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

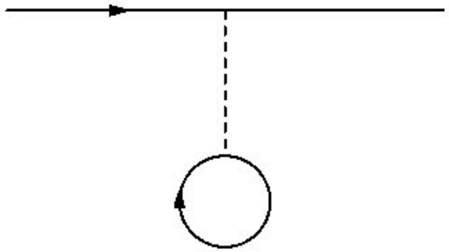
→ Correlation and occupation numbers

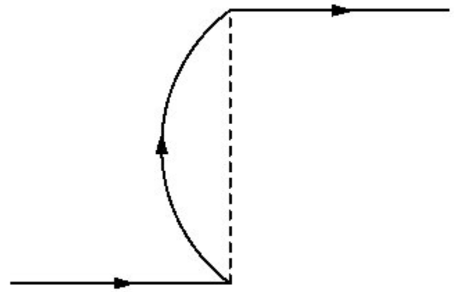
→ Conclusions

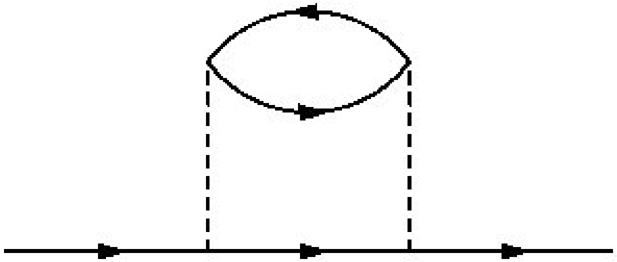
$$\mathcal{G}(1,2) = -i \langle T[\psi(1)\psi^{\dagger}(2)]\rangle$$

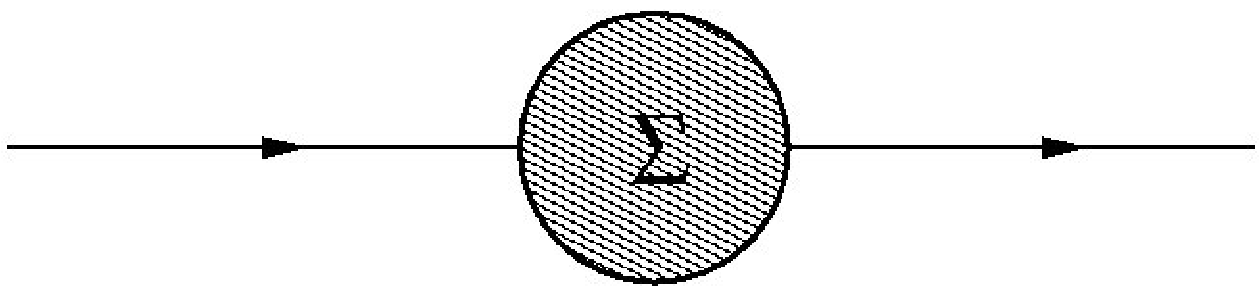
→ The Framework

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

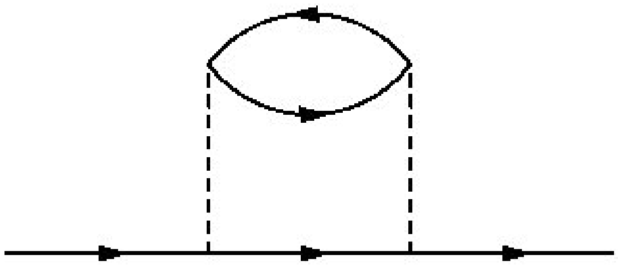








Dyson equation: $\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G}$

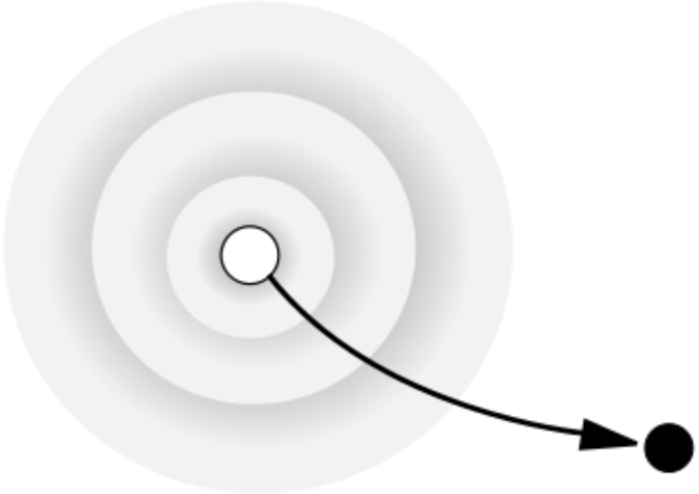


$+ \ldots\ldots\ldots$

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

L. Hedin (1965)

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



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

Hedin's equations

$$\Sigma_{\mathrm{xc}}(1,2) = iG(1,\bar{4})W(1^{+},\bar{3})\tilde{\Gamma}(\bar{4},2;\bar{3})$$

GW

$$W(1,2) = v_c(1,2) + v_c(1,\bar{3})P(\bar{3},\bar{4})W(\bar{4},\bar{2})$$

$$P(1,2) = -iG(1,\bar{3})G(\bar{4},1)\tilde{\Gamma}(\bar{3},\bar{4};2)$$

RPA

$$\tilde{\Gamma}(1,2;3) = \delta(12)\delta(13) + \frac{\delta\Sigma_{\mathrm{xc}}(12)}{\delta G(\bar{4},\bar{5})}G(\bar{4},\bar{6})G(\bar{7},\bar{5})\tilde{\Gamma}(\bar{6},\bar{7};3)$$

$$G(1,2) = G_0(1,2) + G_0(1,\bar{3})\Sigma(\bar{3},\bar{4})G(\bar{4},2)$$

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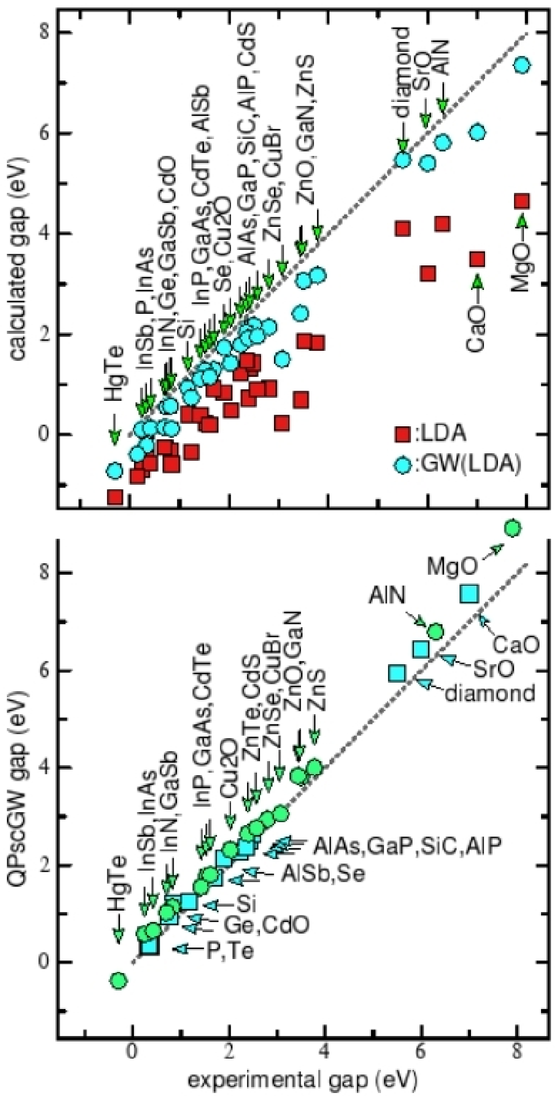
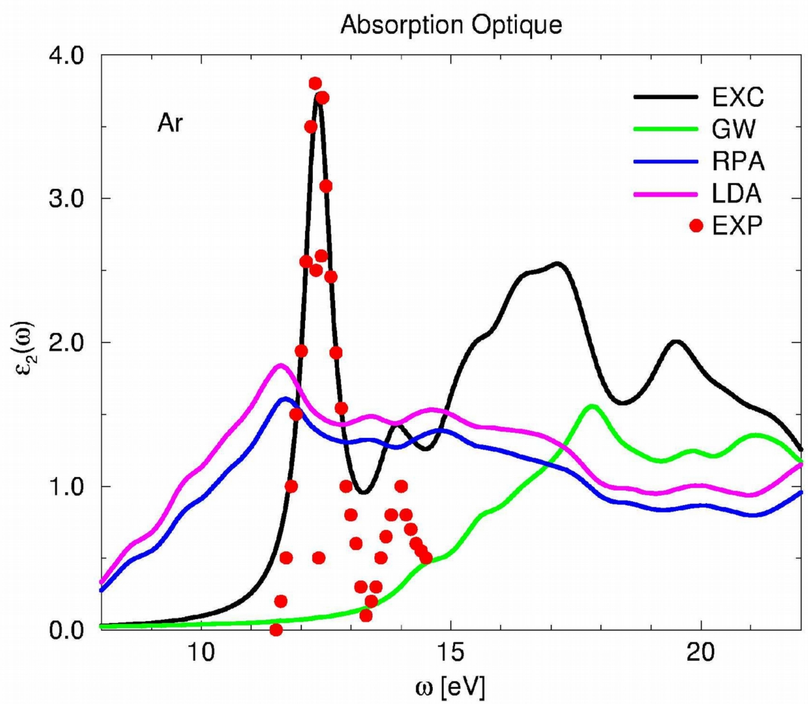
BSE

$$G(1,2) = G_0(1,2) + G_0(1,\bar{3})\Sigma(\bar{3},\bar{4})G(\bar{4},2)$$

iGW

Successes of GW + BSE: Qps, optics





V. Olevano et al. (2000)
(bulk silicon 1998)

van Schilfgaarde, Kotani, Faleev,
Phys. Rev. Lett. 96, 226402 (2006)

Calculating the one-body G

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*

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

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

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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: $\mathcal{W} = \varepsilon^{-1} v_c$

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

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"

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

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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

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

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

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

$$y(z) = \left[\frac{1}{y_0(z)} + \frac{v y_0(z)}{2} \left(1 + \frac{y_0(z)\sqrt{\frac{v}{\pi}}\exp\left[-\frac{1}{v y_0^2(z)}\right]}{\mathrm{erf}\left[\frac{1}{\sqrt{v y_0^2(z)}}\right] - \frac{1}{C\left(v,\, y_0^0\right)}} \right)^{-1} \right]^{-1}$$

$$C(v,\, y_0^0) = 0 \text{ for all } v$$

$$y_v(z) = \frac{2 y_0(z)}{2 + v y_0^2(z)} \qquad y_v(z) = y_0(z) \sum_{n=0}^{\infty} \left(-\frac{y_0^2(z)}{2} v \right)^n$$

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

Perturbation theory

Power of the 1-point model: structure of MBPT

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

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

$$y = y_0 + y_0 s[y, u] y$$

Working with dressed GFs

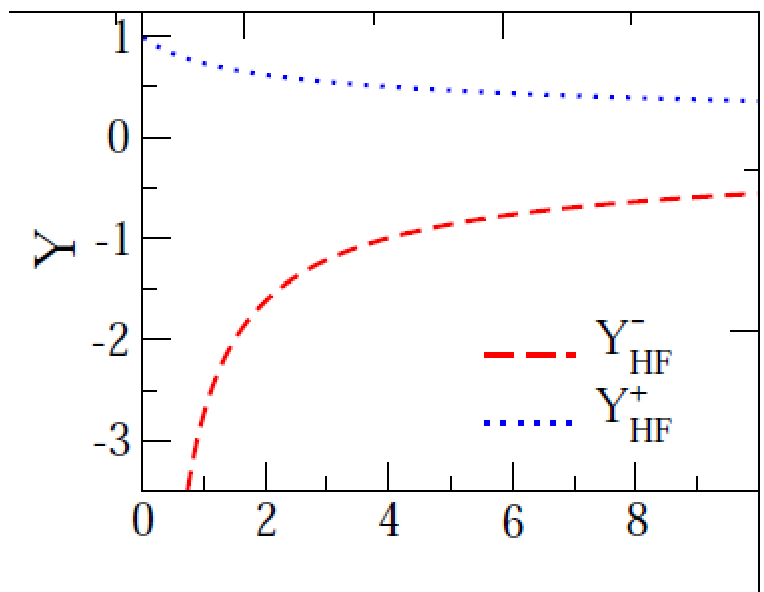
$$s^{HF}[y, u] = -\tfrac{1}{2} u y$$

$$Y_{HF}^{\pm} = \frac{1}{V} \left[-1 \pm \sqrt{1 + 2V} \right] \qquad Y = y / y_0 \qquad V = u y_0^2$$

+ : Physical

- : Unphysical

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



Y
1
0
-1
-2
-3
0
2
4
6
8
Y^-_{HF}
Y^+_{HF}

How to get the physical solution in practice?

$$y = y_0 + y_0 s[y,u]y \qquad s^{HF}[y,u] = -\tfrac{1}{2}uy$$

$$Y = y/y_0 \qquad V = uy_0^2$$

2Y = 2 – VY Y

VY = 2/Y - 2

$$Y^{(n+1)} = \frac{2}{2+VY^{(n)}}\ (\mathbf{I});\ Y^{(n+1)} = \frac{2}{VY^{(n)}} - \frac{2}{V}\ (\mathbf{II})$$

Physical

$$\sqrt{1+x} = 1 + \frac{x/2}{1+\frac{x/4}{1+\frac{x/4}{1+\cdots}}}$$

Unphysical

$$Y_{HF}^{\pm} = \frac{1}{V}\left[-1 \pm \sqrt{1+2V}\right]$$

How to get the physical solution in practice?

$$y = y_0 + y_0 s[y,u] y \qquad s^{HF}[y,u] = -\tfrac{1}{2} u y$$

$$Y = y/y_0 \qquad V = u y_0^2$$

2Y = 2 – VY Y VY = 2/Y - 2

Solution depends on iteration scheme!

$$Y^{(n+1)} = \frac{2}{2 + VY^{(n)}} \ (\mathbf{I}); \ Y^{(n+1)} = \frac{2}{VY^{(n)}} - \frac{2}{V} \ (\mathbf{II})$$

Physical

$$\sqrt{1+x} = 1 + \frac{x/2}{1 + \frac{x/4}{1 + \frac{x/4}{1 + \cdots}}}$$

Unphysical

$$Y_{HF}^{\pm} = \frac{1}{V}\left[-1 \pm \sqrt{1 + 2V}\right]$$

What about real life?

Hedin's equations

$$\Sigma_{\mathrm{xc}}(1,2) = iG(1,\bar{4})W(1^+,\bar{3})\tilde{\Gamma}(\bar{4},2;\bar{3})$$

$$W(1,2) = v_c(1,2) + v_c(1,\bar{3})P(\bar{3},\bar{4})W(\bar{4},\bar{2})$$

$$P(1,2) = -iG(1,\bar{3})G(\bar{4},1)\tilde{\Gamma}(\bar{3},\bar{4};2)$$

$$\tilde{\Gamma}(1,2;3) = \delta(12)\delta(13) + \frac{\delta\Sigma_{\mathrm{xc}}(12)}{\delta G(\bar{4},\bar{5})}G(\bar{4},\bar{6})G(\bar{7},\bar{5})\tilde{\Gamma}(\bar{6},\bar{7};3)$$

BSE

$$G(1,2) = G_0(1,2) + G_0(1,\bar{3})\Sigma(\bar{3},\bar{4})G(\bar{4},2)$$

iGW

What about real life?

