A direct approach to the calculation of many-body Green' s functions

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A direct approach
to the calculation of many-body Green’ s functions

→ The Framework; MBPT

→ A direct approach

→ Power of the 1-point model: structure of MBPT

→ W and satellites, a life beyond the GWA

→ Conclusions

Calculating the one-body G

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

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

Equation of motion (EOM)

$$G(1,2) = G_0(1,2) - i \int d3d4\, G_0(1,3) v(4,3^+) \underbrace{G_2(3,4;2,4^+)}_{\text{Unknown}}$$

Closing the hierarchy of G_n

- $G_2 \leftrightarrow G_3 \cdots \leftrightarrow \cdots G_n$
- $G(1,2) \rightarrow G(1,2;[\varphi])$, φ time-dependent external potential
- Schwinger's relation (exact): $G_2 \leftrightarrow \dfrac{\delta G([\varphi])}{\delta \varphi}$

Set of *coupled non-linear* functional **differential equations**

$$G(1,2;[\varphi]) = G_0(1,2) + \int d3\, G_0(1,3) V_H(3;[\varphi]) G(3,2;[\varphi]) + \int d3\, G_0(1,3)\varphi(3) G(3,2;[\varphi]) + i \int d4d3\, G_0(1,3) v(3^+,4) \underbrace{\frac{\delta G(3,2;[\varphi])}{\delta \varphi(4)}}_{\text{As mind-blogging as } G_2}$$

Many-body perturbation theory

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

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

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

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

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

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

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

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

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W

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

Many-body perturbation theory: GW

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

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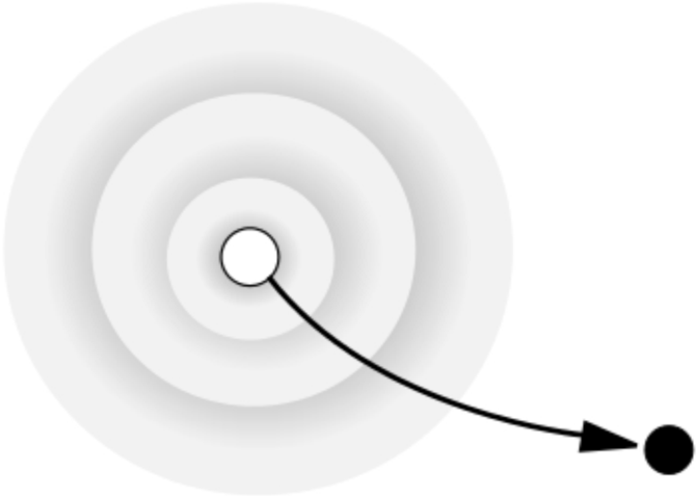
$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G}$

W

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

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

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



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L. Hedin (1965)

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

A direct approach to the calculation of many-body Green' s functions : Differential Equation

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

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(Linearized)

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Molinari L G 2005 *Phys. Rev.* B **71** 113102

Molinari L G and Manini N 2006 *Eur. Phys. J.* B **51** 331

Pavlyukh Y and Hübner W 2007 *J. Math. Phys.* **48** 052109

$$y(z) = y_0^0 - v y_0^0 y^2(z) + y_0^0 z y(z) + \lambda v y_0^0 y'(z) \qquad \lambda = 1/2$$

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

Berger et al., New J. Phys. 16, 113025 (2014)

Stan et al., http://arxiv.org/abs/1503.07742

(Non-linearized)

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A. Berger

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→ test of GW and beyond

→ multiple solutions of Dyson equations, and how to do ok

→ questionning the LW functional

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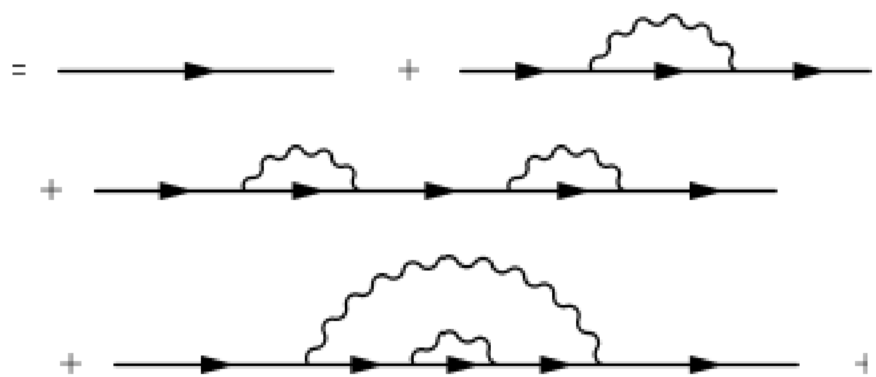
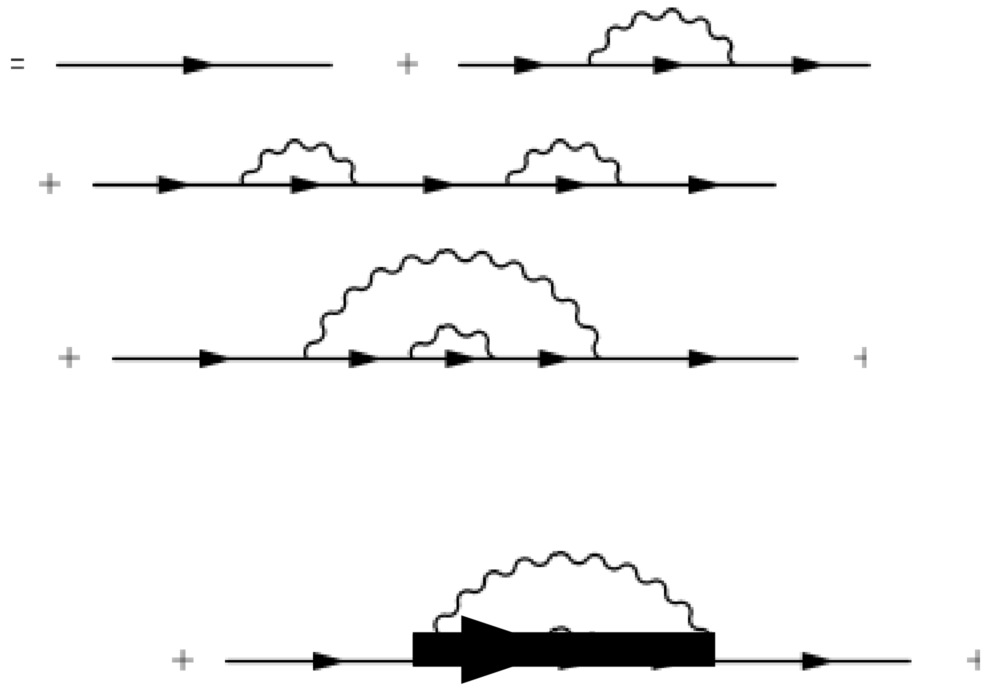




Luttinger Ward

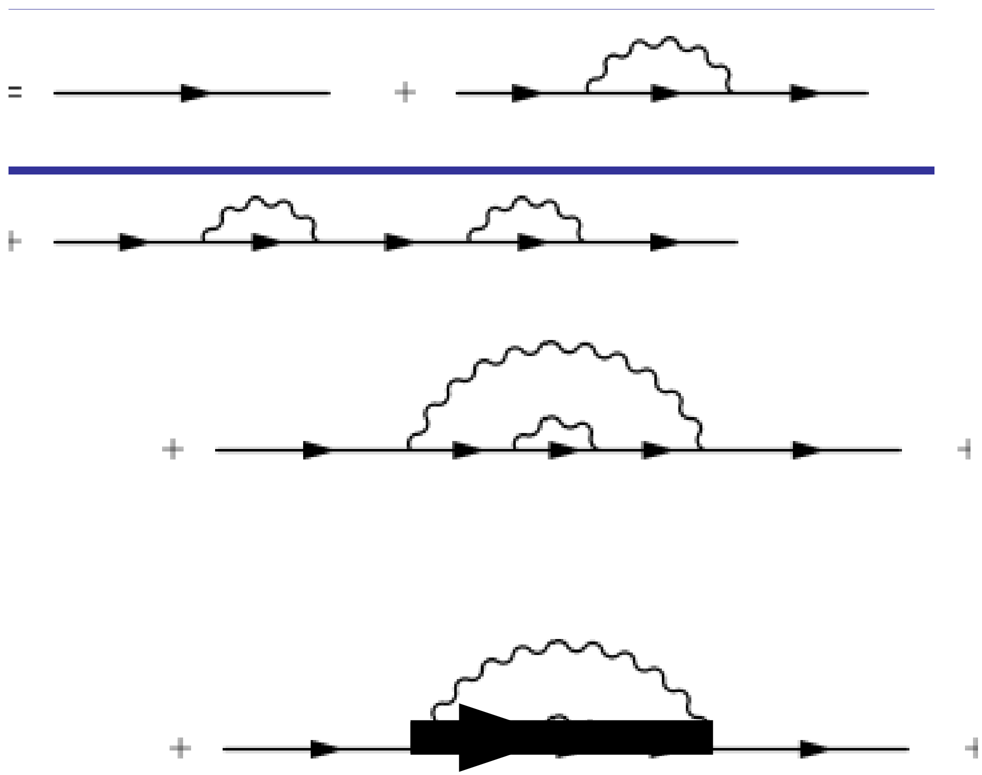
Strange observations in models.......
...suspicions about LW functional.....

Schaefer et al., PRL 110, 246405 (2013)

“Divergent Precursors of the Mott-Hubbard Transition at the Two-Particle Level”

Kozik et al., PRL 114, 156402 (2105)

“Nonexistence of the Luttinger-Ward Functional and Misleading Convergence of Skeleton Diagrammatic Series for Hubbard-Like Models”



$$\tilde{\Sigma}[G_0,v] \rightarrow \tilde{\Sigma}[G_0[G],v] = \Sigma[G,v]$$

$G_0 \rightarrow G$ map $G_0 \leftarrow G$

M. Potthoff, Condensed Matter Physics 9, 557 (2006).

$y_0 \rightarrow y$ $G_0 \rightarrow G$ $\longrightarrow$ map $G_0 \leftarrow G$

$$y[y_0, u] = \frac{y_0}{1 + \frac{1}{2} u y_0^2} \quad \text{and} \quad \tilde{s}[y_0, u] = -\frac{1}{2} u y_0$$

Exact

$$y = y_0 + y_0 \, \tilde{s}[y_0, u] \, y \qquad y = y_0 + y_0 s[y, u] y$$

$$z_0 = y + \frac{1}{2} u y z_0^2$$

$$z_0^{\pm} = \frac{1}{uy}\left(1 \pm \sqrt{1 - 2uy^2}\right) \Rightarrow Z_0^{\pm} = \frac{2 + V \pm \sqrt{(2-V)^2}}{2V}$$

$$V = u y_0^2$$

$y_0 \to y$ $G_0 \to G$ $\longrightarrow$ map $G_0 \leftarrow G$

$$y[y_0, u] = \frac{y_0}{1 + \frac{1}{2} u y_0^2} \quad \text{and} \quad \tilde{s}[y_0, u] = -\frac{1}{2} u y_0$$

Exact

$$y = y_0 + y_0\, \tilde{s}[y_0, u]\, y \qquad y = y_0 + y_0\, s[y, u]\, y$$

$$z_0 = y + \frac{1}{2} u y z_0^2 \qquad y_0[y] = ?$$

$$z_0^{\pm} = \frac{1}{uy}\left(1 \pm \sqrt{1 - 2uy^2}\right) \Rightarrow Z_0^{\pm} = \frac{2 + V \pm \sqrt{(2 - V)^2}}{2V}$$

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With exact y yields $Z_0 = z_0 / y_0 = 1$???

