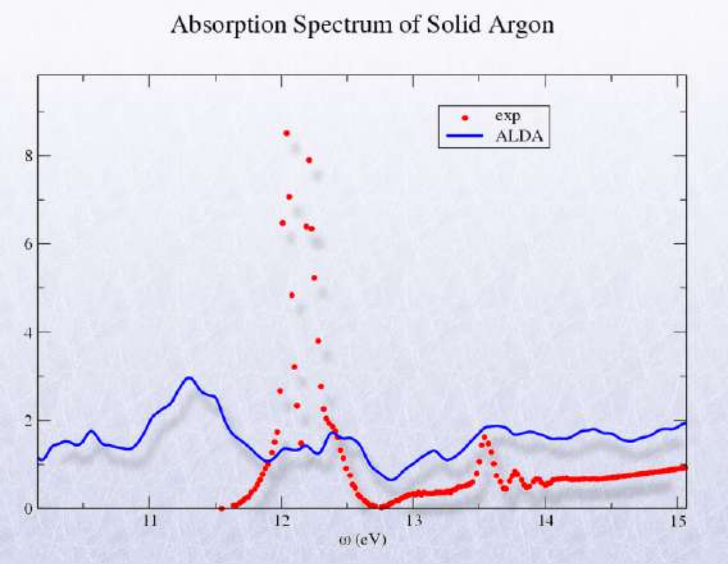

Outline

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Many Body Perturbation Theory

Hedin's equations

$$\Sigma(1,2) = i \int d(34) G(1,3) \tilde{\Gamma}(3,2,4) W(4,1^+)$$

$$G(1,2) = G^0(1,2) + \int d(34) G^0(1,3) \Sigma(3,4) G(4,2)$$

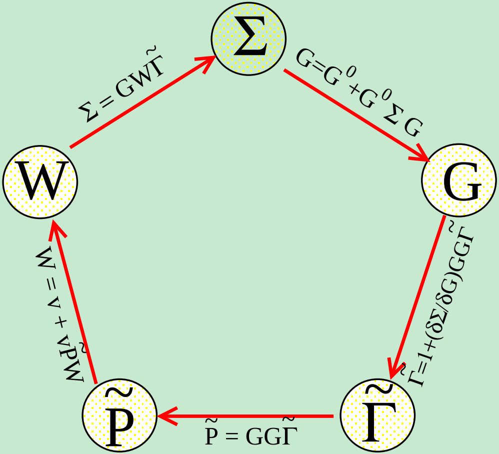
$$\tilde{\Gamma}(1,2,3) = \delta(1,2)\delta(1,3) + \int d(4567) \frac{\delta \Sigma(1,2)}{\delta G(4,5)} G(4,6) G(7,5) \tilde{\Gamma}(6,7,3)$$

$$\tilde{P}(1,2) = -i \int d(34) G(1,3) G(4,1^+) \tilde{\Gamma}(3,4,2)$$

$$W(1,2) = v(1,2) + \int d(34) v(1,3) \tilde{P}(3,4) W(4,2)$$

Many Body Perturbation Theory

Hedin's pentagon



Many Body Perturbation Theory

Polarizability $\tilde{P}$ is *irreducible*

$$\tilde{P} = \frac{\delta n}{\delta U} \qquad ; \qquad U = V_{ext} + V_H$$

$$\tilde{\Gamma} = \frac{\delta G^{-1}}{\delta U} = 1 + \frac{\delta \Sigma}{\delta U}$$

Irreducible $\tilde{P}$ and Reducible χ

$$\tilde{P} = \frac{\delta n}{\delta U} \qquad ; \qquad \chi = \frac{\delta n}{\delta V_{ext}}$$

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

Different quantities

$$\tilde{P}, \tilde{\Gamma}, G \quad = \quad \text{time-ordered}$$
$$\chi^0, \chi \quad = \quad \text{retarded}$$

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Different quantities

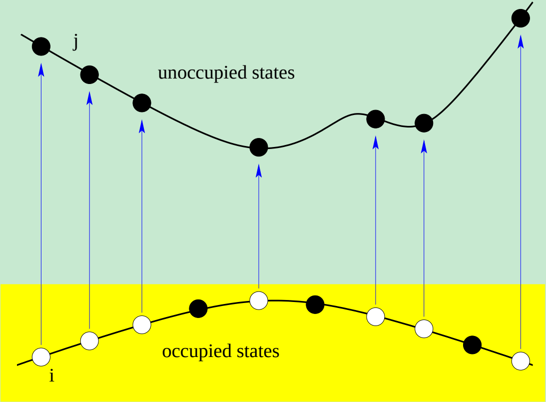
$\tilde{P}, \tilde{\Gamma}, G$	$=$	time-ordered
χ^0, χ	$=$	retarded

