The Bethe-Salpeter Equation

An Introduction

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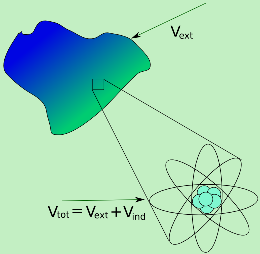
Outline

Outline

1. Generalities of Linear Response Approach
2. The Bethe-Salpeter equation
   - Polarizability in MBPT
   - Definition of BSE
   - BSE in practice
3. Results
4. The EXC Code

Linear Response Approach

System subject to an external perturbation



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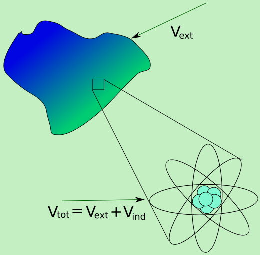

$$V_{tot} = \varepsilon^{-1} V_{ext}$$

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

Linear Response Approach

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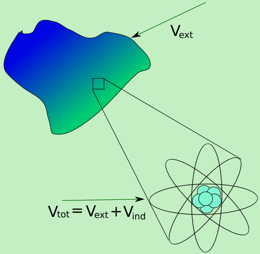

$$V_{tot} = \varepsilon^{-1} V_{ext}$$

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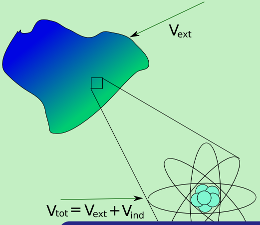
$$\mathbf{E} = \varepsilon^{-1} \mathbf{D}$$

Linear Response Approach

System subject to an external perturbation



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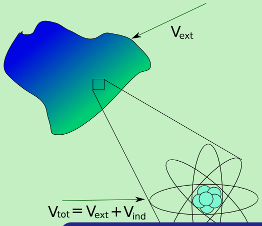
Dielectric function ε

$$\varepsilon$$

Linear Response Approach

System subject to an external perturbation



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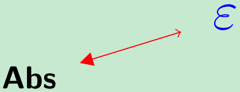

Linear Response Approach

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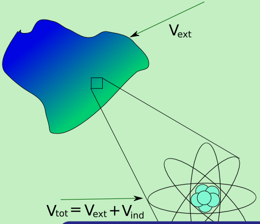

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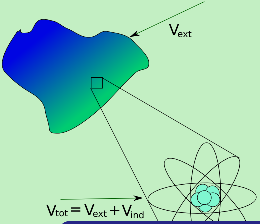
Dielectric function ε

EELS $\leftrightarrow$ ε $\leftrightarrow$ **Abs**

Linear Response Approach

System subject to an external perturbation



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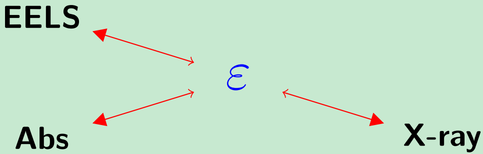
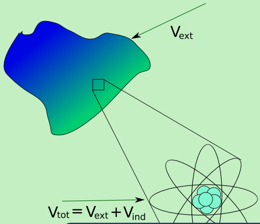


Linear Response Approach

System subject to an external perturbation



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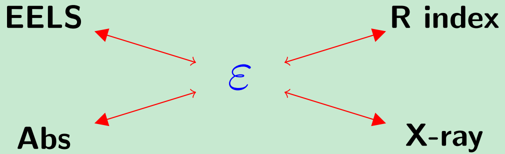


Linear Response Approach

Definition of polarizability

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

χ is the polarizability of the system

Linear Response Approach

Polarizability

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

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

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)

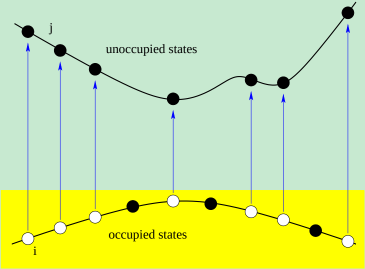
Linear Response Approach

Polarizability

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

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

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



Linear Response Approach

First approximation: IP-RPA

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

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

Linear Response Approach

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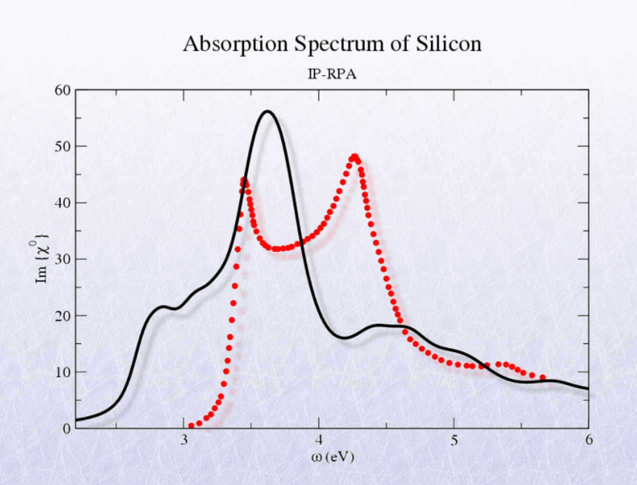

Linear Response Approach

How to go beyond χ^0 ?