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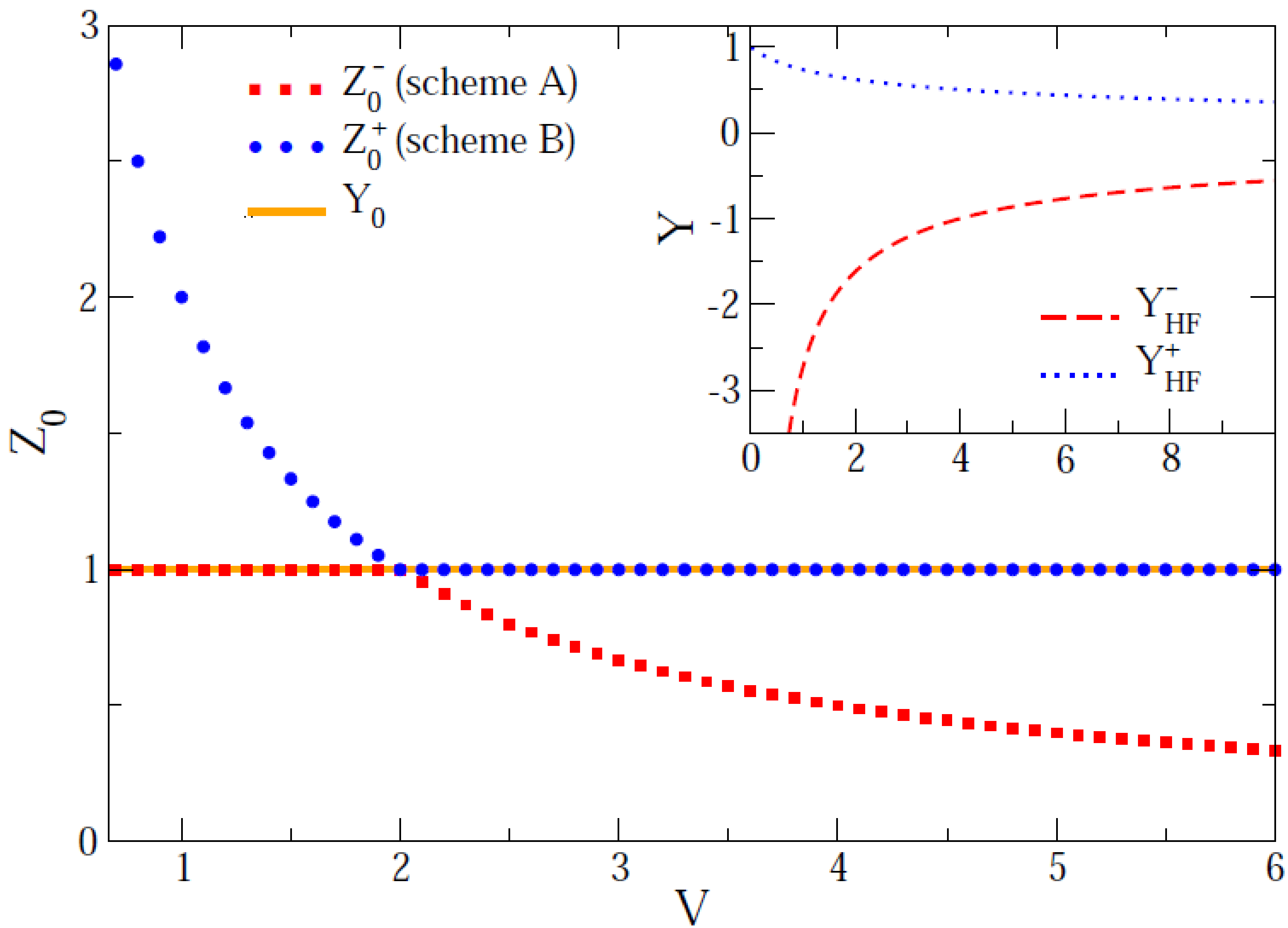
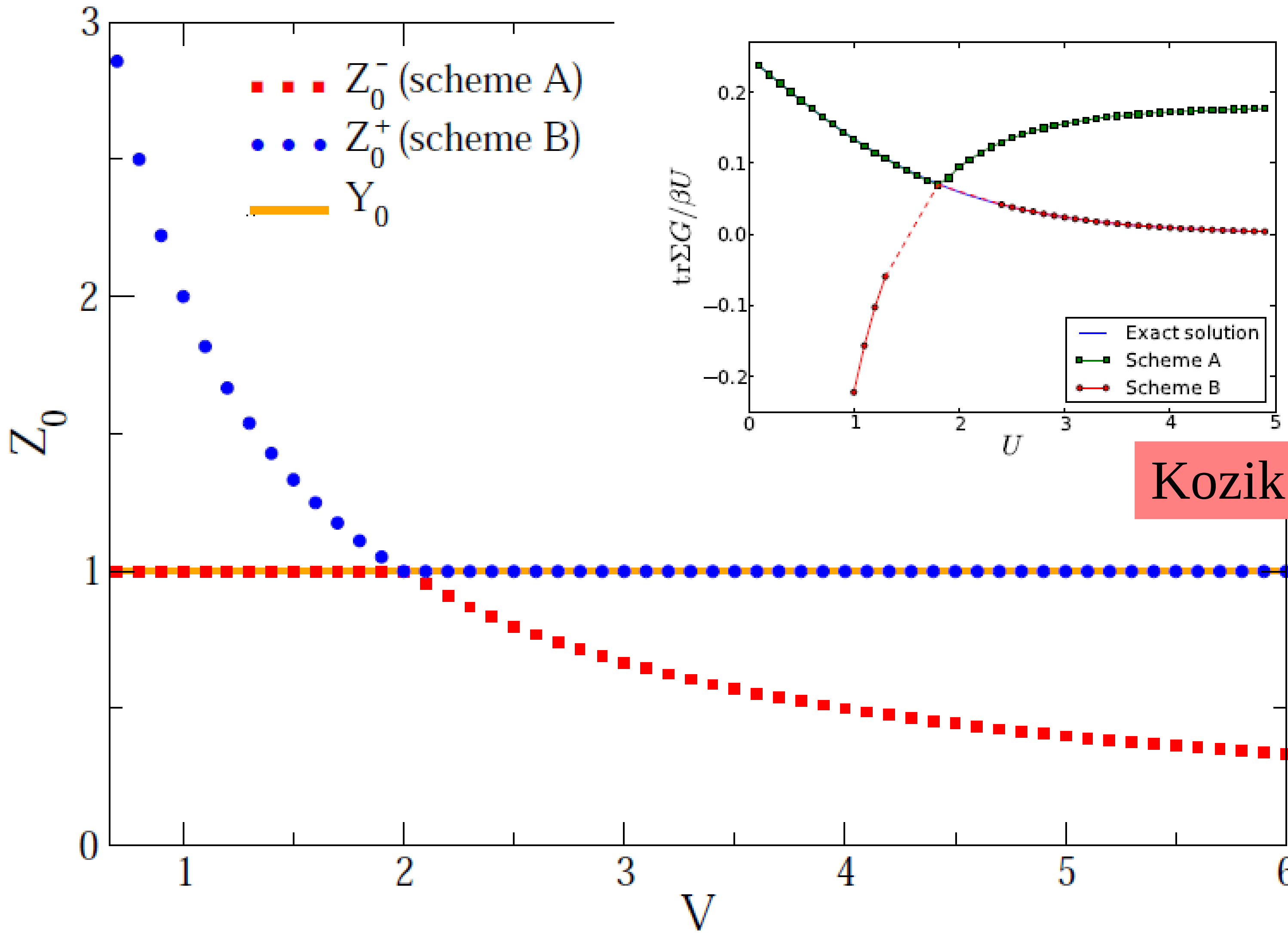
$$V = u y_0^2$$

Continuity requires change of sign!
Otherwise Z_0 is not Y_0!!!



3
2
1
0
1
2
3
4
5
6
V
Z0
Z0− (scheme A)
Z0+ (scheme B)
Y0
Y
1
0
-1
-2
-3
0
2
4
6
8
Y−HF
Y+HF



Kozik et al

Also observations of Schaefer et al. explained

Functional of the dressed G? (→ LW)

$$\tilde{s}[y_0,u] = -\frac{1}{2}uy_0 \qquad z_0^{\pm} = \frac{1}{uy}\left(1 \pm \sqrt{1-2uy^2}\right)$$

exact

$$s^{\pm}[y,u] = -\frac{1}{2y}\left(1 \pm \sqrt{1-2uy^2}\right)$$

2 branches!