TDDFT

$$\chi(\omega) = \chi_0(\omega) + \chi_0(\omega)\left[v_c + f_{xc}\right]\chi(\omega)$$

$$f_{xc} = \frac{1 + v_c\chi(\omega = 0)}{\chi_0(\omega = 0)}$$

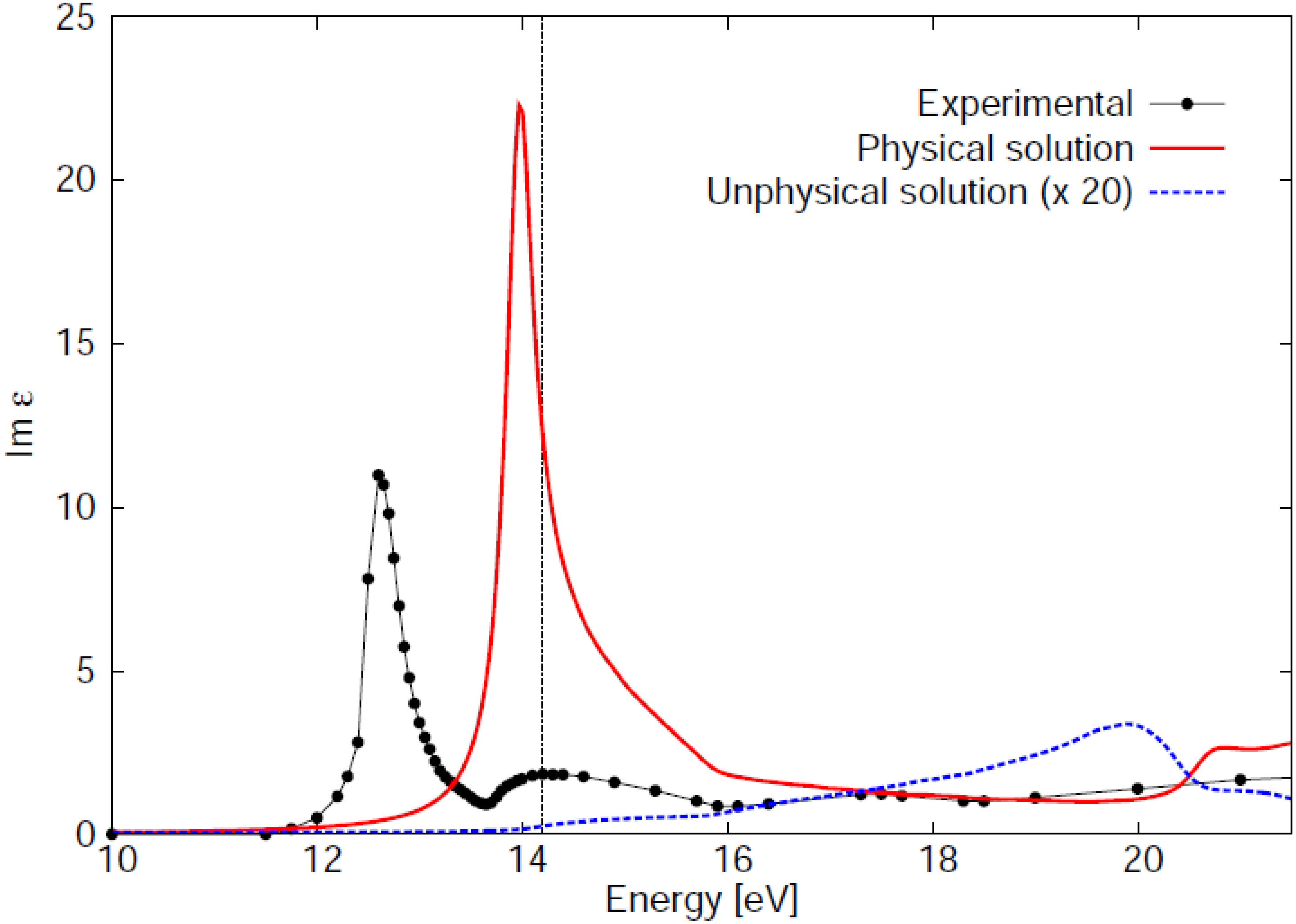
S. Sharma, J. K. Dewhurst, A. Sanna, and E. K. U. Gross, Phys. Rev. Lett. 107, 186401 (2011)

$$\chi(\omega) = \chi_0(\omega) + \chi_0(\omega)\left[v_c + \frac{1 + v_c\chi(\omega = 0)}{\chi_0(\omega = 0)}\right]\chi(\omega)$$

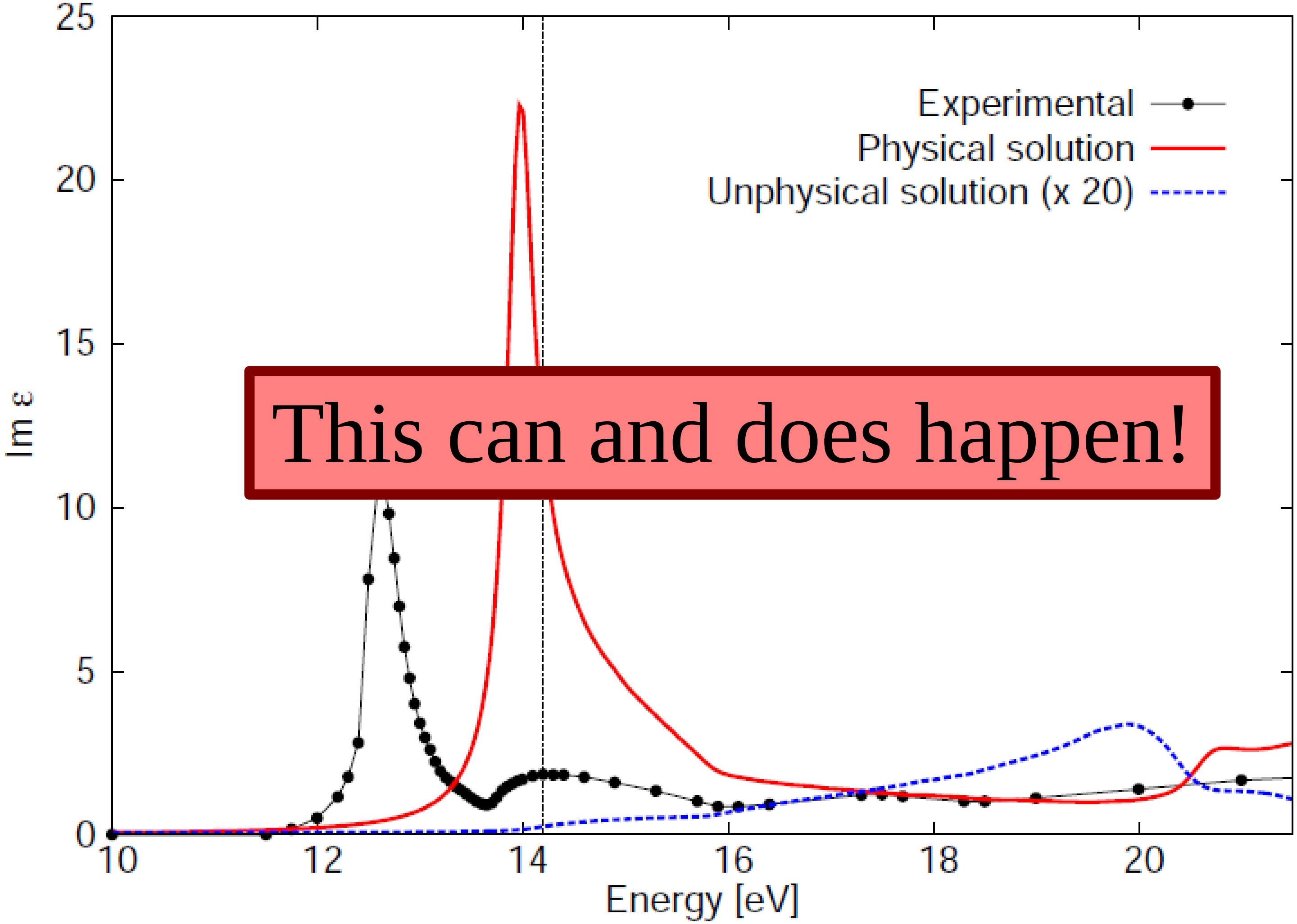
$$\chi^{\pm} = -\frac{\chi_0}{2} \pm \sqrt{\left(\frac{\chi_0}{2}\right)^2 - \frac{\chi_0}{v_c}}$$

$$= -\frac{\chi_0}{2} \pm \left|\frac{\chi_0}{2}\right|\sqrt{1 - \frac{4}{v_c\chi_0}}$$

Physical: fxc → 0
For large screening



Absorption spectrum of LiF, ab initio



This can and does happen!

Absorption spectrum of LiF, ab initio

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

$y_0 \to y$

$$\tilde{s}[y_0, u] = -\frac{1}{2} u y_0$$

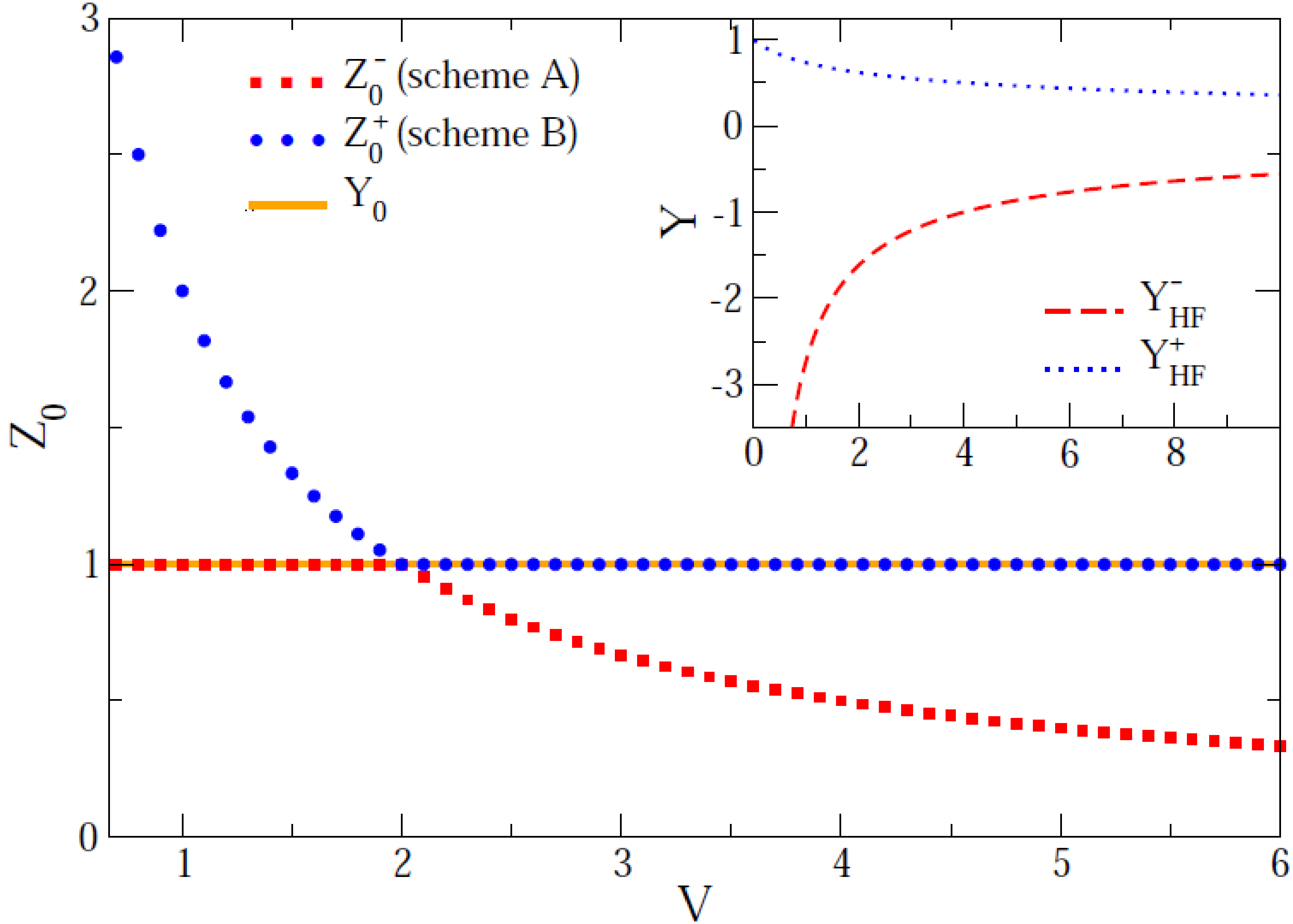
$$y = y_0 + y_0 s[y, u] y \qquad\qquad z_0 \leftarrow y$$

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

leads to $z_0 = y_0$?

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

Continuity requires change of sign!



Z0− (scheme A)
Z0+ (scheme B)
Y0
Z0
V
Y
Y−HF
Y+HF

Iteration?

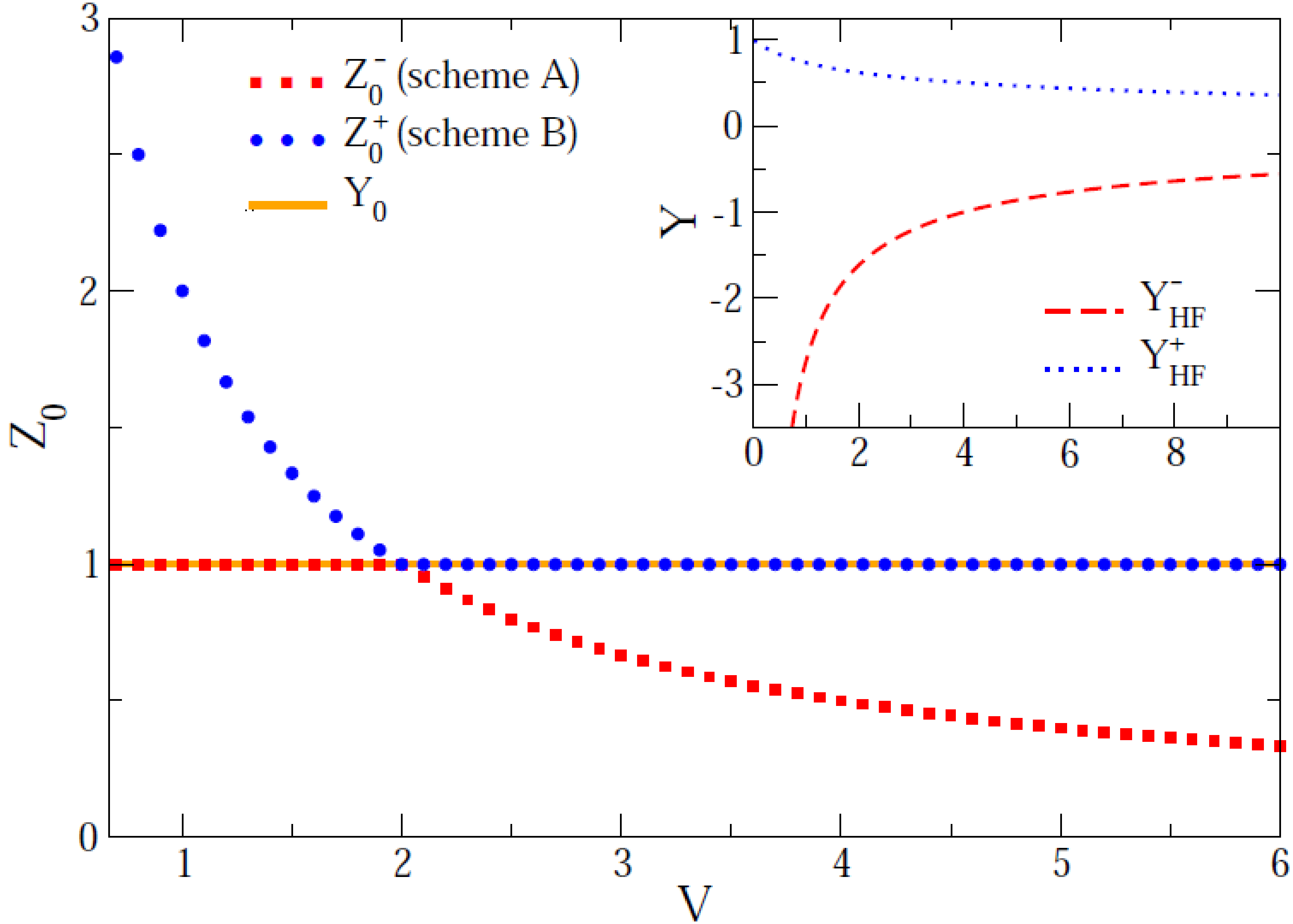
In analogy to:

