What is this ?
An introduction to Theoretical Spectroscopy

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$$
\begin{aligned}
i\theta(t_2-t_1) &= -i\int_{t_1}^{\infty} dt_3 \int dt_4 t_7 W(t_3,t_4) g(t_3,t_2;[\varphi]) W^{-1}(t_4,t_7)\varphi(t_7) \\
&+ \int_{t_1}^{\infty} dt_3 \int dt_6 t_{\bar{1}} t_8 j(t_3,t_6)\epsilon(t_6;[\varphi]) g(t_{\bar{1}},t_2;[\varphi]) j^{-1}(t_6,t_{\bar{1}})\epsilon^{-1}(t_6,[\varphi])\frac{j(t_8,t_6)}{j(t_3,t_6)}\theta^{-1}(t_3,t_8) \\
&+ i\int_{t_1}^{\infty} dt_3 \int dt_4 W(t_3,t_4) g(t_3,t_2;[\varphi])\theta(t_2-t_4)\theta(t_4-t_3) && (13) \\
&= -i\int_{t_1}^{\infty} dt_3 g(t_3,t_2;[\varphi])\varphi(t_3) + \int_{t_1}^{\infty} dt_3 \int dt_6 t_8 g(t_{\bar{1}},t_2;[\varphi]) j^{-1}(t_6,t_{\bar{1}}) j(t_8,t_6)\theta^{-1}(t_3,t_8) \\
&+ i\int_{t_1}^{\infty} dt_3 \int dt_4 W(t_3,t_4) g(t_3,t_2;[\varphi])\theta(t_2-t_4)\theta(t_4-t_3) && (14) \\
&= -i\int_{t_1}^{\infty} dt_3 g(t_3,t_2;[\varphi])\varphi(t_3) + \int_{t_1}^{\infty} dt_3 \int dt_{\bar{1}} g(t_{\bar{1}},t_2;[\varphi])\theta^{-1}(t_3,t_{\bar{1}}) \\
&+ i\int_{t_1}^{\infty} dt_3 \int dt_4 W(t_3,t_4) g(t_3,t_2;[\varphi])\theta(t_2-t_4)\theta(t_4-t_3) && (15) \\
&= -i\int_{t_1}^{\infty} dt_3 g(t_3,t_2;[\varphi])\varphi(t_3)\theta(t_3-t_1) + \int_{t_1}^{\infty} dt_3 \int dt_{\bar{1}} g(t_{\bar{1}},t_2;[\varphi])\theta^{-1}(t_3,t_{\bar{1}})\theta(t_3-t_1) \\
&+ i\int_{t_1}^{\infty} dt_3 \int dt_4 W(t_3,t_4) g(t_3,t_2;[\varphi])\theta(t_2-t_4)\theta(t_4-t_3)\theta(t_3-t_1) && (16) \\
&= -i\int_{t_1}^{\infty} dt_3 g(t_3,t_2;[\varphi])\varphi(t_3)\theta(t_3-t_1) + g(t_1,t_2;[\varphi]) + i\int_{t_1}^{\infty} dt_3 \int_{t_1}^{t_2} dt_4 W(t_3,t_4) g(t_3,t_2;[\varphi]) && (17)
\end{aligned}
$$

and finally we obtain a more compact expression:

$$
i\theta(t_2-t_1) = i\int dt_3 g(t_3,t_2;[\varphi])\Big\{-\varphi(t_3)\theta(t_3-t_1) + \int_{t_3}^{t_2} dt_4 W(t_3,t_4)\theta(t_3-t_1) - i\delta(t_1,t_3)\Big\} \quad (18)
$$

Now, if we manipulate Eq. 1, with the change of variable $y \to g$ and performing explicitely $\dfrac{\delta g(t_3,t_2;[\varphi])}{\delta\varphi(t_4)}$ we get:

$$
g(t_1,t_2;[\varphi]) = i\theta(t_2-t_1) + i\int_{t_1}^{\infty} dt_3 \varphi(t_3) g(t_3,t_2;[\varphi]) + i^2\int_{t_1}^{\infty} dt_3 \int dt_4 W(t_3,t_4)\theta(t_4-t_3)\theta(t_2-t_4) g(t_3,t_2;[\varphi]) \quad (19)
$$

$$
\begin{aligned}
i\theta(t_2-t_1) = & -i\int_{t_1}^{\infty} dt_3 \int dt_4 t_7 W(t_3,t_4) g(t_3,t_2;[\varphi]) W^{-1}(t_4,t_7)\varphi(t_7) \\
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= & -i\int_{t_1}^{\infty} dt_3 g(t_3,t_2;[\varphi])\varphi(t_3) + \int_{t_1}^{\infty} dt_3 \int dt_6 t_8 g(t_{\bar{1}},t_2;[\varphi]) j^{-1}(t_6,t_{\bar{1}}) j(t_8,t_6)\theta^{-1}(t_3,t_8) \\
& + i\int_{t_1}^{\infty} dt_3 \int dt_4 W(t_3,t_4) g(t_3,t_2;[\varphi])\theta(t_2-t_4)\theta(t_4-t_3) \qquad (14) \\
= & -i\int_{t_1}^{\infty} dt_3 g(t_3,t_2;[\varphi])\varphi(t_3) + \int_{t_1}^{\infty} dt_3 \int dt_{\bar{1}} g(t_{\bar{1}}, \text{[illegible]} \\
& + i\int_{t_1}^{\infty} dt_3 \int dt_4 W(t_3,t_4) g(t_3,t_2; \text{[illegible]} \qquad (15) \\
= & -i\int_{t_1}^{\infty} dt_3 g(t \text{[illegible]} \int_{t_1} dt_3 \int dt_{\bar{1}} g(t_{\bar{1}},t_2;[\varphi])\theta^{-1}(t_3,t_{\bar{1}})\theta(t_3-t_1) \\
& \text{[illegible]} t_4) g(t_3,t_2;[\varphi])\theta(t_2-t_4)\theta(t_4-t_3)\theta(t_3-t_1) \qquad (16) \\
& \text{[illegible]} \int_{t_1} dt_3 g(t_3,t_2;[\varphi])\varphi(t_3)\theta(t_3-t_1) + g(t_1,t_2;[\varphi]) + i\int_{t_1}^{\infty} dt_3 \int_{t_1}^{t_2} dt_4 W(t_3,t_4) g(t_3,t_2;[\varphi]) \qquad (17)
\end{aligned}
$$

Don't worry!!!!!

and finally we obtain a more compact expression:

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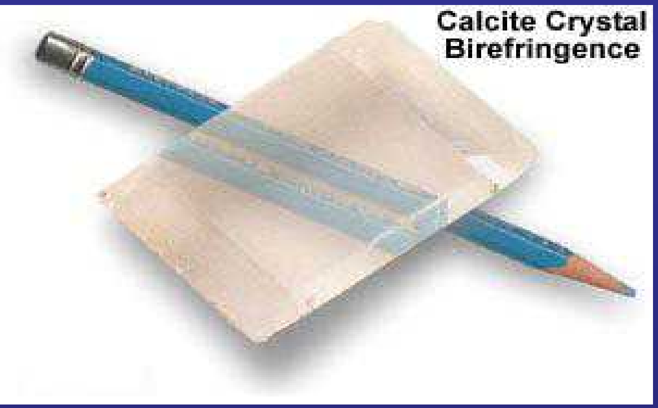
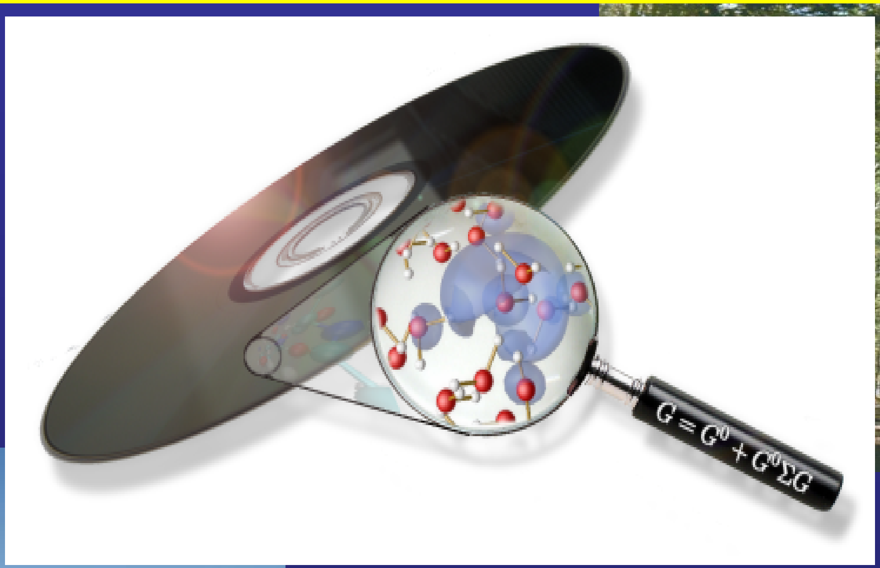
$$

→ Theoretical Spectroscopy, the aim





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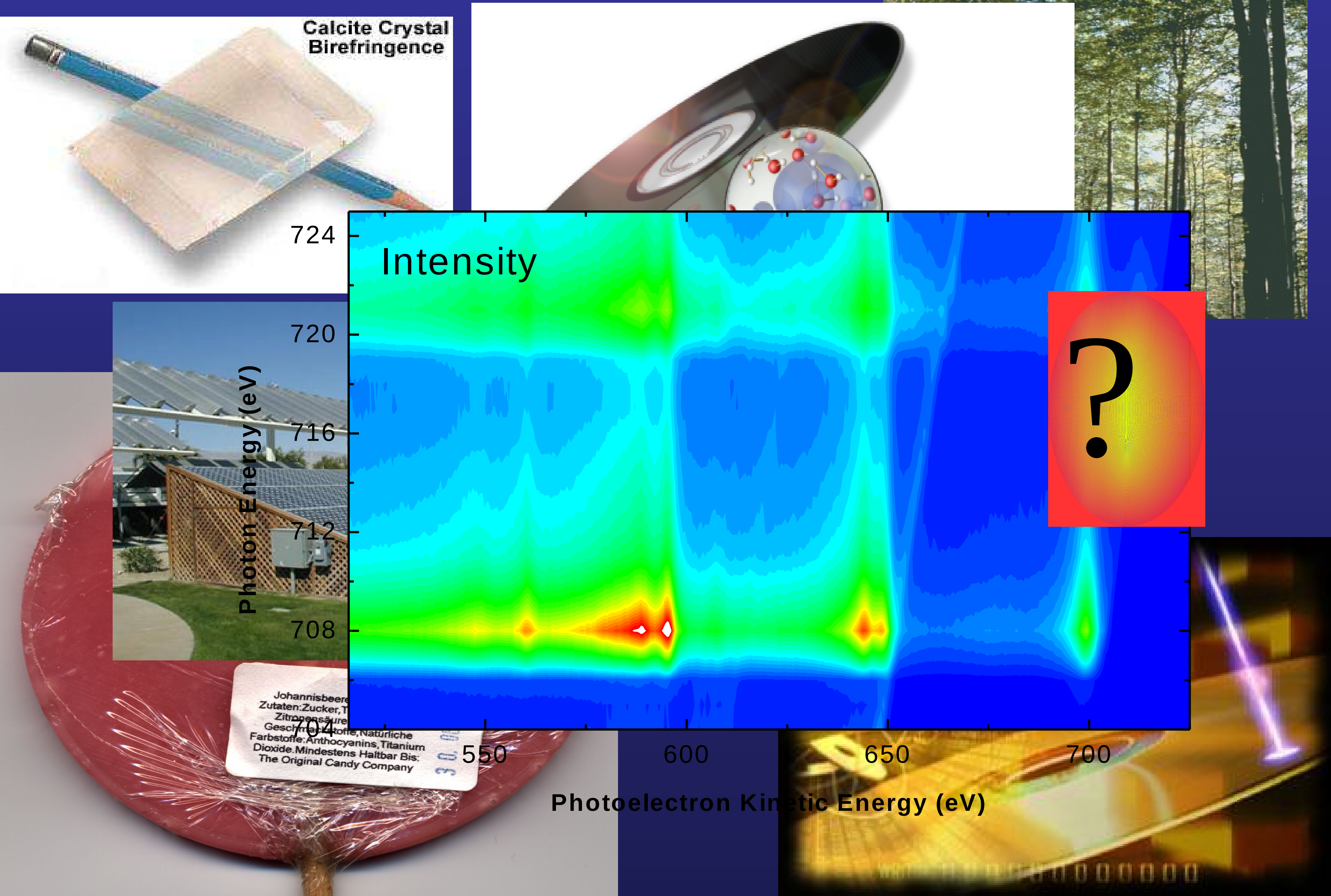
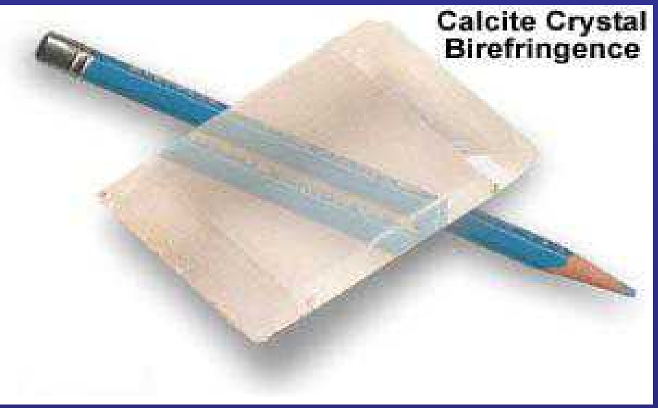
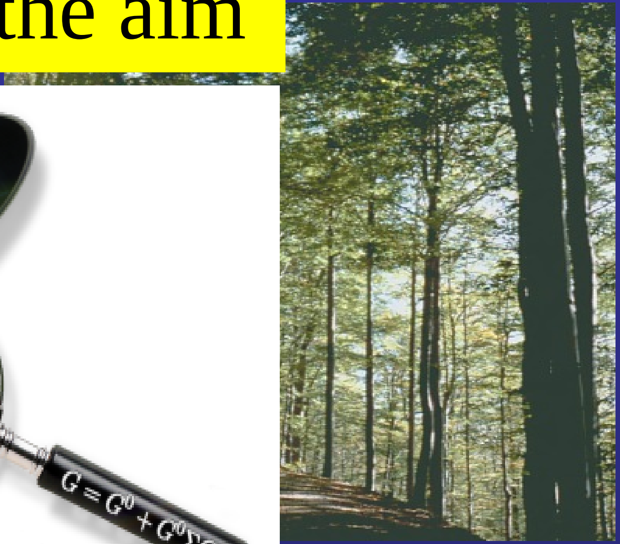
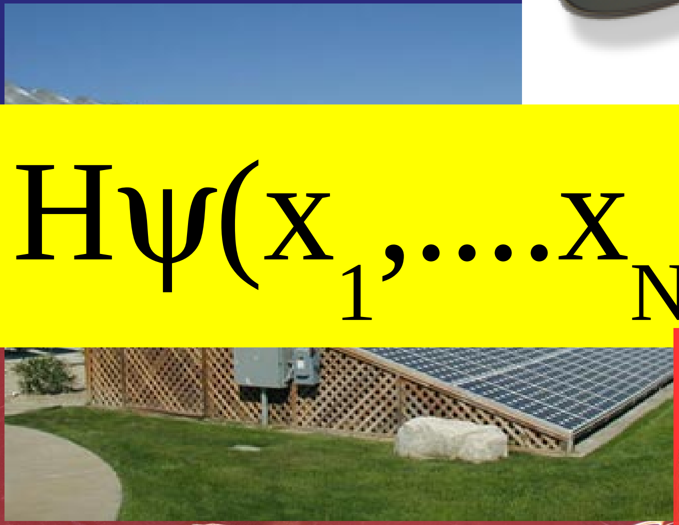