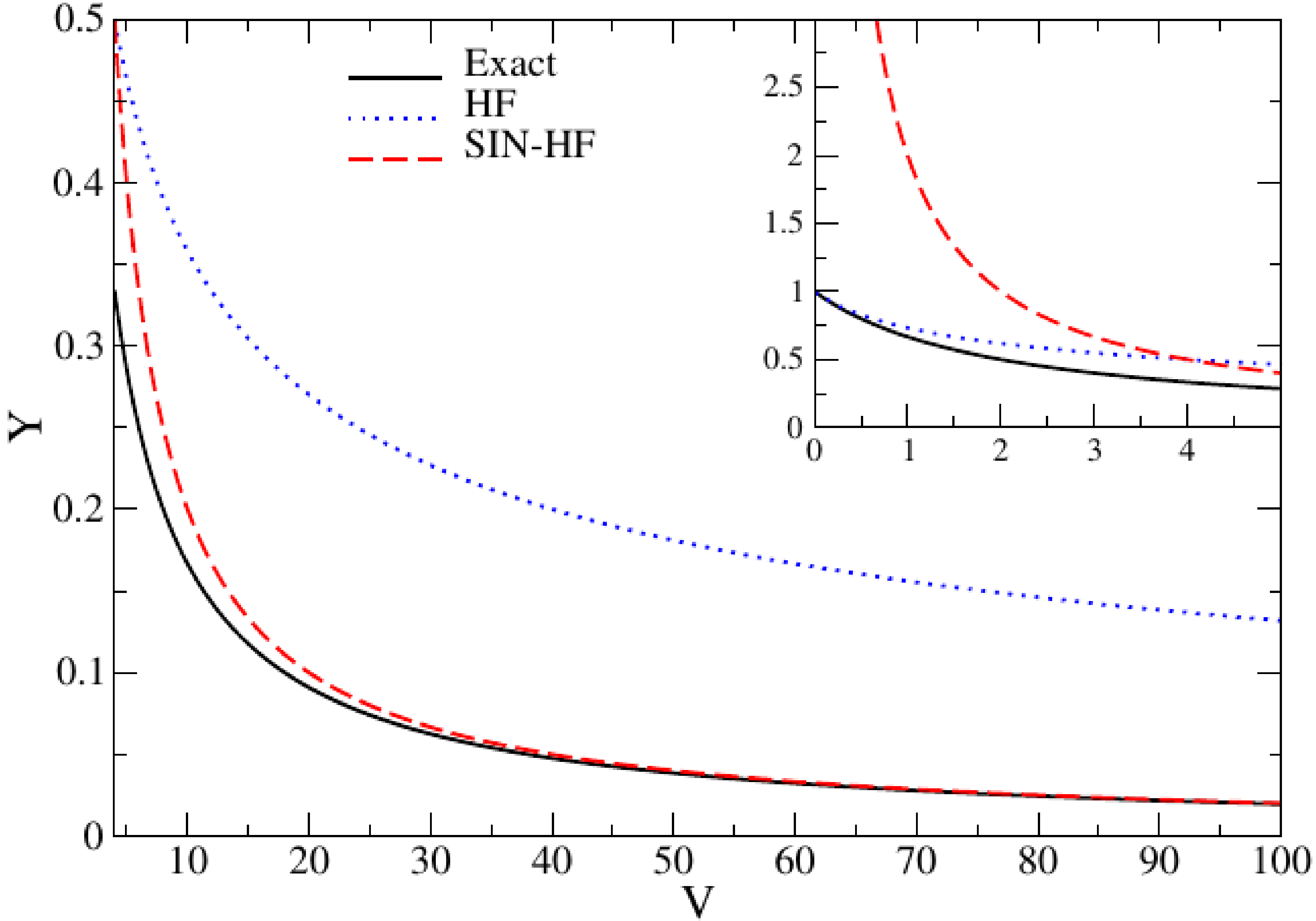
$$= -\frac{1}{2y} \mp \frac{1}{2y} \pm \frac{1}{2}u\left[y + \frac{uy^3}{2} + \frac{u^2y^5}{2} + \dots\right]$$

Change functional at V=2!!!

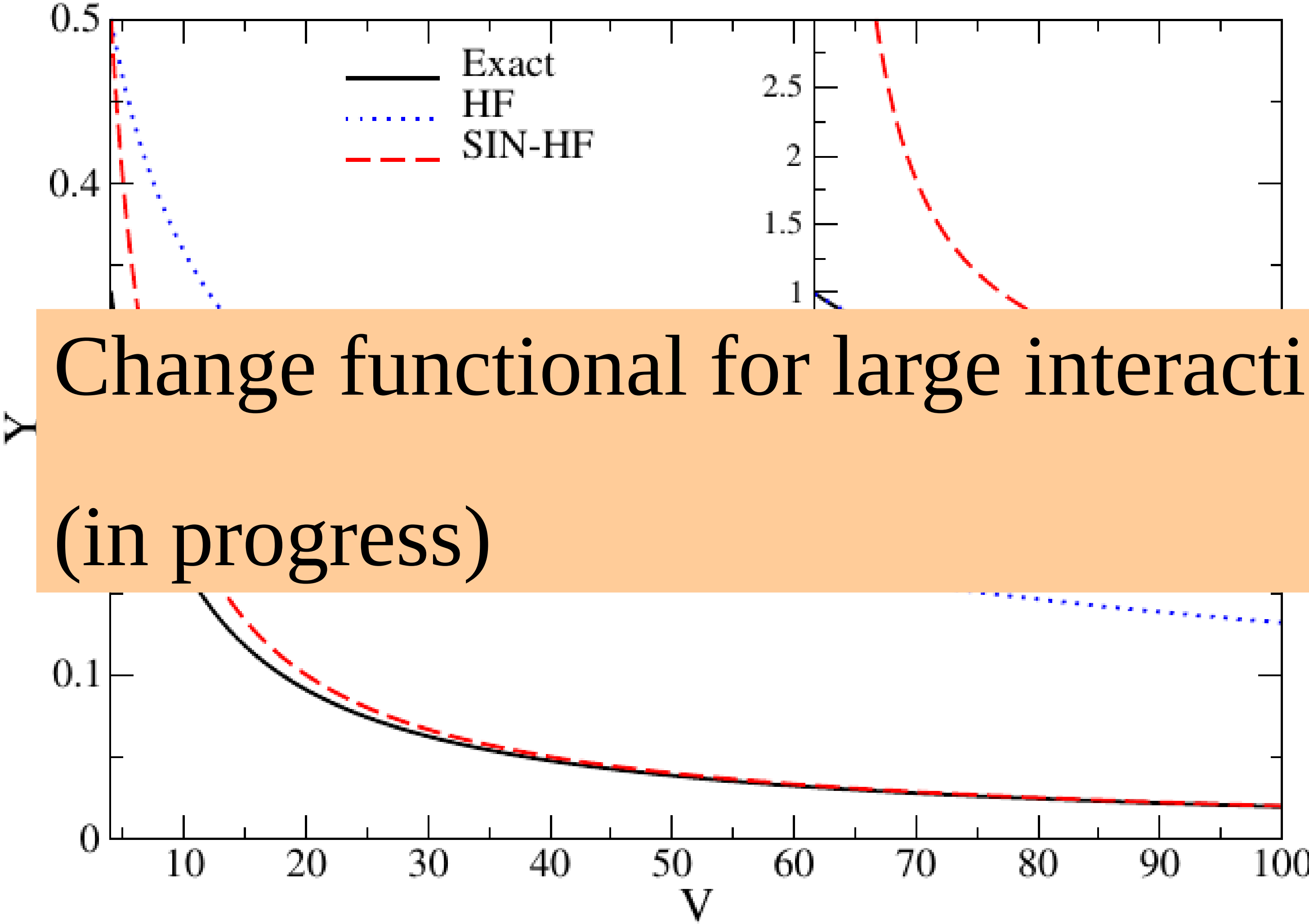
$$0 \lesssim 2uy^2 \leq 1$$

Perturbation expansion always possible!

$$s^{HF} = -\frac{1}{2}uy \qquad s^{\mathrm{SIN-HF}} = -\frac{1}{y} - s^{\mathrm{HF}}$$



Stan, Romaniello, Rigamonti, Reining, Berger,
http://arxiv.org/abs/1503.07742

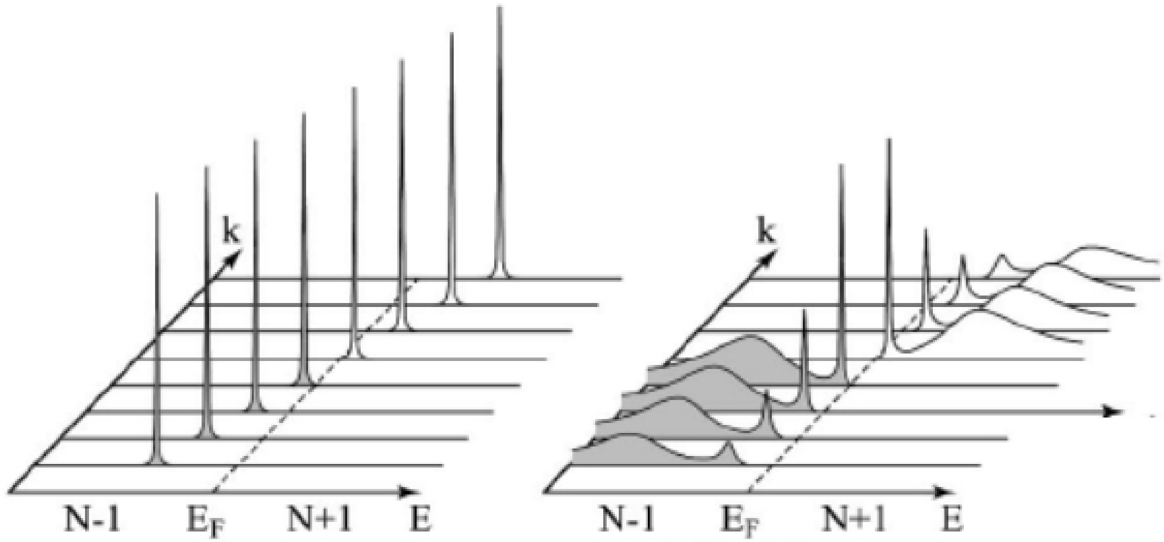


Change functional for large interaction

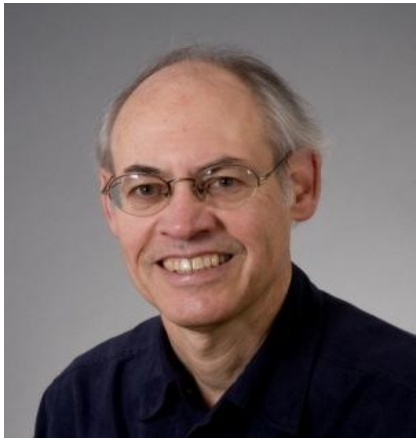
(in progress)