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Outline

Many Body Perturbation Theory

Hedin's equations

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

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

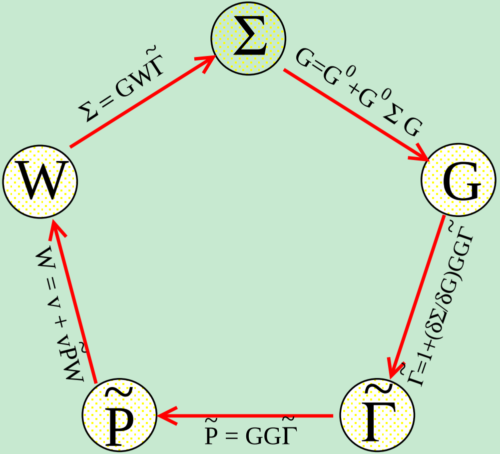
$$\tilde{\Gamma}(1,2,3) = \delta(1,2)\delta(1,3) + \int d(4567)\frac{\delta\Sigma(1,2)}{\delta G(4,5)}G(4,6)G(7,5)\tilde{\Gamma}(6,7,3)$$

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

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

Many Body Perturbation Theory

Hedin's pentagon



Many Body Perturbation Theory

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

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

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

Irreducible $\tilde{P}$ and Reducible χ

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

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

Different quantities

$\tilde{P}, \tilde{\Gamma}, G$ = time-ordered

χ^0, χ = retarded

Many Body Perturbation Theory

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Different quantities

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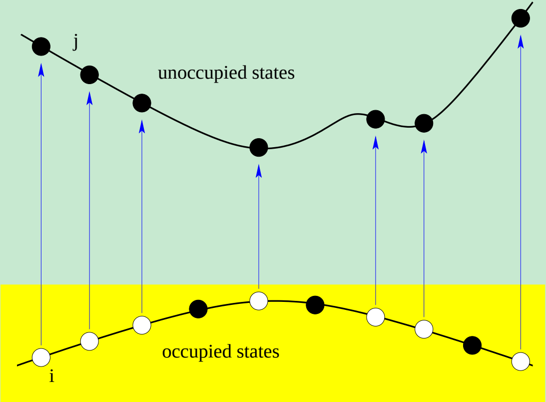
Spectra in MBPT

Spectra in IP picture

IP-RPA

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



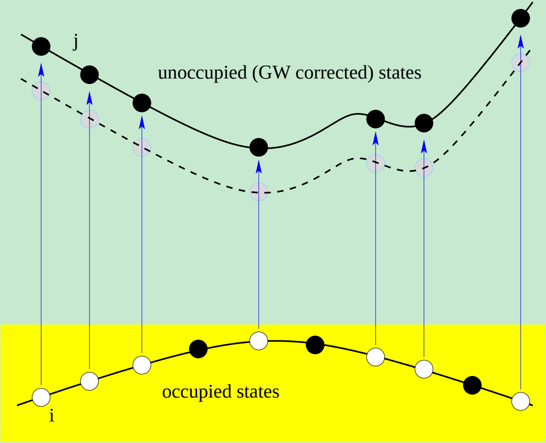
Spectra in MBPT

Spectra in GW approximation

GW-RPA

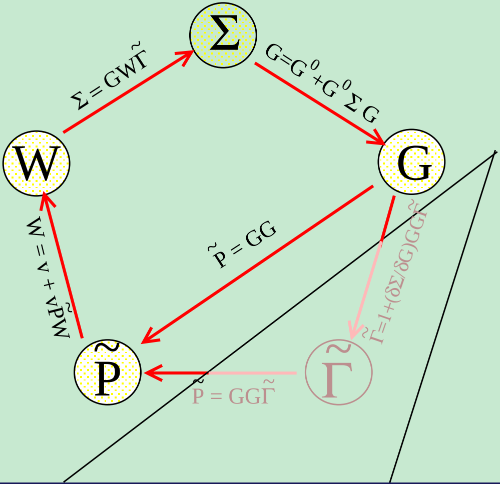
$$\text{Abs} = \text{Im}\ \chi^0_{\text{GW}}$$

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



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

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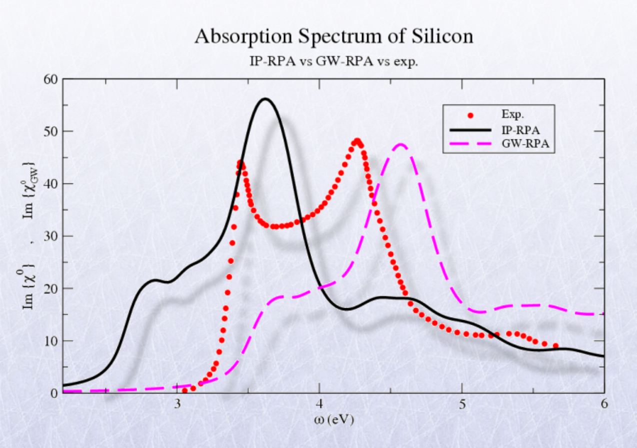
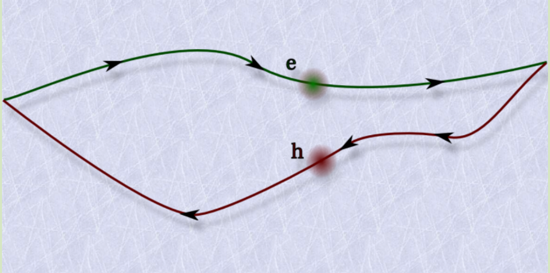


Spectra in MBPT

GG Polarizability

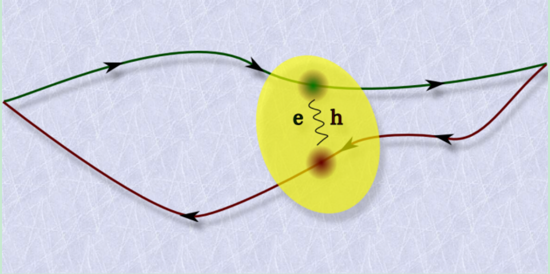
$$\tilde{P}(1,2) = -i \quad G(1,2)G(2,1^+)$$



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

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

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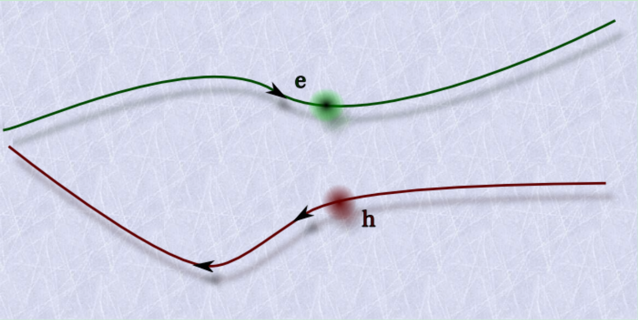
Bethe-Salpeter Equation

Towards the Bethe-Salpeter Equation

From electron and hole propagation ... ..