→ Theoretical Spectroscopy, the aim







$$H\psi(x_1,....x_N) = E\,\psi(x_1,....x_N)$$

→ Calculate only what you want,
………………..so that you can understand!

$$H\psi_n(x_1,....x_N) = E_n\, \psi_n(x_1,....x_N)$$

Want: → total energy E_0

→ expectation values like

* density
* spectral functions
* dielectric function

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

Do not want: → all many-body $\psi_n(x_1,....x_N)$

Effective quantities in an effective world

A practical example, simulate zero gravity

→ Calculate only what you want,
……...............so that you can understand!

$$H\psi_n(x_1,....x_N) = E_n\ \psi_n(x_1,....x_N)$$

Want: → total energy E_0

→ expectation values like

* density
* spectral functions
* dielectric function

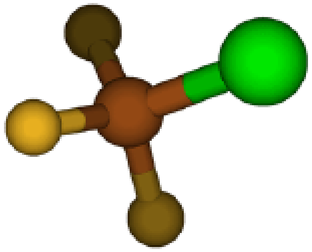
$$V_{tot}(\omega) = \varepsilon^{-1}(\omega) V_{ext}(\omega)$$

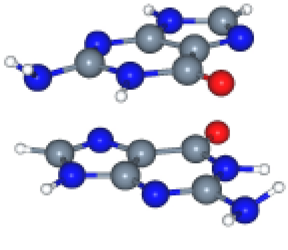
Do not want: → all many-body $\psi_n(x_1,....x_N)$

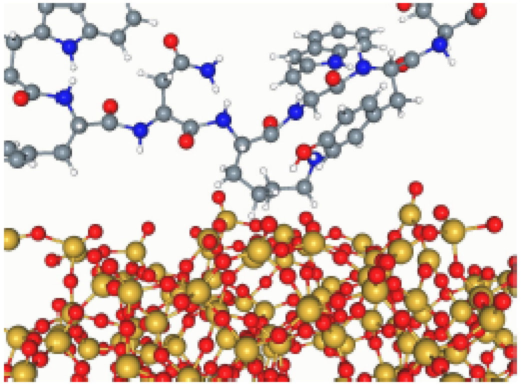
→ The effective quantities:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, .., \mathbf{r}_N, t) \quad \longrightarrow \quad G(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) \quad \longrightarrow \quad \rho(\mathbf{r}, t)$$

CI, QMC — GF methods (GW, BSE) — DF







→ Density Functional versus Propagators

→ The effective world:

$$\left(-\frac{1}{2}\nabla^2 + v_{\text{eff}}(\mathbf{r})\right)\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})$$

LDA or so

$$v_{\text{eff}}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) + v_{\text{H}}([n],\mathbf{r}) + v_{\text{xc}}([n],\mathbf{r}).$$

Designed for density and top valence

NOT for bandgaps, for example!!!

Giorgia

Kohn-Sham

→ The effective world:

$$\left(-\frac{1}{2}\nabla^2 + v_{\text{eff}}(\mathbf{r})\right)\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})$$

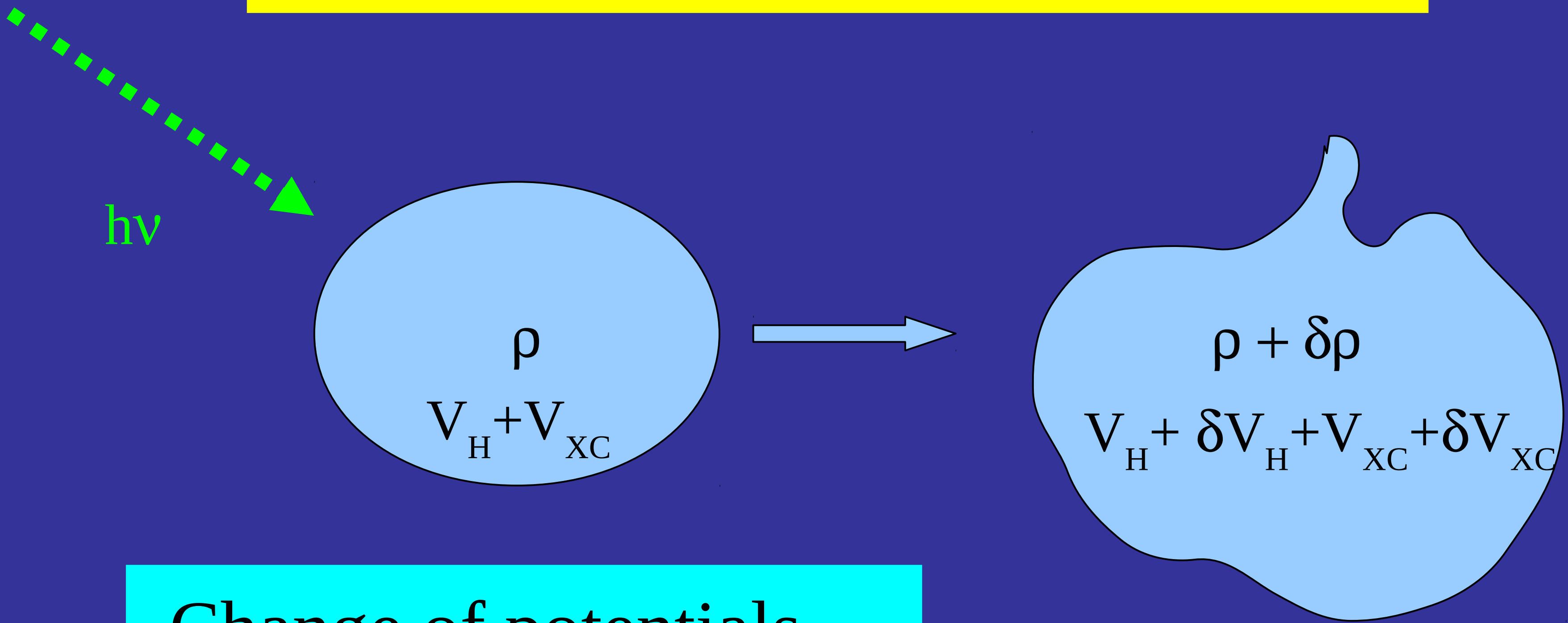
$$v_{\text{eff}}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) + v_{\text{H}}([n],\mathbf{r}) + v_{\text{xc}}([n],\mathbf{r})$$

$$\Sigma(\mathbf{r},\mathbf{r}',\varepsilon_i)$$

Designed for electron addition and removal spectra (bandstructure, lifetimes, satellites,....,density,...)

Other: DMFT $\Sigma_{\iota\iota}(\omega)$

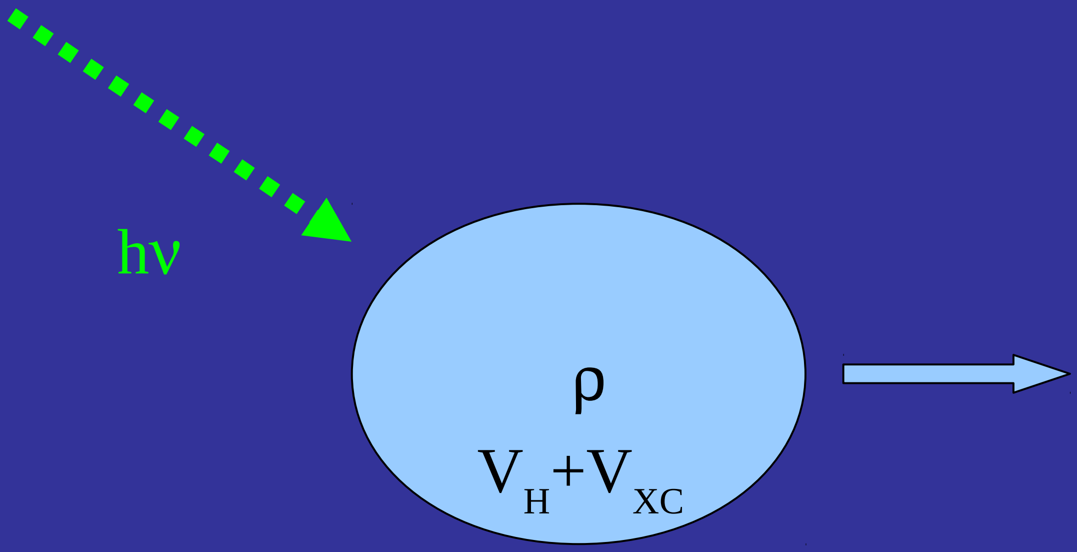
- DFT point of view: moving density

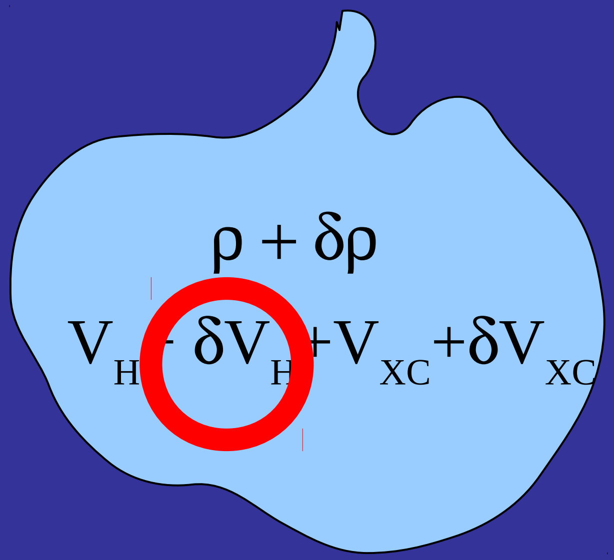


Change of potentials

Excitation ?

→ Induced potentials



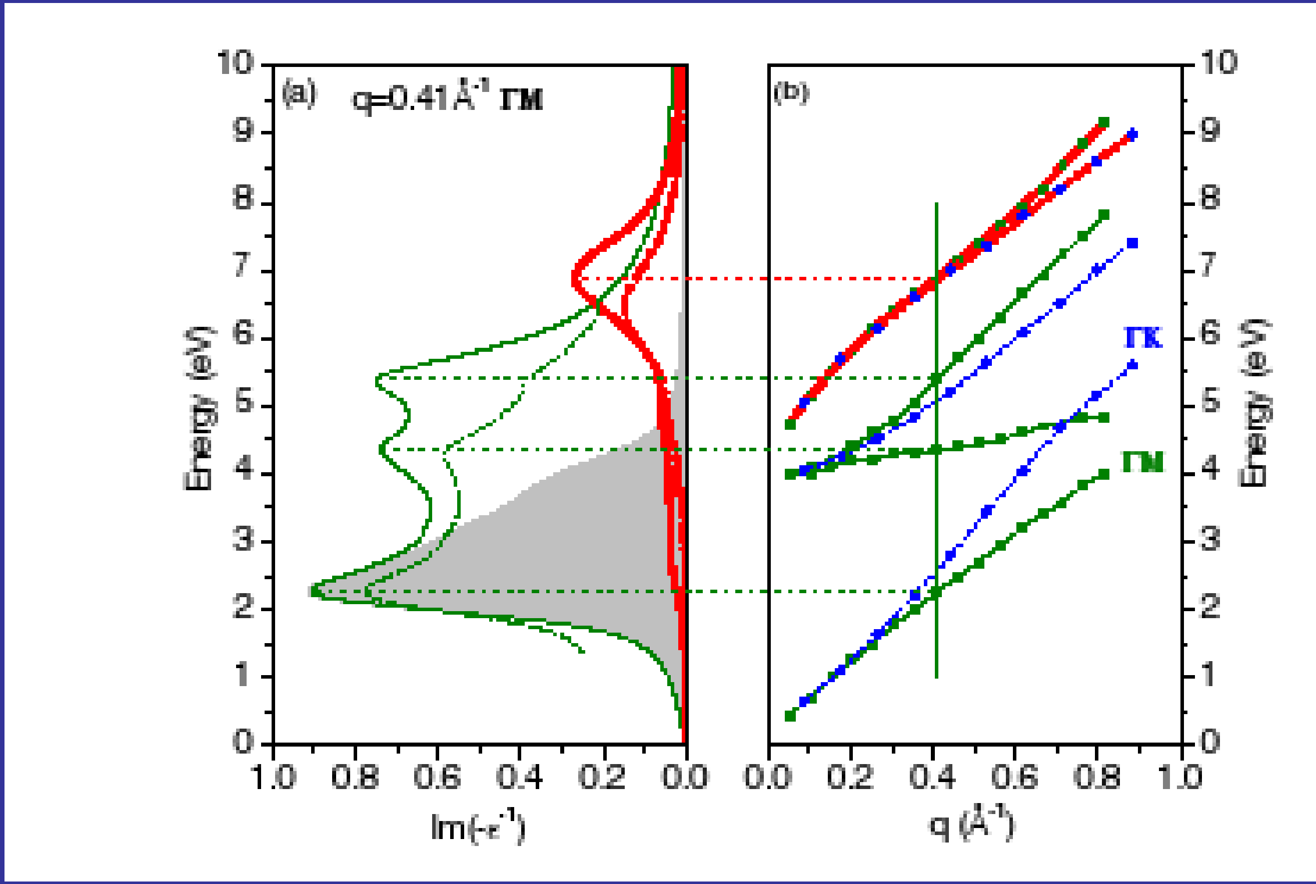


Change of potentials

Induced Hartree: long-range and local field effects

RPA

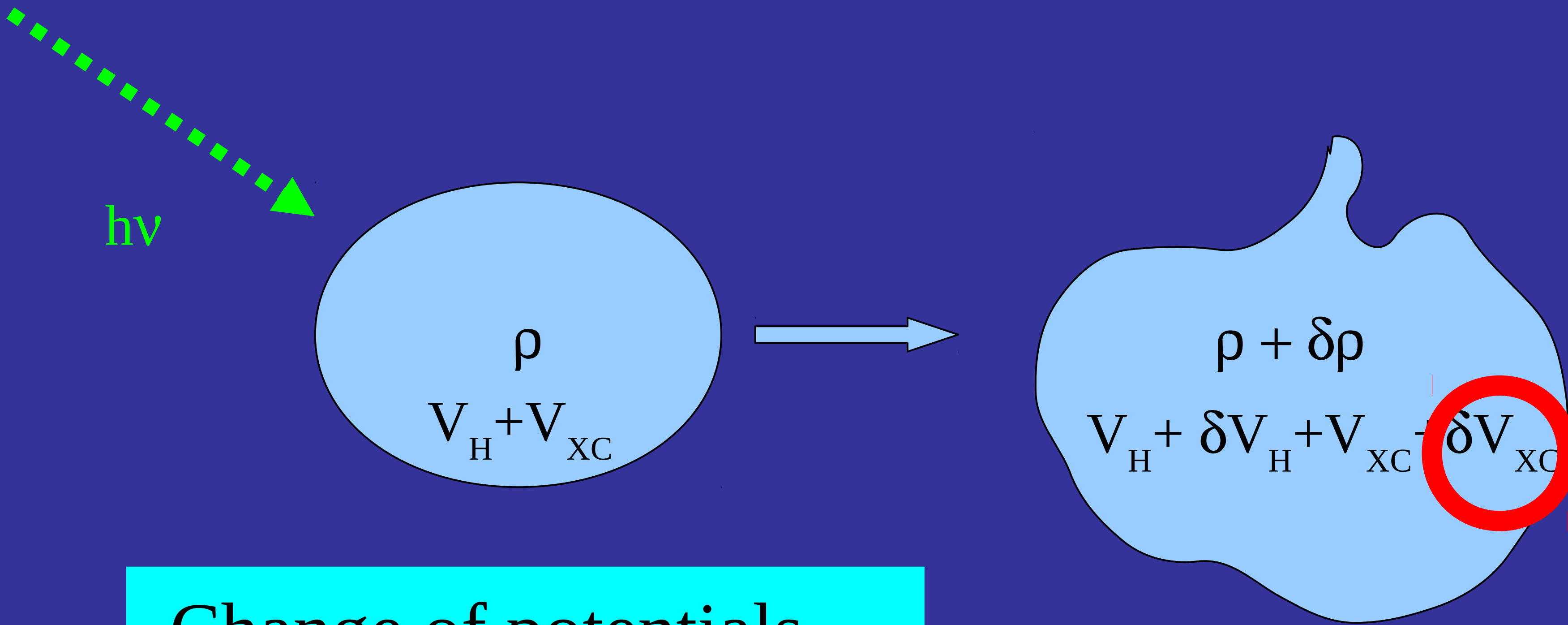
Graphene, π plasmon



C. Kramberger et al., PRL 100, 196803 (2008)

Excitation ?

