Many-body Perturbation Theory II. Bethe-Salpeter equation: electron-hole excitations and optical spectra

Ilya Tokatly

European Theoretical Spectroscopy Facility (ETSF)
University of the Basque Country - UPV/EHU San Sebastián - Spain
IKERBASQUE, Basque Foundation for Science - Bilbao - Spain
ilya.tokatly@ehu.es

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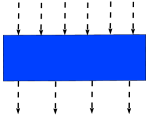
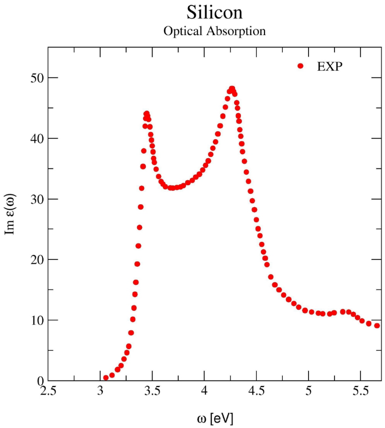
Outline

Outline

Optical absorption: Experiment and Phenomenology





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

Light is absorbed: $I = I_0 e^{-\alpha(\omega)x}$

Classical electrodynamics

$$E = E_0 e^{-i(\omega t - qx)}, \qquad q^2 = \frac{\omega^2}{c^2}\epsilon_M(\omega)$$

$$\epsilon_M(\omega) = \epsilon'_M(\omega) + i\epsilon''_M(\omega)$$

$$q \approx \frac{\omega}{c}\sqrt{\epsilon'_M} + i\frac{\omega}{2c\sqrt{\epsilon'_M}}\epsilon''_M$$

$\sqrt{\epsilon'_M} = n_r$ – index of refraction

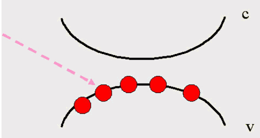
$$I \sim |E|^2 = |E_0|^2 e^{-\alpha(\omega)x}$$

$$\alpha(\omega) = \frac{\omega}{cn_r}\epsilon''_M(\omega)$$

$\epsilon''_M(\omega) \sim$ absorption rate

Optical absorption: Microscopic picture

Elementary process of absorption: Photon creates a single e-h pair



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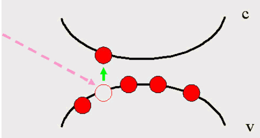

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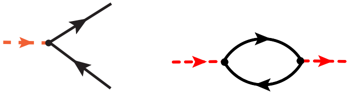
Representation by Feynman diagrams:



- photon creates an e-h pair
- the pair propagates freely
- it recombines and recreates a photon

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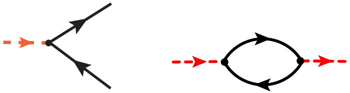

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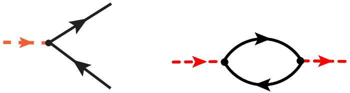

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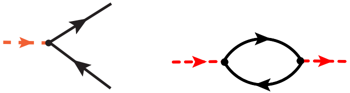

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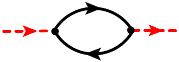
Representation by Feynman diagrams:

- photon creates an e-h pair
- the pair propagates freely
- it recombines and recreates a photon

Absorption rate is given by an imaginary part of the polarization loop

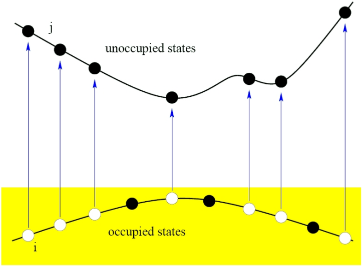
$$W = \frac{2\pi}{\hbar} \sum_{i,j} |\langle \varphi_i | \mathbf{e} \cdot \hat{\mathbf{v}} | \varphi_j \rangle|^2 \delta(\varepsilon_j - \varepsilon_i - \hbar\omega) \sim \mathrm{Im}\epsilon(\omega)$$