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

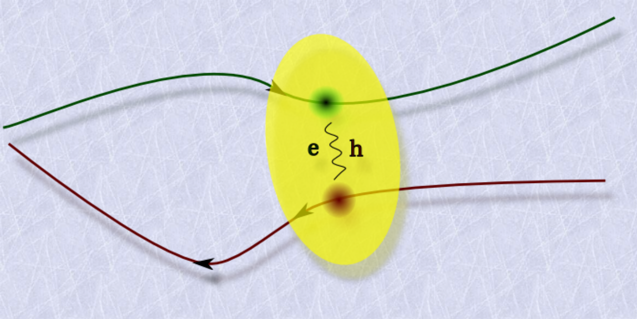


Bethe-Salpeter Equation

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

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

$$L(1234) = \frac{\delta G(12)}{\delta \tilde{V}_{ext}(34)}$$

Bethe-Salpeter Equation

Comparison with Linear Response quantities

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

$$L(1133) = \frac{\delta G(11)}{\delta \tilde{V}_{ext}(33)}$$

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

First point: Choosing Σ

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

Coulomb term

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

$\Rightarrow$ **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} ; $\varepsilon^{-1}_{\mathrm{RPA}}(\mathbf{r}, \mathbf{r}', \omega)$; $W(\mathbf{r}, \mathbf{r}', \omega) = \varepsilon^{-1}_{\mathrm{RPA}} v$

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

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

Bethe-Salpeter Equation

Choice of $\Sigma = GW$

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Bethe-Salpeter Equation

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Bethe-Salpeter Equation

Choice of $\Sigma = GW$

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$\Longrightarrow$ ground state calculation $\longrightarrow \quad \phi_i, \epsilon_i$

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

$\Longrightarrow$ $\Sigma(\mathbf{r},\mathbf{r}',\omega) = \int d\omega' G^0_{\mathrm{KS}}(\mathbf{r},\mathbf{r}',\omega') W(\mathbf{r},\mathbf{r}',\omega+\omega')$

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

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Bethe-Salpeter Equation

Choice of $\Sigma = GW$

Everything should be coherently chosen

$\Rightarrow$ ground state calculation $\longrightarrow \quad \phi_i, \epsilon_i$

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

$\Rightarrow$ $\Sigma(\mathbf{r}, \mathbf{r}', \omega) = \int d\omega' G^0_{\mathrm{KS}}(\mathbf{r}, \mathbf{r}', \omega') W(\mathbf{r}, \mathbf{r}', \omega + \omega')$

$\Rightarrow$ $E_i = \epsilon_i + \Delta_i^{\mathrm{GW}} \quad ; \quad \psi_i \simeq \phi_i$

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

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} ; $\varepsilon^{-1}_{\mathrm{RPA}}(\mathbf{r}, \mathbf{r}', \omega)$; $W(\mathbf{r}, \mathbf{r}', \omega) = \varepsilon^{-1}_{\mathrm{RPA}} v$

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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

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

$\Rightarrow$ 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

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

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

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

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Bethe-Salpeter Equation

Macroscopic Quantity from the contracted L

1. $L(1234,\omega) \Longrightarrow L(\mathbf{r},\mathbf{r},\mathbf{r}',\mathbf{r}',\omega)$

2. $\varepsilon_{\mathrm{M}}(\omega) = 1 - \lim_{\mathbf{q}\to 0} v(\mathbf{q}) \int d\mathbf{r}d\mathbf{r}'\, e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} L(\mathbf{r},\mathbf{r},\mathbf{r}',\mathbf{r}',\omega)$

   $\varepsilon_{\mathrm{M}}(\omega) = 1 - \lim_{\mathbf{q}\to 0} v(\mathbf{q}) L(\mathbf{G}=0,\mathbf{G'}=0,\omega)$

Bethe-Salpeter Equation

Macroscopic Quantity from the contracted L

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Bethe-Salpeter Equation

BSE (4 space points - 1 frequency)

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

How to solve it ?

Really invert 4-point function for every frequency?

Bethe-Salpeter Equation

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Outline

Bethe-Salpeter Equation

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

Bethe-Salpeter Equation

$$L(1234,\omega) = L^0(1234,\omega) + L^0(1256,\omega)K(5678)L(7834,\omega)$$

Bethe-Salpeter Equation

$$L(1234,\omega) = L^0(1234,\omega) + L^0(1256,\omega)K(5678)L(7834,\omega)$$

We work in transition space...

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

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

Bethe-Salpeter Equation

$$L(1234,\omega) = L^0(1234,\omega) + L^0(1256,\omega)K(5678)L(7834,\omega)$$

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Clever choice of the basis ϕ_n

Bethe-Salpeter Equation in transition space

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = L^{0\,(n_3 n_4)}_{(n_1 n_2)}(\omega) + L^{0\,(n_5 n_6)}_{(n_1 n_2)}(\omega) K^{(n_7 n_8)}_{(n_5 n_6)} L^{(n_3 n_4)}_{(n_7 n_8)}(\omega)$$

... some "trivial" mathematical arzigogoli ...