→ Induced potentials

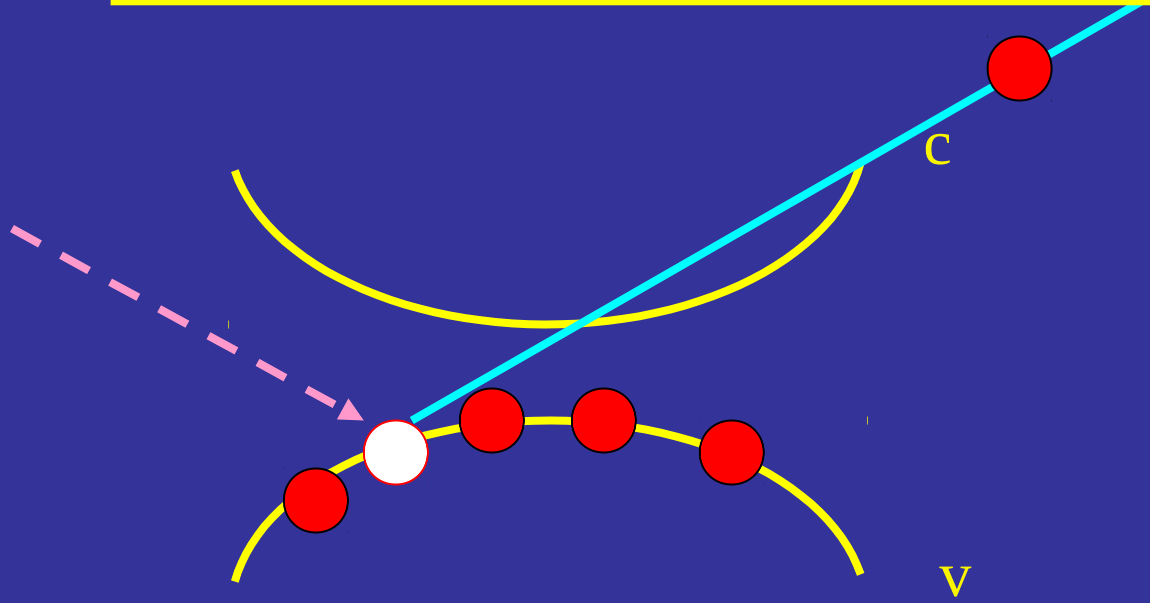


Change of potentials

Plus induced xc: excitons ???………..

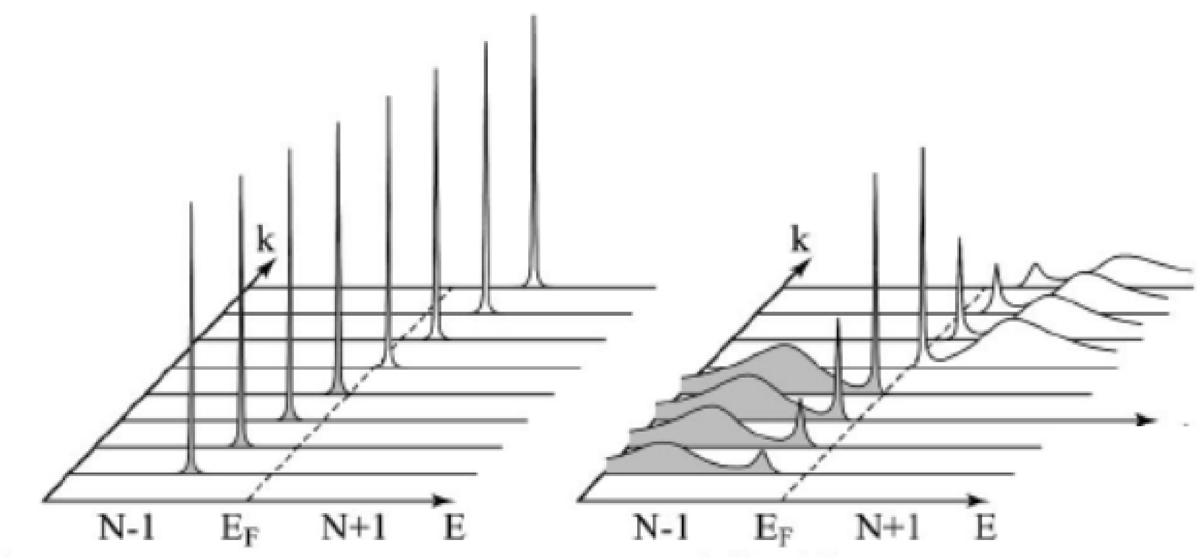
TD-LDA ……..

Propagators (example photoemission)



Hole - (N-1) (excited) electrons

$A(\omega) \sim \mathrm{Im}[\mathcal{G}(\omega)]$



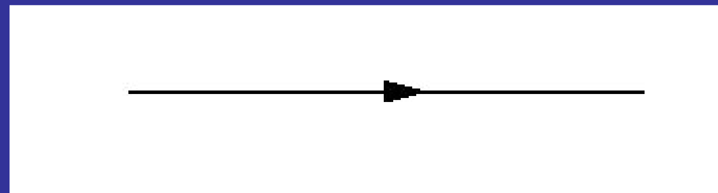
From Damascelli et al., RMP 75, 473 (2003)

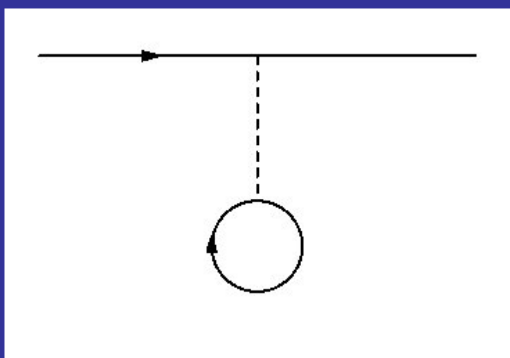
Coupling to other excitations!

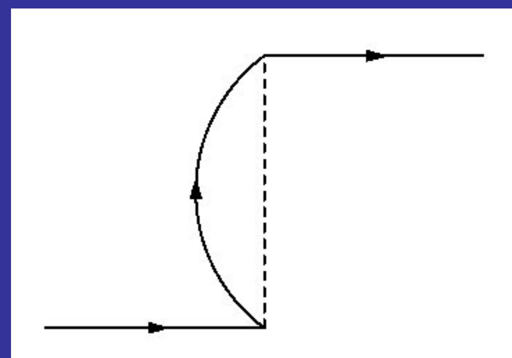
+......

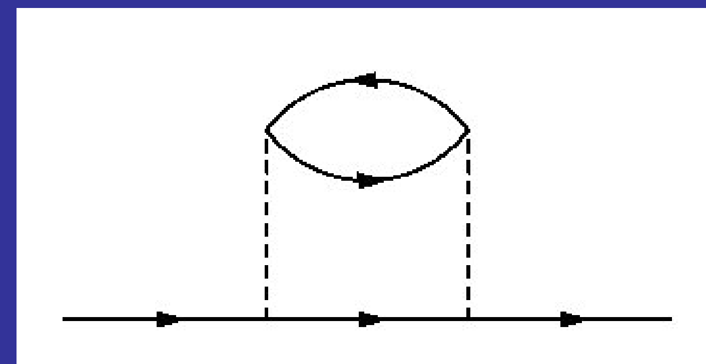
$\mathcal{G}(1,2) = -i \langle T[\psi(1)\psi^\dagger(2)] \rangle$

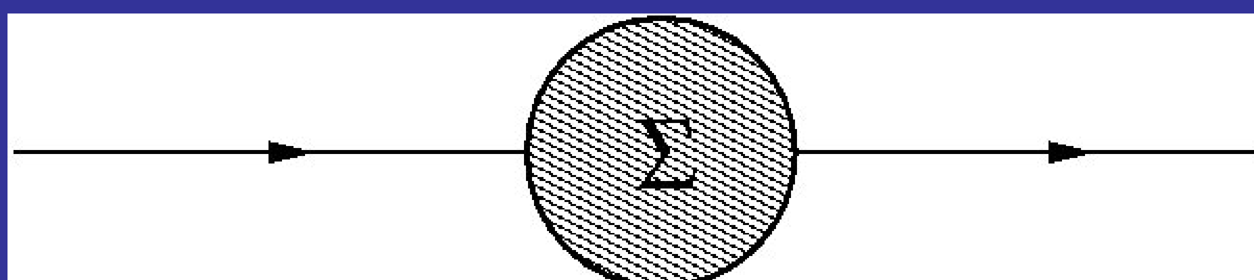
$1=(r_1,\sigma_1,t_1)$



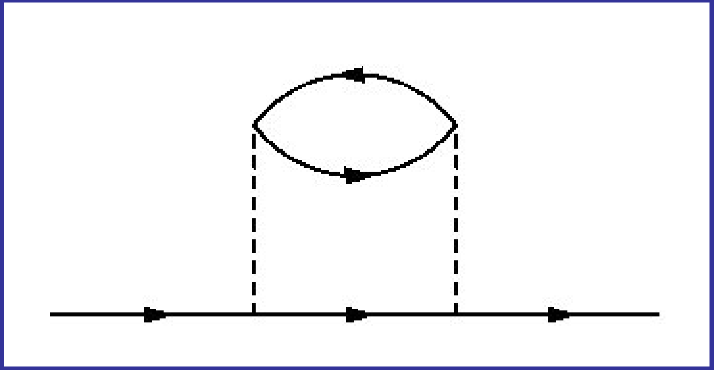








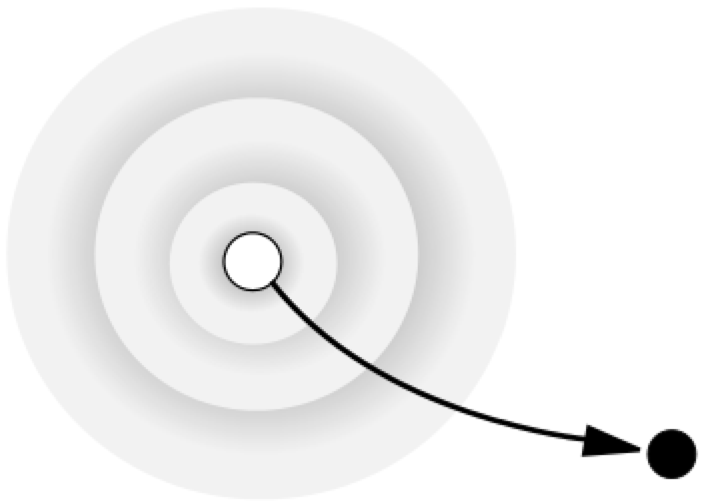
Dyson equation: $\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \, \Sigma \, \mathcal{G}$



$\rightarrow \Sigma \sim i\,WG$ “GW”