Stan, Romaniello, Rigamonti, Reining, Berger,
http://arxiv.org/abs/1503.07742

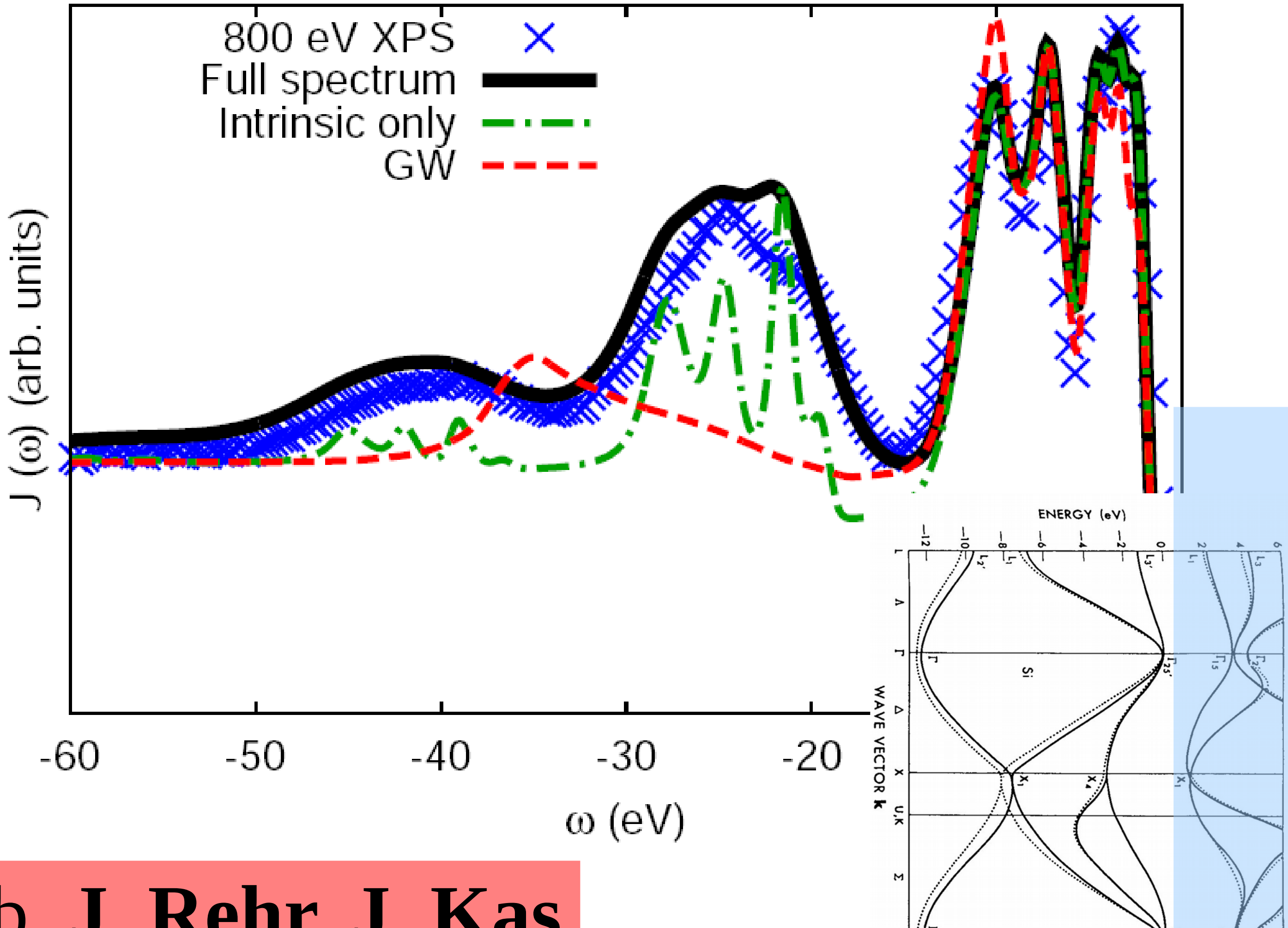
Real Spectroscopy?



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



→ W and satellites, a life beyond the GWA

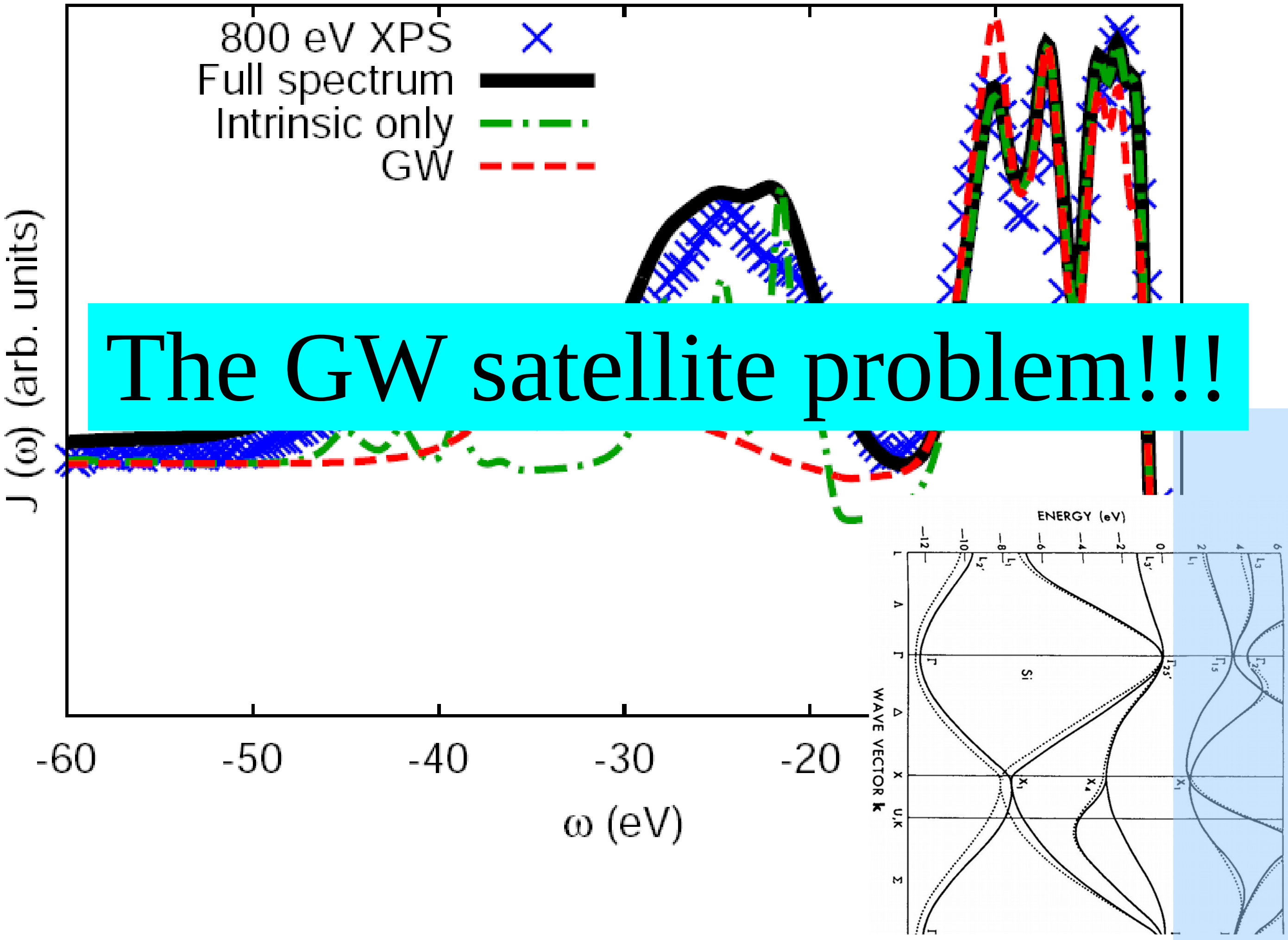


Collab. **J. Rehr, J. Kas**

Cohen and Chelikowsky: "Electronic Structure and Optical Properties of Semiconductors" Solid-State Sciences 75, Springer-Verlag 1988)

M. Guzzo et al., PRL 107, 166401 (2011)

→ W and satellites, a life beyond the GWA



The GW satellite problem!!!

Cohen and Chelikowsky: “Electronic Structure and Optical Properties of Semiconductors” Solid-State Sciences 75, Springer-Verlag 1988)

M. Guzzo et al., PRL 107, 166401 (2011)

We need frequencies → time

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

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

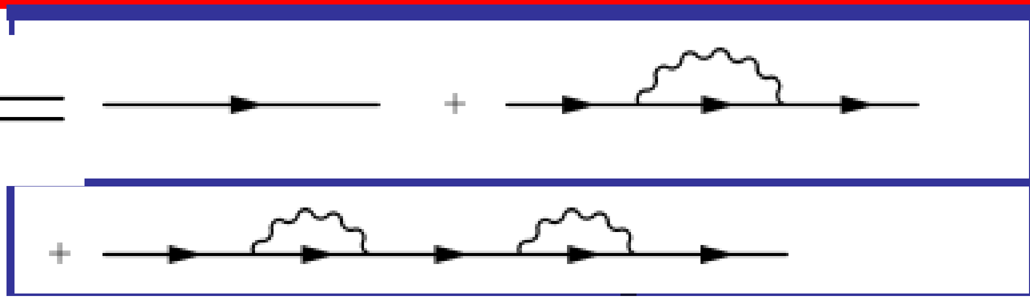
1. Linearization $V_H[\varphi] = V_H^0 + v_c \chi \varphi$ .....

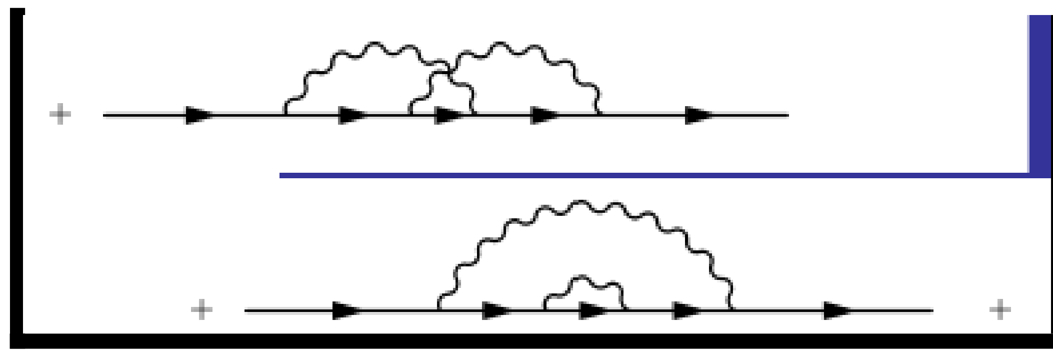
$$\begin{aligned}\mathcal{G}(t_1 t_2) &= \mathcal{G}_H(t_1 t_2) + \mathcal{G}_H(t_1 t_3)\bar{\varphi}(t_3)\mathcal{G}(t_3 t_2) \\ &+ i\mathcal{G}_H(t_1 t_3)\mathcal{W}(t_3 t_4)\frac{\delta \mathcal{G}(t_3 t_2)}{\delta \bar{\varphi}(t_4)},\end{aligned}$$

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

$$\mathcal{G}(t_1 t_2) = \mathcal{G}_{\Delta}(\tau) e^{i\Delta^{QP}\tau} e^{i\int_{t_1}^{t_2} dt' [\bar{\varphi}(t') - \int_{t'}^{t_2} dt'' \mathcal{W}(t't'')]}$$

$\mathcal{G} =$





$$A(\omega) = \frac{\Gamma}{\pi} e^{-\frac{\lambda}{\omega_p^2}} \Bigg[\frac{1}{(\omega - \varepsilon^{QP})^2 + \Gamma^2} + \frac{\lambda}{\omega_p^2} \frac{1}{(\omega - \varepsilon^{QP} + \omega_p)^2 + \Gamma^2} + \frac{1}{2}\left(\frac{\lambda}{\omega_p^2}\right)^2 \frac{1}{(\omega - \varepsilon^{QP} + 2\omega_p)^2 + \Gamma^2} + \frac{1}{6}\left(\frac{\lambda}{\omega_p^2}\right)^3 \frac{1}{(\omega - \varepsilon^{QP} + 3\omega_p)^2 + \Gamma^2} + \dots \Bigg]$$