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = \left[(E_{n_2} - E_{n_1} - \omega)\delta_{n_1 n_3}\delta_{n_2 n_4} + K^{(n_3 n_4)}_{(n_1 n_2)} \right]^{-1}$$

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = [(E_{n_2} - E_{n_1} - \omega)\delta_{n_1 n_3}\delta_{n_2 n_4} + \ll v \gg - \ll W \gg]^{-1}$$

Bethe-Salpeter Equation in transition space

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = L^{0\,(n_3 n_4)}_{(n_1 n_2)}(\omega) + L^{0\,(n_5 n_6)}_{(n_1 n_2)}(\omega) K^{(n_7 n_8)}_{(n_5 n_6)} L^{(n_3 n_4)}_{(n_7 n_8)}(\omega)$$

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Bethe-Salpeter Equation in transition space

$$L_{(n_1 n_2)}^{(n_3 n_4)}(\omega) = L_{(n_1 n_2)}^{0\,(n_3 n_4)}(\omega) + L_{(n_1 n_2)}^{0\,(n_5 n_6)}(\omega) K_{(n_5 n_6)}^{(n_7 n_8)} L_{(n_7 n_8)}^{(n_3 n_4)}(\omega)$$

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Bethe-Salpeter Equation in transition space

The Excitonic Hamiltonian

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = \left[(E_{n_2} - E_{n_1} - \omega)\delta_{n_1 n_3}\delta_{n_2 n_4} + \ll v \gg - \ll W \gg\right]^{-1}$$

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = \frac{1}{H^{exc} - \omega}$$

$$H^{exc} = (E_{n_2} - E_{n_1})\delta_{n_1 n_3}\delta_{n_2 n_4} + \ll v \gg - \ll W \gg$$

Resonant vs Coupling

$n_1, n_2, n_3, n_4 = v, c \quad (\mathbf{k})$

$$H^{reso} = (E_c - E_v)\delta_{vv'}\delta_{cc'} + \ll v \gg - \ll W \gg$$

Bethe-Salpeter Equation in transition space

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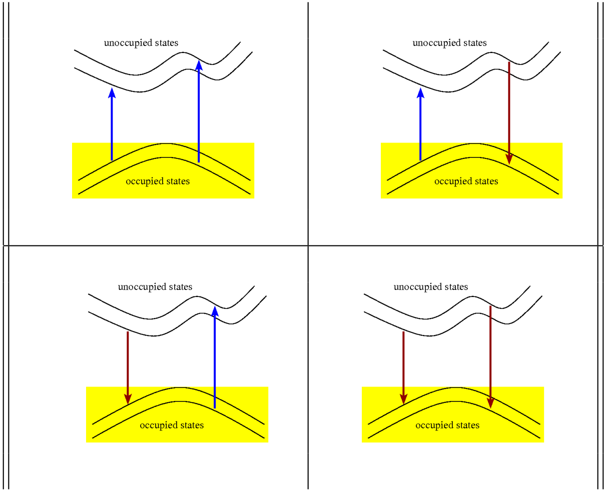
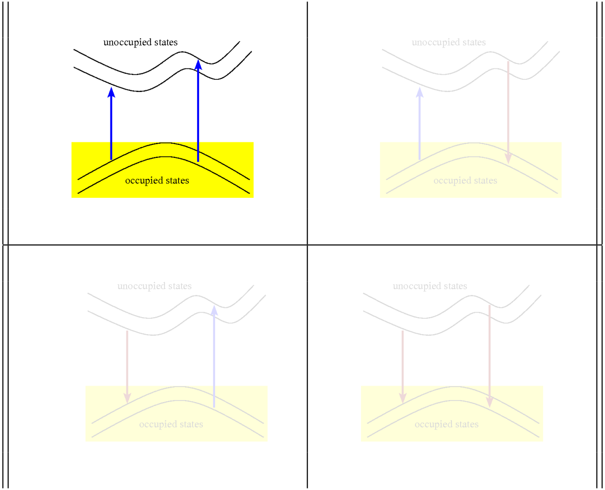
Bethe-Salpeter Equation in transition space



Bethe-Salpeter Equation in transition space



Bethe-Salpeter Equation in transition space

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) \Longrightarrow L(\mathbf{r},\mathbf{r}',\omega) = \sum_{\substack{(n_1 n_2)\\(n_3 n_4)}} L^{(n_3 n_4)}_{(n_1 n_2)}(\omega)\phi_{n_1}(\mathbf{r})\phi^*_{n_2}(\mathbf{r})\phi_{n_3}(\mathbf{r}')\phi^*_{n_4}(\mathbf{r}')$$

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) \Longrightarrow L(\mathbf{G},\mathbf{G'},\omega) = \sum_{\substack{(n_1 n_2)\\(n_3 n_4)}} L^{(n_3 n_4)}_{(n_1 n_2)}(\omega)\int \phi_{n_1}(\mathbf{r})e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}}\phi^*_{n_2}(\mathbf{r})\phi_{n_3}(\mathbf{r}')e^{i(\mathbf{q}+\mathbf{G}')\mathbf{r}'}\phi^*_{n_4}(\mathbf{r}')$$

Bethe-Salpeter Equation in transition space

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Bethe-Salpeter Equation in transition space

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Bethe-Salpeter Equation in transition space