Spectra in MBPT

Spectra in IP picture

IP-RPA

$$\text{Abs} = \text{Im}\ \chi^0$$



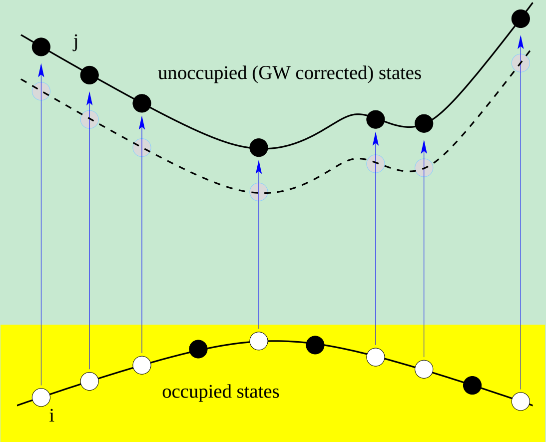
Spectra in MBPT

Spectra in GW approximation

GW-RPA

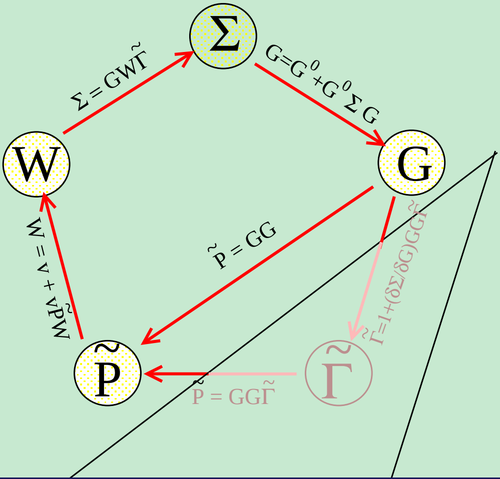
$$\text{Abs} = \text{Im}\ \chi^0_{\text{GW}}$$

$$\chi^0_{\text{GW}} = P = -iGG$$



Spectra in MBPT

GW pentagon



Spectra in MBPT

Spectra in GW-RPA

$$\chi^0 = \sum_{ij} \frac{\phi_i(\mathbf{r})\phi_j^*(\mathbf{r})\phi_i^*(\mathbf{r}')\phi_j(\mathbf{r}')}{\omega - (\epsilon_i - \epsilon_j)}$$

$$\Downarrow$$

$$\chi^0_{\mathrm{GW}} = \sum_{ij} \frac{\phi_i(\mathbf{r})\phi_j^*(\mathbf{r})\phi_i^*(\mathbf{r}')\phi_j(\mathbf{r}')}{\omega - \left[\left(\epsilon_i + \Delta_i^{\mathrm{GW}}\right) - \left(\epsilon_j + \Delta_j^{\mathrm{GW}}\right)\right]}$$

Spectra in MBPT

Spectra in GW-RPA

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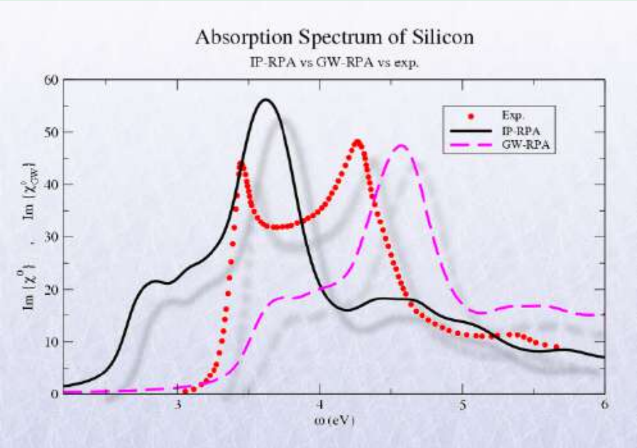
Spectra in MBPT

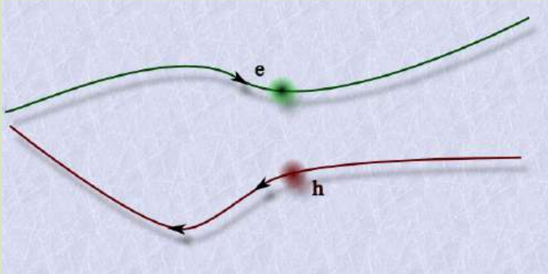
Spectra in GW-RPA



Spectra in MBPT

GG Polarizability

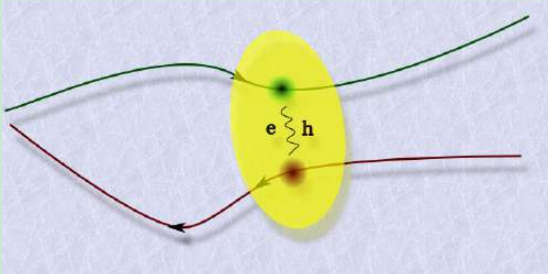
$$\tilde{P}(1,2) = -i \quad G(1,2)G(2,1^+)$$