Exponential solution: ↔ cumulant expansion

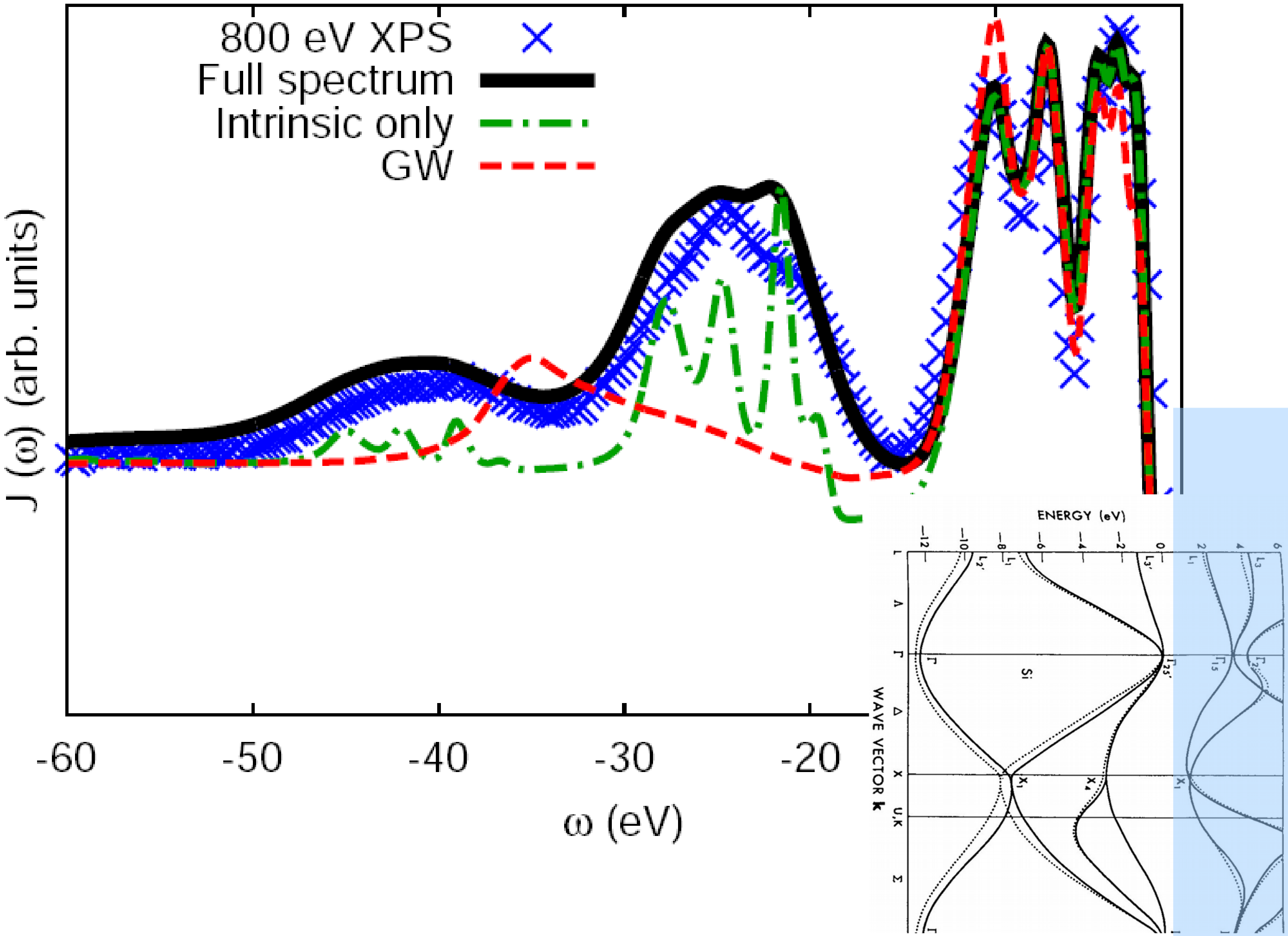
L. Hedin, Physica Scripta **21**, 477 (1980), ISSN 0031-8949.
L. Hedin, J. Phys.: Condens. Matter **11**, R489 (1999).
P. Nozieres and C. De Dominicis, Physical Review **178**, 1097 (1969), ISSN 0031-899X.
D. Langreth, Physical Review B **1**, 471 (1970).

Sodium: Aryasetiawan et al., PRL 77, 1996)

Silicon: Kheifets et al., PRB 68, 2003

Here: the first in a series of approximations

→ W and satellites, a life beyond the GWA



Cohen and Chelikowsky: “Electronic Structure and Optical Properties of Semiconductors” Solid-State Sciences 75, Springer-Verlag 1988)

M. Guzzo et al., PRL 107, 166401 (2011)

Now:

→ how to go beyond?

→ Total energies?

→ G or G_0?

→ which W?

Now:

→ how to go beyond?

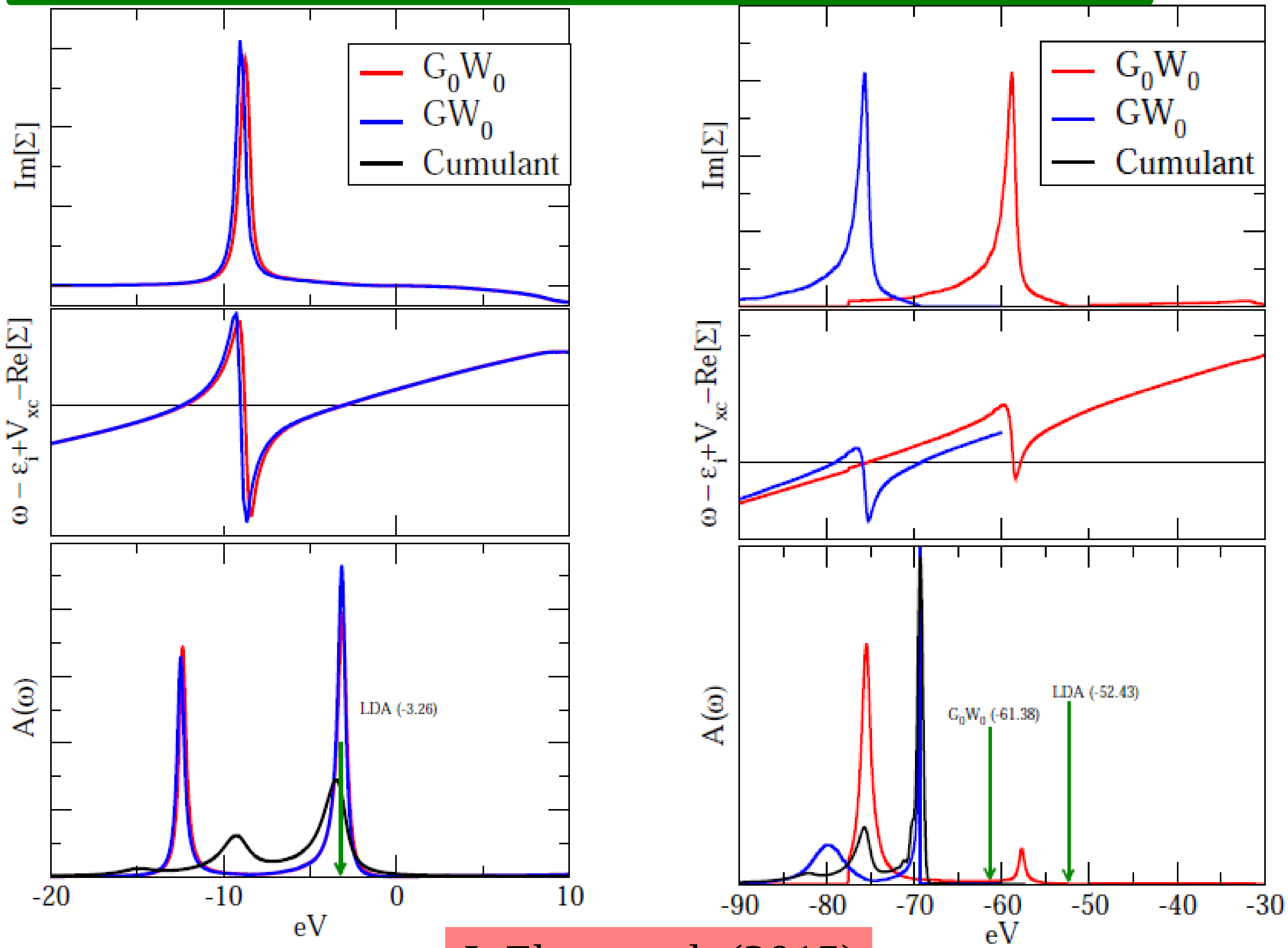
Sky Jianqiang Zhou

→ Total energies?

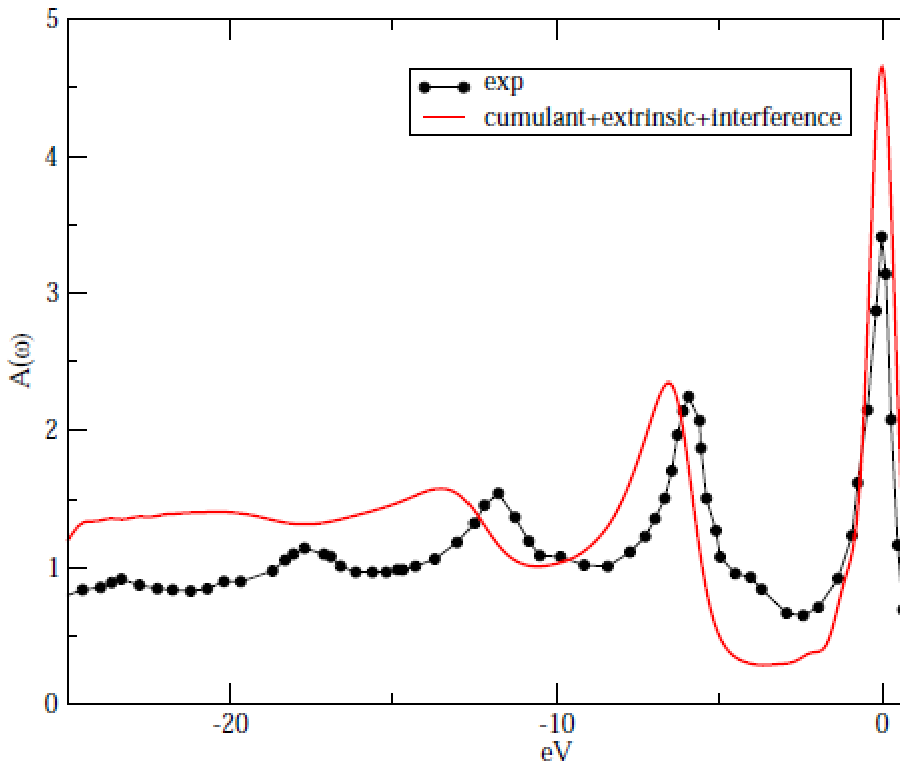
→ G or G_0? → G!!!

→ which W? → the best!!!