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = \left[(E_{n_2} - E_{n_1} - \omega)\delta_{n_1 n_3}\delta_{n_2 n_4} + \ll v \gg - \ll W \gg\right]^{-1}$$

$$L^{(n_3 n_4)}_{(n_1 n_2)}(\omega) = \left[H^{exc} - \omega\right]^{-1}$$

$$H^{exc} = \left[(E_{n_2} - E_{n_1})\delta_{n_1 n_3}\delta_{n_2 n_4} + \ll v \gg - \ll W \gg\right]$$

Diagonalization

Iterative inversion

Bethe-Salpeter Equation in transition space

$$L_{(n_1 n_2)}^{(n_3 n_4)}(\omega) = \left[(E_{n_2} - E_{n_1} - \omega)\delta_{n_1 n_3}\delta_{n_2 n_4} + \ll v \gg - \ll W \gg\right]^{-1}$$

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Diagonalization

Iterative inversion

Bethe-Salpeter Equation in transition space

Diagonalization case (only resonant approx)

$$L_{vc}^{v'c'} = [(E_c - E_v)\,\delta_{vv'}\delta_{cc'} - \omega + \ll v \gg - \ll W \gg]^{-1}$$

$$\frac{1}{H - \omega I} = \sum_{\lambda} \frac{|A_\lambda >< A_\lambda|}{E_\lambda - \omega}$$

Spectrum within BSE

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

Bethe-Salpeter Equation in transition space

Diagonalization case (only resonant approx)

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Bethe-Salpeter Equation in transition space

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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)

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

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

Bethe-Salpeter Equation

BSE - creating and diagonalizing a (big) matrix

$\Longrightarrow$ $H^{exc}_{(vc)(v'c')}$

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

Bethe-Salpeter Equation

BSE - creating and diagonalizing a (big) matrix

$$\Rightarrow \; H^{exc}_{(vc)(v'c')} = (E_c - E_v)\,\delta_{vv'}\delta_{cc'} + v^{v'c'}_{vc} - W^{v'c'}_{vc}$$

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

Bethe-Salpeter Equation

BSE - creating and diagonalizing a (big) matrix

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

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

Bethe-Salpeter Equation

BSE - creating and diagonalizing a (big) matrix

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

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

Bethe-Salpeter Equation

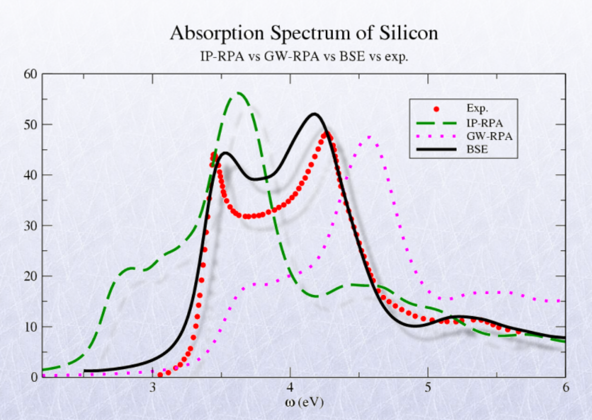
Standard Approximations for BSE

- 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

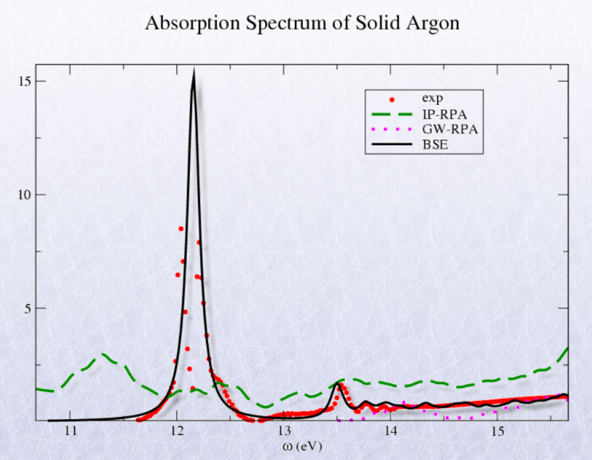
Outline

Bethe-Salpeter equation results: Semiconductors



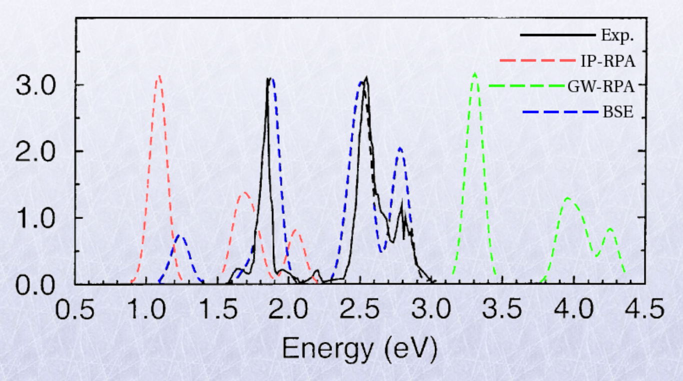
Albrecht *et al.*, PRL **80**, 4510 (1998)

Bethe-Salpeter equation results: Insulators



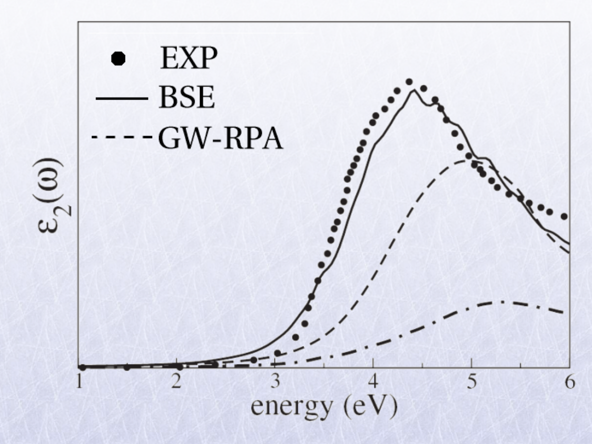
Sottile, Marsili, *et al.*, PRB (2007).