Spectra in MBPT

GGΓ Polarizability

$$\tilde{P}(1,2) = -i \int d(34) G(1,3) G(4,1^+) \tilde{\Gamma}(3,4,2)$$



Outline

Bethe-Salpeter Equation

$$\tilde{\Gamma}(1,2,3) = \delta(1,2)\delta(1,3) + \\ + \int d(4567) \frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6) G(7,5) \tilde{\Gamma}(6,7,3)$$

Bethe-Salpeter Equation

Towards the Bethe-Salpeter

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

$$G G \tilde{\Gamma} = G G + G G \frac{\delta \Sigma}{\delta G} G G \tilde{\Gamma}$$

$$\tilde{L} = L^0 + L^0 \frac{\delta \Sigma}{\delta G} \tilde{L}$$

$$\tilde{L}(1234) = L^0(1234) + L^0(1256) \frac{\delta \Sigma(56)}{\delta G(78)} \tilde{L}(7834)$$

Bethe-Salpeter Equation

Towards the Bethe-Salpeter

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

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

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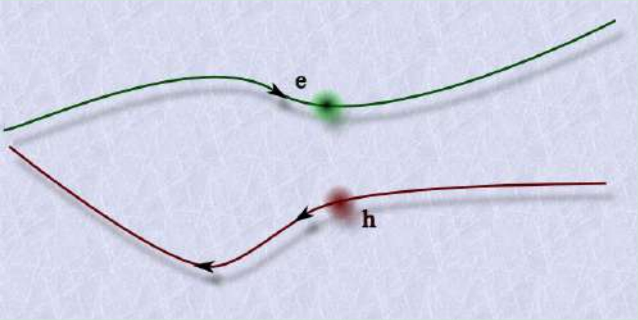
Bethe-Salpeter Equation

Towards the Bethe-Salpeter Equation

From electron and hole propagation ... ..

$$L^0(1234) = G(13)G(42) \qquad \ldots$$

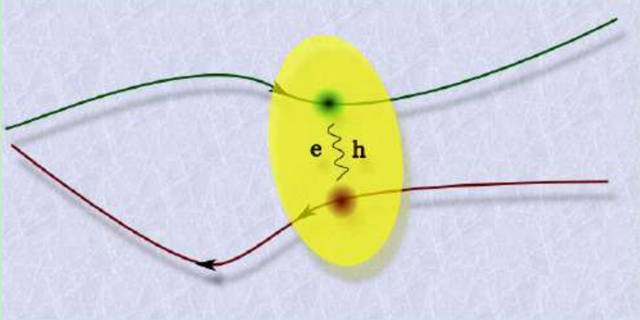


Bethe-Salpeter Equation

Towards the Bethe-Salpeter Equation

From electron and hole propagation to **the electron-hole interaction**

$$\tilde{L}(1234) = L^0(1234) + L^0(1256)\frac{\delta\Sigma(56)}{\delta G(78)}\tilde{L}(7834)$$



Bethe-Salpeter Equation

Irreducible form of the Bethe-Salpeter equation

$$\tilde{L}(1234) = L^0(1234) + L^0(1256)\frac{\delta\Sigma(56)}{\delta G(78)}\tilde{L}(7834)$$

Reducible quantity

$$L = \tilde{L} + \tilde{L}vL$$

Bethe-Salpeter Equation

Bethe-Salpeter Equation

$$L(1234) = L^0(1234) + L^0(1256)\left[v(57)\delta(56)\delta(78) + \frac{\delta\Sigma(56)}{\delta G(78)} \right] L(7834)$$

Bethe-Salpeter Equation

Comparison with Linear Response quantities

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

Bethe-Salpeter Equation

Comparison with Linear Response quantities

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

$$L(1234) =$$

Bethe-Salpeter Equation

Comparison with Linear Response quantities

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Bethe-Salpeter Equation

Comparison with Linear Response quantities

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

$$L(1133) = \frac{\delta G(11)}{\delta V_{ext}(33)}$$

Bethe-Salpeter Equation

Comparison with Linear Response quantities

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

$$L(1133) = \frac{\delta n(1)}{\delta V_{ext}(3)}$$

Bethe-Salpeter Equation

We have the (4-point) Bethe-Salpeter equation.
And now ?