E. Kozik, M. Ferrero, and A. Georges, arXiv:1407.5687 (2014).

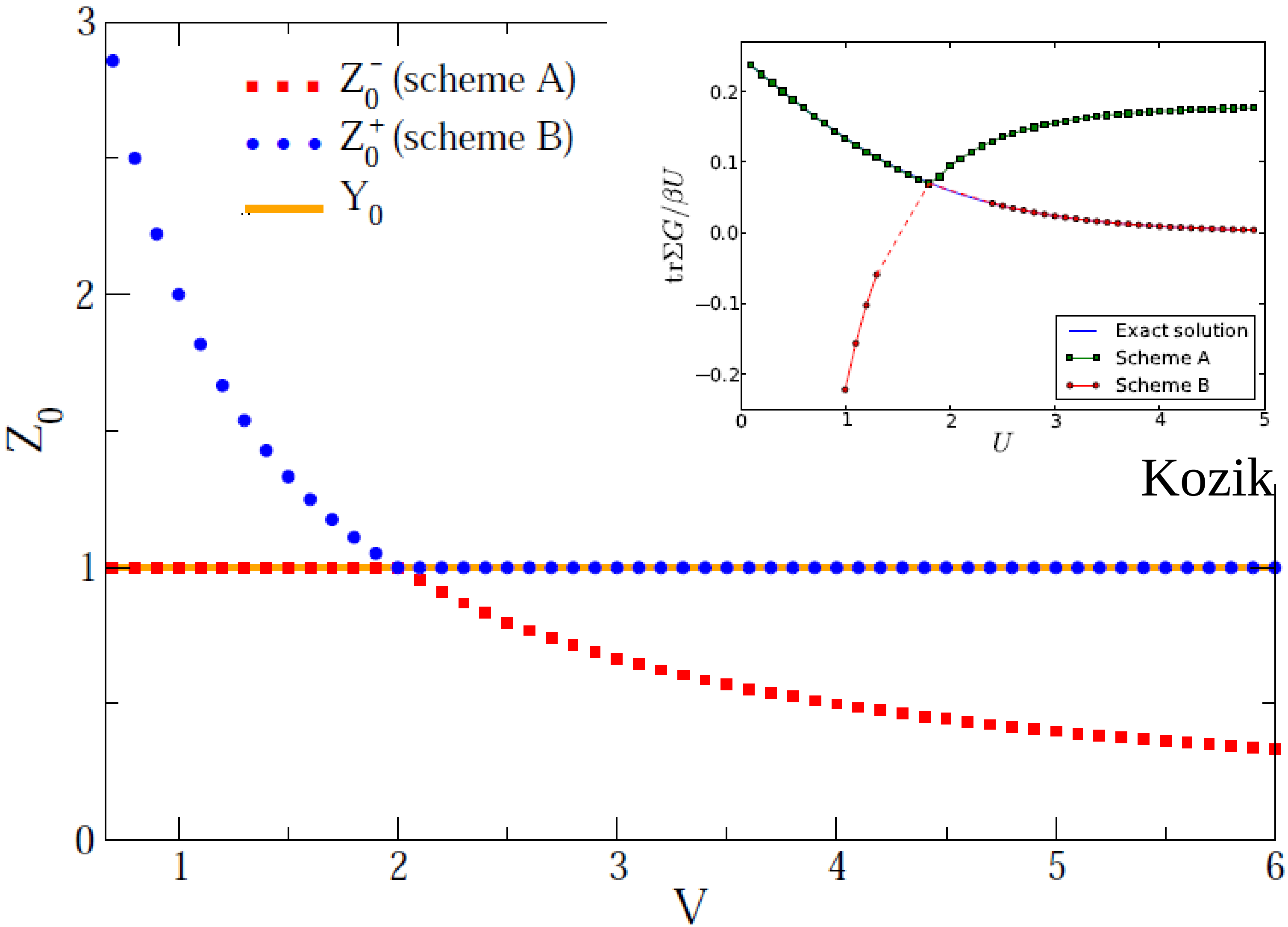
$$\frac{1}{Z_0^{(n+1)}} = 1 + \frac{1}{2} V (1 - Z_0^{(n)}) \qquad (\mathbf{A})$$

$$\frac{1}{Z_0^{(n+1)}} = -1 - \frac{1}{2} V (1 - Z_0^{(n)}) + \frac{2}{Z_0^{(n)}} \qquad (\mathbf{B}).$$

Hubbard atom, 2D Hubbard, AIM



Z_0^- (scheme A)
Z_0^+ (scheme B)
Y_0
Z_0
V
Y
Y_{HF}^-
Y_{HF}^+



Z_0^- (scheme A)
Z_0^+ (scheme B)
Y_0
Z_0
V
Exact solution
Scheme A
Scheme B
$\mathrm{tr}\Sigma G/\beta U$
U

Kozik et al

Functional of the dressed G?

$$\tilde{s}[y_0, u] = -\frac{1}{2} u y_0$$

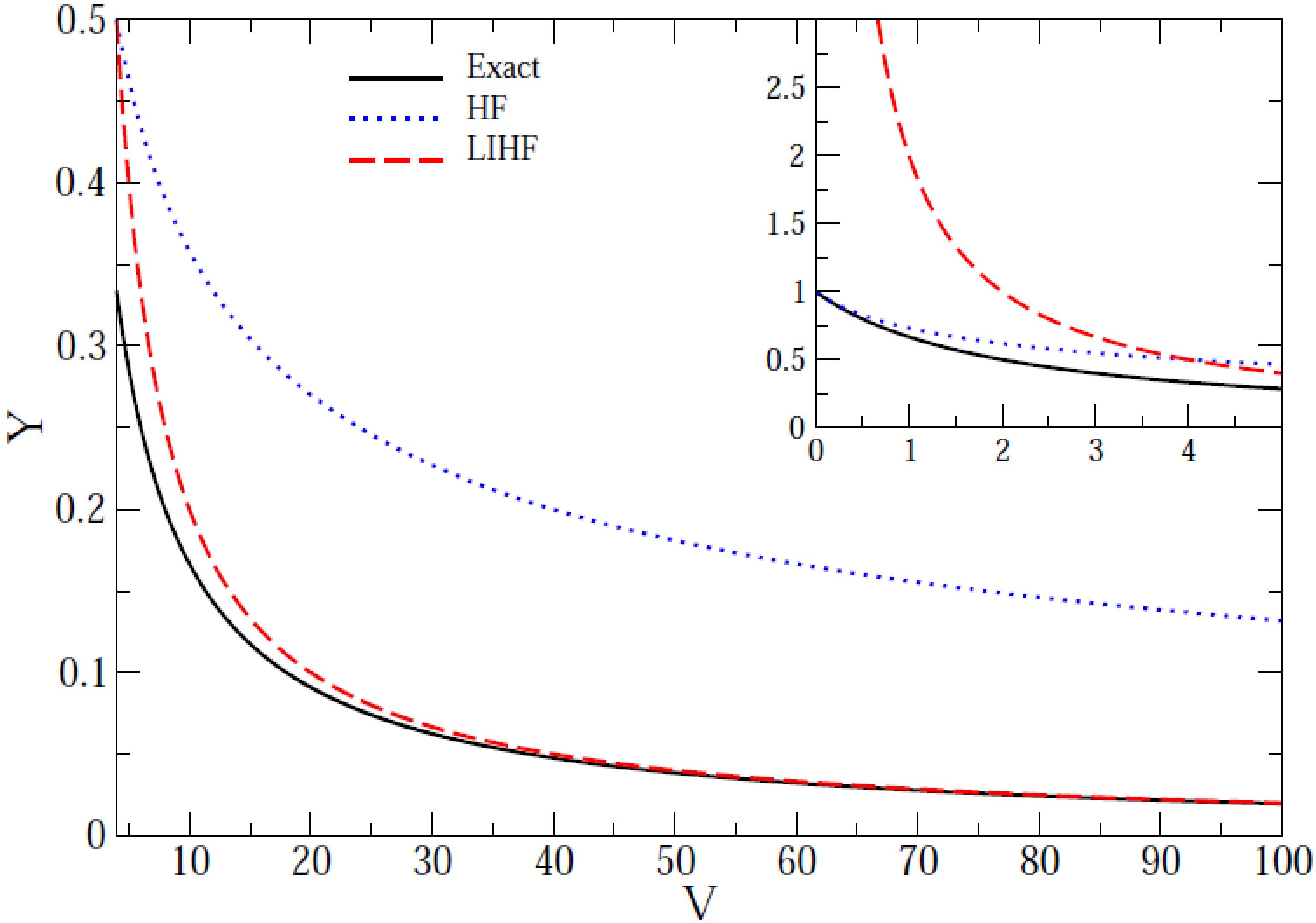
$$z_0^{\pm} = \frac{1}{uy}\left(1 \pm \sqrt{1 - 2uy^2}\right)$$

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

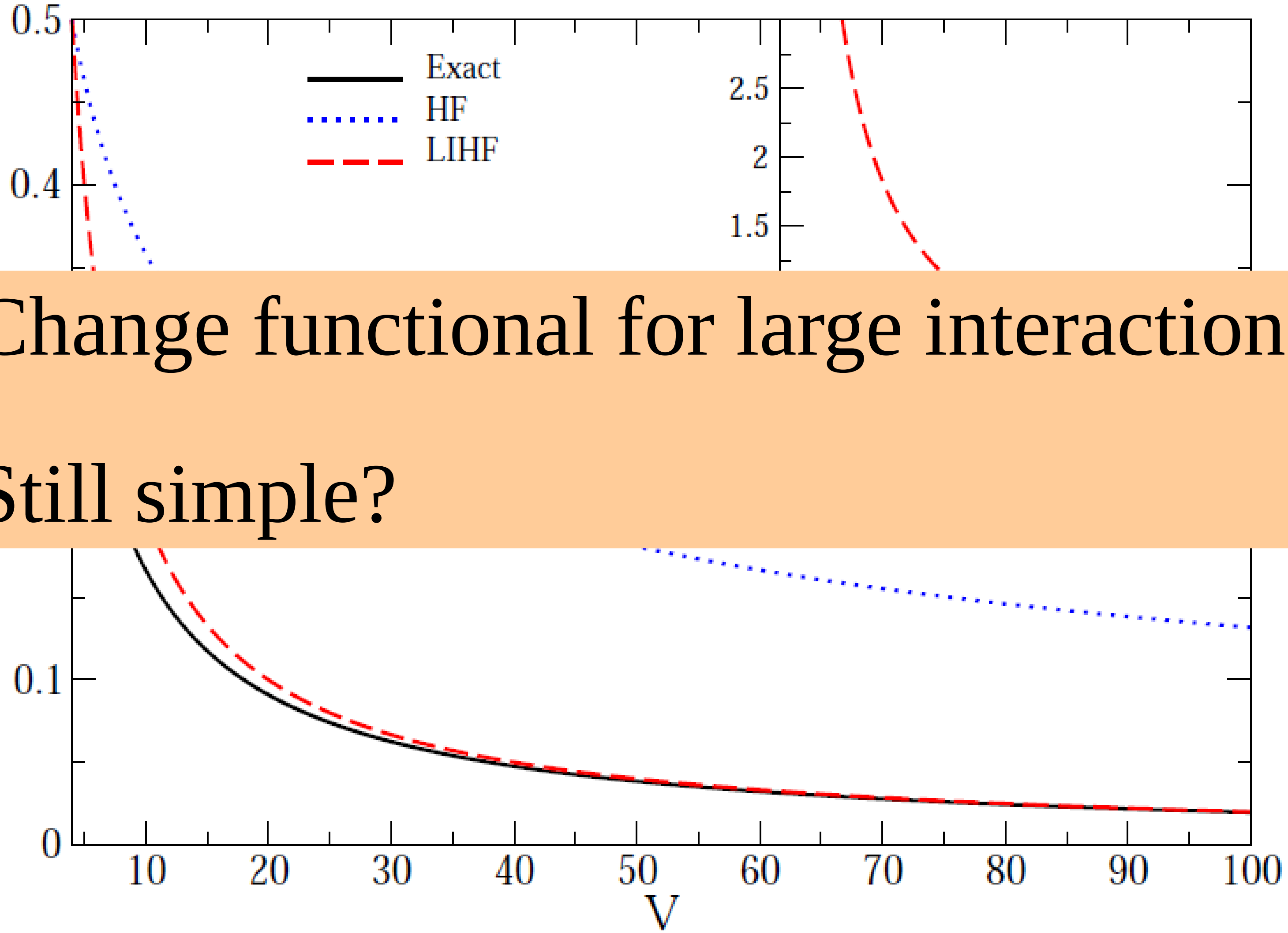
$$= -\frac{1}{2y} \mp \frac{1}{2y} \pm \frac{1}{2} u \left[y + \frac{uy^3}{2} + \frac{u^2 y^5}{2} + \ldots \right]$$

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

$$s^{HF} = -\tfrac{1}{2} uy \qquad s^{LIHF} = -\tfrac{1}{y} - s^{HF}$$



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

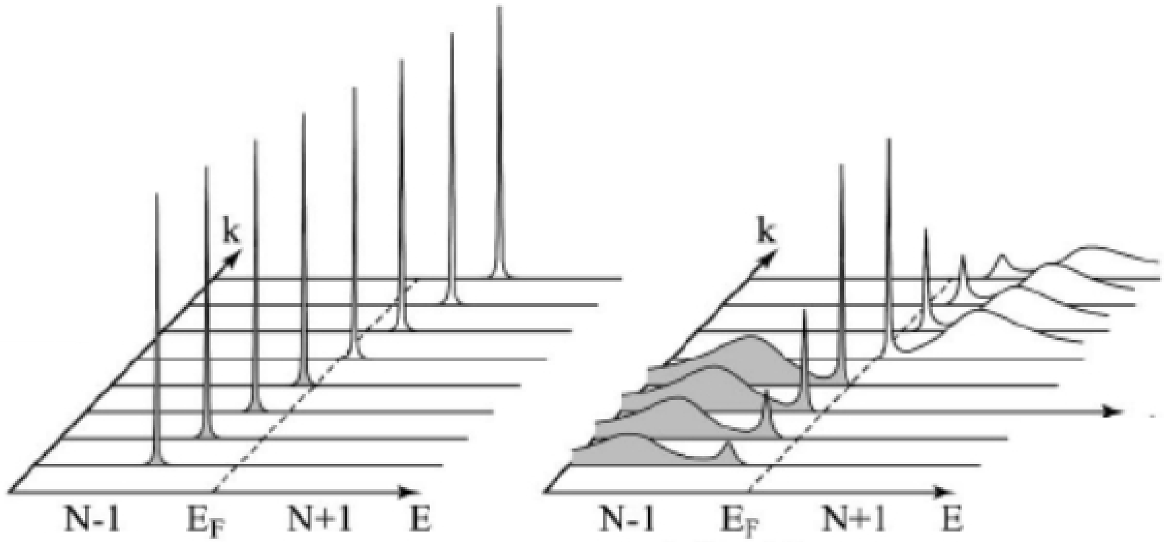


Change functional for large interaction

Still simple?