L. Hedin (1965)

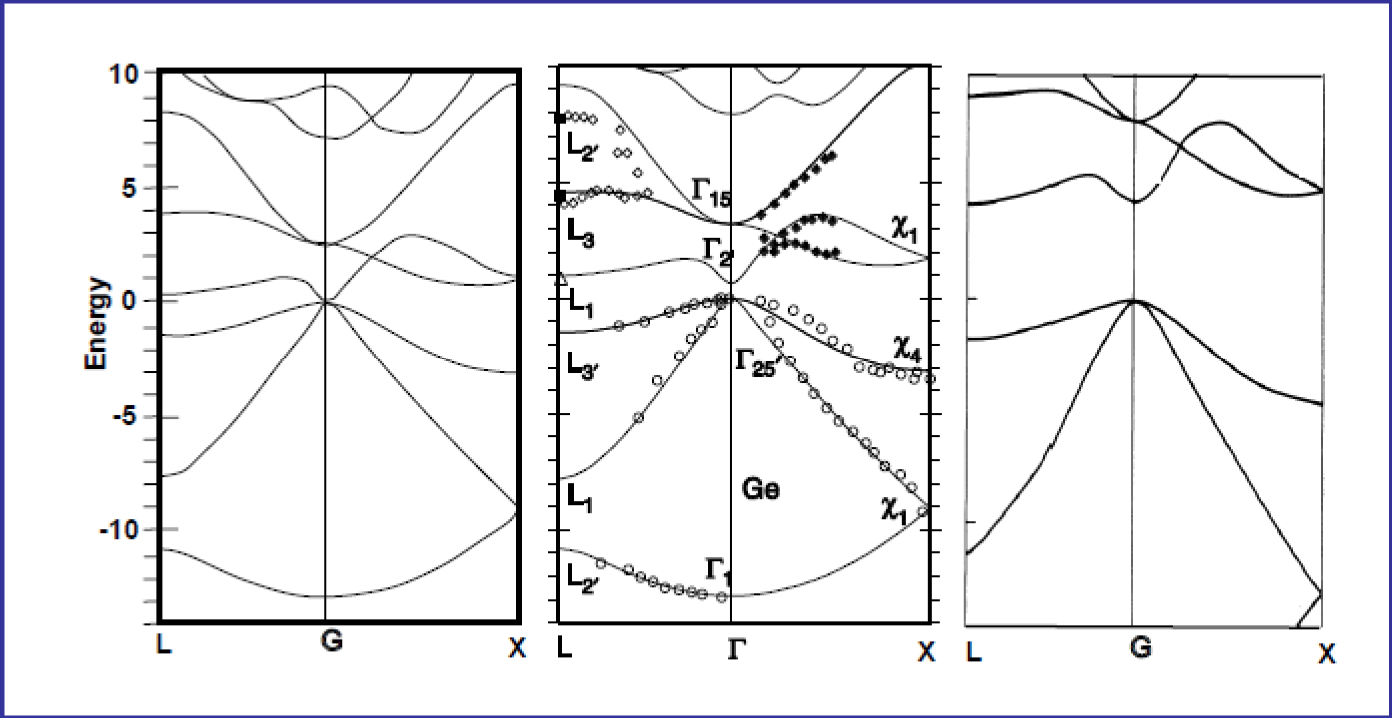
$W = \varepsilon^{-1}(\omega)\, v$



Model $W(r,r',\omega)$

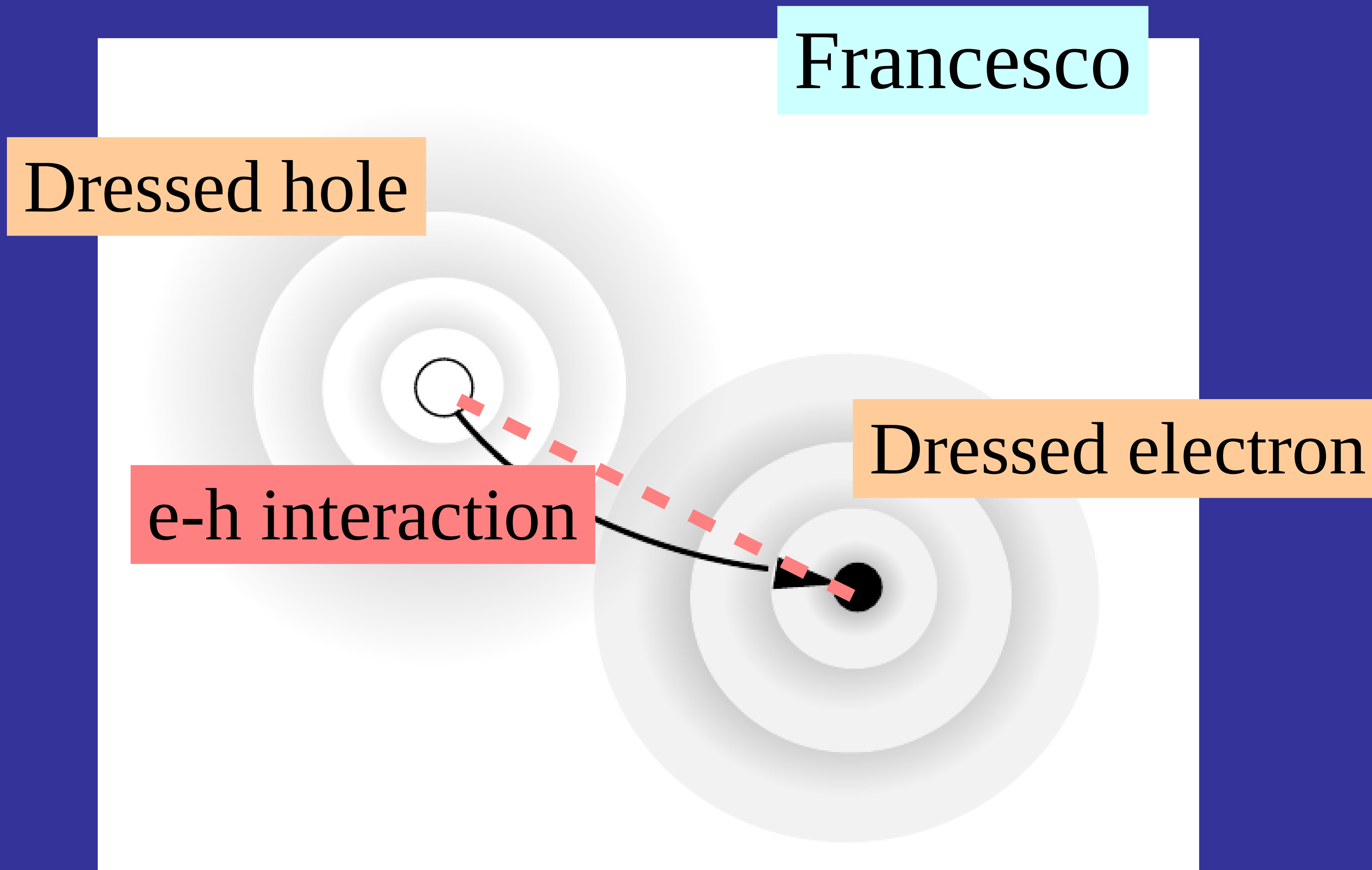
Ab initio $W(r,r',\omega)$

LDA GW HF



GW calculations, Rohlfing et al., PRB 48, 17791 (1993)

Matteo and Claudia



Correlation induces many additional excitations

e-h problem: Bethe-Salpeter equation

→ Theory and Experiment

$$+\, i \int_{t_1}^{\infty} dt_3 \int dt_4 W(t_3,t_4) g(t_3,t_2;[\varphi])\theta(t_2-t_4)\theta(t_4-t_3)$$

$$= -i \int_{t_1}^{\infty} dt_3 g(t_3,t_2;[\varphi])\varphi(t_3)\theta(t_3-t_1) + \int_{t_1}^{\infty} dt_3 \int dt_{\bar{1}} g(t_{\bar{1}},t_2;[\varphi])$$

$$+\, i \int_{t_1}^{\infty} dt_3 \int dt_4 W(t_3,t_4) g(t_3,t_2;[\varphi])\theta(t_2-t_4)\theta(t_4-t_3)\theta(t_3-t_1)$$

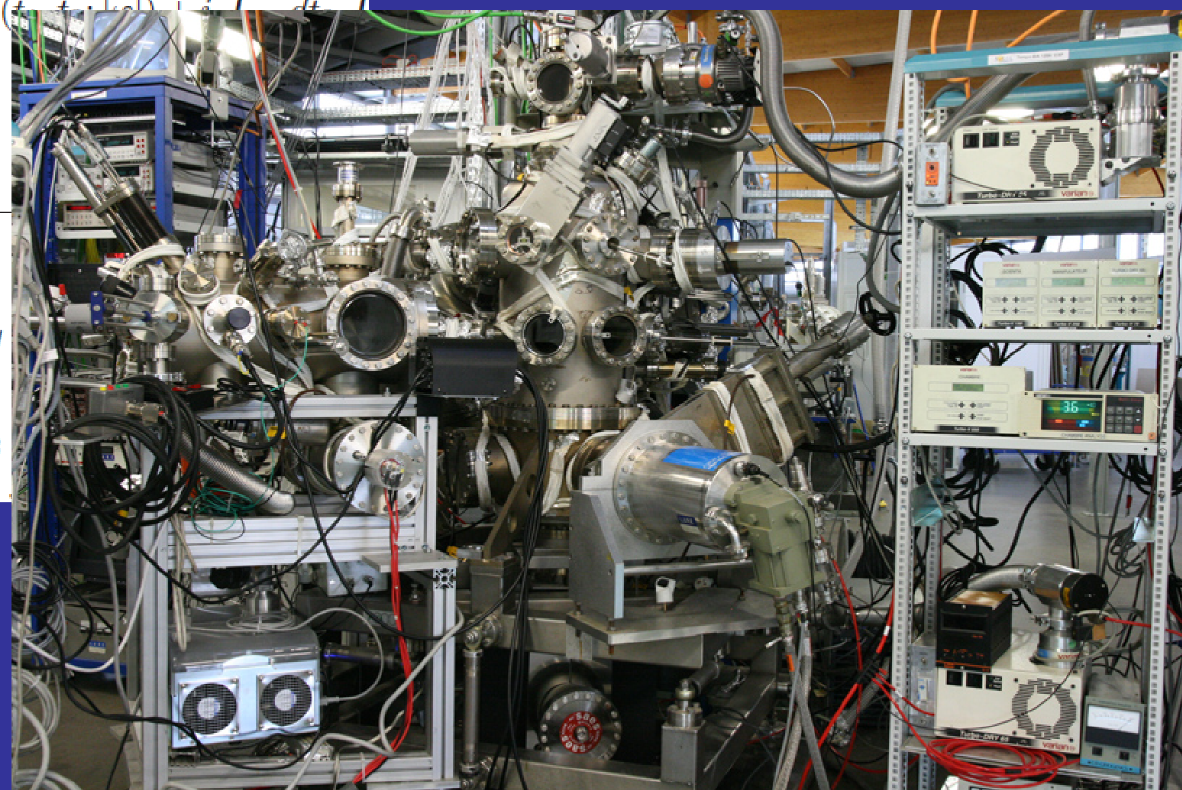
$$= -i \int_{t_1}^{\infty} dt_3 g(t_3,t_2;[\varphi])\varphi(t_3)\theta(t_3-t_1) + g(t \ldots$$

obtain a more compact expression:

$$\theta(t_2-t_1) = i \int dt_3 g(t_3,t_2;[\varphi])\Big\{ -\varphi(t_3)\theta(t_3 - \ldots$$

nipulate Eq. 1, with the change of variable y

$$= i\theta(t_2-t_1) + i \int_{t_1}^{\infty} dt_3 \varphi(t_3) g(t_3,t_2;[\varphi]) + i^2 \ldots$$



→ Theory and Experiment

$$+\,i\int_{t_1}^{\infty} dt_3 \int dt_4 W(t_3,t_4) g(t_3,t_2;[\varphi])\theta(t_2-t_4)\theta(t_4-t_3)$$

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$$= -i\int_{t_1}^{\infty} dt_3 g(t_3,t_2;[\varphi])\varphi(t_3)\theta(t_3$$

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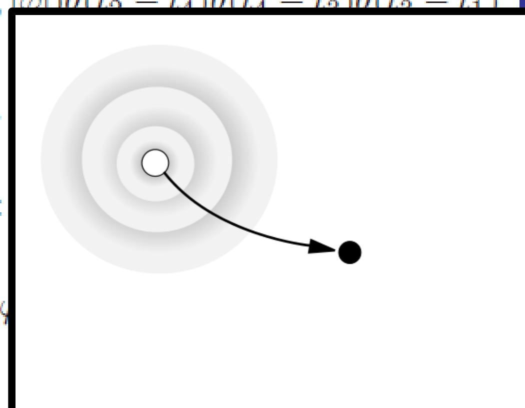
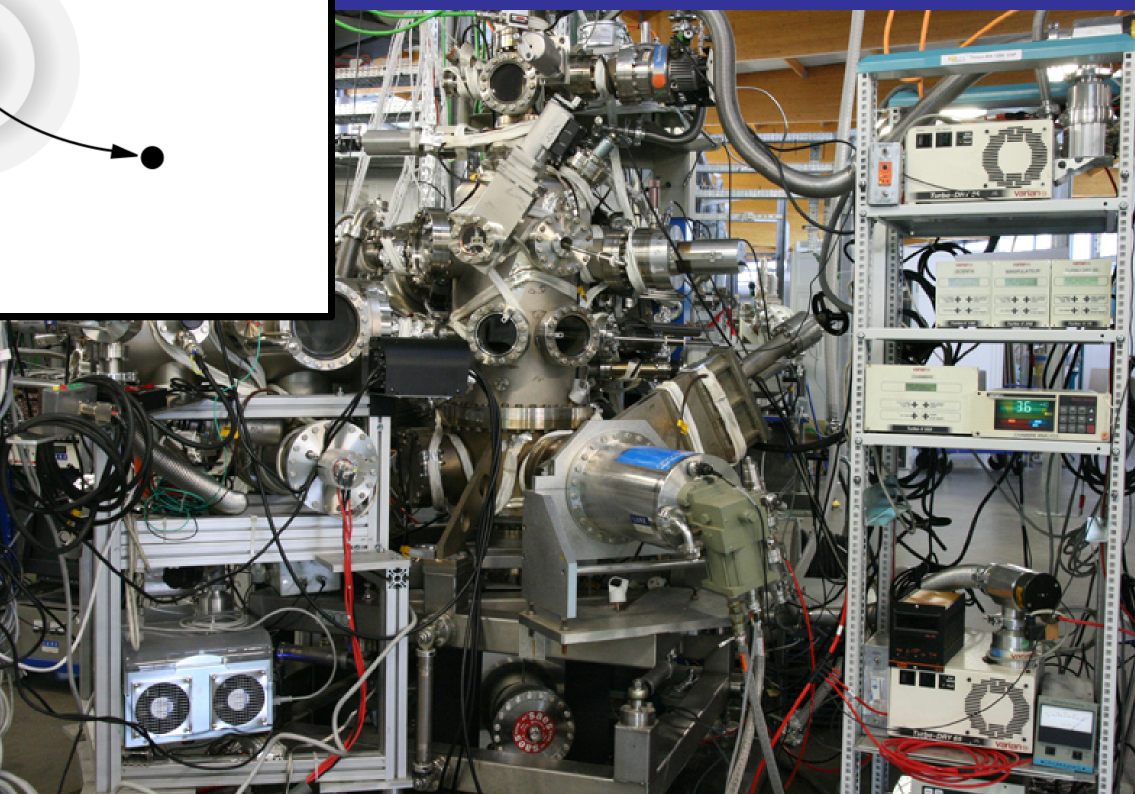




→ Theory and Experiment

$$+ i \int_{t_1}^{\infty} dt_3 \int dt_4 W(t_3, t_4) g(t_3, t_2; [\varphi]) \theta(t_2 - t_4) \theta(t_4 - t_3)$$

$$= -i \int_{t_1}^{\infty} dt_3 g(t_3, t_2; [\varphi]) \varphi(t_3) \theta(t_3 - t_1) + \int_{t_1}^{\infty} dt_3 \int dt_{\bar{1}} g(t_{\bar{1}}, t_2; [\varphi])$$

$$+ i \int_{t_1}^{\infty} dt_3 \int dt_4 W(t_3, t_4) g(t_3,$$

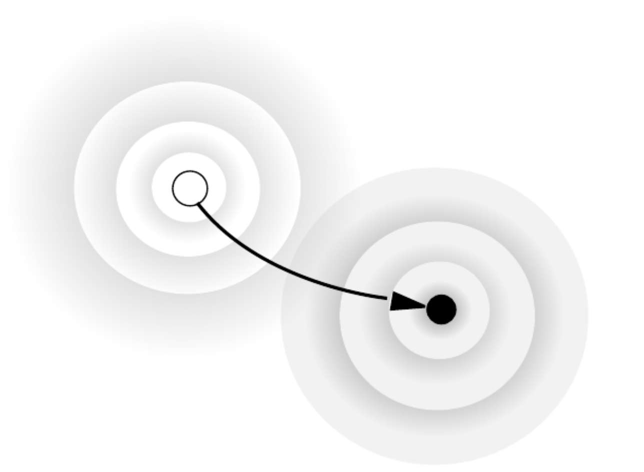
$$= -i \int_{t_1}^{\infty} dt_3 g(t_3, t_2; [\varphi]) \varphi(t_3) \theta$$