Bethe-Salpeter Equation

First point: Choosing Σ

$$L(1234) = L^0(1234) + L^0(1256)\left[v(57)\delta(56)\delta(78) + \frac{\delta\Sigma(56)}{\delta G(78)}\right]L(7834)$$

BSE

Bethe-Salpeter Equation

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Coulomb term

$$\Sigma_x(1,2) = G(12)v(21)$$

$\Rightarrow$ **Time-Dependent Hartree-Fock**

BSE

Bethe-Salpeter Equation

First point: Choosing Σ

$$L(1234) = L^0(1234) + L^0(1256)\left[v(57)\delta(56)\delta(78) + \frac{\delta\Sigma(56)}{\delta G(78)}\right]L(7834)$$

Screened Coulomb term

$$\Sigma^{\mathrm{GW}}(1,2) = -iG(12)W(21)$$

$\Rightarrow$ **Standard Bethe-Salpeter equation (Time-Dependent Screened Hartree-Fock)**

▸ BSE

Bethe-Salpeter Equation

Choice of $\Sigma = GW$

Everything should be coherently chosen

$\Longrightarrow$ ground state calculation $\longrightarrow$ ϕ_i, ϵ_i

$\Longrightarrow$ G^0_{KS} ; $\varepsilon^{-1}_{\text{RPA}}(\mathbf{r}, \mathbf{r}', \omega)$; $W(\mathbf{r}, \mathbf{r}', \omega) = \varepsilon^{-1}_{\text{RPA}} v$

$\Longrightarrow$ $E_i = \epsilon_i + \Delta_i^{\text{GW}}$; $\psi_i \simeq \phi_i$

$\Longrightarrow$ $G^{\text{GW}}(\mathbf{r}, \mathbf{r}', \omega)$

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$\Rightarrow$ $G^{\text{GW}}(\mathbf{r}, \mathbf{r}', \omega)$

Bethe-Salpeter Equation

$$L = L^0 + L^0 \left[v + \frac{\delta \Sigma}{\delta G} \right] L$$

$\Rightarrow$ Approx. $\frac{\delta W}{\delta G} = 0$

Bethe-Salpeter Equation

$$L = GG + GG \left[v - \frac{\delta \left[GW \right]}{\delta G} \right] L$$

$\Rightarrow$ Approx. $\frac{\delta W}{\delta G} = 0$

Bethe-Salpeter Equation

$$L = GG + GG\left[v - W\right]L$$

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Bethe-Salpeter Equation

Bethe-Salpeter Equation

$$L = L^0 + L^0 \left[v - W \right] L$$

Bethe-Salpeter Equation

Bethe-Salpeter Equation

$$L(1234) = L^0(1234) + \\ + L^0(1256)\left[v(57)\delta(56)\delta(78) - W(56)\delta(57)\delta(68)\right]L(7834)$$

Bethe-Salpeter Equation

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$$L(1234) = L^0(1234) + \\ + L^0(1256)\left[v(57)\delta(56)\delta(78) - W(56)\delta(57)\delta(68)\right] L(7834)$$

Intrinsic 4-point equation

Correct!

It describes the (coupled) progation of two particles, the electron and the hole !

Bethe-Salpeter Equation

Bethe-Salpeter Equation

$$L(1234) = L^0(1234) + $$
$$+ L^0(1256)\left[v(57)\delta(56)\delta(78) - W(56)\delta(57)\delta(68)\right]L(7834)$$

Exercise

Show that, if $W = 0$, the equation for $L(1133)$ is a two-point equation!

Int

It describes the (coupled) progation of two particles, the electron and the hole !

Bethe-Salpeter Equation

Bethe-Salpeter equation (4-points - space and time)

$$L(1234) = L^0(1234) + \\ + L^0(1256)\left[v(57)\delta(56)\delta(78) - W(56)\delta(57)\delta(68)\right] L(7834)$$

$$W(12) = W(\mathbf{r}_1, \mathbf{r}_2)\delta(t_1 t_2)$$

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

Bethe-Salpeter Equation

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Bethe-Salpeter Equation

BSE (4 space points - 1 frequency)

$$L(1234,\omega) = L^0(1234,\omega) + $$
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How to solve it ?

Really invert 4-point function for every frequency?

Bethe-Salpeter Equation

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Outline

1. Spectra in Linear Response Approach
   - Generalities
   - Polarizability in TDDFT
2. The Bethe-Salpeter equation
   - Polarizability in MBPT
   - Definition of BSE
   - BSE in practise
3. Results

Bethe-Salpeter Equation

We work in transition space...

$$L(1234,\omega) \Rightarrow L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) =$$

$$= \int d(1234) L(1234,\omega) \phi_{n_1}(1) \phi^*_{n_2}(2) \phi_{n_3}(3) \phi^*_{n_4}(4)$$

... and go back in real space.