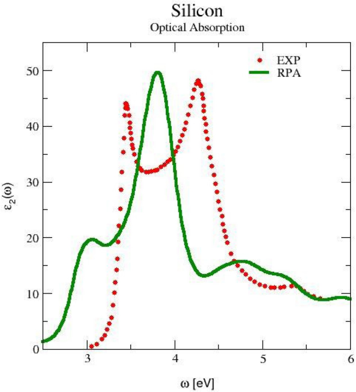
Absorption by independent Kohn-Sham particles



Independent transitions:

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





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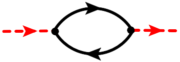

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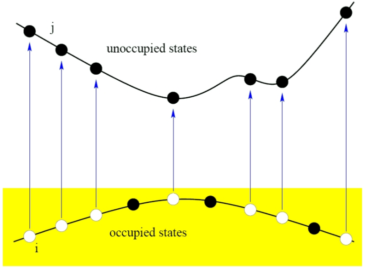
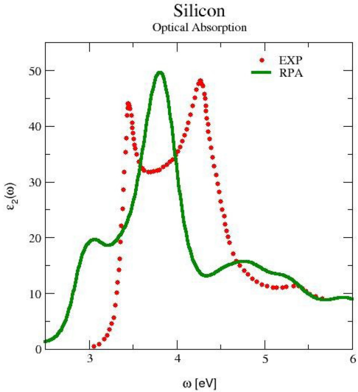
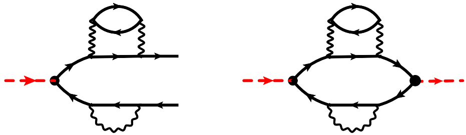




Particles are interacting!

Interaction effects: self-energy corrections

1st class of interaction corrections:



Created electron and hole interact with other particles in the system, but do not touch each other

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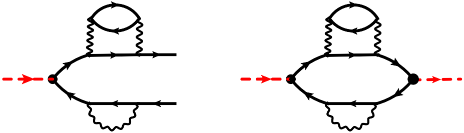

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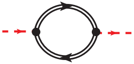
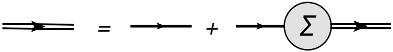
Absorption by “dressed” particles





Bare propagator G_0 is replaced by the full propagator
$G = G_0 + G_0 \Sigma G$

$$[\omega - \hat{h}_0(\mathbf{r})]G(\mathbf{r}, \mathbf{r}', \omega) + \int d\mathbf{r}_1 \Sigma(\mathbf{r}, \mathbf{r}_1, \omega) G(\mathbf{r}_1, \mathbf{r}', \omega) = \delta(\mathbf{r} - \mathbf{r}')$$

Self-energy corrections

Perturbative GW corrections

$$\hat{h}_0(\mathbf{r})\varphi_i(\mathbf{r}) + V_{xc}(\mathbf{r})\varphi_i(r) = \epsilon_i\varphi_i(\mathbf{r})$$

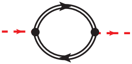
$$\hat{h}_0(\mathbf{r})\phi_i(\mathbf{r}) + \int d\mathbf{r}' \; \Sigma(\mathbf{r},\mathbf{r}',\omega = E_i) \; \phi_i(\mathbf{r}') = E_i \, \phi_i(\mathbf{r})$$

First-order perturbative corrections with $\Sigma = GW$:

$$E_i - \epsilon_i = \langle\varphi_i|\Sigma - V_{xc}|\varphi_i\rangle$$

Hybersten and Louie, PRB **34** (1986);
Godby, Schlüter and Sham, PRB **37** (1988)

Optical absorption: Independent quasiparticles



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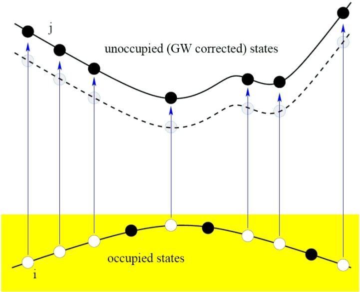
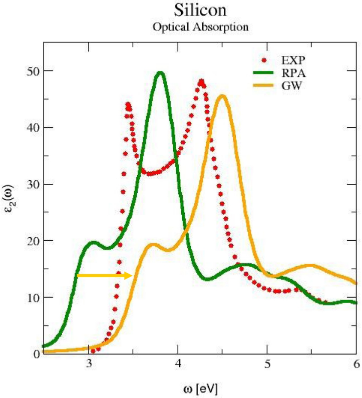
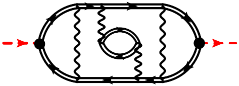