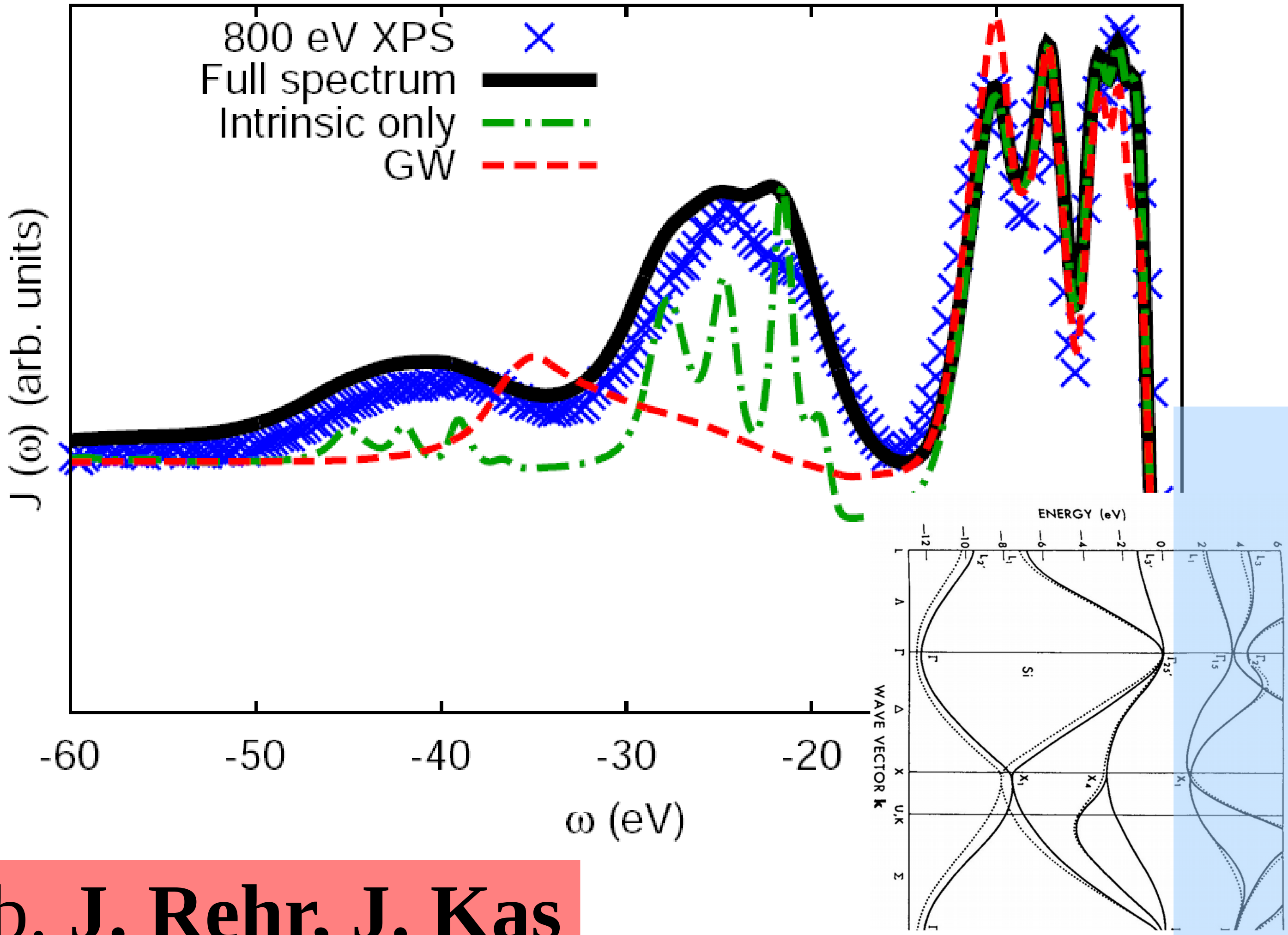
Stan, Romaniello, Rigamonti, Reining, Berger,
http://arxiv.org/abs/1503.07742

What is interesting in real materials?



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

→ W and satellites, a life beyond the GWA

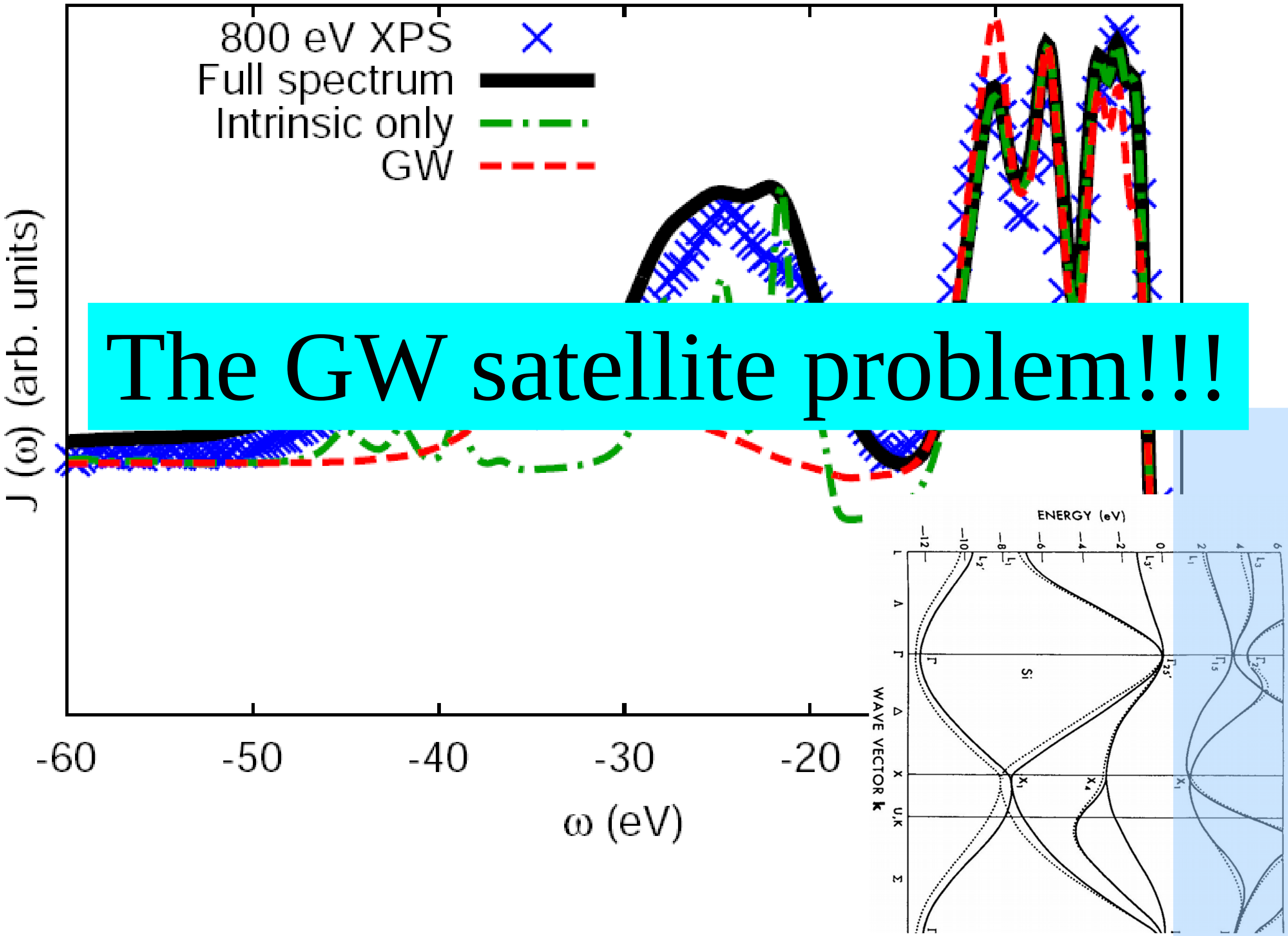


Collab. **J. Rehr, J. Kas**

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)

I - Removing nonlinearity

Approximating the Hartree potential

$$V_H(3;[\varphi]) \approx -i\int d4\, v(3^+,4)G(4,4^+;[\varphi])\Big|_{\varphi=0} - i\int d4\, d5\, v(3^+,4)\frac{\delta G(4,4^+;[\varphi])}{\delta\varphi(5)}\Big|_{\varphi=0}\varphi(5)+\cdots$$

Set of coupled **linearized** DEs (N-points)

$$\boxed{G(1,2;[\bar\varphi]) = G_H^0(1,2) + \int d3d5\, G_H^0(1,3)\bar\varphi(3)G(3,2;[\bar\varphi]) + i\int d3d5\, G_H^0(1,3)W(3^+,5)\frac{\delta G(3,2;[\bar\varphi])}{\delta\bar\varphi(5)}}$$

$\bar\varphi = \varphi\cdot\epsilon^{-1}$, $W = v\cdot\epsilon^{-1}$ and $G_H^0(1,2)$ is a Hartree G @ zero-potential

How good/bad the linearization is?

Working out $\frac{\delta G([\bar\varphi])}{\delta\bar\varphi}$ assuming $\frac{\delta\Sigma}{\delta\bar\varphi} = 0$

$$G(1,2;[\bar\varphi]) = G_H^0(1,2) + \int d3\, G_H^0(1,3)\bar\varphi(3)G(3,2;[\bar\varphi]) + i\int d3d5\, G_H^0(1,3)\underbrace{W(3^+,5)G(3,5;[\bar\varphi])}_{\Sigma_{GW}(3,5)}G(5,2;[\bar\varphi])$$

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

Relaxing 1-point in time → N-times

Decoupled differential equation

$$G(t_1,t_2;[\bar{\varphi}]) = G_H^0(t_1,t_2) + \int dt_3 G_H^0(t_1,t_3)\bar{\varphi}(t_3)G(t_3,t_2;[\bar{\varphi}]) + i\int dt_3 dt_5\, G_H^0(t_1,t_3)W(t_{3^+},t_5)\frac{\delta G(t_3,t_2;[\bar{\varphi}])}{\delta\bar{\varphi}(t_5)}$$

Iteration of the equation & ansatz for the solution

The iteration suggests an ansatz in the form

$$\tilde{y}(t_1,t_2;[\bar{\varphi}]) = \tilde{y}_{\varphi}(t_1,t_2)\cdot F_W(t_1,t_2)$$

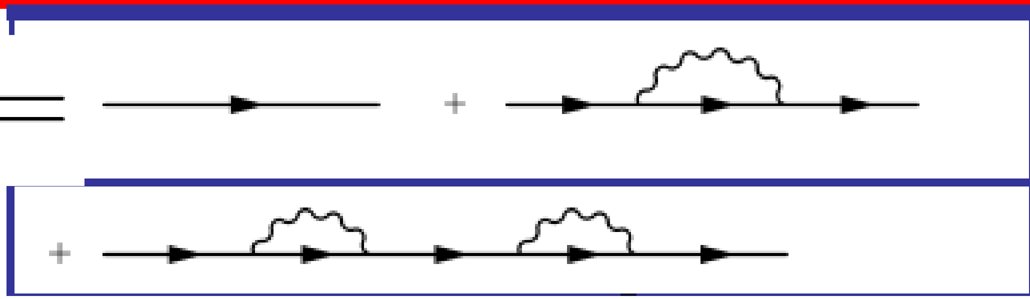
$$G(t_1,t_2)_{\bar{\varphi}=0} = G_H^0(t_1,t_2)e^{-i\int_{t_1}^{t_2} dt \int_t^{t_2} dt_4 W(t,t_4)}$$

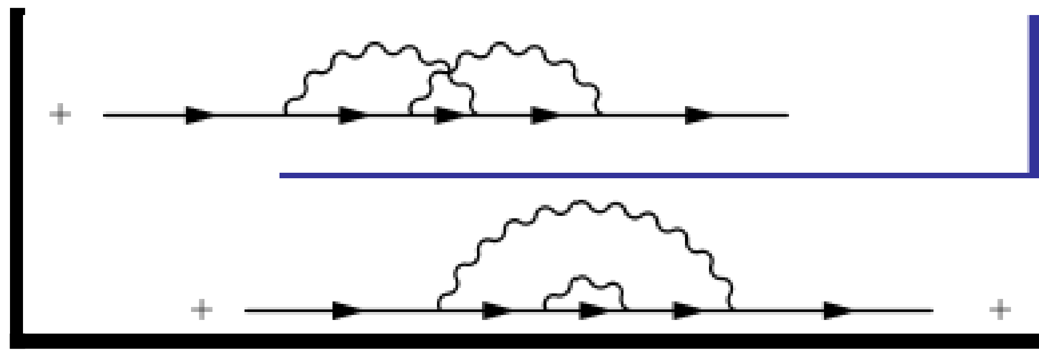
What can we use the exact exponential G for?

- Expanding the *exponential* G yields a *series of plasmon satellites*: beyond G_0W_0 spectral function[8]
- Exact G provides insights to tackle the full functional DE!

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

$\mathcal{G} =$





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

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

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

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

Exponential solution: ↔ cumulant expansion

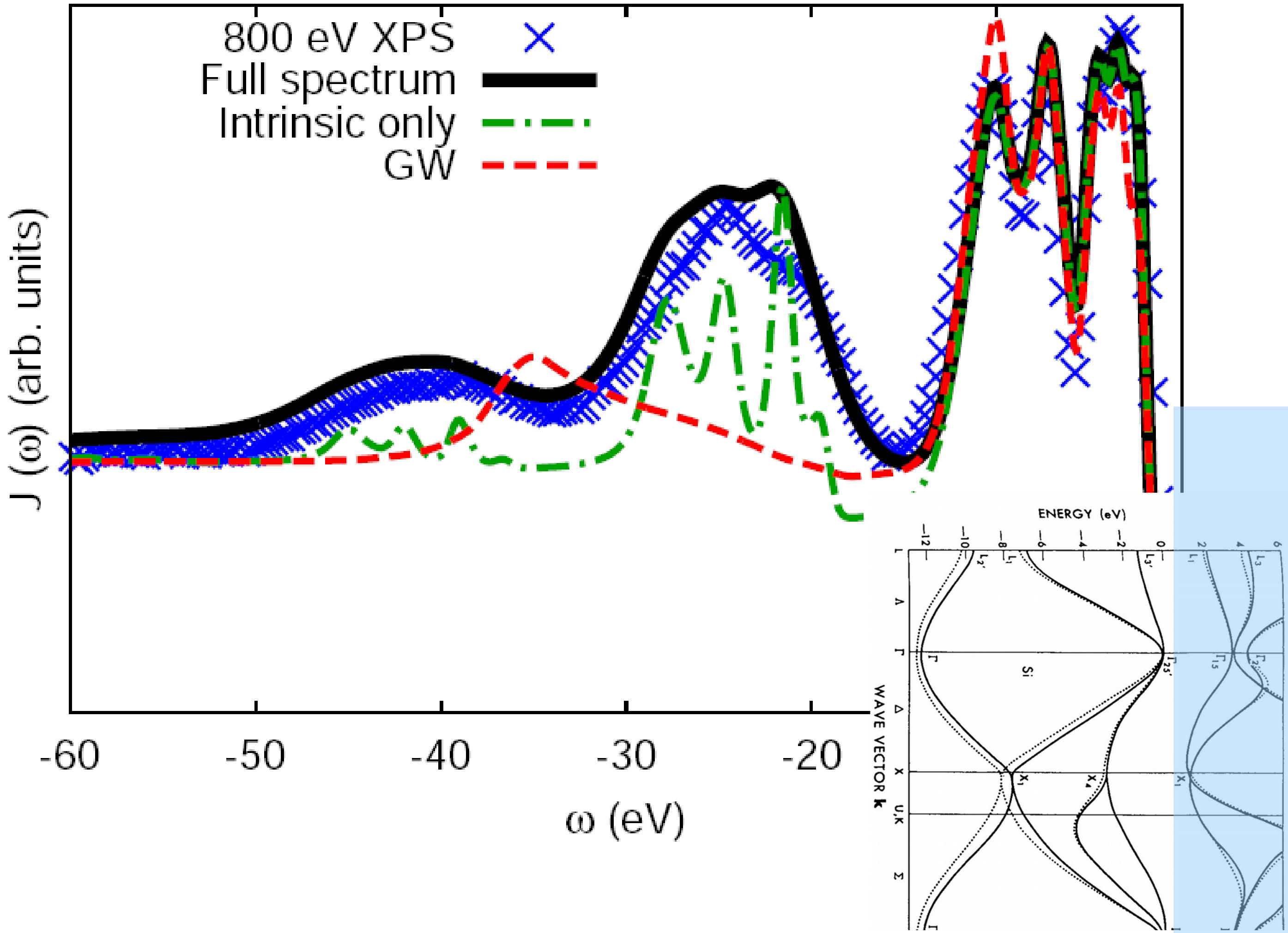
L. Hedin, Physica Scripta **21**, 477 (1980), ISSN 0031-8949.
L. Hedin, J. Phys.: Condens. Matter **11**, R489 (1999).
P. Nozieres and C. De Dominicis, Physical Review **178**, 1097 (1969), ISSN 0031-899X.
D. Langreth, Physical Review B **1**, 471 (1970).