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) \Rightarrow L(1234,\omega)$$

$$\phi_{KS}(\mathbf{r})$$

Bethe-Salpeter Equation

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$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) \Rightarrow L(1234,\omega)$$

$$\phi_{KS}(\mathbf{r})$$

Bethe-Salpeter Equation

Polarizability in BSE (only resonant)

$$L(\mathbf{r},\mathbf{r}',\omega) = \sum_{\lambda} \frac{\sum_{vc} A_{\lambda}^{(vc)} \phi_v(\mathbf{r}) \phi_c^*(\mathbf{r}) \phi_v^*(\mathbf{r}') \phi_c(\mathbf{r}') A_{\lambda}^{*(vc)}}{\omega - E_{\lambda}^{exc} + i\eta}$$

Onida, Reining, Rubio, RMP **74**, 601 (2002)
http://theory.polytechnique.fr/people/sottile/Tesi_dot.pdf

Bethe-Salpeter Equation

$E_\lambda,\ A_\lambda$ solution of the BSE in transition space

$$H^{2p,exc}_{(vc)(v'c')} A^{(v'c')}_\lambda = E^{exc}_\lambda A^{(vc)}_\lambda$$

Only resonant approximation

Bethe-Salpeter Equation

$E_\lambda, \ A_\lambda$ solution of the BSE in transition space

$$H^{2p,exc}_{(vc)(v'c')} A_\lambda^{(v'c')} = E_\lambda^{exc} A_\lambda^{(vc)}$$

Only resonant approximation

Bethe-Salpeter Equation

BSE - creating and diagonalizing a (big) matrix

$\Rightarrow$ $H^{exc}_{(vc)(v'c')} A^{(v'c')}_\lambda = E^{exc}_\lambda A^{(vc)}_\lambda$

$\Rightarrow$ $L^{(v'c')}_{(vc)}(\omega) = \sum_\lambda \frac{A^{(vc)}_\lambda A^{*(v'c')}_\lambda}{\omega - E^{exc}_\lambda + i\eta}$

Bethe-Salpeter Equation

BSE - creating and diagonalizing a (big) matrix

$$\Rightarrow \quad H^{exc}_{(vc)(v'c')} A_\lambda^{(v'c')} = E_\lambda^{exc} A_\lambda^{(vc)}$$

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Bethe-Salpeter Equation

BSE - creating and diagonalizing a (big) matrix

$$\Rightarrow H^{exc}_{(vc)(v'c')} A^{(v'c')}_{\lambda} = E^{exc}_{\lambda} A^{(vc)}_{\lambda}$$

$$\Rightarrow L^{(v'c')}_{(vc)}(\omega) = \sum_{\lambda} \frac{A^{(vc)}_{\lambda} A^{*(v'c')}_{\lambda}}{\omega - E^{exc}_{\lambda} + i\eta}$$

Bethe-Salpeter Equation

Spectrum in BSE (only resonant)

$$L(\mathbf{r},\mathbf{r}',\omega) = \sum_{\lambda} \frac{\sum_{vc} A_{\lambda}^{(vc)} \phi_v(\mathbf{r})\phi_c^*(\mathbf{r})\phi_v^*(\mathbf{r}')\phi_c(\mathbf{r}') A_{\lambda}^{*(vc)}}{\omega - E_{\lambda}^{exc} + i\eta}$$

$$\chi^0(\mathbf{r},\mathbf{r}',\omega) = \sum_{vc} \frac{\phi_v(\mathbf{r})\phi_c^*(\mathbf{r})\phi_v^*(\mathbf{r}')\phi_c(\mathbf{r}')}{\omega - (\epsilon_c - \epsilon_v) + i\eta}$$

Bethe-Salpeter Equation

Spectrum in BSE (only resonant)

$$L(\mathbf{r},\mathbf{r}',\omega) = \sum_{\lambda} \frac{\sum_{vc} A_{\lambda}^{(vc)} \phi_v(\mathbf{r}) \phi_c^*(\mathbf{r}) \phi_v^*(\mathbf{r}') \phi_c(\mathbf{r}') A_{\lambda}^{*(vc)}}{\omega - E_{\lambda}^{exc} + i\eta}$$

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Bethe-Salpeter Equation

Spectrum in BSE (only resonant)

$$\text{Abs}^{\text{BSE}}(\omega) = Im\,\langle L(\omega)\rangle = \sum_{\lambda} \left| \sum_{vc} A_{\lambda}^{(vc)} \langle c|D|v\rangle \right|^2 \delta\left(\omega - E_{\lambda}^{exc}\right)$$

$$\text{Abs}^{\text{IP-RPA}}(\omega) = Im\,\left\langle \chi^0(\omega)\right\rangle = \sum_{vc} \left|\langle c|D|v\rangle\right|^2 \delta\left(\omega - (\epsilon_c - \epsilon_v)\right)$$