Bethe-Salpeter equation results: Molecule (Na_4)



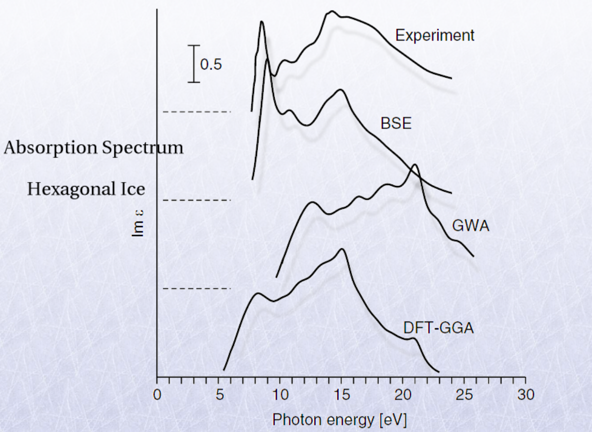
Onida *et al.*, PRL **75**, 818 (1995)

Bethe-Salpeter equation results: Silicon Nanowires



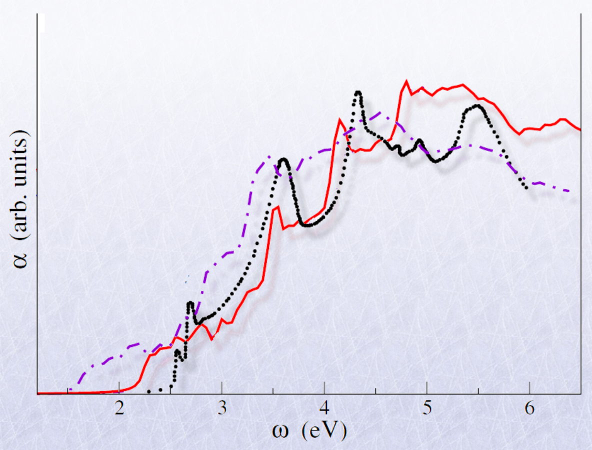
Bruno *et al.*, PRL **98**, 036807 (2007)

Bethe-Salpeter equation results: Hexagonal Ice



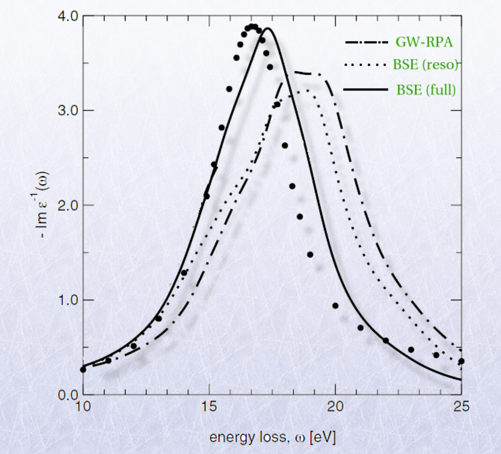
Hahn *et al.*, PRL **94**, 37404 (2005)

Bethe-Salpeter equation results: Cu_2O



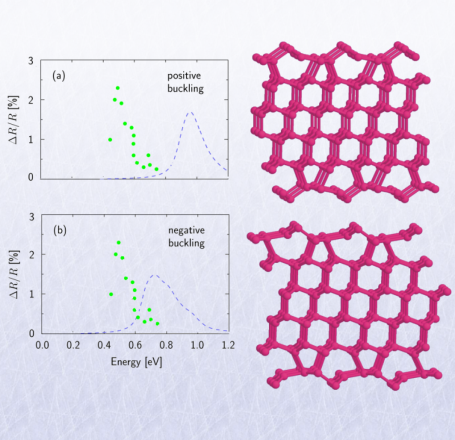
Bruneval *et al.*, PRL **97**, 267601 (2006)

Bethe-Salpeter equation results: EELS of Silicon



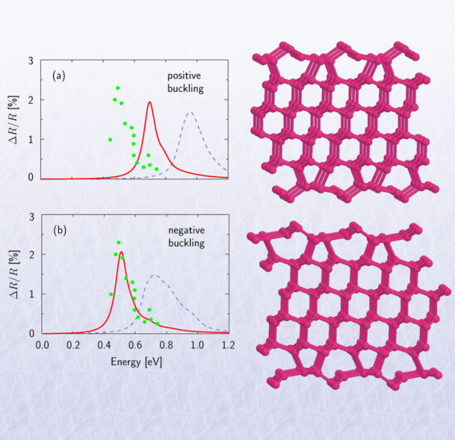
Olevano and Reining, PRL **86**, 5962 (2001)

Bethe-Salpeter equation results: Surface



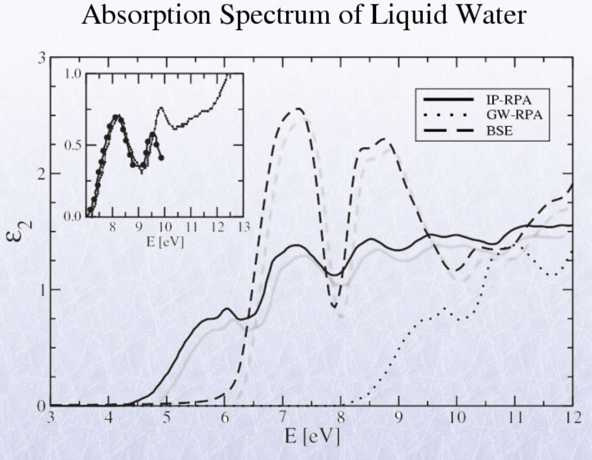
Rohlfing *et al.*, PRL **85**, 005440 (2000)