Interaction effects: vertex (excitonic) corrections

2nd class of interaction corrections:



includes all direct and indirect interactions between electron and hole created by a photon

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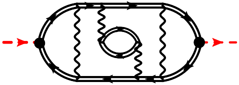

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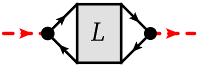
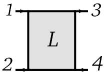
Summing up all such interaction processes we get:





Empty polarization loop is replaced by the full two-particle propagator $L(\mathbf{r}_1t_1;\mathbf{r}_2t_2;\mathbf{r}_3t_3;\mathbf{r}_4t_4) = L(1234)$ with joined ends

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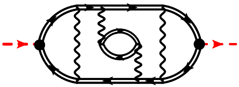

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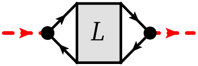
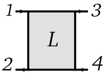
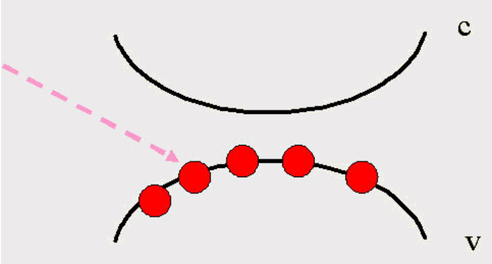




Empty polarization loop is replaced by the full two-particle propagator $L(\mathbf{r}_1 t_1; \mathbf{r}_2 t_2; \mathbf{r}_3 t_3; \mathbf{r}_4 t_4) = L(1234)$ with joined ends

Equation for L(1234) is the Bethe-Salpeter equation!

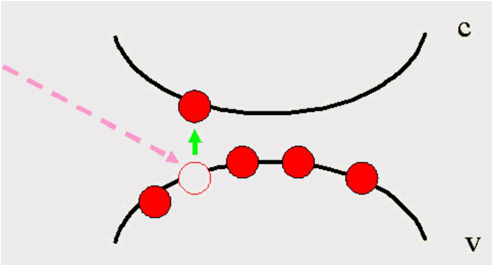
Absorption



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

Excitonic effects = electron - hole interaction

Absorption



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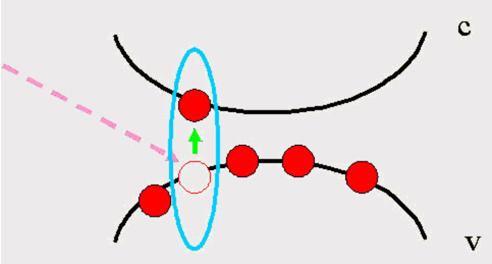

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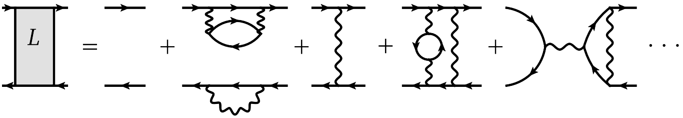
Excitonic effects = electron - hole interaction

Outline

Derivation of the Bethe-Salpeter equation (1)

Propagator of e-h pair in a many-body system:



- Solid lines stand for bare one-particle Green's functions

$$G_0(12) = G_0(\mathbf{r}_1, \mathbf{r}_2, t_1 - t_2)$$

- Wiggled lines correspond to the interaction (Coulomb) potential

$$v(12) = v(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_1 - t_2) = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}\delta(t_1 - t_2)$$

- Integration over space-time coordinates of all intermediate points in each graph is assumed