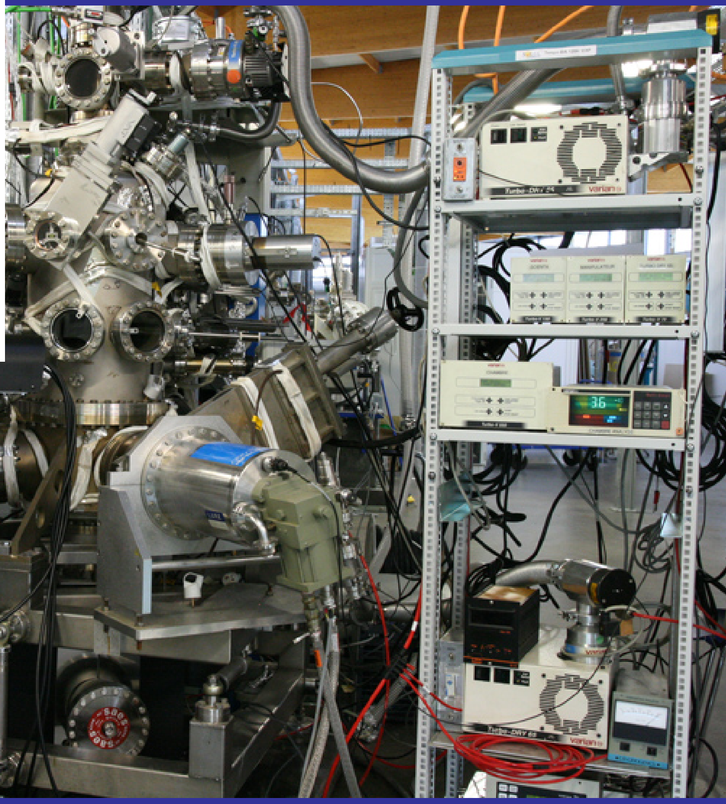
obtain a more compact expressi

$$\theta(t_2 - t_1) = i \int dt_3 g(t_3, t_2; [\varphi]) \Big\{$$

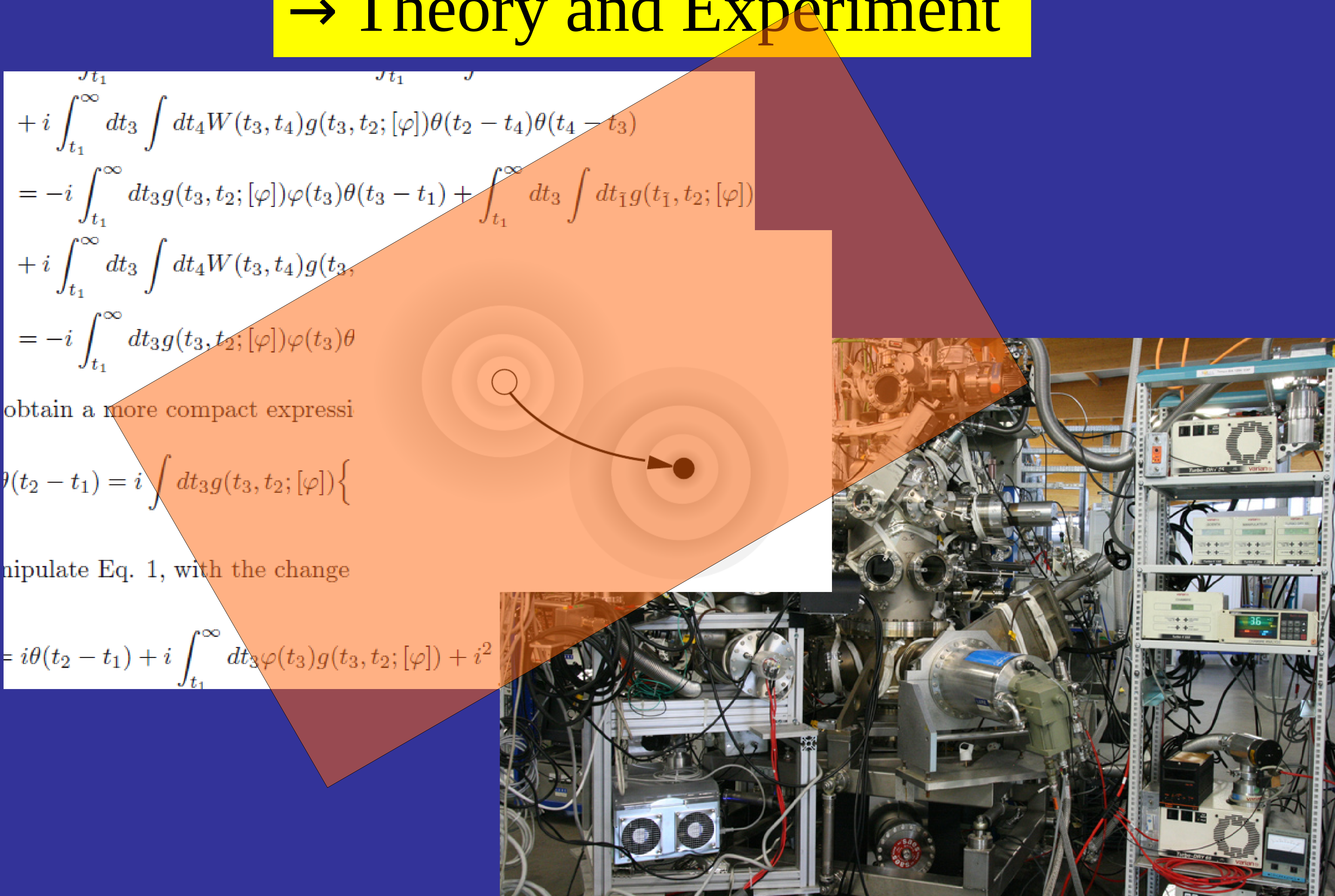
nipulate Eq. 1, with the change

$$= i\theta(t_2 - t_1) + i \int_{t_1}^{\infty} dt_3 \varphi(t_3) g(t_3, t_2; [\varphi]) + i^2$$

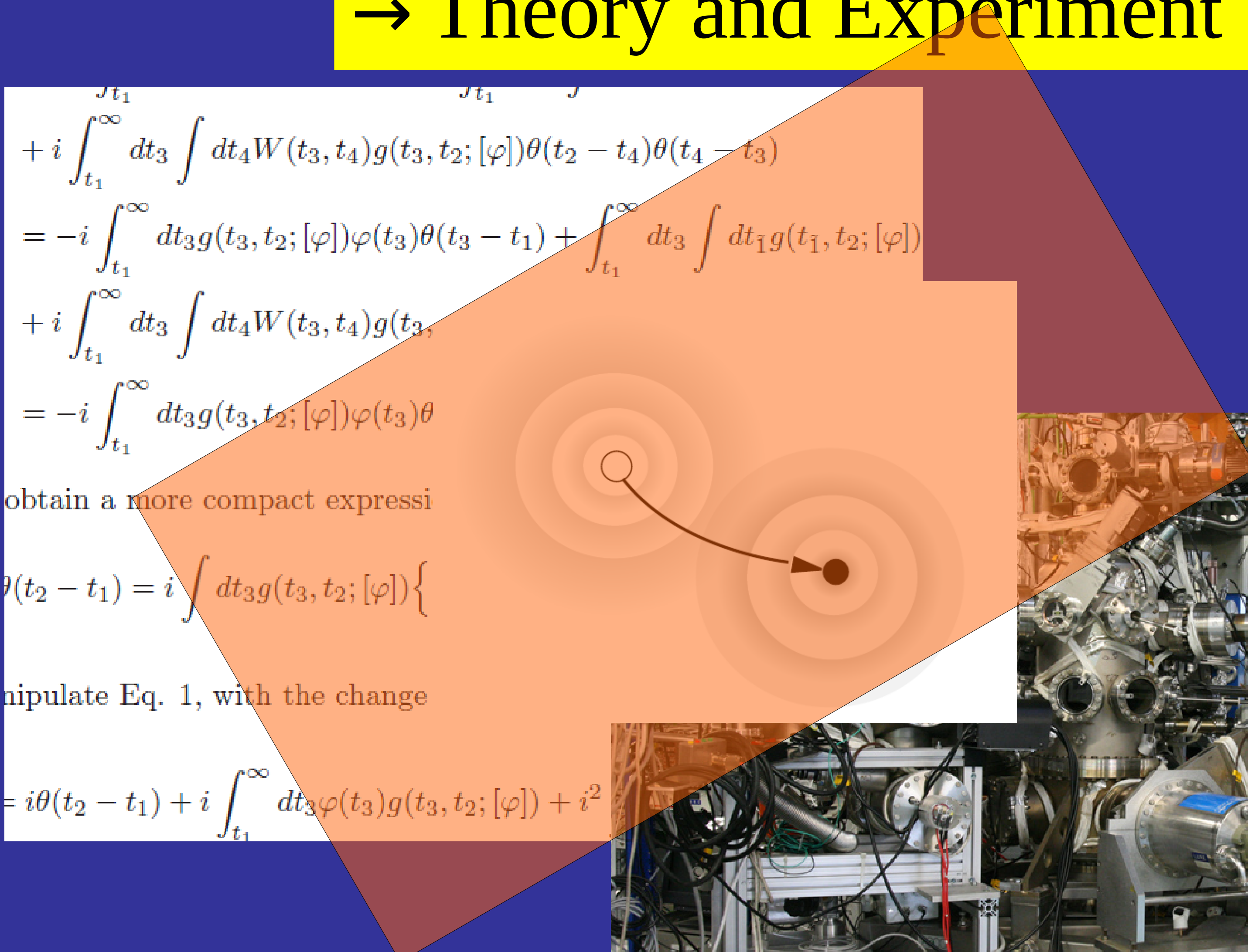


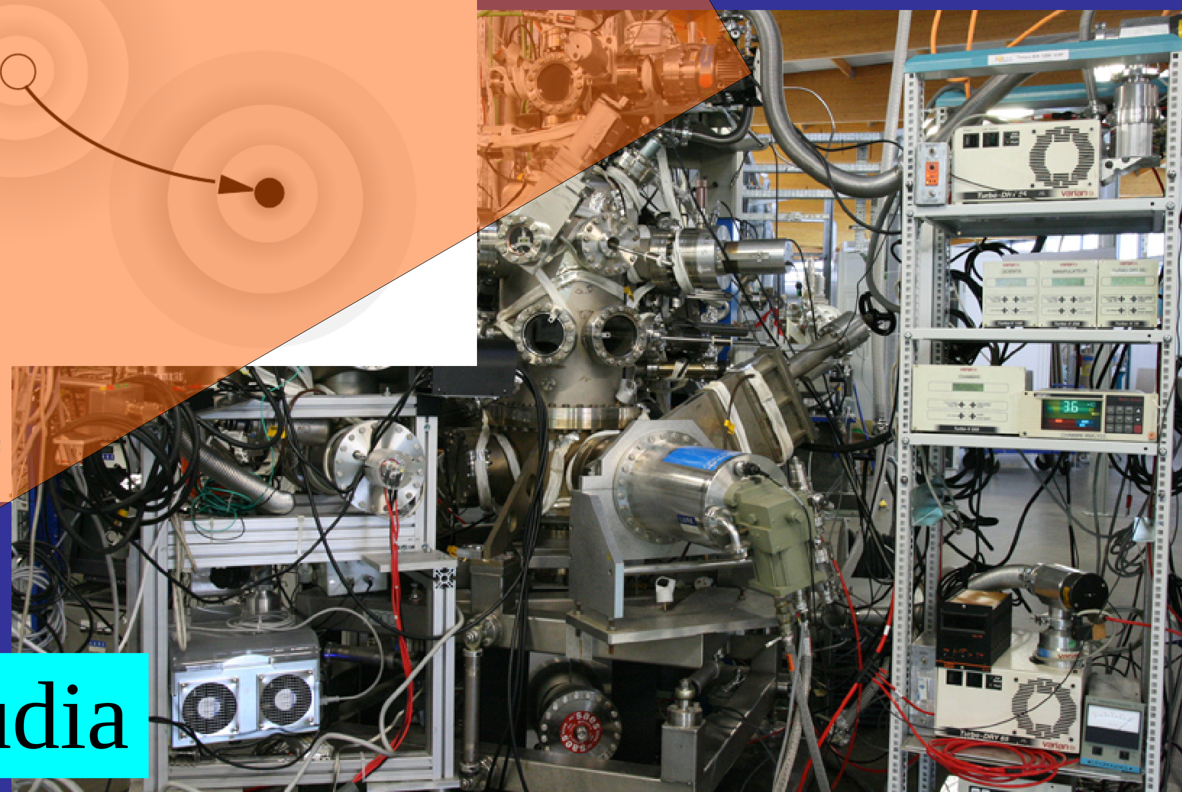


→ Theory and Experiment



→ Theory and Experiment





Matteo and Claudia

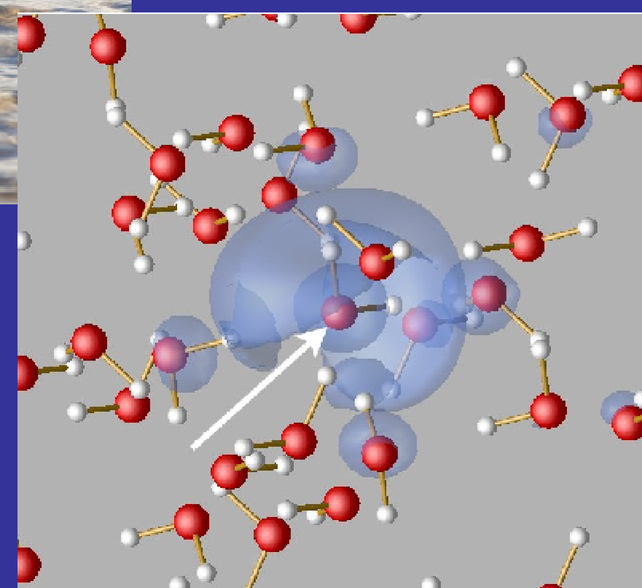
→ Model or ab initio?

→ Technical realization of the theory?

We are all theoreticians
→ models (predictive?)

Ab initio is:
→ not materials specific
→ ab initio code running (standard)
→ be predictive
→ face discrepancies
→ get new physics out of discrepancies

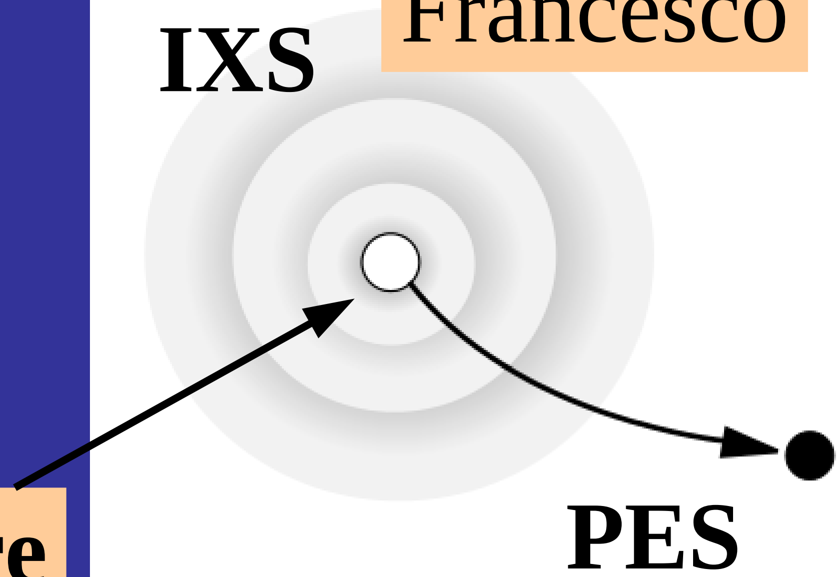

shutterstock



→ Experiment and Experiment

Our theory is:
decomposition into different experiments!