Bethe-Salpeter Equation

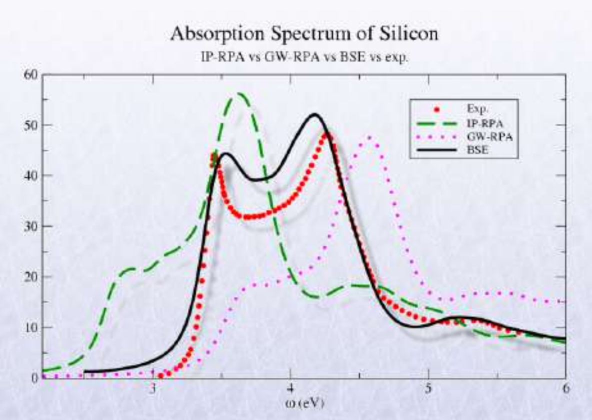
Standard Approximations for BSE

- Ground-state
  - pseudopotential
  - V_{xc} local density approximation
- Quasi-particle Many-Body Theory
  - GW approximation for Σ
  - W rpa, plasmon-pole model
  - $\psi_{\mathrm{GW}} = \phi_{\mathrm{KS}}$
- Bethe-Salpeter equation
  - $\frac{\delta W}{\delta G} = 0$
  - W rpa, static
  - only resonant term

The Bethe-Salpeter Soup

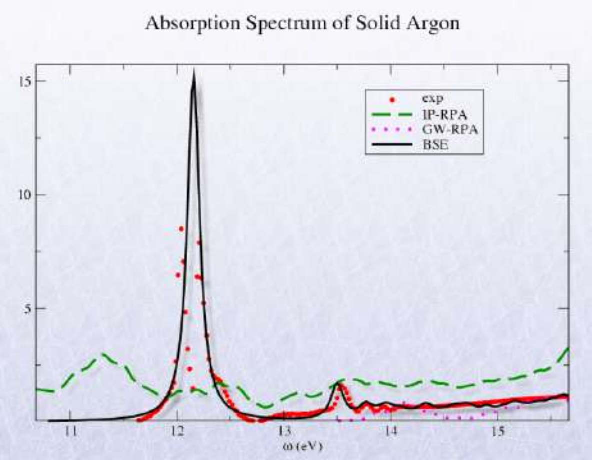
Outline

Bethe-Salpeter equation results: Semiconductors



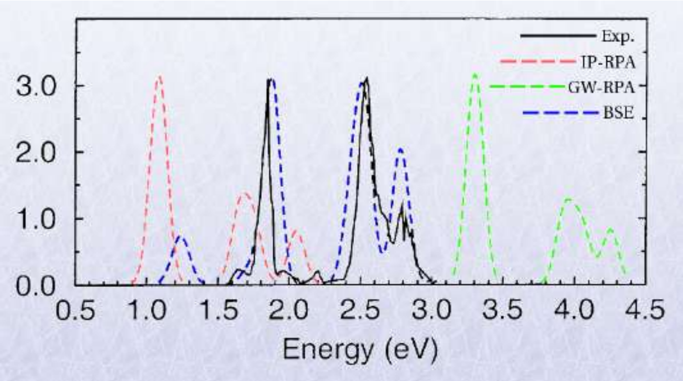
Albrecht *et al.*, PRL **80**, 4510 (1998)

Bethe-Salpeter equation results: Insulators



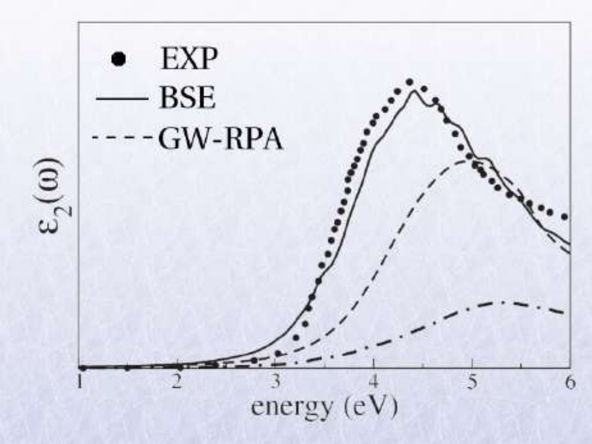
Sottile *et al.*, submitted to PRL.