Bethe-Salpeter equation results: Surface

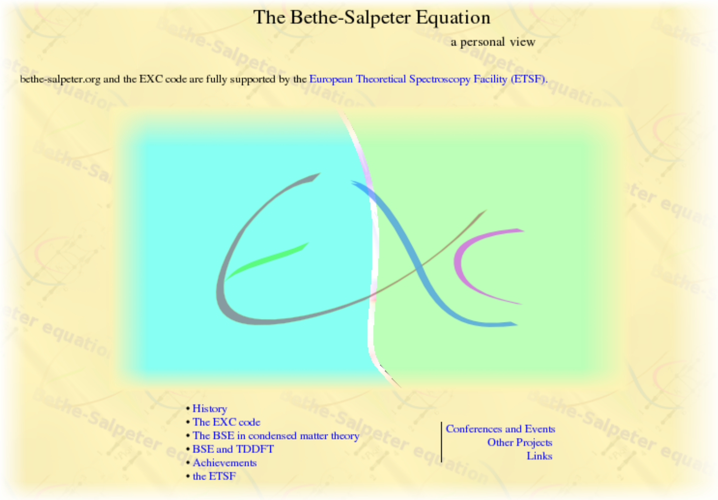


Rohlfing *et al.*, PRL **85**, 005440 (2000)

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

$\surd$ several spectroscopies

$\surd$ variety of systems

$\times$ Cumbersome Calculations

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

- DFT - ground state
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$\surd$ several spectroscopies

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$\times$ Cumbersome Calculations

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

Some references

- Hanke and Sham, PRB **21**, 4656 (1980)
- Onida, Reining, Rubio, RMP **74**, 601 (2002)
- Strinati, Riv Nuovo Cimento **11**, 1 (1988)

Outline

What do we calculate ?

Dielectric function (only resonant case)

$$\varepsilon_M(\omega) = 1 - \lim_{\mathbf{q}\to 0} v_0(\mathbf{q}) \sum_{\lambda} \left[\sum_{(vc)} \frac{\left| \left\langle c \middle| e^{-i\mathbf{q}\cdot\mathbf{r}} \middle| v \right\rangle A_{\lambda}^{(vc)} \right|^2}{E_{\lambda}^{exc} - \omega - i\eta} \right]$$

diagonalize excitonic Hamiltonian

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

$$H = \begin{array}{cc} & (v'c') \\ (vc) & \begin{bmatrix} \cdots & \cdots & & \\ & \ddots & & \\ & & \ddots & \\ \cdots & & & \cdots \end{bmatrix} \end{array}$$

Hamiltonian:

$$H^{2p}_{(vc)(v'c')} = (E_c - E_v)\delta_{vv'}\delta_{cc'} + [v - W]^{(v'c')}_{(vc)}$$

E_i = quasiparticle energies (GW)

$W = \varepsilon^{-1} v$ screened Coulomb interaction

What do we calculate ?

Dielectric function (only resonant case)

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Dielectric function (only resonant case)

$$\varepsilon_M(\omega) = 1 - \lim_{\mathbf{q}\to 0} v_0(\mathbf{q}) \sum_{\lambda} \left[\sum_{(vc)} \frac{\left| \langle c | e^{-i\mathbf{q}\cdot\mathbf{r}} | v \rangle A_\lambda^{(vc)} \right|^2}{E_\lambda^{exc} - \omega - i\eta} \right]$$

diagonalize excitonic Hamiltonian

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

$$\begin{array}{cc} & (\mathrm{v'c'}) \\ H = (\mathrm{vc}) & \begin{bmatrix} \dots & \dots & & \\ & \ddots & & \\ \dots & & \ddots & \\ & & & \dots \end{bmatrix} \end{array}$$

Hamiltonian:

$$H^{2p}_{(vc)(v'c')} = (E_c - E_v)\delta_{vv'}\delta_{cc'} + [v - W]^{(v'c')}_{(vc)}$$

$$\begin{aligned} E_i &= \text{quasiparticle energies (GW)} \\ W &= \varepsilon^{-1} v \quad \text{screened Coulomb interaction} \end{aligned}$$

What do we need ?

structure, screening, quasiparticle files + input file

- $|v\rangle$ gs (LDA) wfs `kss file`
- E_v Quasi-Particle energies `gw file`
- ε^{-1} for the screened interaction `scr file`

The excitonic Hamiltonian

$$H^{2p}_{(vc)(v'c')} = \left(E_c - E_v\right)\delta_{vv'}\delta_{cc'} + [v - W]_{(vc)(v'c')}$$

- $H^{2p}_{(vc)(v'c')} = (\epsilon_c - \epsilon_v)\,\delta_{vv'}\delta_{cc'}$ RPA-NLF
- $H^{2p}_{(vc)(v'c')} = (\epsilon_c - \epsilon_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')}$ RPA
- $H^{2p}_{(vc)(v'c')} = (E_c - E_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')}$ GW
- $H^{2p}_{(vc)(v'c')} = (E_c - E_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')} + W_{(vc)(v'c')}$ BSE

The excitonic Hamiltonian

$$H^{2p}_{(vc)(v'c')} = \Big((\epsilon_c + \Delta_c^{\mathrm{GW}}) - (\epsilon_v + \Delta_v^{\mathrm{GW}})\Big)\delta_{vv'}\delta_{cc'} + [v - W]_{(vc)(v'c')}$$