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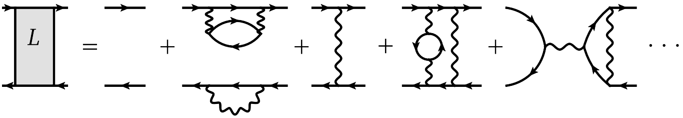
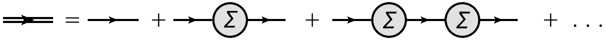
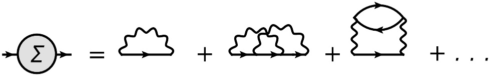


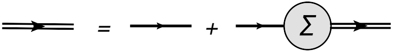
1st step: Dressing one-particle propagators



Self-energy Σ is a sum of all 1-particle irreducible diagrams

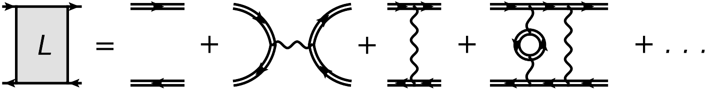


Full 1-particle Green's function satisfies the Dyson equation



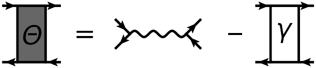
Derivation of the Bethe-Salpeter equation (2)

Propagation of dressed interacting electron and hole:

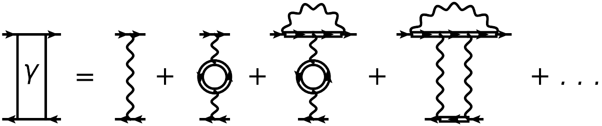


2nd step: Classification of scattering processes

At this stage we identify two-particle irreducible blocks

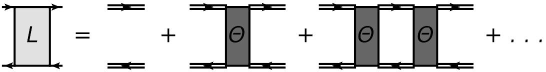


where $\gamma(1234)$ of the electron-hole stattering amplitude

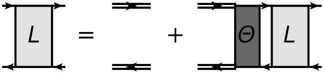


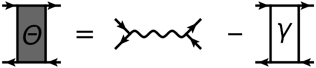
Derivation of the Bethe-Salpeter equation (3)

Final step: Summation of a geometric series



The result is the Bethe-Salpeter equation





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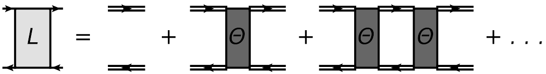

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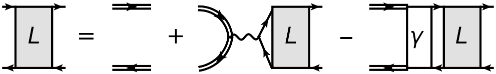
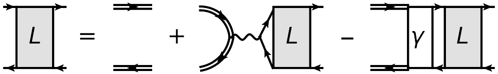


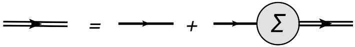
Analytic form of the Bethe-Salpeter equation ($j = \{\mathbf{r}_j, t_j\}$)

$$L(1234) = L_0(1234) + \int L_0(1256)[v(57)\delta(56)\delta(78) - \gamma(5678)]L(7834)d5d6d7d8$$

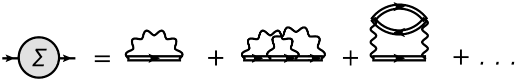
Closed set of equations in a diagrammatic form



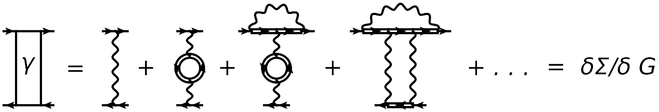
- 1-particle Green's function $G(12)$ satisfies the Dyson equation



- $\Sigma(12)$ is a sum of all 1-particle irreducible diagrams



- $\gamma(1234)$ – sum of all e-h and interaction irreducible diagrams



Outline

Response to external potential

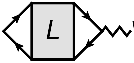
$$V^{ext} \longmapsto n^{ind} \longmapsto V^{ind}(\mathbf{r}) = \int d\mathbf{r}' v(\mathbf{r}-\mathbf{r}') n^{ind}(\mathbf{r}') = v n^{ind}$$