Bethe-Salpeter equation results: Molecule (Na_4)



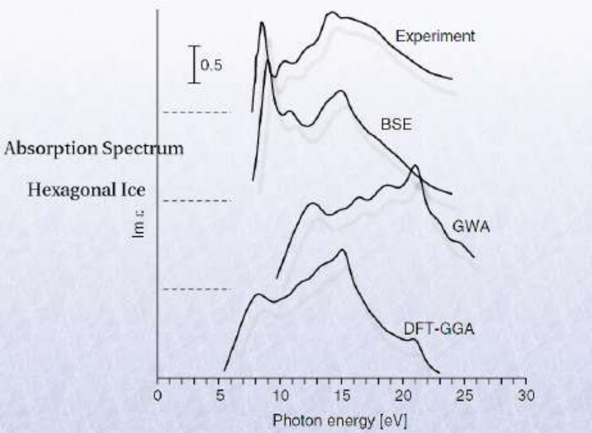
Onida *et al.*, PRL **75**, 818 (1995)

Bethe-Salpeter equation results: Silicon Nanowires



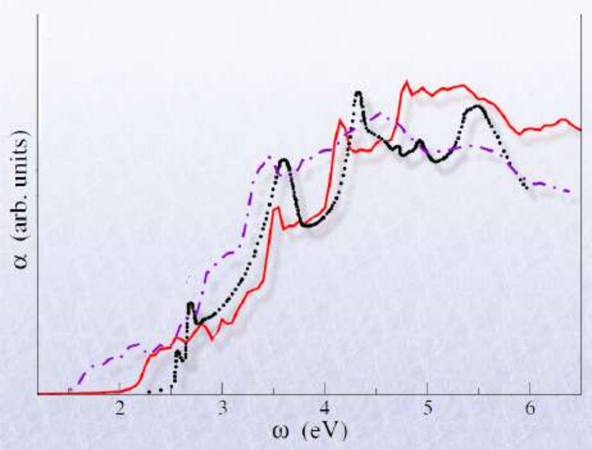
Bruno *et al.*, PRL **98**, 036807 (2007)

Bethe-Salpeter equation results: Hexagonal Ice



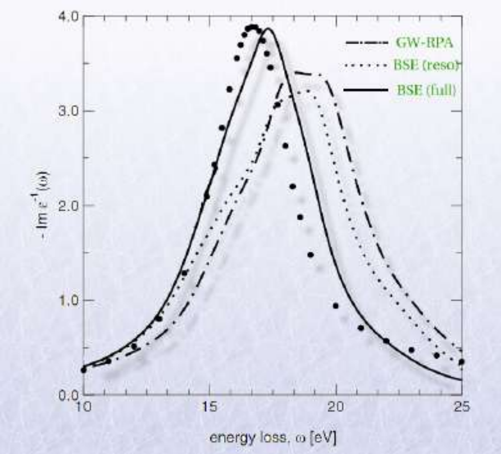
Hahn *et al.*, PRL **94**, 37404 (2005)

Bethe-Salpeter equation results: Cu_2O



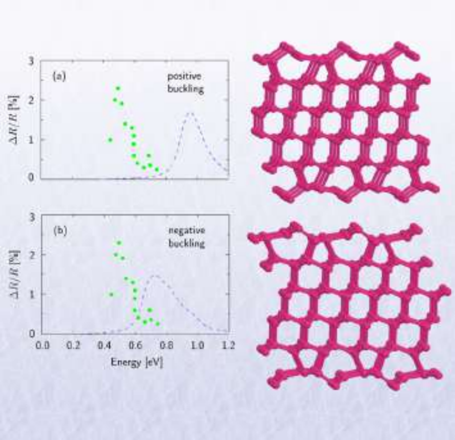
Bruneval *et al.*, PRL **97**, 267601 (2006)

Bethe-Salpeter equation results: EELS of Silicon



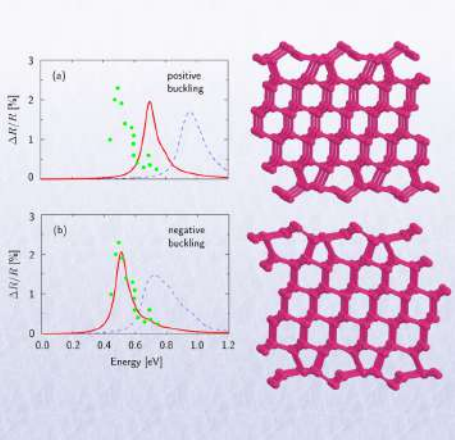
Olevano and Reining, PRL **86**, 5962 (2001)

Bethe-Salpeter equation results: Surface



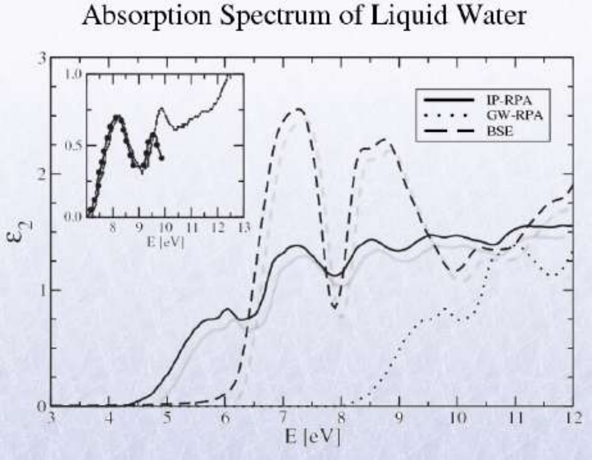
Rohlfing *et al.*, PRL **85**, 005440 (2000)