- $H^{2p}_{(vc)(v'c')} = (\epsilon_c - \epsilon_v)\,\delta_{vv'}\delta_{cc'}$ RPA-NLF
- $H^{2p}_{(vc)(v'c')} = (\epsilon_c - \epsilon_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')}$ RPA
- $H^{2p}_{(vc)(v'c')} = (E_c - E_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')}$ GW
- $H^{2p}_{(vc)(v'c')} = (E_c - E_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')} + W_{(vc)(v'c')}$ BSE

The excitonic Hamiltonian

$$H^{2p}_{(vc)(v'c')} = \Big((\epsilon_c + \Delta_c^{\mathrm{GW}}) - (\epsilon_v + \Delta_v^{\mathrm{GW}}) \Big) \delta_{vv'} \delta_{cc'} + [v - W]_{(vc)(v'c')}$$

- $H^{2p}_{(vc)(v'c')} = (\epsilon_c - \epsilon_v)\,\delta_{vv'}\delta_{cc'}$ RPA-NLF
- $H^{2p}_{(vc)(v'c')} = (\epsilon_c - \epsilon_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')}$ RPA
- $H^{2p}_{(vc)(v'c')} = (E_c - E_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')}$ GW
- $H^{2p}_{(vc)(v'c')} = (E_c - E_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')} + W_{(vc)(v'c')}$ BSE

The excitonic Hamiltonian

$$H^{2p}_{(vc)(v'c')} = \left(\left(\epsilon_c + \Delta^{\mathrm{GW}}_c\right) - \left(\epsilon_v + \Delta^{\mathrm{GW}}_v\right)\right)\delta_{vv'}\delta_{cc'} + [v - W]_{(vc)(v'c')}$$

- $H^{2p}_{(vc)(v'c')} = (\epsilon_c - \epsilon_v)\,\delta_{vv'}\delta_{cc'}$ RPA-NLF
- $H^{2p}_{(vc)(v'c')} = (\epsilon_c - \epsilon_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')}$ RPA
- $H^{2p}_{(vc)(v'c')} = (E_c - E_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')}$ GW
- $H^{2p}_{(vc)(v'c')} = (E_c - E_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')} + W_{(vc)(v'c')}$ BSE

The excitonic Hamiltonian

$$H^{2p}_{(vc)(v'c')} = ((\epsilon_c + \Delta_c^{\mathrm{GW}}) - (\epsilon_v + \Delta_v^{\mathrm{GW}}))\,\delta_{vv'}\delta_{cc'} + [v - W]_{(vc)(v'c')}$$

- $H^{2p}_{(vc)(v'c')} = (\epsilon_c - \epsilon_v)\,\delta_{vv'}\delta_{cc'}$ RPA-NLF
- $H^{2p}_{(vc)(v'c')} = (\epsilon_c - \epsilon_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')}$ RPA
- $H^{2p}_{(vc)(v'c')} = (E_c - E_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')}$ GW
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The excitonic Hamiltonian

$$H^{2p}_{(vc)(v'c')} = \Big(E_c - E_v\Big)\delta_{vv'}\delta_{cc'} + [v + W]_{(vc)(v'c')}$$

- $H^{2p}_{(vc)(v'c')} = (\epsilon_c - \epsilon_v)\,\delta_{vv'}\delta_{cc'}$ RPA-NLF
- $H^{2p}_{(vc)(v'c')} = (\epsilon_c - \epsilon_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')}$ RPA
- $H^{2p}_{(vc)(v'c')} = (E_c - E_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')}$ GW
- $H^{2p}_{(vc)(v'c')} = (E_c - E_v)\,\delta_{vv'}\delta_{cc'} + v_{(vc)(v'c')} + W_{(vc)(v'c')}$ BSE

```
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/       )_/  /__\  \__\    )_

  http://www.bethe-salpeter.org

 program EXC version 2.3.4
 built: 06 Dec 2007

 calculate dielectric properties
 Bethe-Salpeter equation code in frequency domain
          reciprocal space on a transitions basis

 Copyright (C) 1992-2007, Lucia Reining, Valerio Olevano,
 Francesco Sottile, Stefan Albrecht, Giovanni Onida.

 This program is free software; you can redistribute it
 and/or modify it under the terms of the GNU General
 Public License.

 This program is distributed in the hope that it will be
```

The input file

rpa, gw, exc (default) .... type of calculation

nlf, lf (default) .... with or w/o local fields

wdiag (default), wfull .... $W_{\mathbf{GG}'}\delta_{\mathbf{GG}'}$ or $W_{\mathbf{GG}'}$

resonant (default), coupling .... coupling reso-antireso or not

soenergy <value> (default=0.0) ...... scissor operator energy [eV]

matsh <value> (default=all) .... number of G-shell for the $\varepsilon_{\mathbf{GG}'}$

wfnsh <value> (default=all) ..... plane waves shells for the $\psi_{n\mathbf{k}}(\mathbf{G})$

nbands <value> (default=all) last band included in the calculation

lomo <value> (default=1) ..... first band included in the calculation

omegai <value> (default=0.0) .... frequency initial point [eV]

omegae <value> (default=10.0) .... frequency end point [eV]

domega <value> (default=0.01) .... frequency step [eV]

broad <value> (default=domega) .... lorentzian broadening [eV]

haydock .... iterative diagonalization scheme

niter <value> (default=100) .... iterations for haydock scheme

The input file

- rpa, gw, exc (default) ....type of calculation
- nlf, lf (default) ....with or w/o local fields
- wdiag (default), wfull .... $W_{\mathbf{GG'}}\delta_{\mathbf{GG'}}$ or $W_{\mathbf{GG'}}$
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The input file

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wdiag (default), wfull .... $W_{GG'}\delta_{GG'}$ or $W_{GG'}$

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- `resonant (default), coupling` .... coupling reso-antireso or not
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- `omegae <value> (default=10.0)` .... frequency end point [eV]
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