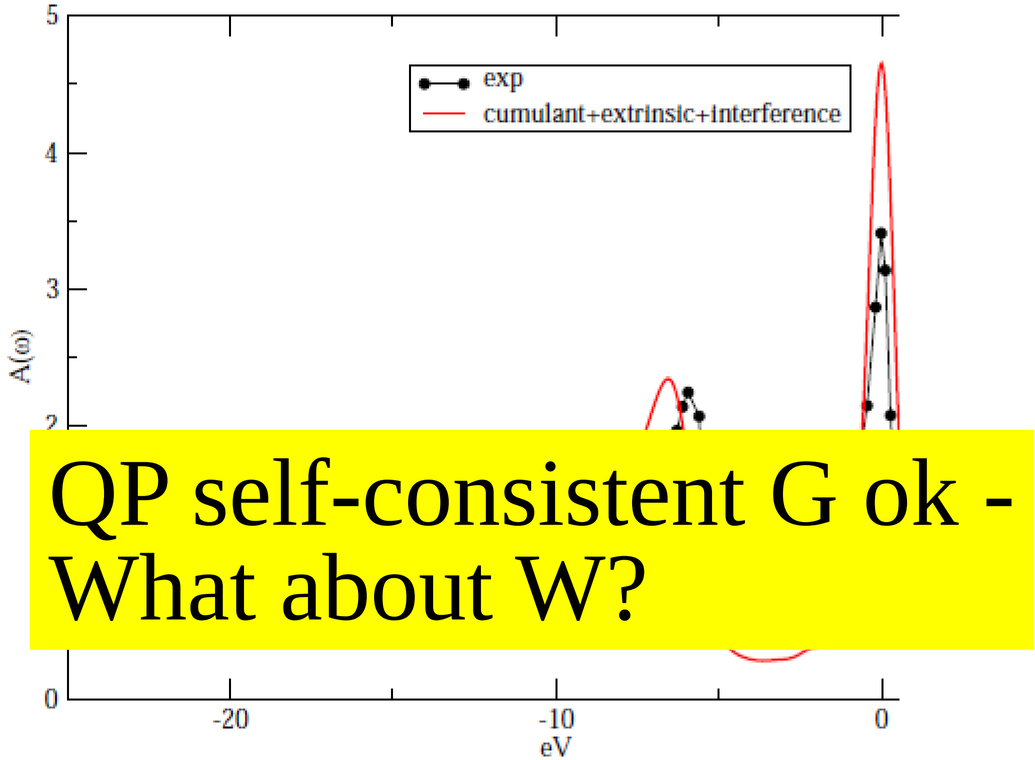
Sodium valence................................and 2s semi-core



J. Zhou et al. (2015)



Na 2s

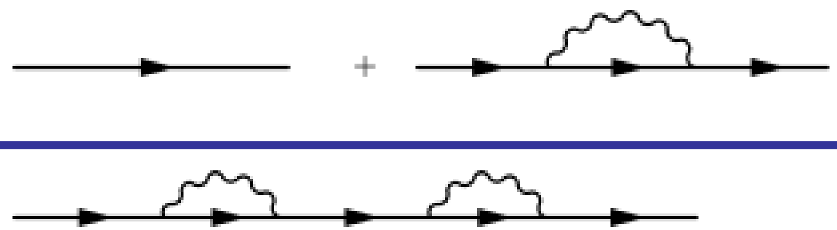


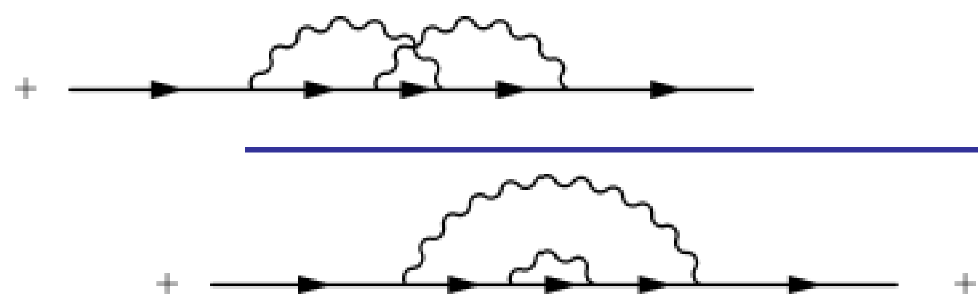
QP self-consistent G ok - What about W?

Na 2s

$$\mathcal{G}(t_{12}) = \mathcal{G}^0_{\mathrm{H}}(t_{12}) \exp\left[-i \int_{t_1}^{t_2} dt' \int_{t'}^{t_2} dt'' \, \mathcal{W}(t't'')\right]$$

$\mathcal{G} =$





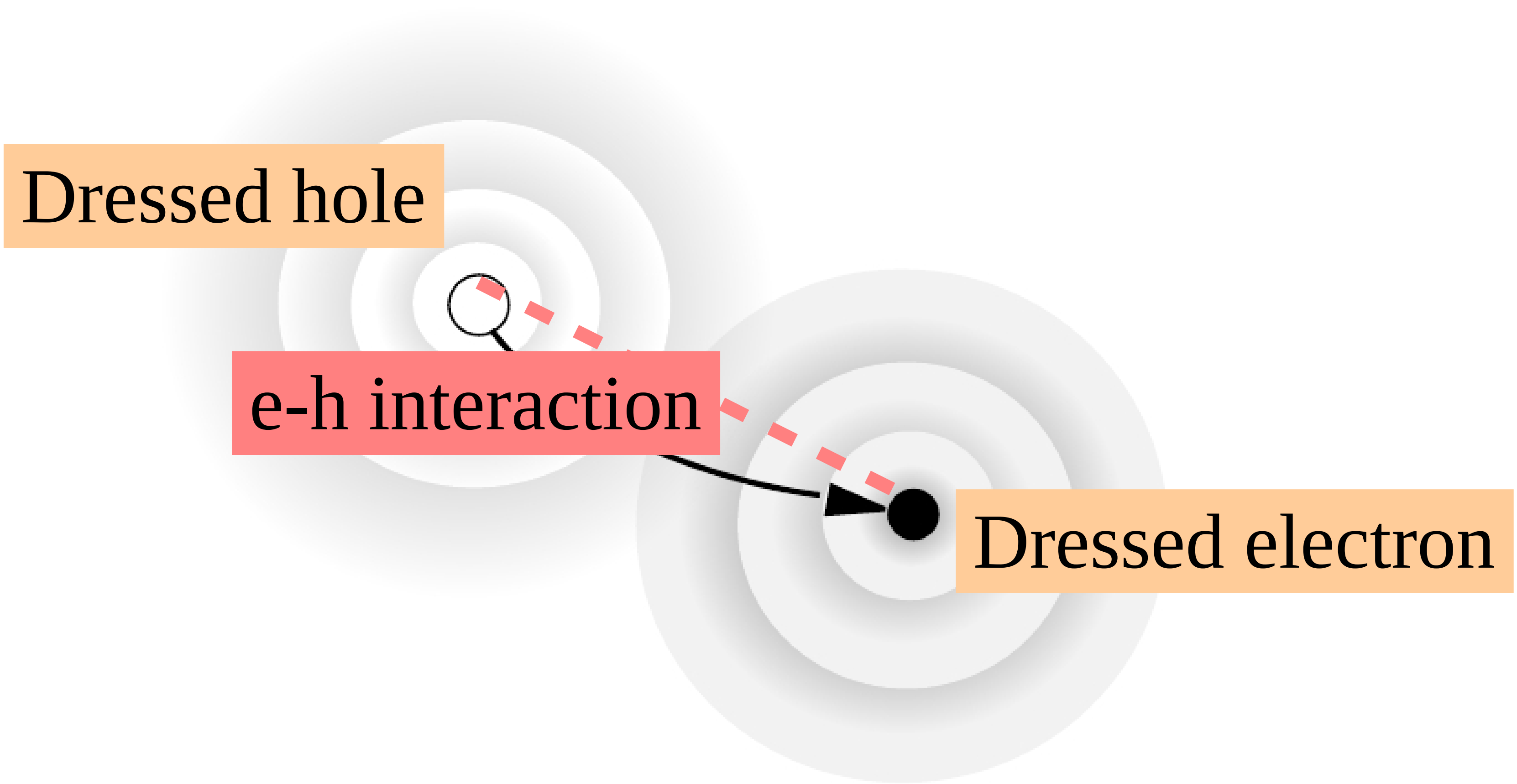
$$A(\omega) = \frac{\Gamma}{\pi} e^{-\frac{\lambda}{\omega_p^2}} \left[\frac{1}{(\omega - \varepsilon^{QP})^2 + \Gamma^2} + \right.$$

$$+ \frac{\lambda}{\omega_p^2} \frac{1}{(\omega - \varepsilon^{QP} + \omega_p)^2 + \Gamma^2} +$$

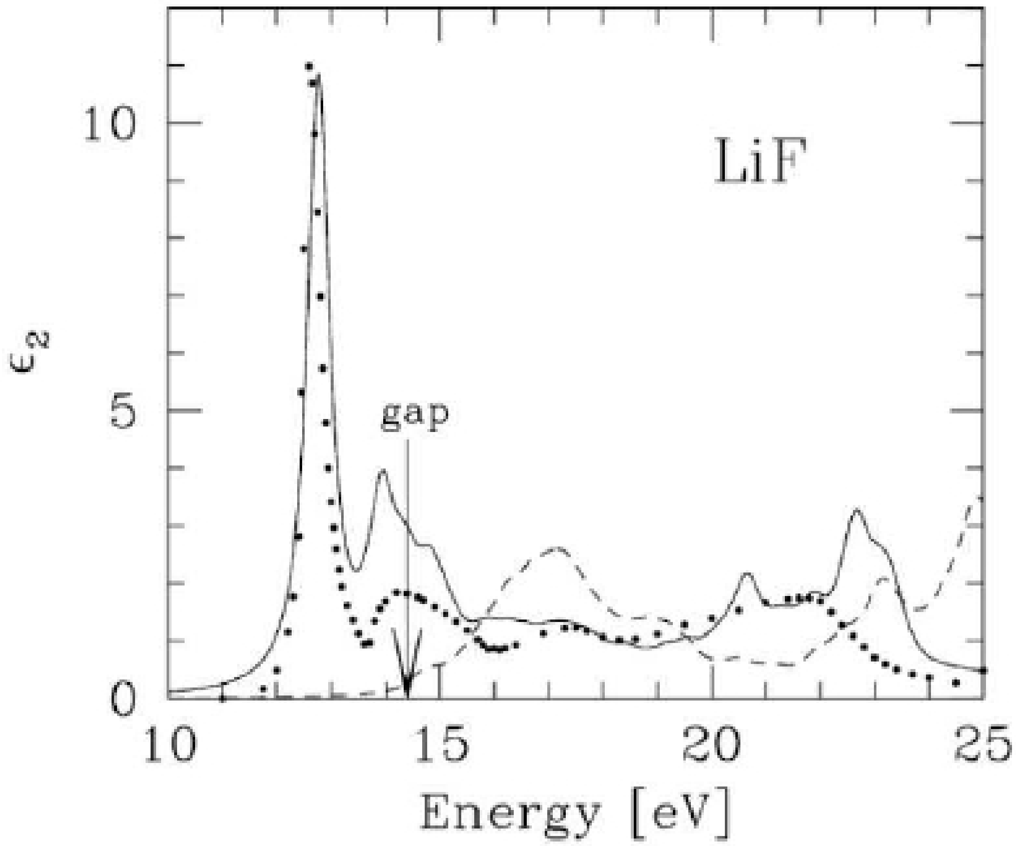
$$+ \frac{1}{2} \left(\frac{\lambda}{\omega_p^2} \right)^2 \frac{1}{(\omega - \varepsilon^{QP} + 2\omega_p)^2 + \Gamma^2} +$$

$$\left. + \frac{1}{6} \left(\frac{\lambda}{\omega_p^2} \right)^3 \frac{1}{(\omega - \varepsilon^{QP} + 3\omega_p)^2 + \Gamma^2} + \ldots \right]$$