Bethe-Salpeter equation results: Surface

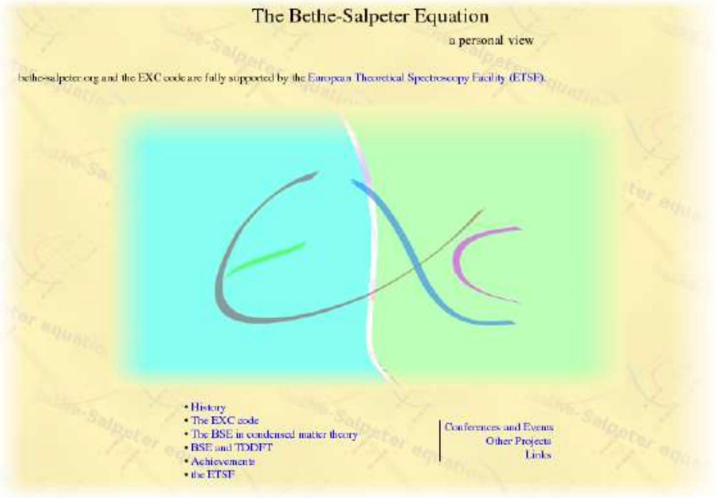


Rohlfing *et al.*, PRL **85**, 005440 (2000)

Bethe-Salpeter equation results: liquid Water



Garbuio *et al.*, PRL **97**, 137402 (2006)



- The EXC code - Sottile, Reining, Olevano, Onida, Albrecht
  `http://www.bethe-salpeter.org`

Bethe-Salpeter equation: State-of-the-art

- DFT - ground state
- GW - quasiparticle energies
- BSE - optical and dielectric properties

√ several spectroscopies

√ variety of systems

× Cumbersome Calculations

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Bethe-Salpeter Equation

from BSE to TDDFT

$$\chi = \chi^0 + \chi^0 \left[v + f_{xc} \right] \chi$$ Nice 2-point

$$L = L^0 + L^0 \left[v - W \right] L$$ Nasty 4-point

$$^4 f_{xc} = {}^4 \left[\left(\chi^0\right)^{-1} - \left(L^0\right)^{-1} - W \right]$$

$$^4 f_{xc} \longrightarrow f_{xc}^{\mathrm{BSE}}$$

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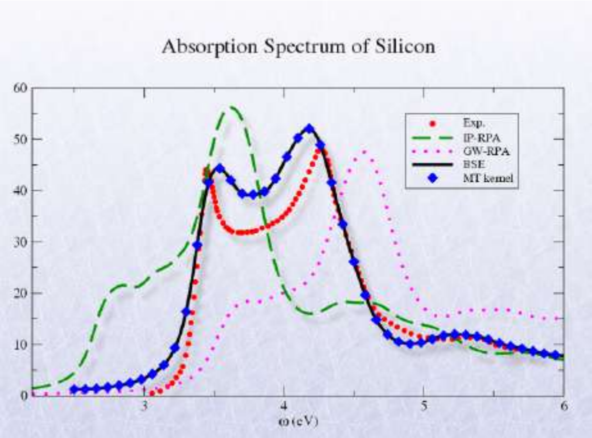
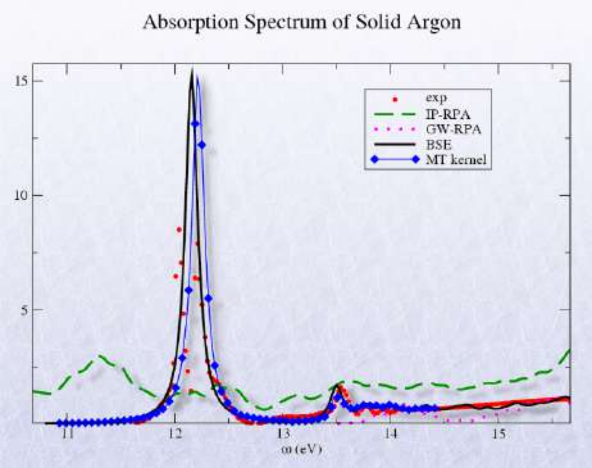
TDDFT kernel from BSE



Sottile *et al.*, PRL **91**, 56402 (2003)

TDDFT kernel from BSE



Sottile *et al.*, submitted to PRL.

TDDFT kernel from BSE

⇒ Palaiseau, mapping theory, PRL **91**, 56402 (2003)

⇒ Rome, perturbation theory PRL **91**, 256402 (2003)

⇒ Erlangen, diagrammatic expansion, PRB **70** 245119 (2004)