Total field acting on particles in the system : $V^{tot} = V^{ext} + V^{ind}$

Linear response theory: Definition of the dielectric function

$$n^{ind}(1) = \int d2 \chi(12) V^{ext}(2) \quad \longmapsto \quad V^{tot} = (1 + v\chi) V^{ext} \equiv \epsilon^{-1} V^{ext}$$

The density response function $\chi(12)$ is related to the e-h propagator L

$n^{ind} =$ 

V^{ext}

$$\chi(12) = \chi(\mathbf{r}_1, \mathbf{r}_2, t_1 - t_2) = L(1122) = L(\mathbf{r}_1\mathbf{r}_1\mathbf{r}_2\mathbf{r}_2, t_1 - t_2)$$

Macroscopic response in solids

Optical absorption is determined by Im$\epsilon_M(\omega)$. How we calculate it?

$$V^{ext}(\mathbf{r},t) = V^{ext}(\mathbf{q})e^{-i(\omega t - \mathbf{qr})}, \qquad q \ll G$$

In a periodic system V^{ind} contains all components with $\mathbf{k} = \mathbf{q} + \mathbf{G}$

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

Fourier component of the total potential in a solid:

$$V^{tot}_{\mathbf{G}}(\mathbf{q}) = \delta_{\mathbf{G},0}V^{ext}(\mathbf{q}) + V^{ind}_{\mathbf{G}}(\mathbf{q}) = \left[\delta_{\mathbf{G},0} + v_{\mathbf{G}}(\mathbf{q})\chi_{\mathbf{G},0}(\mathbf{q},\omega)\right]V^{ext}(\mathbf{q})$$

Macroscopic field and macroscopic dielectric function

- Macroscopic (averaged) potential: $V^{tot}_M(\mathbf{q}) = V^{tot}_{\mathbf{G}=0}(\mathbf{q})$
- Macroscopic dielectric function: $V^{ext}(\mathbf{q}) = \epsilon_M(\mathbf{q},\omega)V^{tot}_M(\mathbf{q})$

$$\epsilon_M(\mathbf{q},\omega) = \frac{1}{1 + v_{\mathbf{G}=0}(\mathbf{q})\chi_{0,0}(\mathbf{q},\omega)}$$

Macroscopic dielectric function from BSE (1)

1st possibility:

- Calculate $L(1234)$ by solving the Bethe-Salpeter equation

$$L = L_0 + L_0(v - \gamma)L$$

- Join electron-hole ends and perform a Fourier transform in time

$$L(1122) = L(\mathbf{r}_1\mathbf{r}_1\mathbf{r}_2\mathbf{r}_2, t_1 - t_2) \mapsto L(\mathbf{r}_1\mathbf{r}_1\mathbf{r}_2\mathbf{r}_2, \omega) = \chi(\mathbf{r}_1, \mathbf{r}_2, \omega)$$

- Go to the momentum representation

$$\chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q}, \omega) = \int d\mathbf{r}_1 d\mathbf{r}_2 e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}_1} L(\mathbf{r}_1\mathbf{r}_1\mathbf{r}_2\mathbf{r}_2, \omega) e^{-i(\mathbf{q}+\mathbf{G}')\mathbf{r}_2}$$

- The “head” of $\chi_{\mathbf{G},\mathbf{G}'}$ (element with $\mathbf{G} = \mathbf{G}' = 0$) determines ϵ_M

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Macroscopic dielectric function and the absorption rate

$$\epsilon_M(\mathbf{q},\omega) = \frac{1}{1 + v_{\mathbf{G}=0}(\mathbf{q})\chi_{0,0}(\mathbf{q},\omega)} \; ; \qquad Abs(\omega) = \lim_{\mathbf{q}\to 0} \epsilon''_M(\mathbf{q},\omega)$$

Macroscopic dielectric function from BSE (2)

2nd possibility:

Define a “long-range part” v_0 of the interaction potential

$$v_{\mathbf{G}}(\mathbf{q}) = v_{\mathbf{G}=0}(\mathbf{q})\delta_{\mathbf{G},0} + \bar{v}_{\mathbf{G}}(\mathbf{q})$$

$$v(r) = \int_{BZ} d\mathbf{q} \sum_{\mathbf{G}} e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}} v_{\mathbf{G}}(\mathbf{q}) = v_0(\mathbf{r}) + \bar{v}(\mathbf{r})$$

Bethe-Salpeter equation for a “proper” e-h propagator $\bar{L}(1234)$
(replace $v \mapsto \bar{v}$ in the full BSE)

$$\bar{L} = L_0 + L_0(\bar{v} - \gamma)\bar{L}$$

The full L-function and the density response function $\chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$

$$L = \bar{L} + \bar{L}v_0 L \quad \Rightarrow \quad \chi = \bar{\chi} + \bar{\chi}v_0\chi$$

Macroscopic dielectric function from BSE (2)

$$L = \bar{L} + \bar{L} v_0 L \quad \Rightarrow \quad \chi(12) = \bar{\chi}(12) + \bar{\chi}(13) v_0(34) \chi(42)$$

In the momentum representation $v_0 \mapsto v_{\mathbf{G}=0}(\mathbf{q}) \delta_{\mathbf{G},0}$

$$\chi_{\mathbf{G},\mathbf{G}'} = \bar{\chi}_{\mathbf{G},\mathbf{G}'} + \bar{\chi}_{\mathbf{G},0} v_{\mathbf{G}=0} \chi_{0,\mathbf{G}'} \quad \Rightarrow \quad \chi_{0,0}(\mathbf{q},\omega) = \frac{\bar{\chi}_{0,0}(\mathbf{q},\omega)}{1 - v_{\mathbf{G}=0}(\mathbf{q}) \bar{\chi}_{0,0}(\mathbf{q},\omega)}$$

Macroscopic dielectric function in terms of proper polarizability

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

$$\bar{\chi}_{0,0}(\mathbf{q},\omega) = \int d\mathbf{r}_1 d\mathbf{r}_2 e^{i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)} \bar{L}(\mathbf{r}_1 \mathbf{r}_1 \mathbf{r}_2 \mathbf{r}_2, \omega)$$

Macroscopic dielectric function from BSE (2)

Optical response from the Bethe-Salpeter equation

- Solve the reduced Bethe-Salpeter equation for $\bar{L}(1234)$

$$\bar{L} = L_0 + L_0(\bar{v} - \gamma)\bar{L}$$

- Calculate the macroscopic dielectric function from $\bar{L}(1122)$

$$\epsilon_M(\mathbf{q},\omega) = 1 - v_{\mathbf{G}=0}(\mathbf{q}) \int d\mathbf{r}_1 d\mathbf{r}_2 e^{i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)} \bar{L}(\mathbf{r}_1\mathbf{r}_1\mathbf{r}_2\mathbf{r}_2,\omega)$$

- Calculate the absorption rate from the imaginary part of $\epsilon_M(\mathbf{q},\omega)$

$$Abs(\omega) = \lim_{\mathbf{q}\to 0} \epsilon''_M(\mathbf{q},\omega)$$

By setting $\bar{v} = 0$ we neglect local field effects – the difference between the macroscopic field $V_M^{tot}(\mathbf{r})$ and the actual field $V^{tot}(\mathbf{r})$

Outline

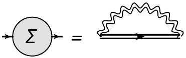
The Bethe-Salpeter equation: Approximations

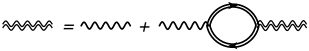
Reminder

BSE determines 2-particle propagator $L(1234)$, provided 1-particle self-energy $\Sigma(12)$ and e-h scattering amplitude $\gamma(1234)$ are given.