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

Silicon: Kheifets et al., PRB 68, 2003

Here: the first in a series of approximations

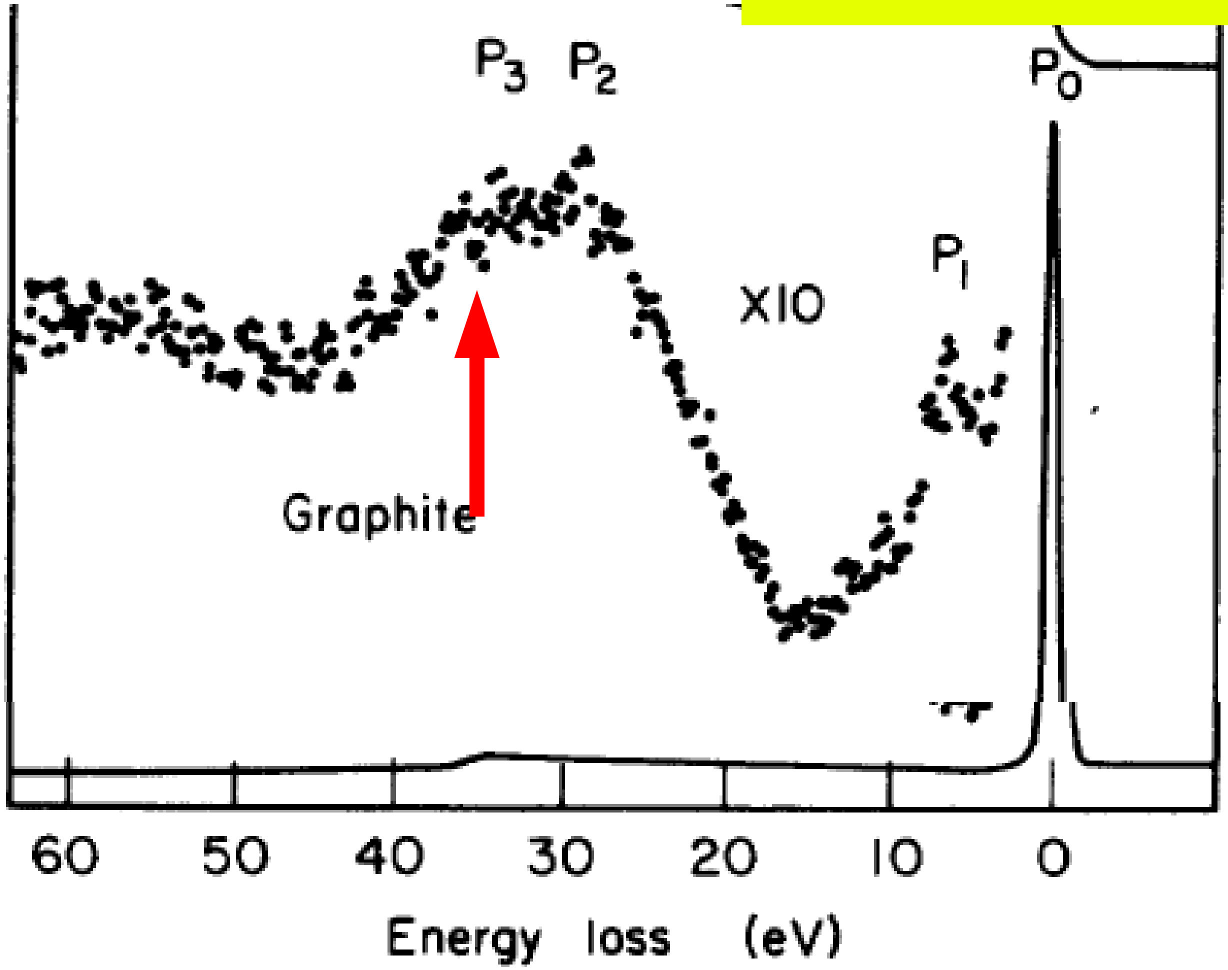
→ W and satellites, a life beyond the GWA



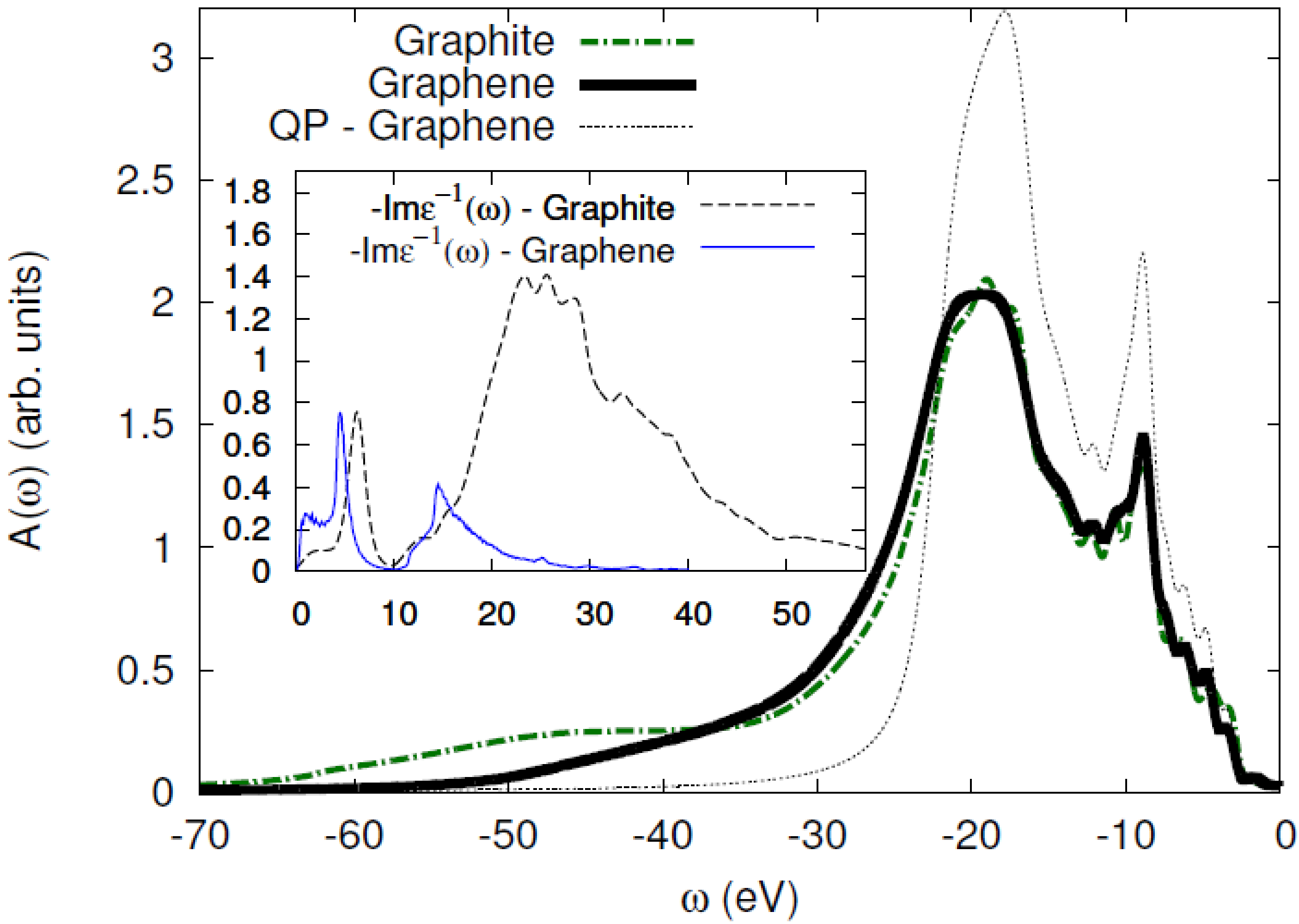
Cohen and Chelikowsky: “Electronic Structure and Optical Properties of Semiconductors” Solid-State Sciences 75, Springer-Verlag 1988)

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

XPS carbon 1s

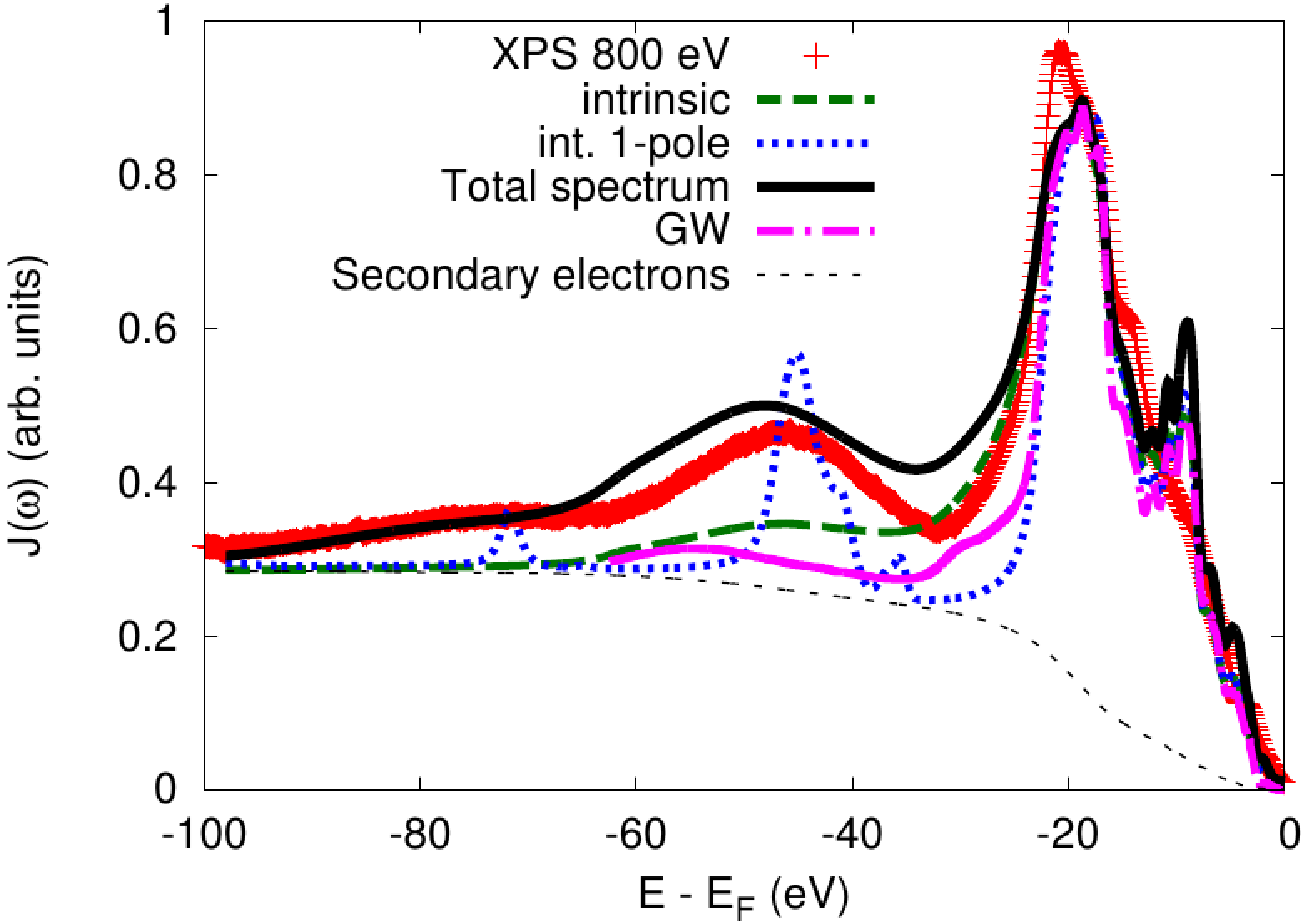


McFeely et al., PRB 9, 5268 (1974)



M. Guzzo et al., Phys. Rev. B 89, 085425 (2014)

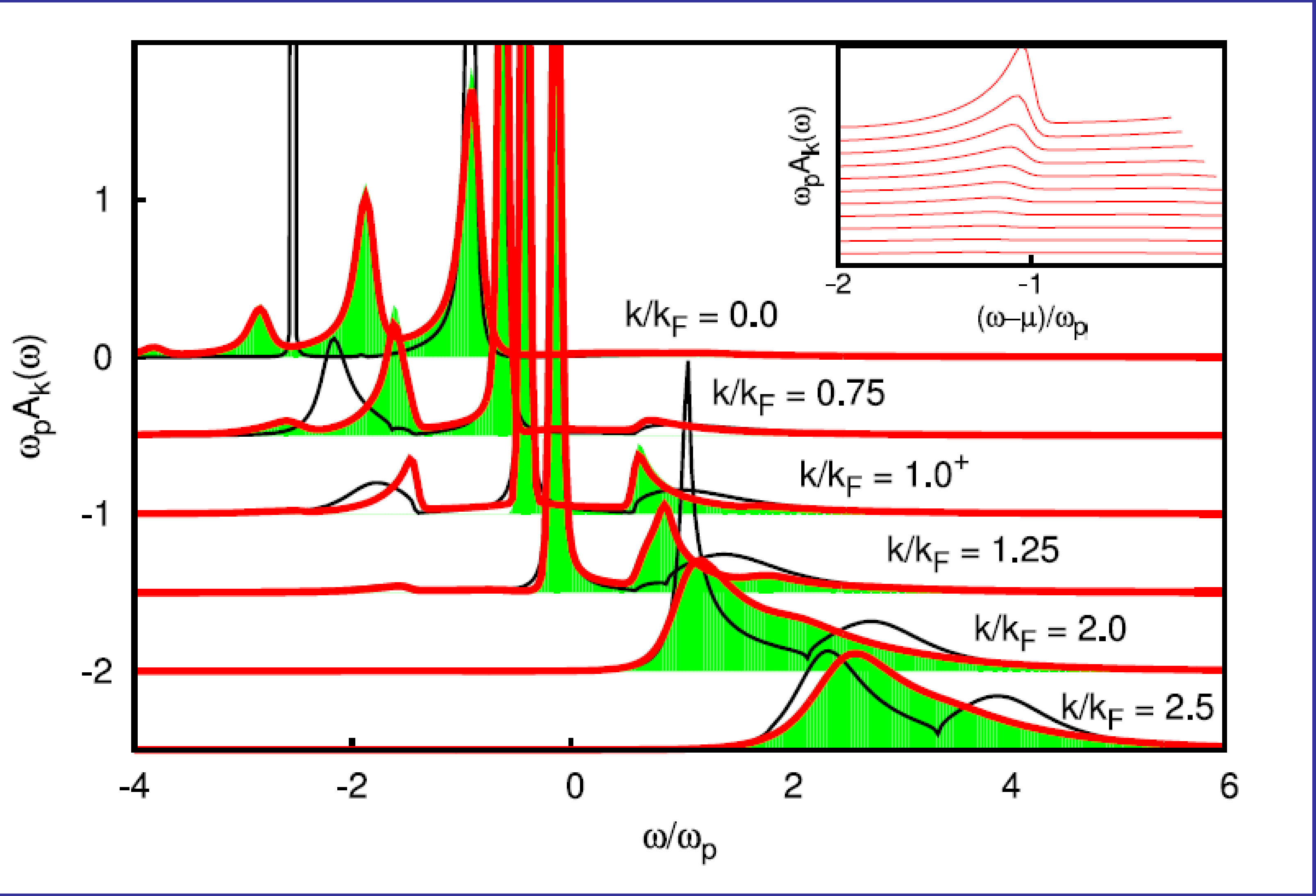
Graphite valence double plasmon: shift + broadening