→ Electron-hole correlation



e-h problem: Bethe-Salpeter equation



Rohlfing and Louie, PRL 81, 2312 (1998)

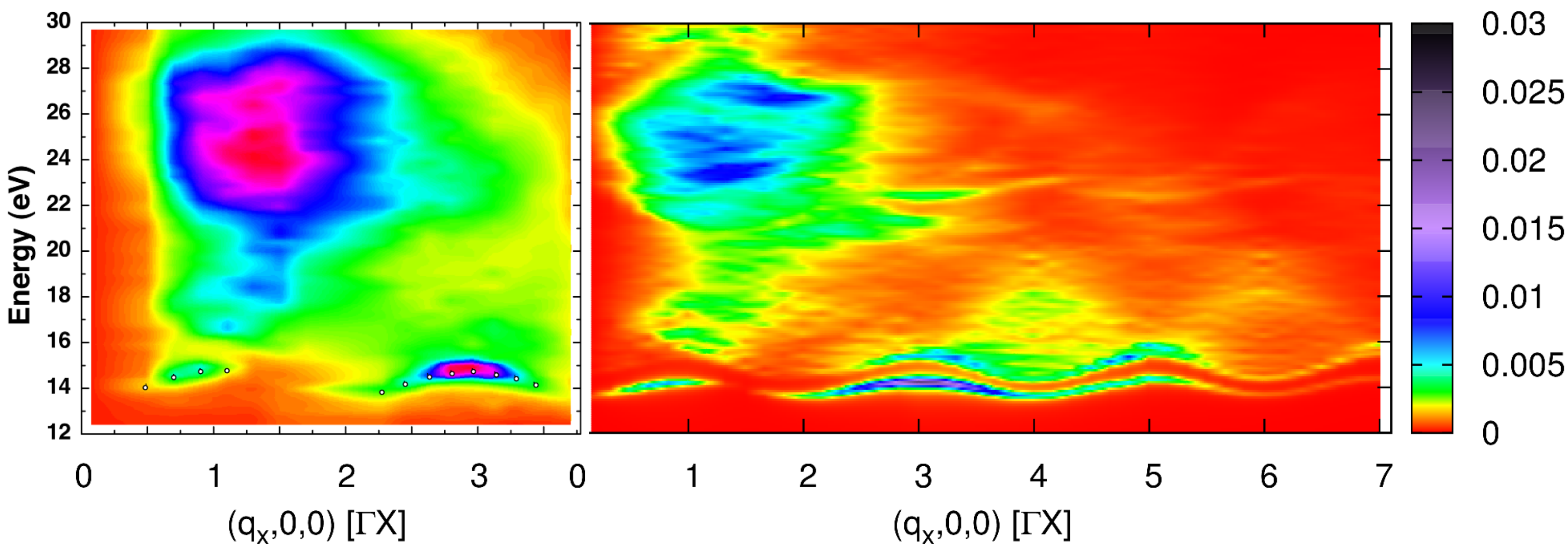
$$\chi(\omega) = \begin{pmatrix} \chi_{00}(q\to 0,\omega) & \chi_{01}(q\to 0,\omega) & . & . \\ \chi_{10}(q\to 0,\omega) & \chi_{11}(q\to 0,\omega) & . & . \\ . & . & & \\ . & . & & \\ . & . & & \end{pmatrix}$$

The whole function?
The whole matrix?

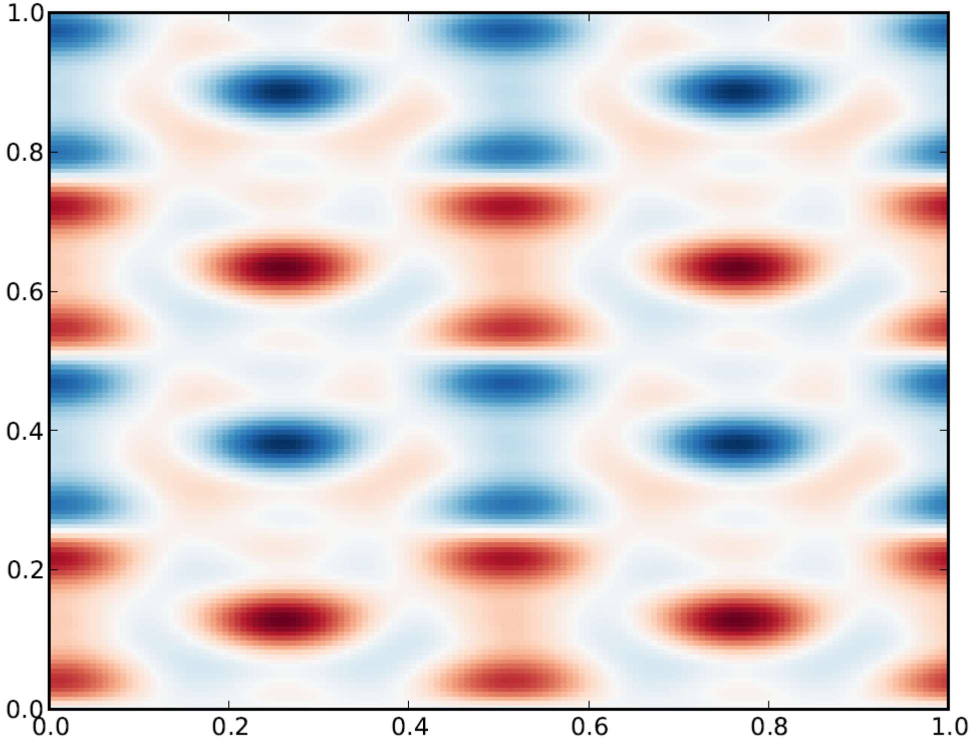
$$\chi(\omega) = \begin{pmatrix} \chi_{00}(q,\omega) & \chi_{01}(q,\omega) & . & . \\ \chi_{10}(q,\omega) & \chi_{11}(q,\omega) & . & . \\ . & . & & \\ . & . & & \\ . & . & & \end{pmatrix}$$

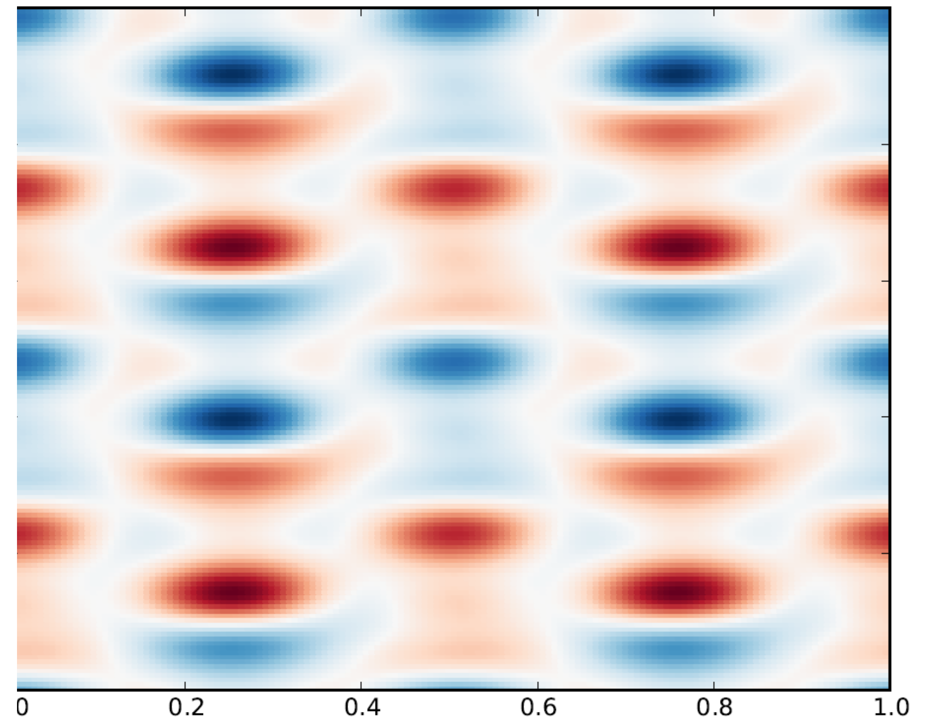
The whole function?
The whole matrix?