Francesco



Core

Matteo and Claudia

John and Keith

What is this ?
An introduction to Theoretical Spectroscopy

→ Theoretical Spectroscopy, the aim

→ Calculate only what you want,
…...................so that you can understand!

→ Density Functional versus Propagators

→ Theory and Experiment

→ Model or ab initio?

→ Experiment and Experiment

10h30-11h00 Coffee break

11h00-11h40 Giorgia Fugallo - Basics of density-functional theory

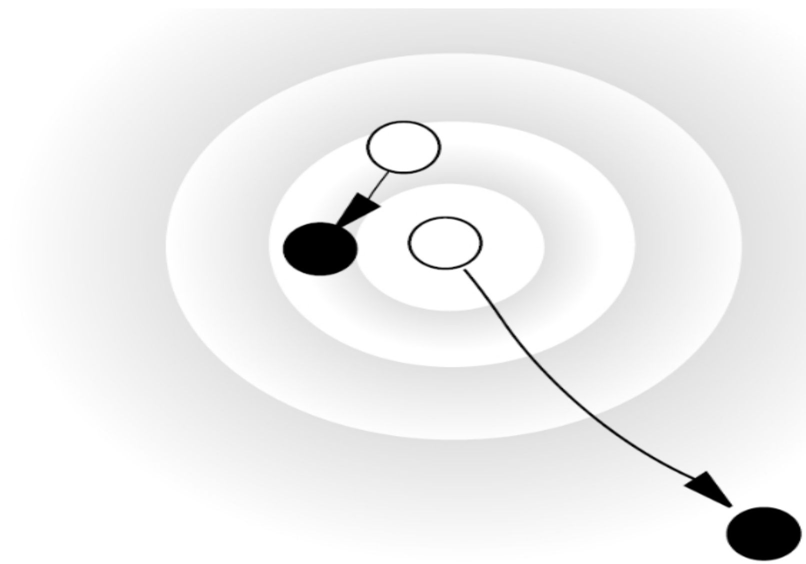
11h40-12h30 Matteo Gatti & Claudia Roedl - Photoelectron spectroscopy

12h30-13h30 Lunch break

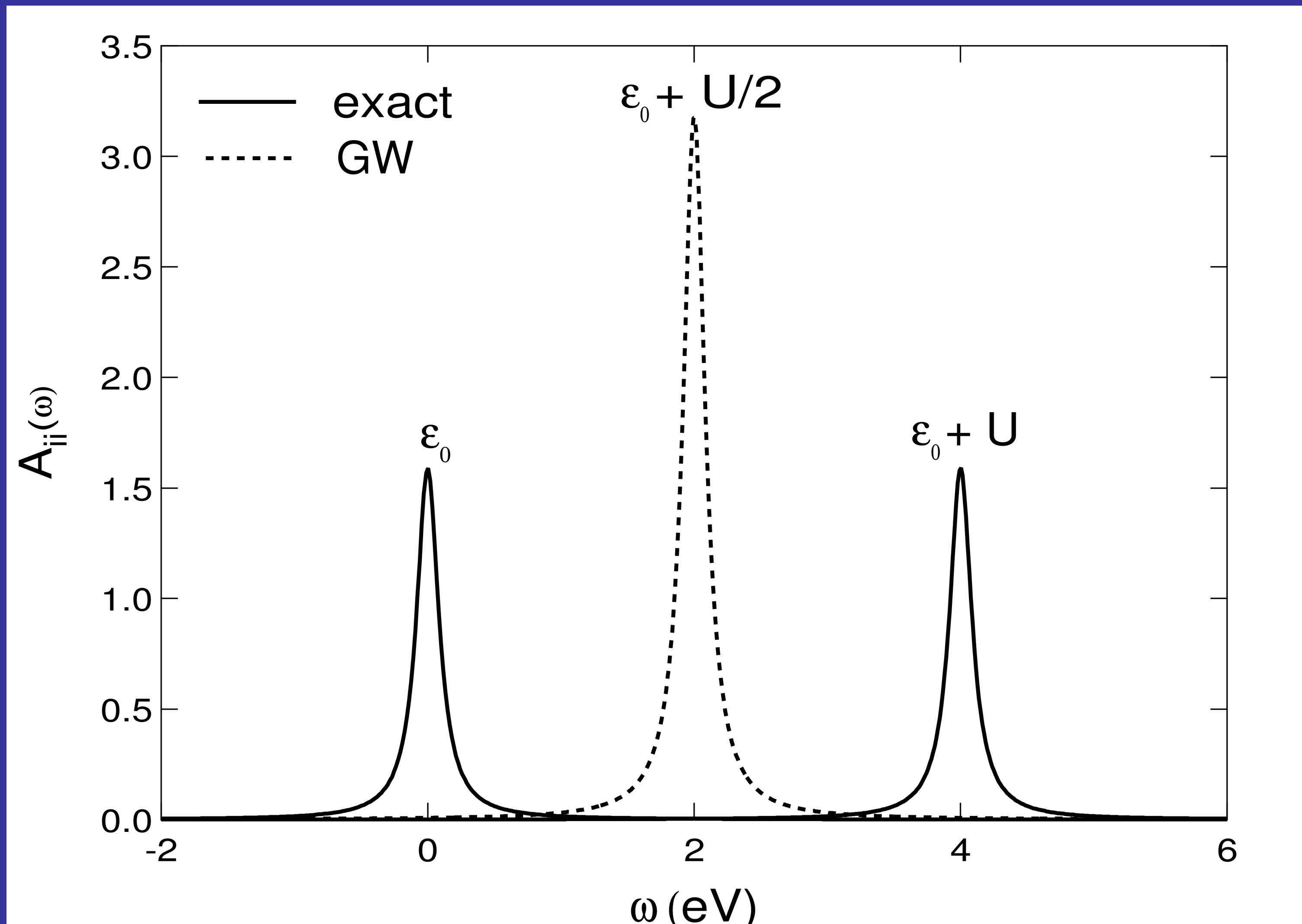
13h30-14h20 Francesco Sottile - Absorption and energy-loss spectroscopy

14h20-15h10 John Rehr - Core-level spectroscopies

15h10-16h00 Poster session

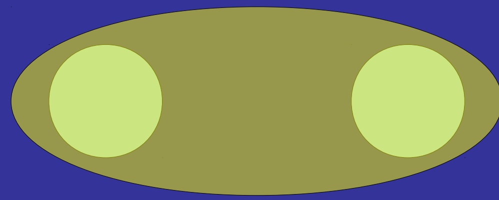


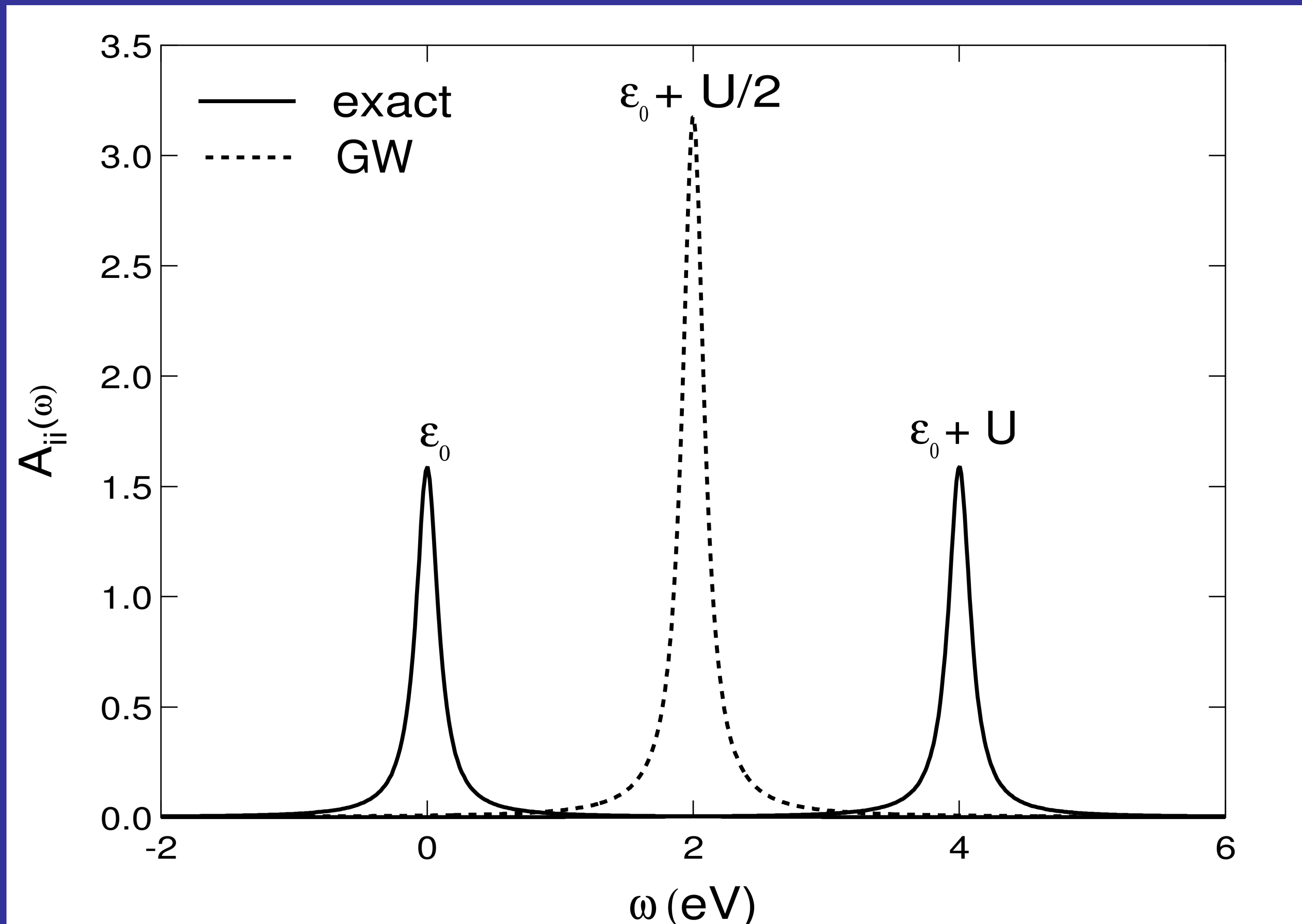
H_2^+



exact
GW
$\varepsilon_0 + U/2$
ε_0
$\varepsilon_0 + U$
$A_{ii}(\omega)$
ω (eV)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-2
0
2
4
6

H_2^+





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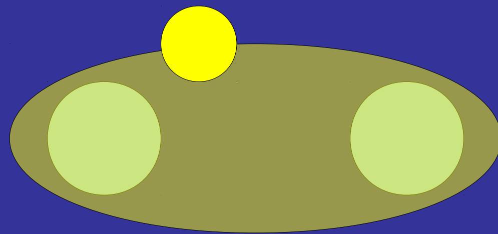

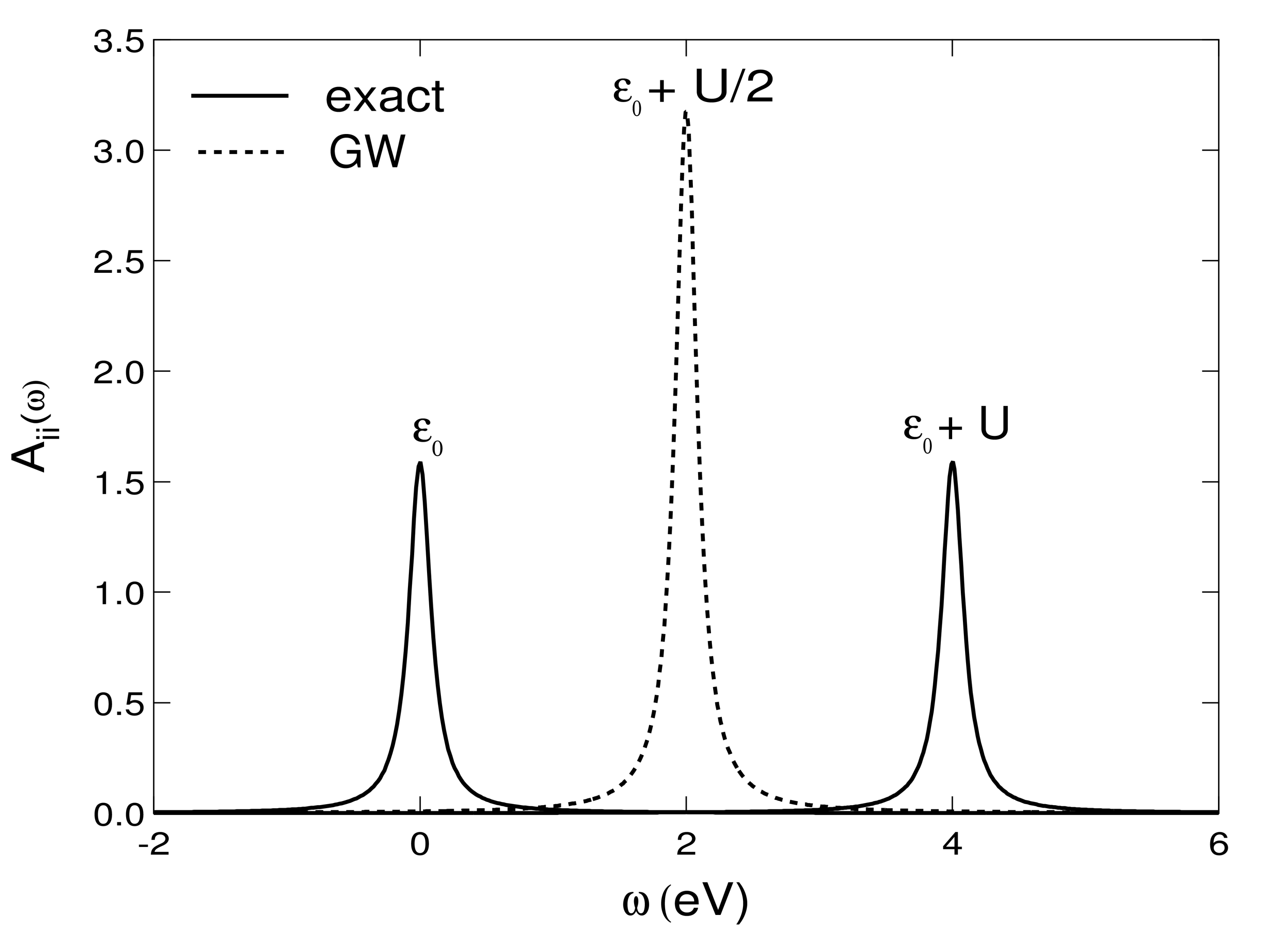

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Many-body perturbation theory: GW