Exp. on TEMPO

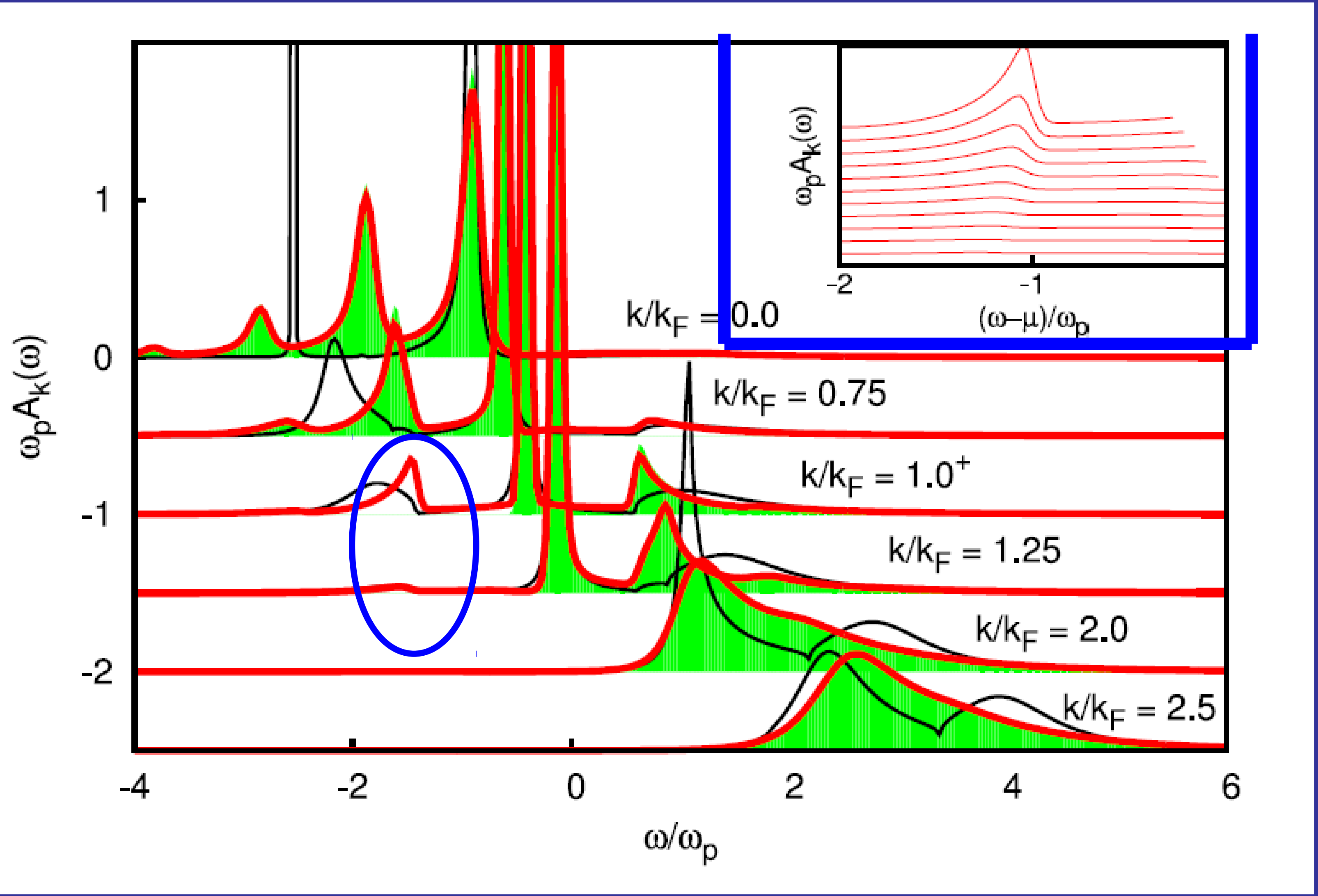
M. Guzzo et al., Phys. Rev. B 89, 085425 (2014)

Coupling occupied and empty states: more correlation

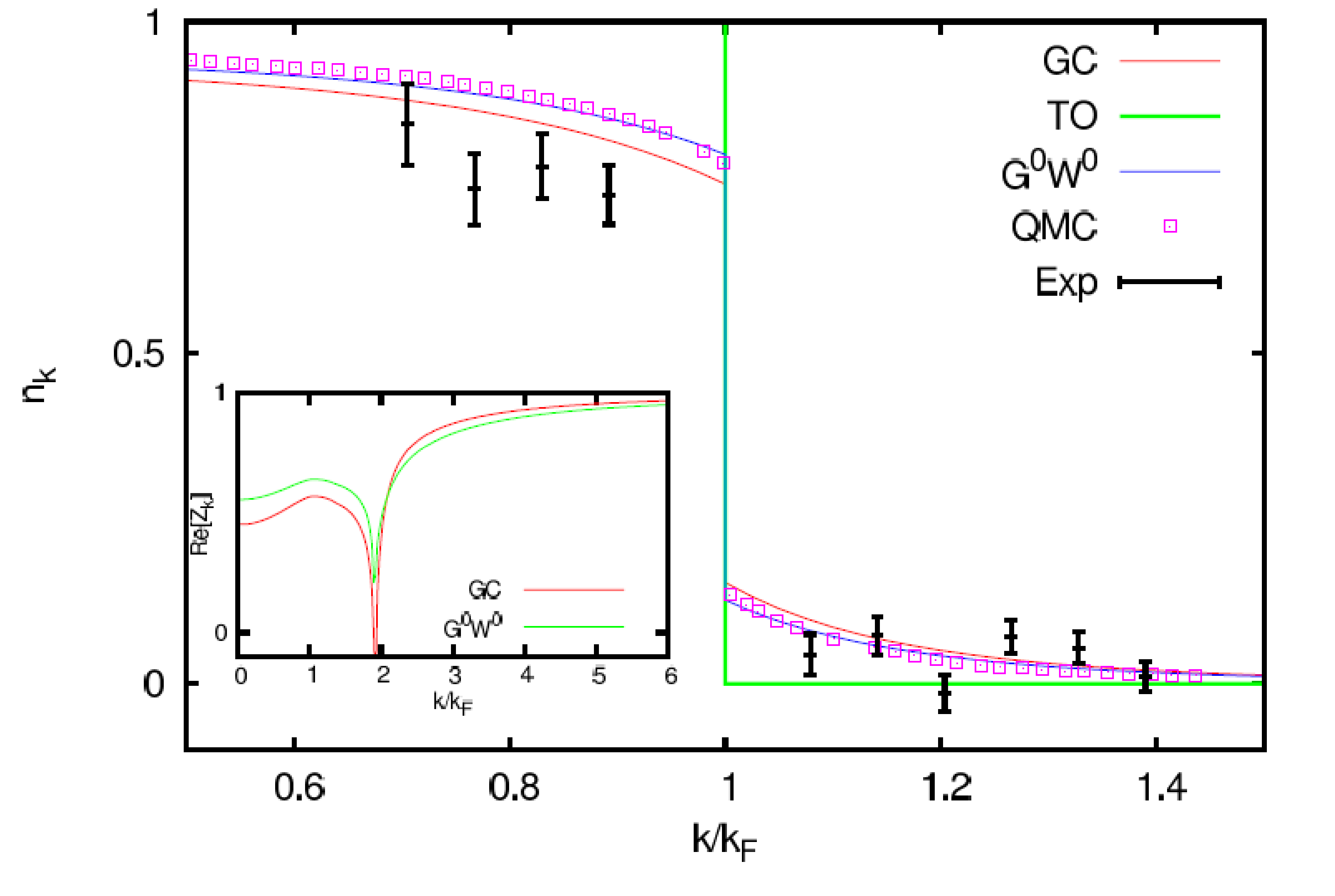


Kas, Rehr, Reining (2014) Phys. Rev. B 90, 085112 (2014)

Coupling occupied and empty states: more correlation



Kas, Rehr, Reining (2014) Phys. Rev. B 90, 085112 (2014)



Kas, Rehr, Reining (2014) Phys. Rev. B 90, 085112 (2014)