On the diagonal, whole fct:
Exciton dispersion in LiF



M. Gatti and F. Sottile, Phys. Rev. B 88, 155113
Exp. P. Abbamonte et al., Proc. Natl. Acad. Sci. USA 105, 12159 (2008).





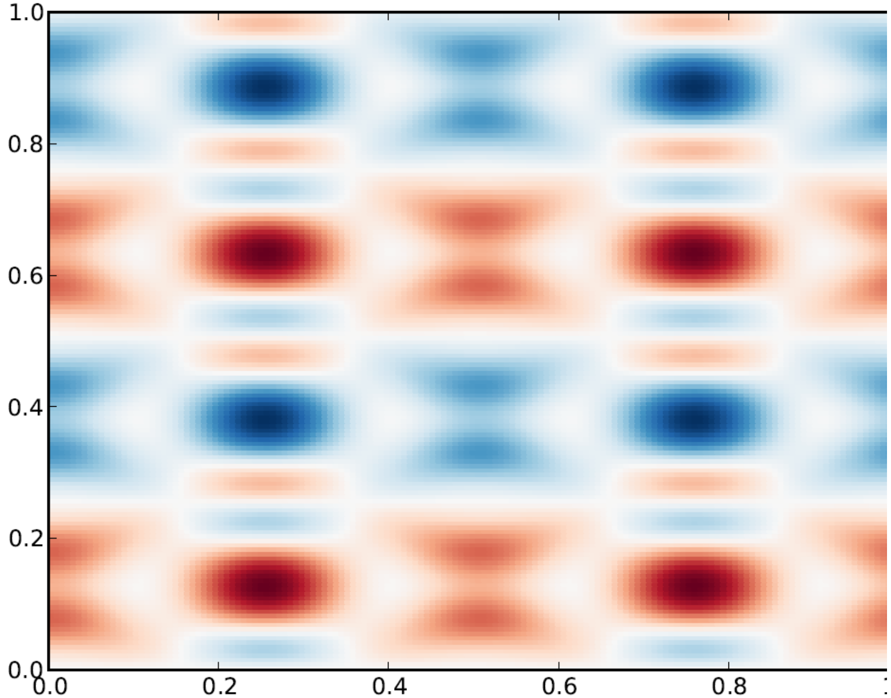
RPA

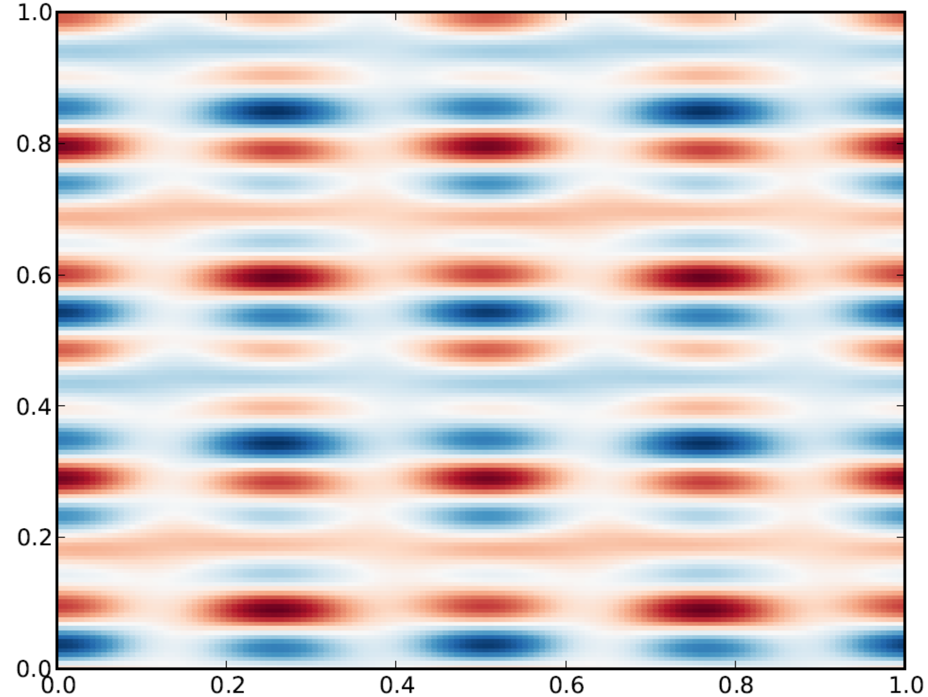
BSE

At 25 eV

The whole matrix → follow excitations in real space and time

PhD thesis I. Reshetnyak





RPA

BSE

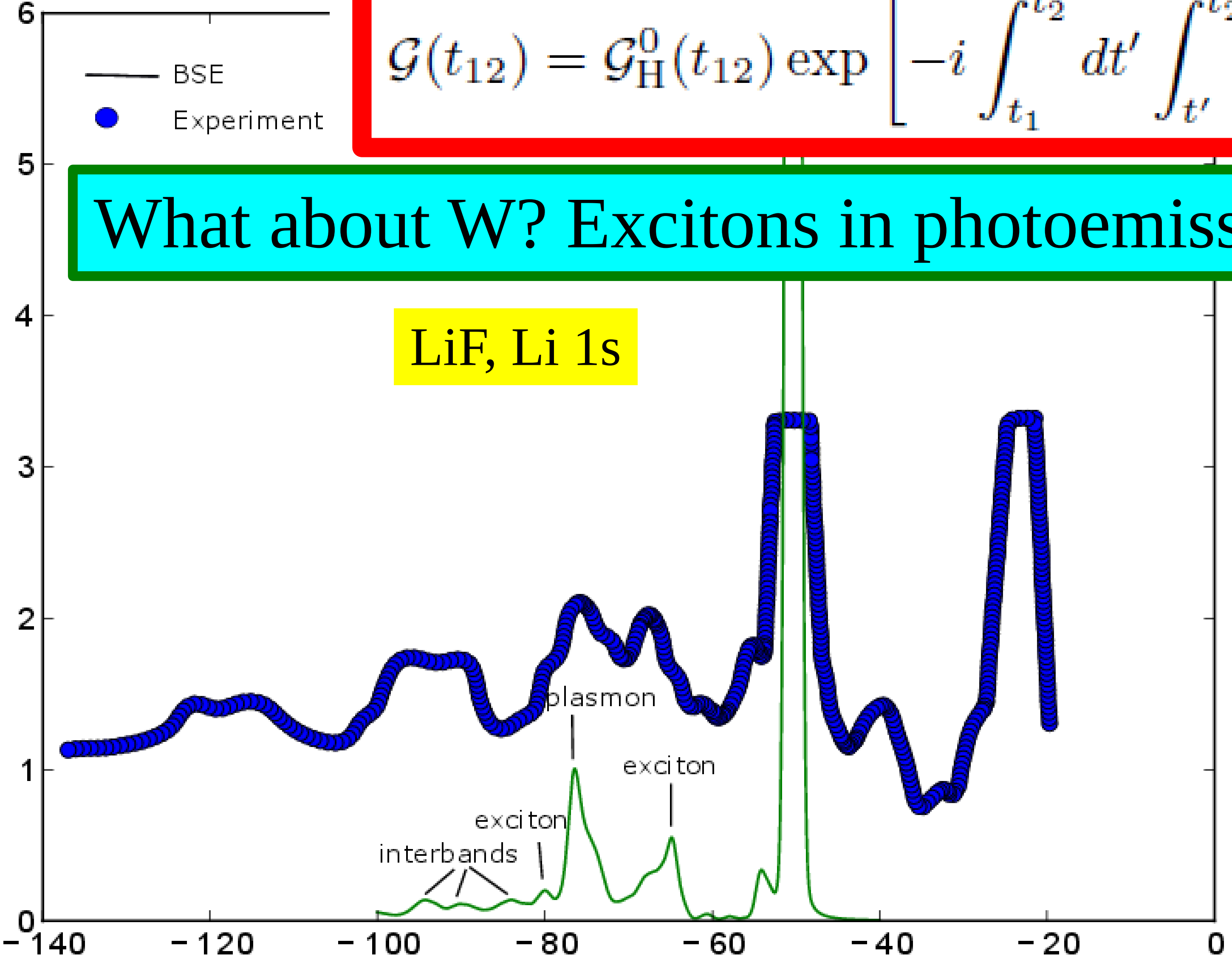
At 14.1 eV

Consequences of excitons?

PhD thesis I. Reshetnyak

$$\mathcal{G}(t_{12}) = \mathcal{G}^0_{\mathrm{H}}(t_{12}) \exp\left[-i\int_{t_1}^{t_2} dt' \int_{t'}^{t_2} dt''\, \mathcal{W}(t't'')\right]$$

What about W? Excitons in photoemission



F. Sottile
M. Gatti

Igor Reshetnyak, PhD thesis

Using: M. Gatti and F. Sottile, Phys. Rev. B 88, 155113

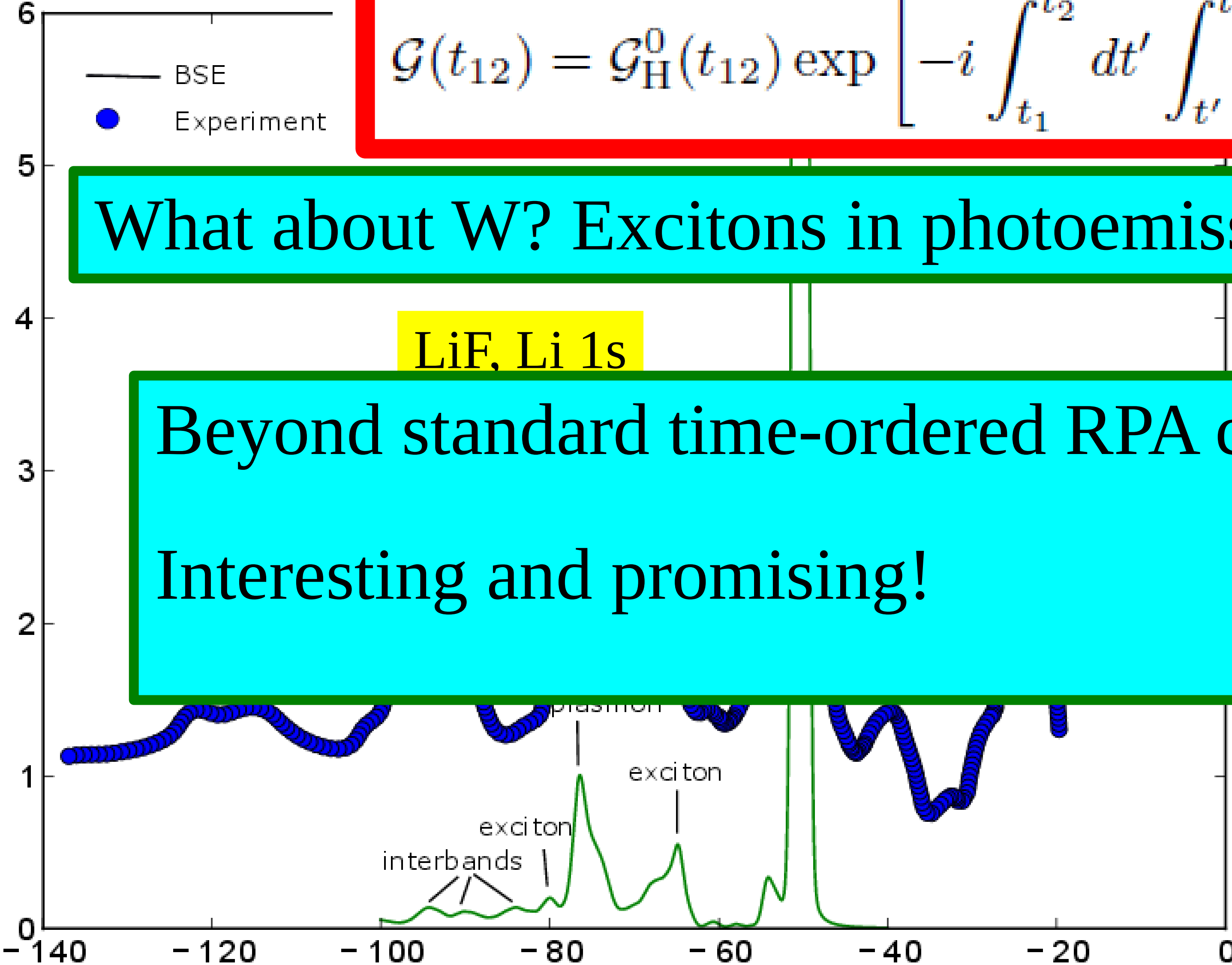
$$\mathcal{G}(t_{12}) = \mathcal{G}_{\mathrm{H}}^{0}(t_{12}) \exp\left[-i \int_{t_1}^{t_2} dt' \int_{t'}^{t_2} dt''\, \mathcal{W}(t't'')\right]$$

What about W? Excitons in photoemission

LiF, Li 1s

Beyond standard time-ordered RPA cumulant:

Interesting and promising!



Igor Reshetnyak, PhD thesis

Using: M. Gatti and F. Sottile, Phys. Rev. B 88, 155113

A direct approach
to the calculation of many-body Green' s functions

→ The Framework; MBPT

→ A direct approach

→ Power of the 1-point model: (no) mysteries of MBPT

→ How to solve a Dyson equation

→ Change fctl for strong interaction!

→ W and satellites, a life beyond the GWA

→ Conclusions

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