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V_H \mathcal{G} + \mathcal{G}_0 \varphi \mathcal{G} + i\mathcal{G}_0 v_c \frac{\delta \mathcal{G}}{\delta \varphi}.$$

L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics*

1. Linearization $V_H[\varphi] = V_H^0 + v_c \chi \varphi$ .....

$$\mathcal{G}(t_1 t_2) = \mathcal{G}_H(t_1 t_2) + \mathcal{G}_H(t_1 t_3)\bar{\varphi}(t_3)\mathcal{G}(t_3 t_2) + i\mathcal{G}_H(t_1 t_3)\mathcal{W}(t_3 t_4)\frac{\delta \mathcal{G}(t_3 t_2)}{\delta \bar{\varphi}(t_4)},$$

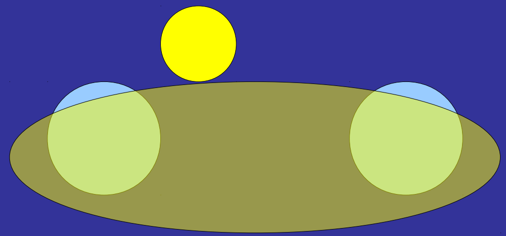
$\sim \mathcal{G}\mathcal{G}$

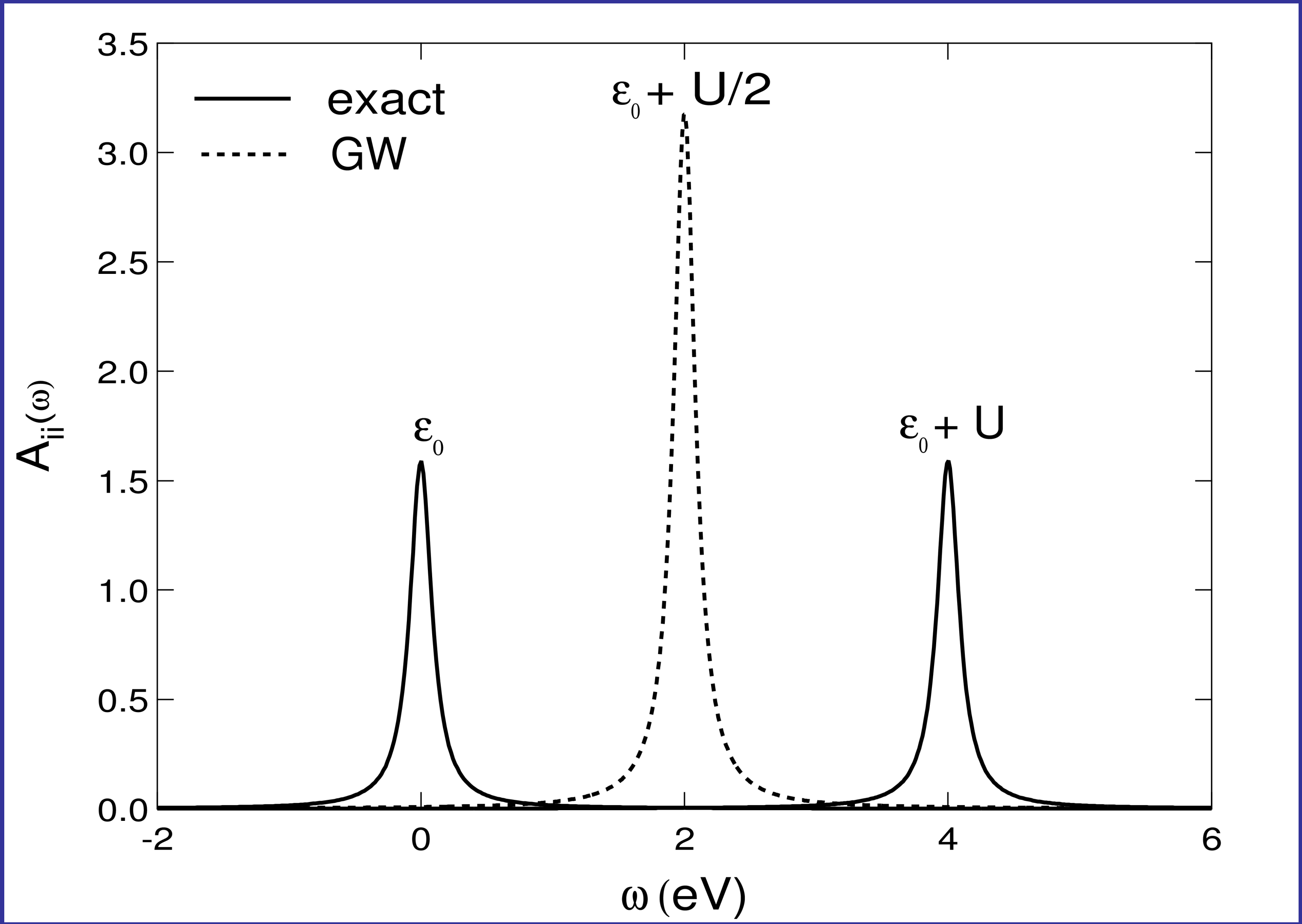
Lani et al., New J. Phys. 14, 013056 (2012)

$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G}$

$\rightarrow \Sigma \sim i\mathcal{W}\mathcal{G}$ “GW”

H_2^+





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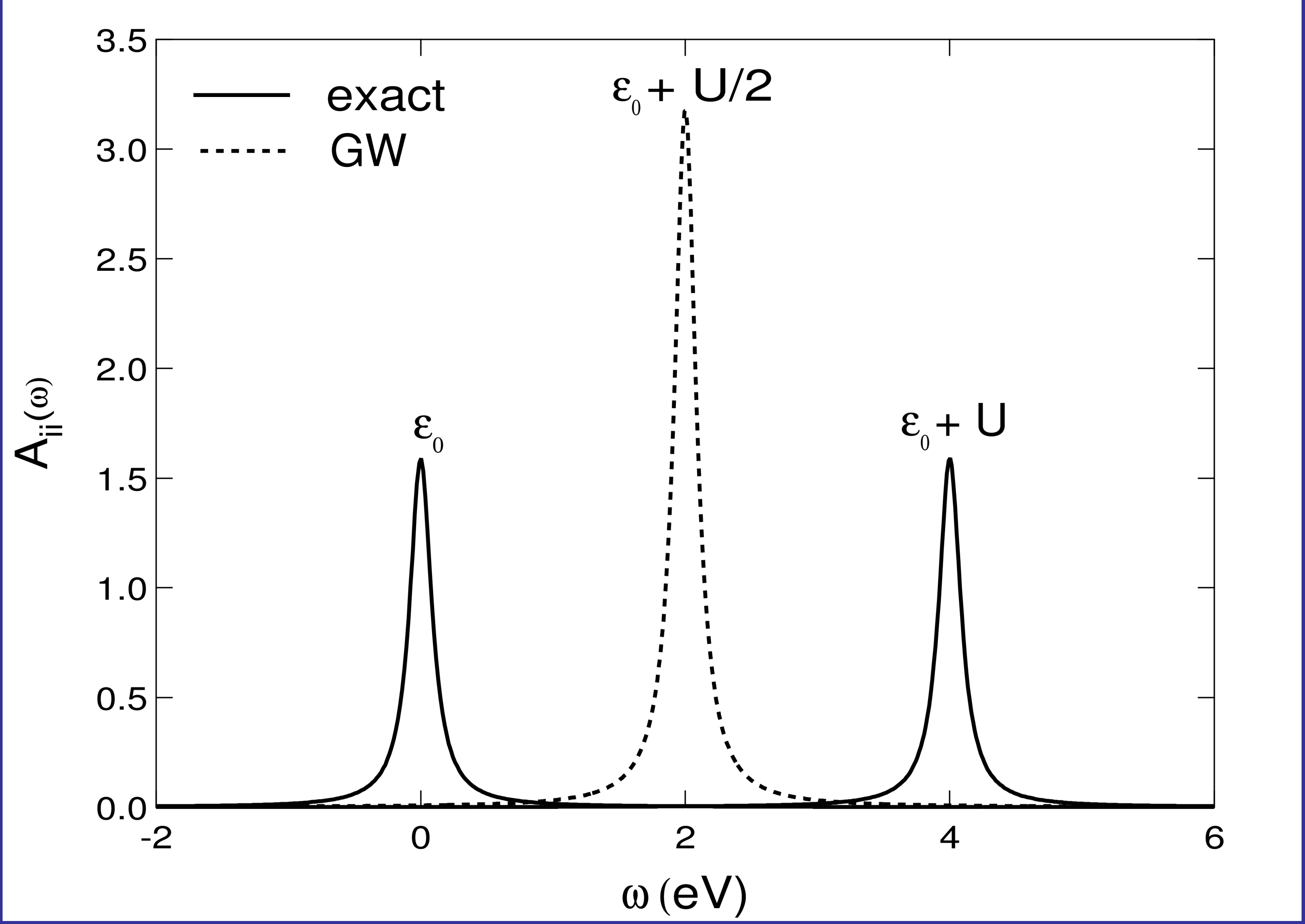

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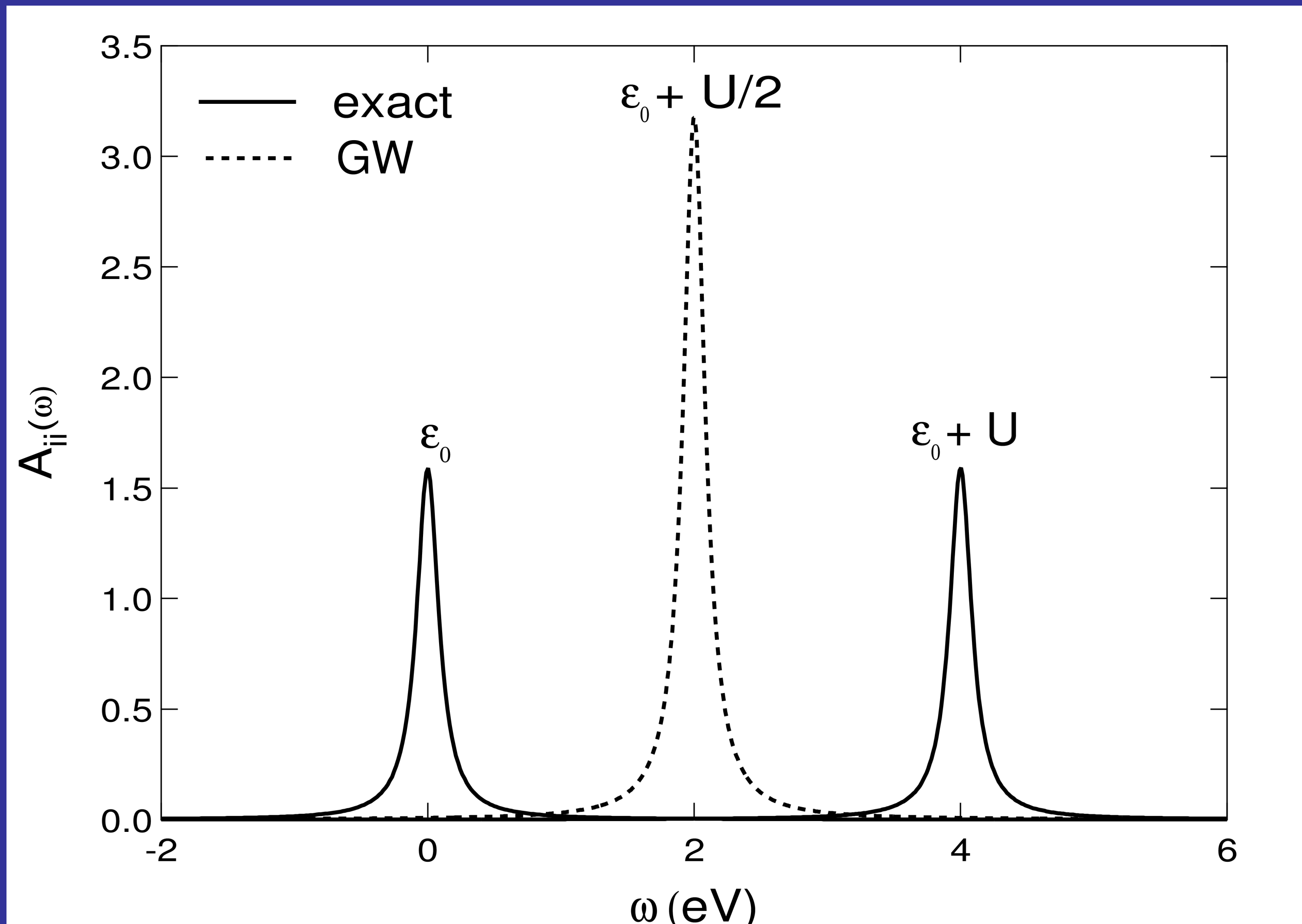

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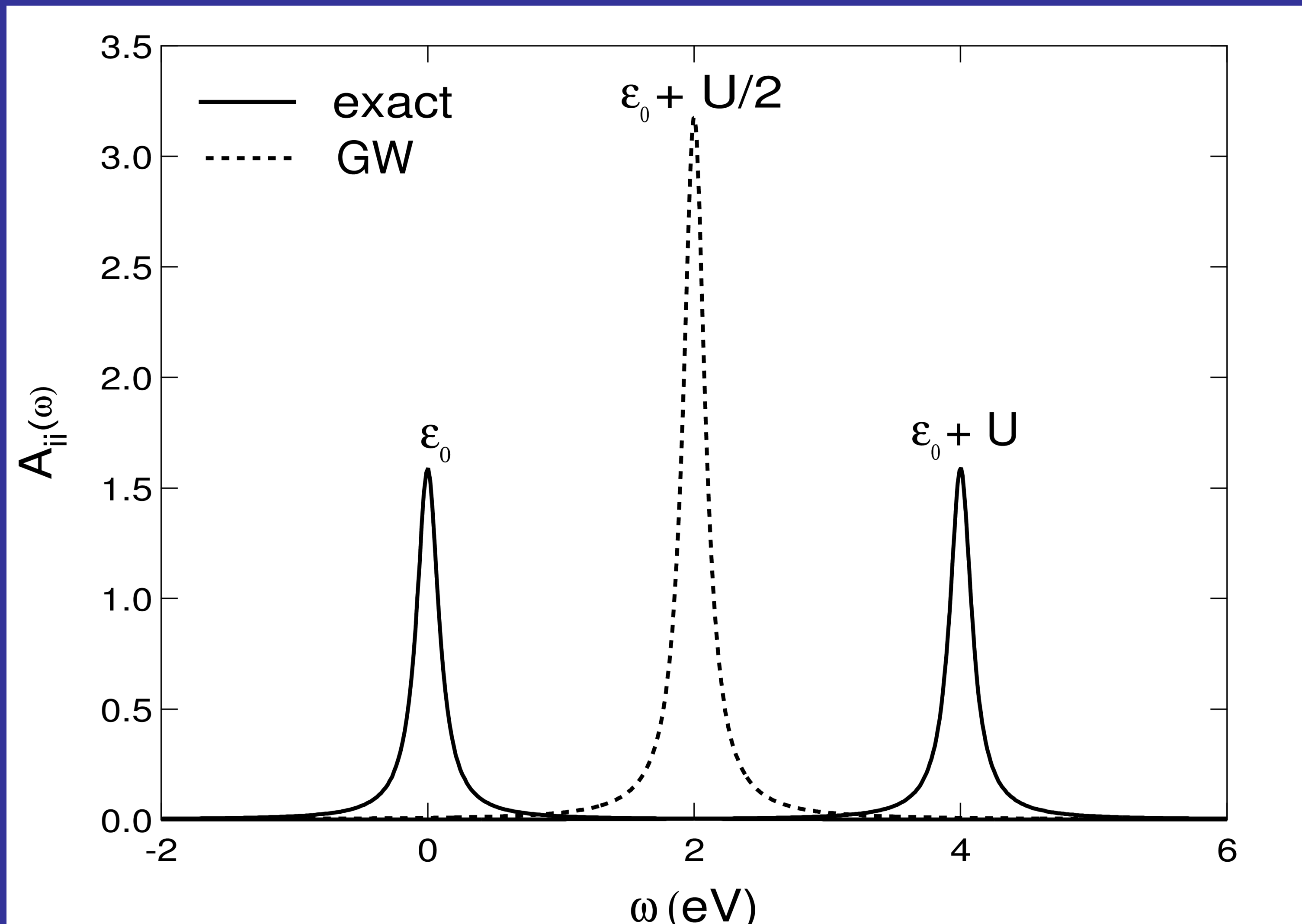