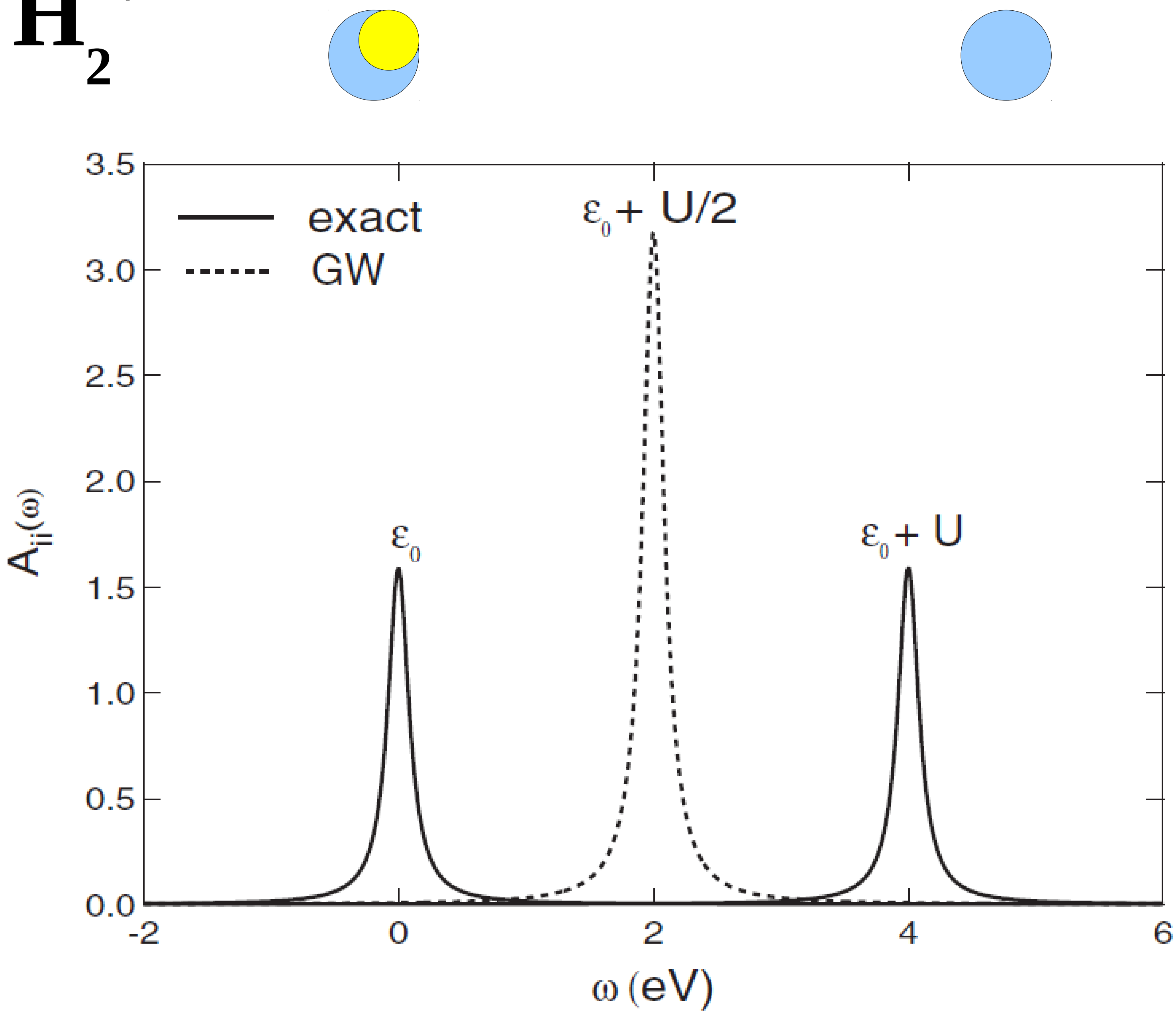
H_2^+

Independent particle excitation

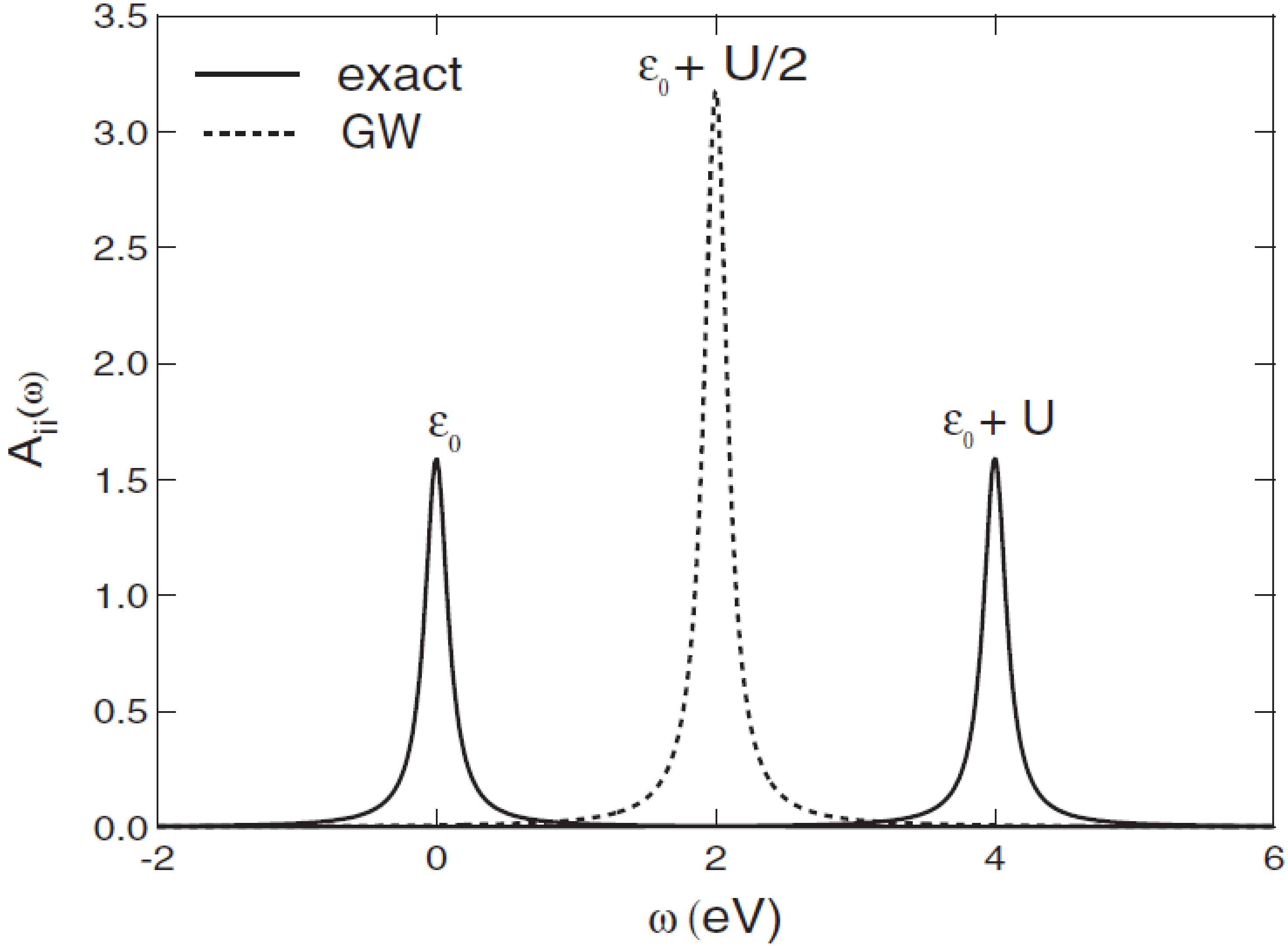
H_2^+

Independent particle excitation

H_2^+

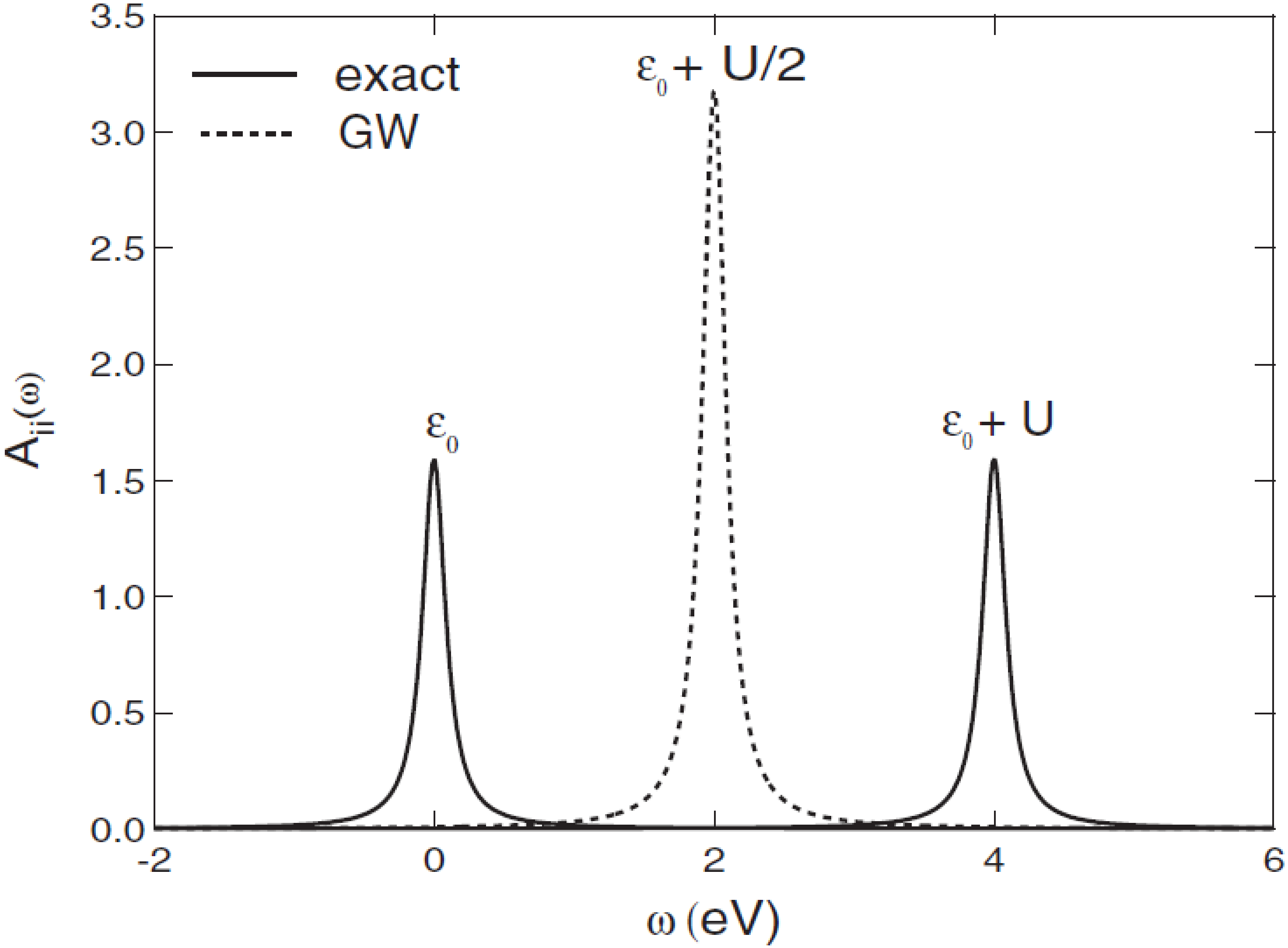


H_2^+

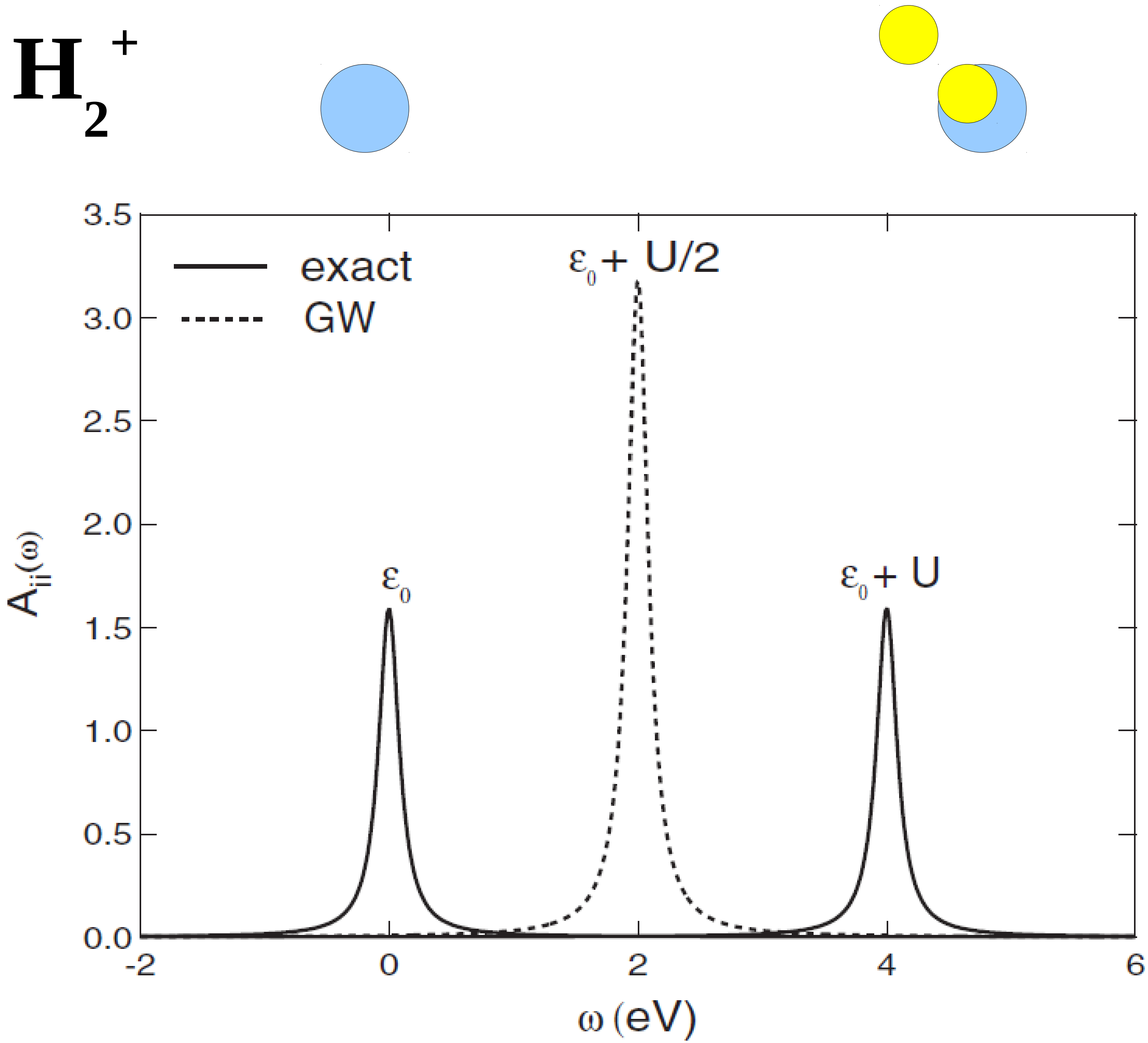


exact
GW
$\varepsilon_0 + U/2$
ε_0
$\varepsilon_0 + U$
$A_{ii}(\omega)$
ω (eV)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-2
0
2
4
6

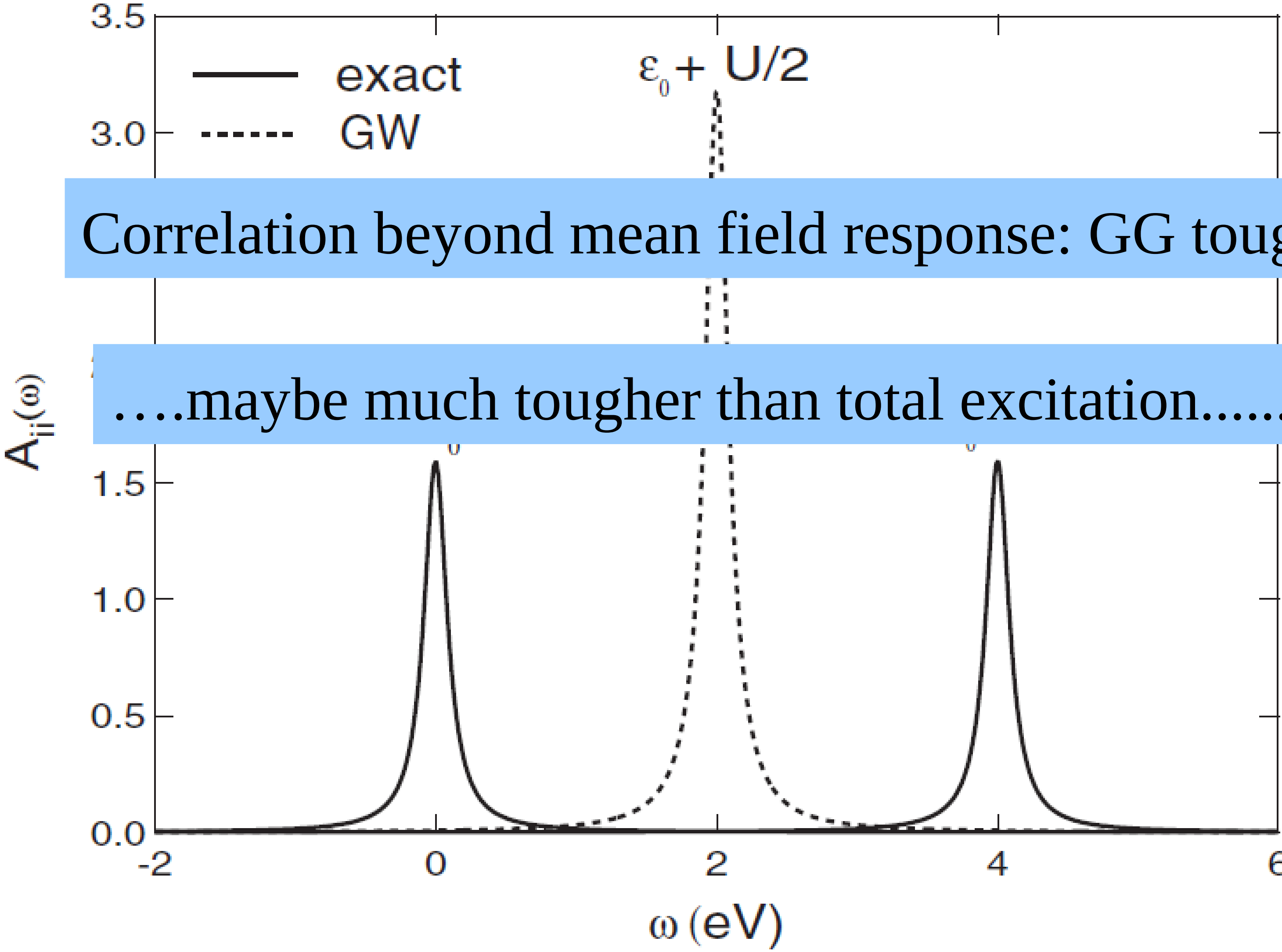
H_2^+



H_2^+



H_2^+



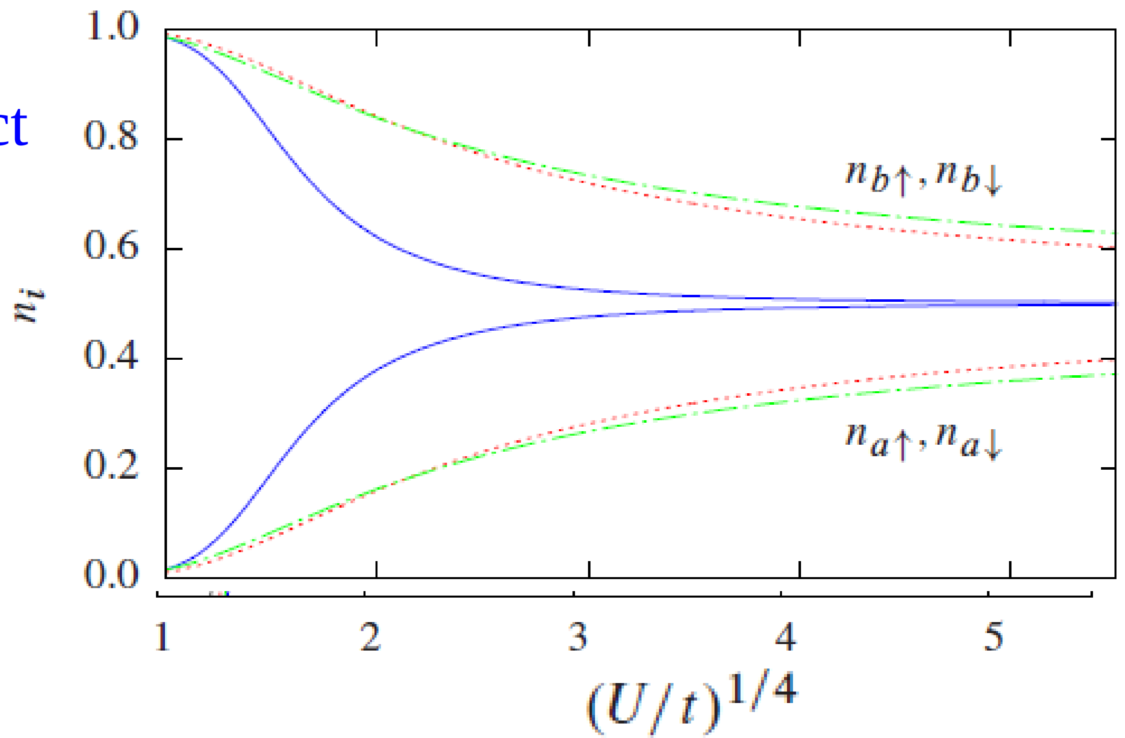
Correlation beyond mean field response: GG tough!

….maybe much tougher than total excitation........

→ Correlation and occupation numbers

exact

GW

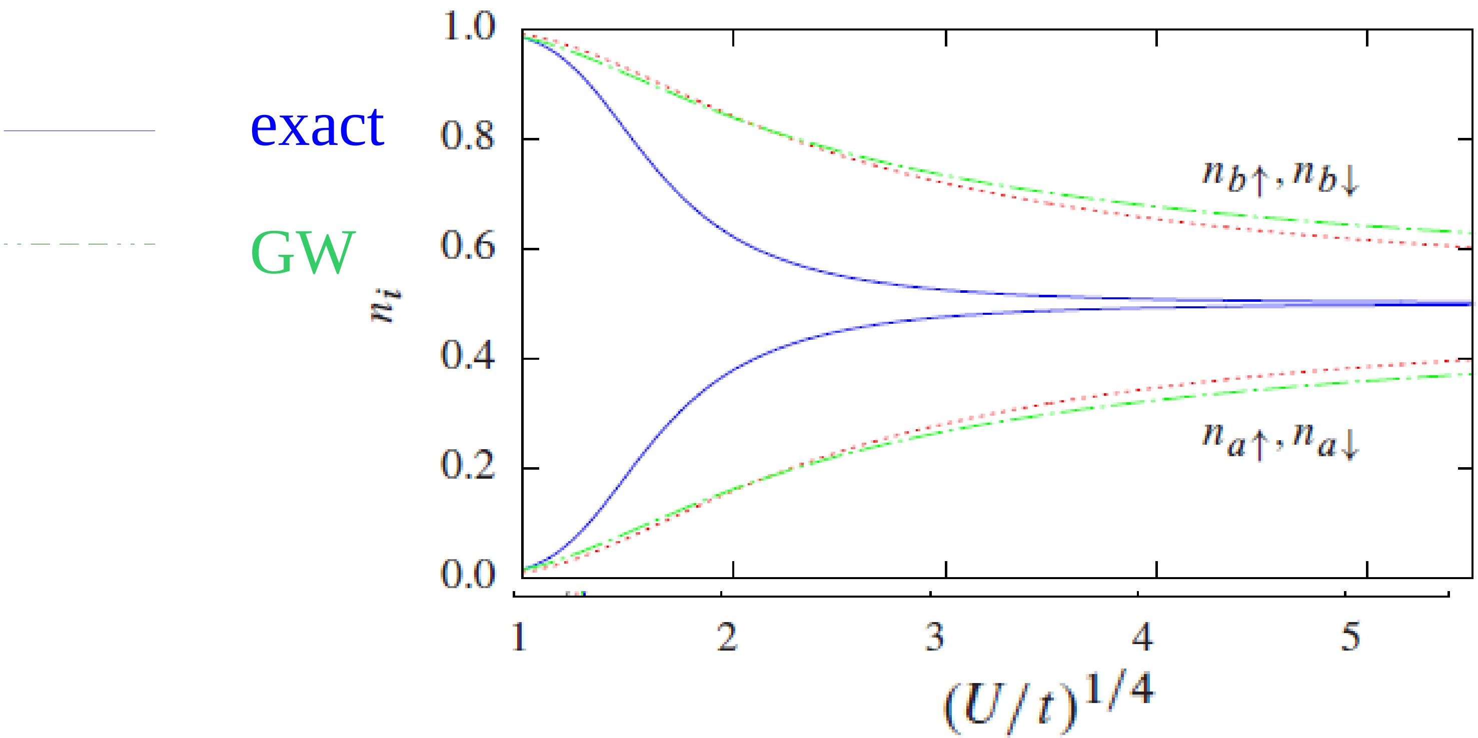


Hubbard,
½ filling

Fractional occupation === we don't know → have to correlate

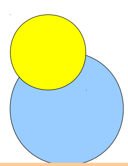
Di Sabatino, Berger, Reining, Romaniello
http://arxiv.org/abs/1409.1008