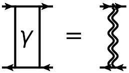
Standard approximations:

- Apprixmating Σ by GW diagram: $\Sigma(12) = G(12)W(12)$



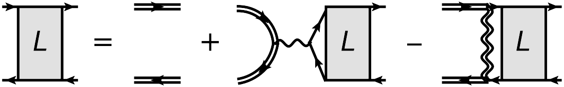


- Approximating γ by W: $\gamma(1234) = W(12)\delta(13)\delta(24)$



The Bethe-Salpeter equation: Approximations

Approximate Bethe-Salpeter equation



Analytic form of the approximate Bethe-Salpeter equation

$$L(1234) = L_0(1234) + \int L_0(1256)[v(57)\delta(56)\delta(78) - W(56)\delta(57)\delta(68)]L(7834)d5d6d7d8$$

$L_0(1234) = G(12)G(43)$ and $W(12)$ come out of the GW calculations

The Bethe-Salpeter equation: Approximations

Reduced BSE for the proper e-h propagator

$$L(1234) = L_0(1234) + \int d5d6d7d8 L_0(1256) \times$$
$$\times \left[v(57)\delta(56)\delta(78) - W(56)\delta(57)\delta(68)\right] L(7834)$$

Further simplifications: Static W

Assumption of the static screening:

$$W(\mathbf{r}_1, \mathbf{r}_2, t_1 - t_2) \Rightarrow W(\mathbf{r}_1, \mathbf{r}_2)\delta(t_1 - t_2)$$

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

The Bethe-Salpeter equation: Approximations

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Optical response in practice

Calculation of the macroscopic dielectric function

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

$$\epsilon_M(\omega) = 1 - \lim_{\mathbf{q}\to 0}\left[v_{\mathbf{G}=0}(\mathbf{q})\int d\mathbf{r}d\mathbf{r}' e^{i\mathbf{q}(\mathbf{r}-\mathbf{r}')}\bar{L}(\mathbf{r},\mathbf{r},\mathbf{r}',\mathbf{r}',\omega)\right]$$

$$L_0(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4,\omega) = \sum_{ij}(f_j - f_i)\frac{\phi_i^*(\mathbf{r}_1)\phi_j(\mathbf{r}_2)\phi_i(\mathbf{r}_3)\phi_j^*(\mathbf{r}_4)}{\omega - (E_i - E_j)}$$

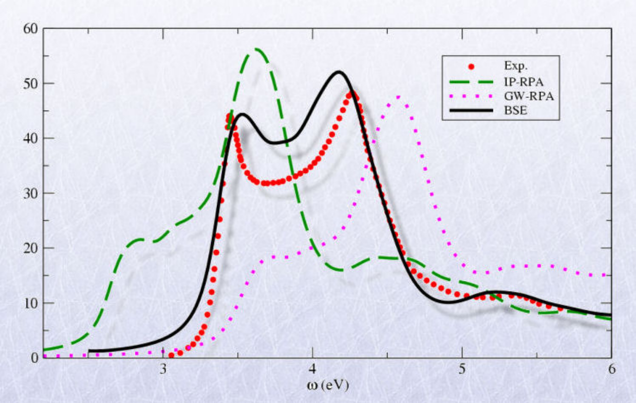
BSE calculations

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 $\bar{L} = L_0 + L_0(\bar{v} - \gamma)\bar{L}$
   $\Rightarrow$ proper e-h propagator $\bar{L}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4\omega)$
   $\Rightarrow$ spectra $\epsilon_M(\omega)$

Results: Continuum excitons (Si)

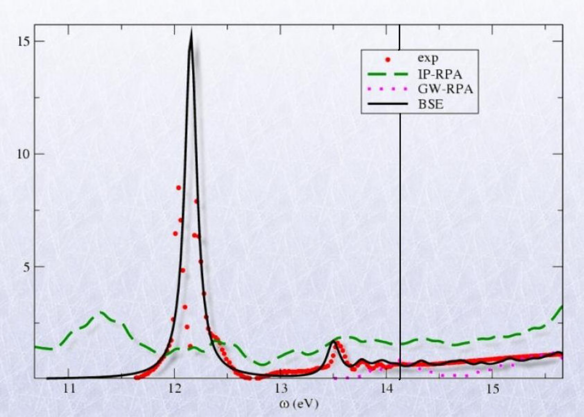
Bulk silicon



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

Results: Bound excitons (solid Ar)

Solid argon



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