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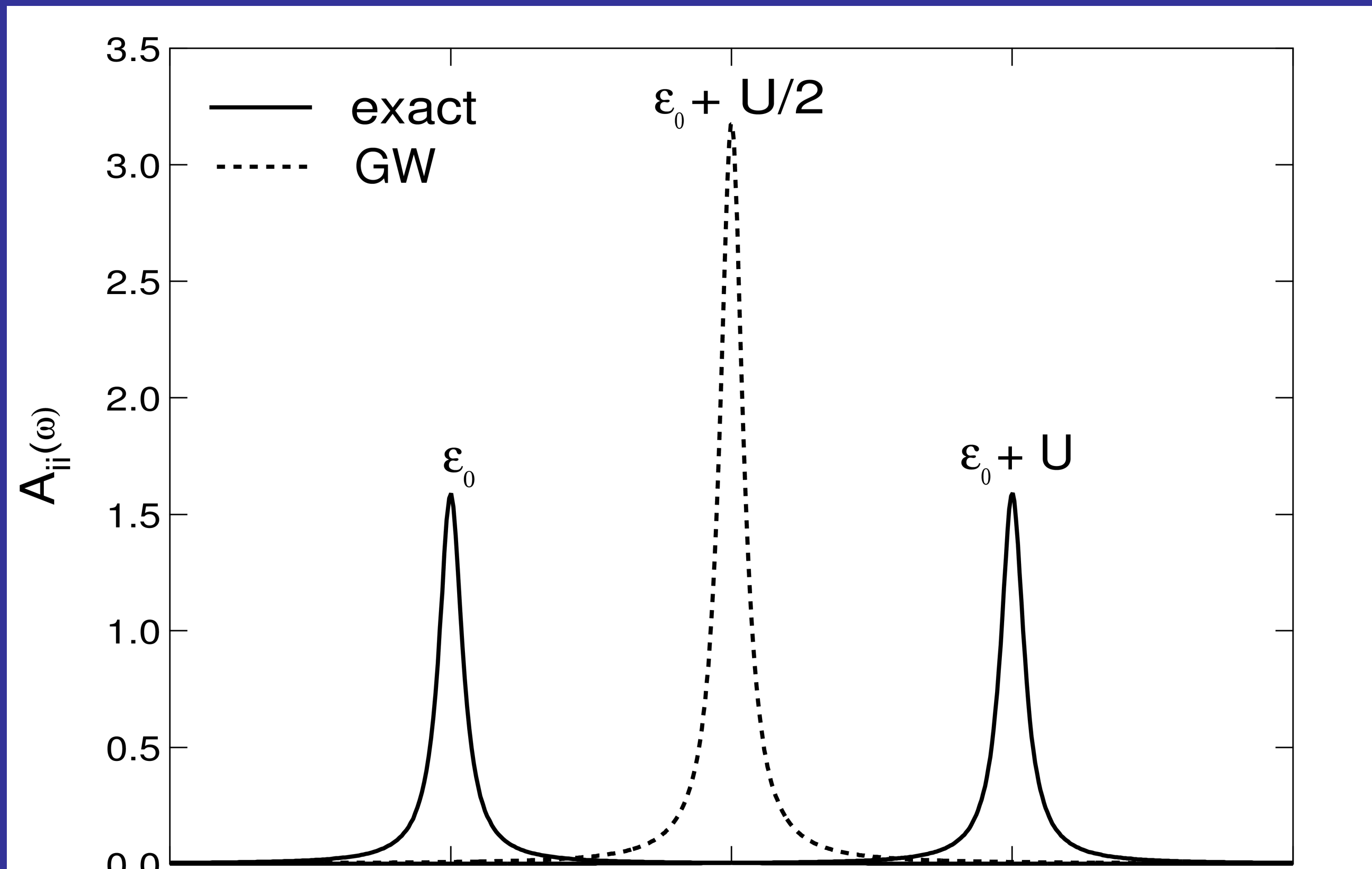

Correlation beyond mean field response

Many-body perturbation theory

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V_H \mathcal{G} + \mathcal{G}_0 \varphi \mathcal{G} + i\mathcal{G}_0 v_c \; L$$

L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics*

$\mathcal{G}(1,2) = -i \langle T[\psi(1)\psi^\dagger(2)] \rangle$

$1=(r_1,\sigma_1,t_1)$

Many-body perturbation theory

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V_H \mathcal{G} + \mathcal{G}_0 \varphi \mathcal{G} + i\mathcal{G}_0 v_c \frac{\delta \mathcal{G}}{\delta \varphi}.$$

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L. P. Kadanoff and G. Baym, *Quantum Stati*

$\sim \mathcal{G}\mathcal{G} \rightarrow$ HF

Dyson equation: $\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G}$

$$\Sigma \sim i v_c \mathcal{G}$$

Many-body perturbation theory: GW

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V_H \mathcal{G} + \mathcal{G}_0 \varphi \mathcal{G} + i\mathcal{G}_0 v_c \frac{\delta \mathcal{G}}{\delta \varphi}.$$

L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics*

1. Linearization $V_H[\varphi] = V_H^0 + v_c \chi \varphi$ .....

$$\begin{aligned} \mathcal{G}(t_1 t_2) &= \mathcal{G}_H(t_1 t_2) + \mathcal{G}_H(t_1 t_3)\bar{\varphi}(t_3)\mathcal{G}(t_3 t_2) \\ &+ i\mathcal{G}_H(t_1 t_3)\mathcal{W}(t_3 t_4)\frac{\delta \mathcal{G}(t_3 t_2)}{\delta \bar{\varphi}(t_4)}, \end{aligned}$$

.......leads to screening: $\mathcal{W} = \varepsilon^{-1} v_c$

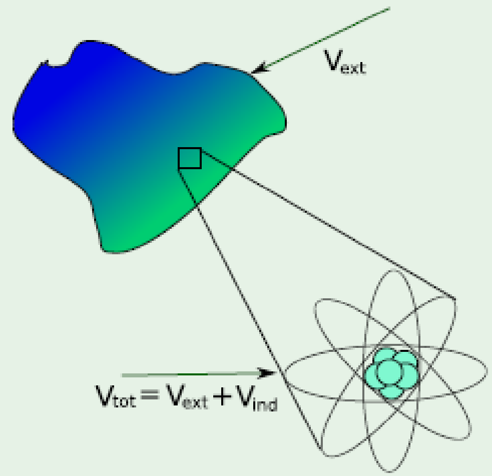
Definition of polarizability

$$\begin{aligned}
\text{not polarizable} \quad &\Rightarrow \quad V_{tot} = V_{ext} \quad \Rightarrow \quad \varepsilon^{-1} = 1 \\
\text{polarizable} \quad &\Rightarrow \quad V_{tot} \neq V_{ext} \quad \Rightarrow \quad \varepsilon^{-1} \neq 1 \\
& \qquad\qquad\qquad\qquad\qquad\quad \varepsilon^{-1} = 1 + v\chi
\end{aligned}$$

χ is the polarizability of the system

Linear Response Approach

System submitted to an external perturbation



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

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

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

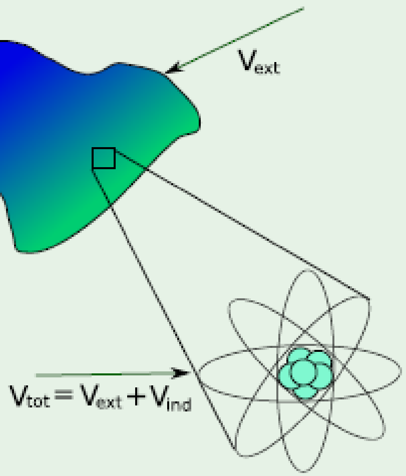
Dielectric function ε

EELS ↔ ε ↔ **R index**

Abs ↔ ε ↔ **X-ray**

Linear Response Approach

System submitted to an external perturbation



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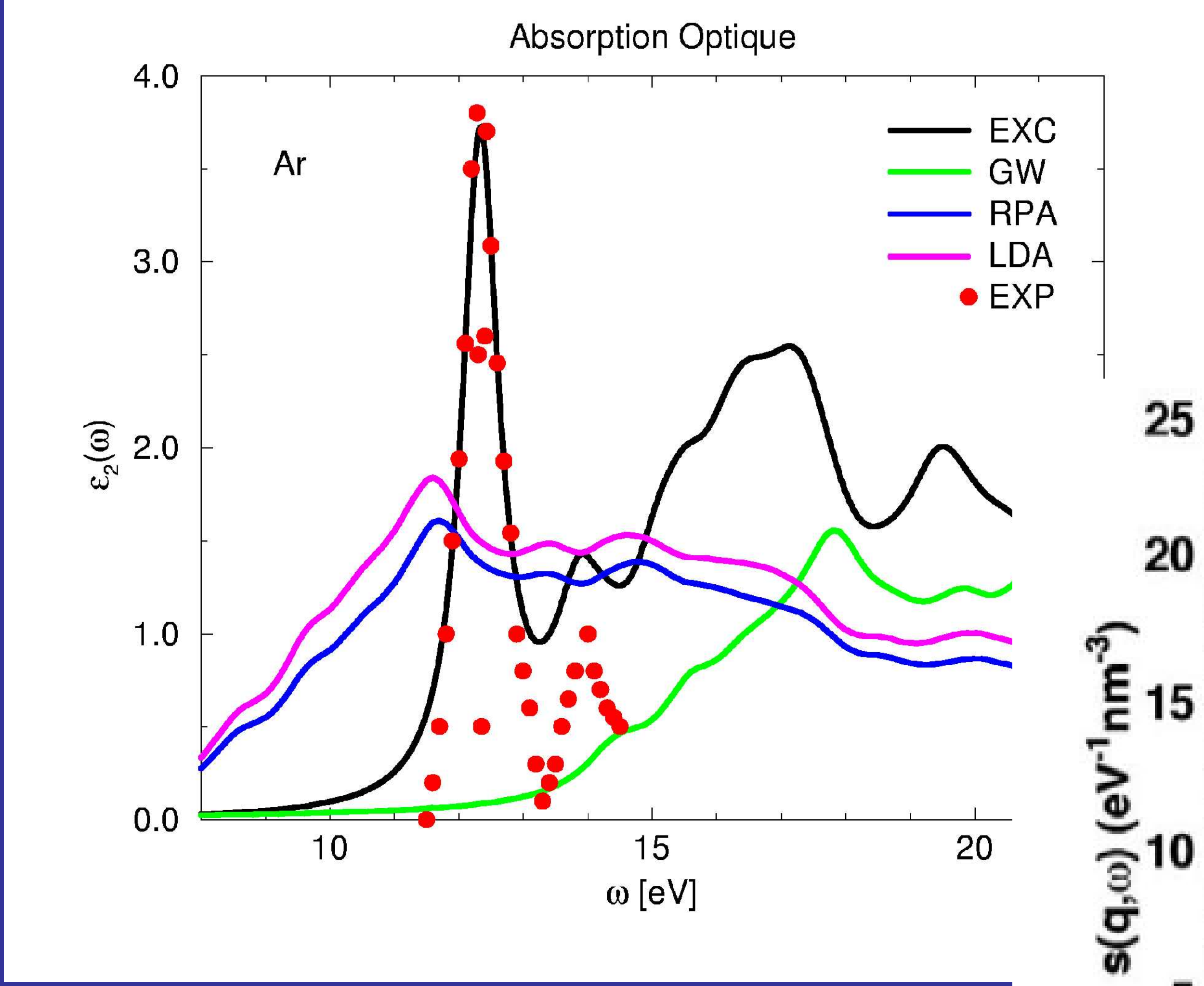
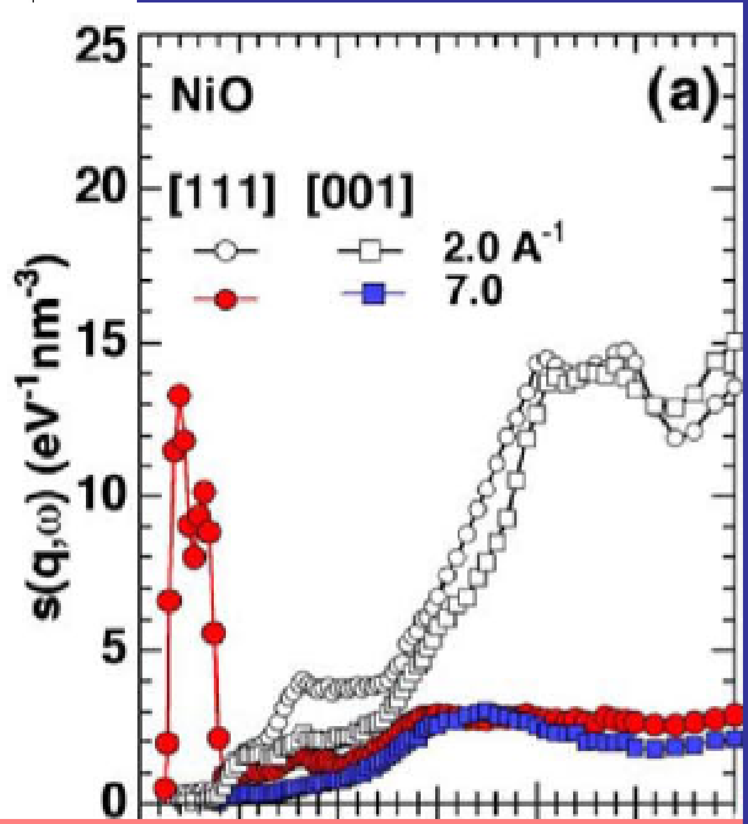
Francesco



V. Olevano et al.



Larson et al., PRL 99, 026401 (2007)

Exciton: Lee, Hsueh, Ku, PRB 82, 081106 (2010)