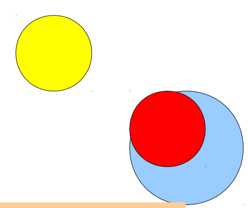
→ Correlation and occupation numbers



Hubbard,
½ filling

Fractional occupation === we don't know → have to correlate





Di Sabatino, Berger, Reining, Romaniello
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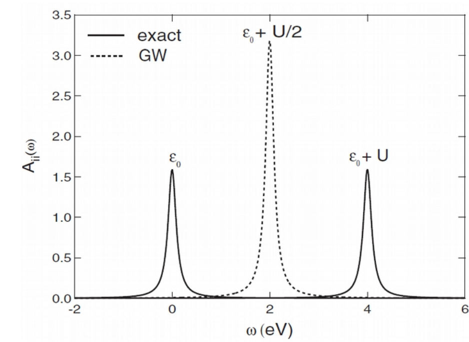


Spectral functions from density matrices?

$$G_{ij}(\omega) = \sum_k \frac{A_{ij}^{k,R}}{\omega - \epsilon_k^R - i\eta} + \sum_k \frac{B_{ij}^{k,A}}{\omega - \epsilon_k^A + i\eta}$$

$$\sum_k \frac{A_{ij}^{k,R}}{\omega - \epsilon_k^R} = \sum_k \frac{A_{ij}^{k,R}}{\omega - \delta_{ij}^R(\omega)}$$

$$A_{ij}^{k,R} = \langle\Psi_0|c_j^\dagger|\Psi_k^{N-1}\rangle\langle\Psi_k^{N-1}|c_i|\Psi_0\rangle$$

$$G_{ii}^{\sigma_i}(\omega) = \frac{n_i}{\omega - \delta_{i\sigma_i}^R(\omega)} + \frac{1 - n_i}{\omega - \delta_{i\sigma_i}^A(\omega)}$$

The “effective energies” δ are approximated
with a series of commutators, following
Berger, Reining, Sottile, PRB 82, 041103 (2010)

$$E_0 - E_k^{N-1} = \epsilon_k^R$$

Using [c,H] = α c + rest

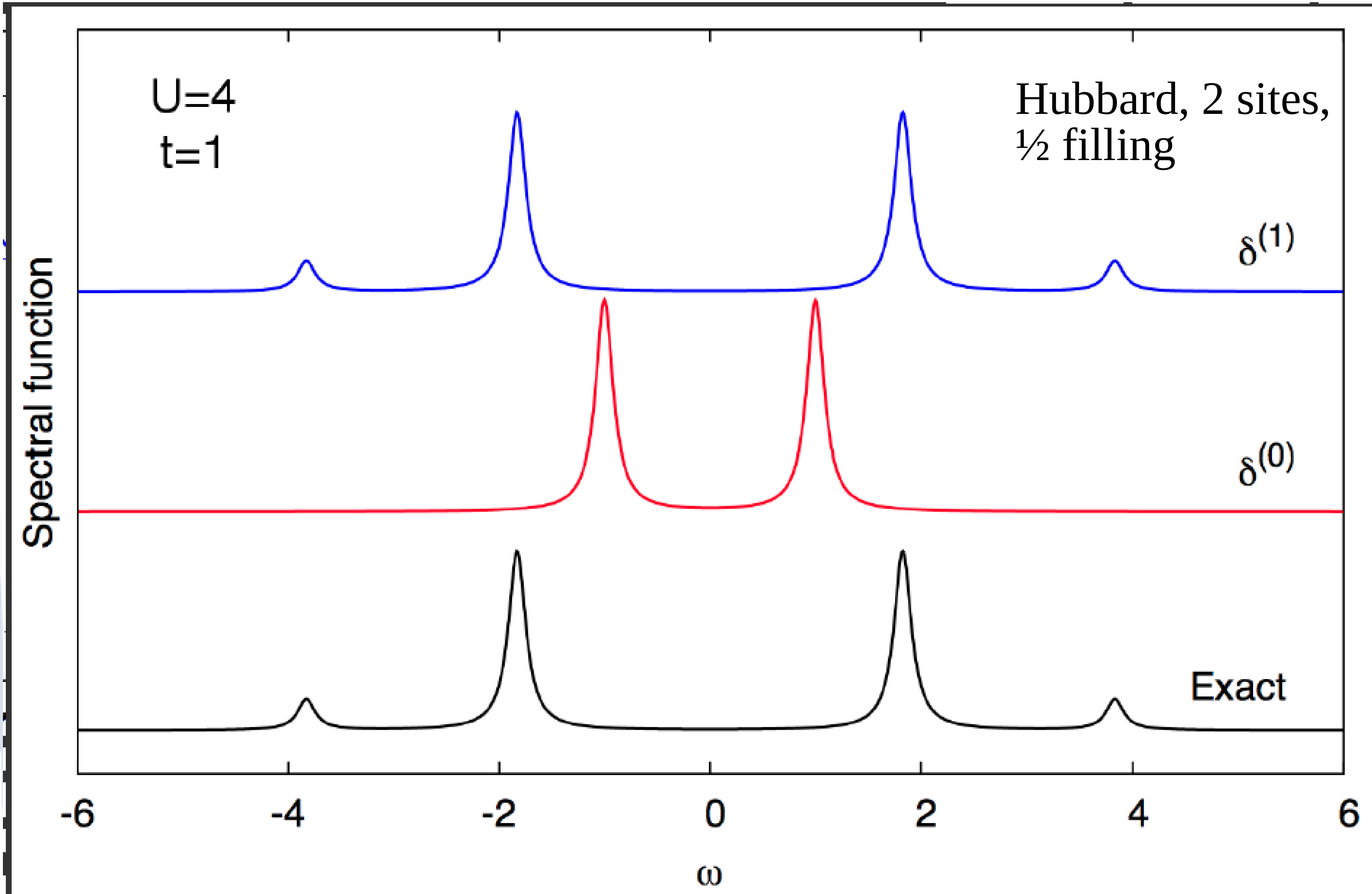
$$\delta^{R,(0)}_{i\sigma_i}(\omega) \;=\; h_{ii}$$

$$\delta^{R,(1)}_{i\sigma_i}(\omega) \;=\; h_{ii} + \frac{\tilde{n}^R_{i\sigma_i}}{n_{i\sigma_i}}$$

$$\delta^{R,(2)}_{i\sigma_i}(\omega) \;=\; h_{ii} + \frac{\tilde{n}^R_{i\sigma_i}}{n_{i\sigma_i}} \frac{\omega - h_{ii} - \frac{\tilde{n}^R_{i\sigma_i}}{n_{i\sigma_i}}}{\omega - h_{ii} - \frac{\tilde{\tilde{n}}^R_{i\sigma_i}}{\tilde{n}^R_{i\sigma_i}}}$$

....

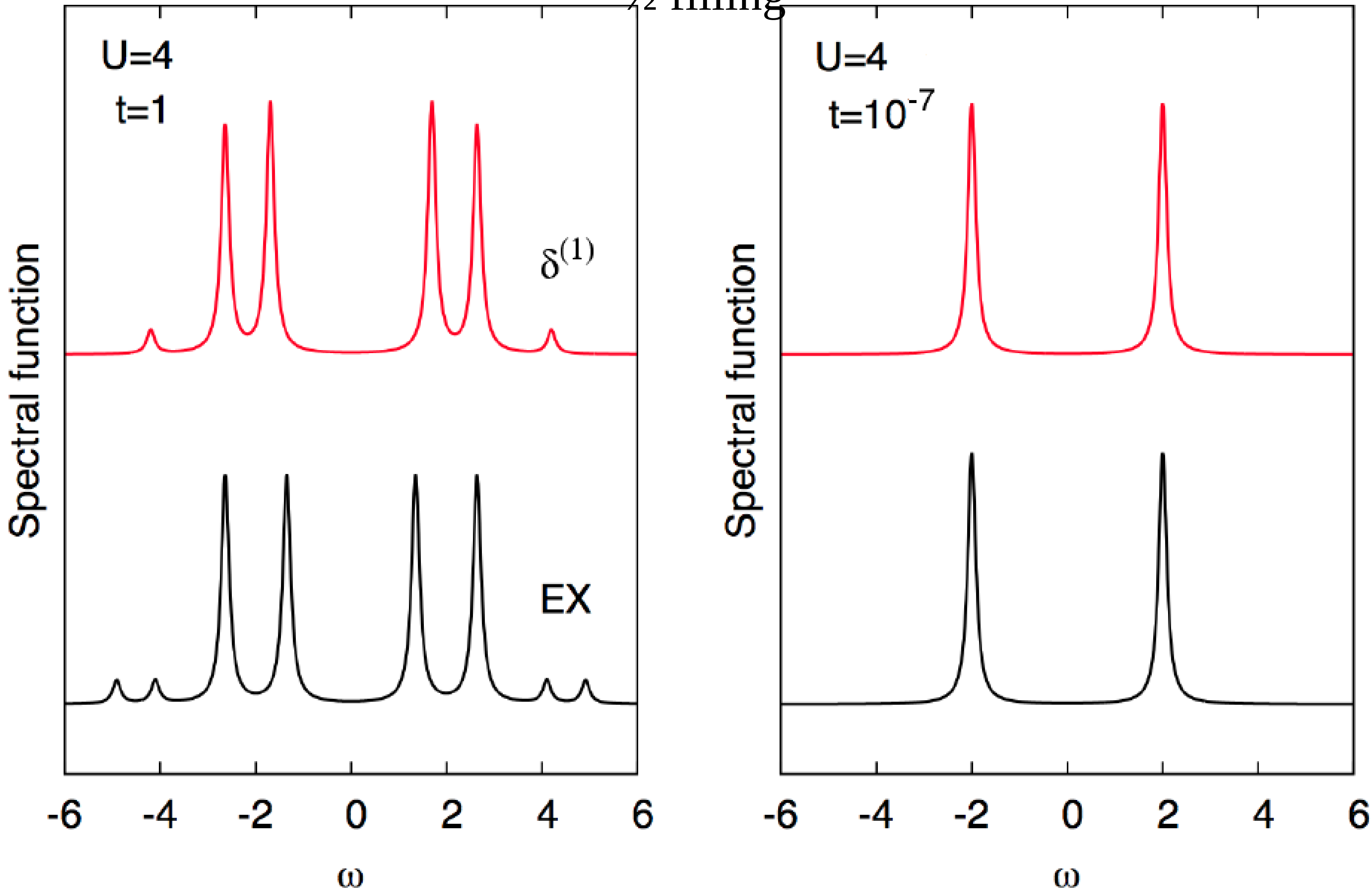
$$\begin{aligned} \tilde{n}^R_n \;&=\; \sum_{jkl} (V_{njkl} - V_{jnkl}) \Gamma_{njlk} \\ &\sim\; \frac{1}{2} \sum_{jkl} (V_{njkl} - V_{jnkl}) \left(n_n n_j \delta_{nk} \delta_{jl} - n^\alpha_n n^\alpha_j \delta_{nl} \delta_{jk} \right) \end{aligned}$$



U=4
t=1
Hubbard, 2 sites,
½ filling
δ(1)
δ(0)
Exact
Spectral function
-6
-4
-2
0
2
4
6
ω

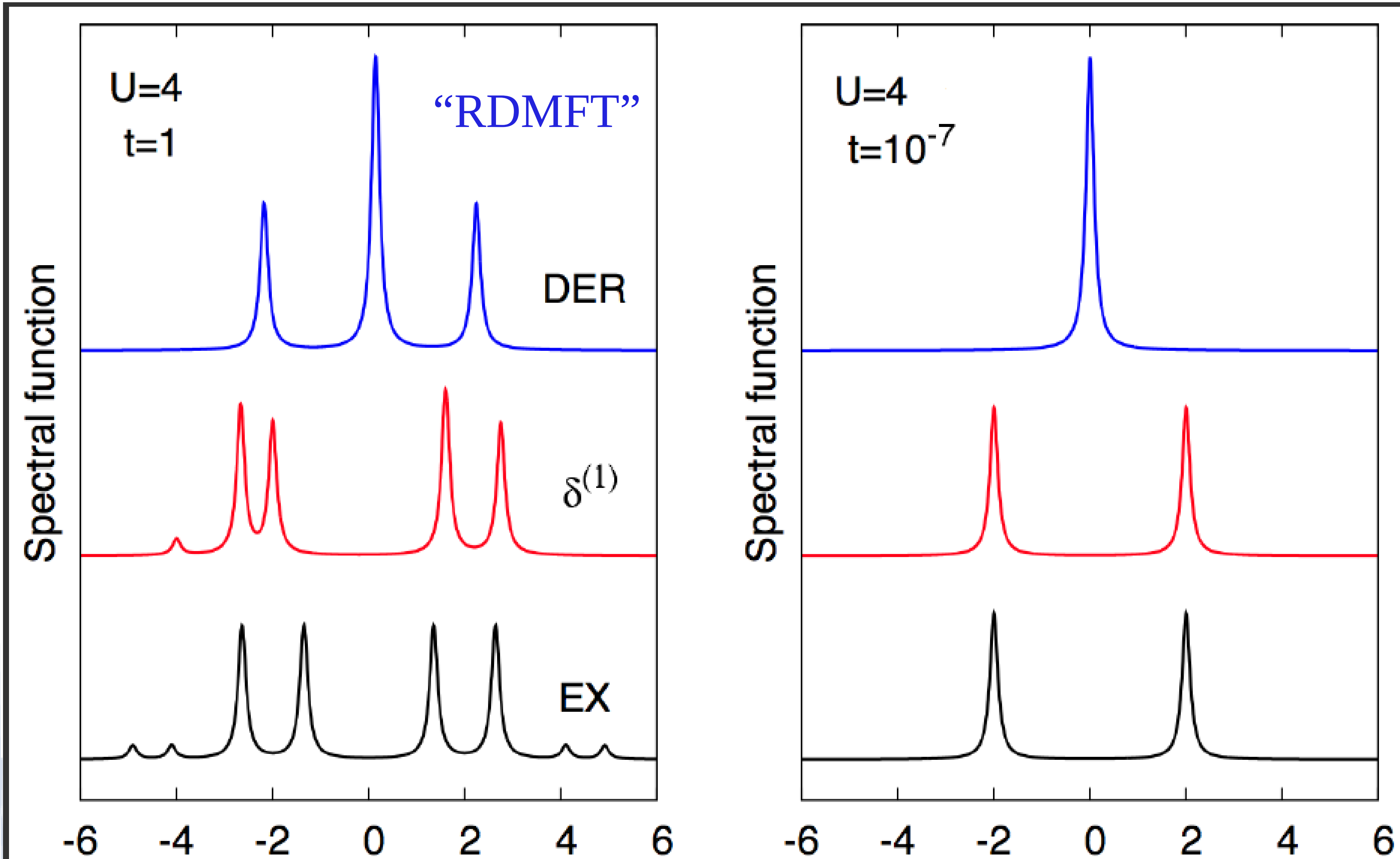
Hubbard, 4 sites,
½ filling

Exact fctl



Hubbard, 4 sites,
½ filling

Mueller fctl



DER: S. Sharma, et al. , Phys. Rev. Lett. 110, 116403 (2013).

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

→ Correlation and occupation numbers

→ Conclusions

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Berlin: **Santiago Rigamonti**
U. Washington: **John Rehr, Joshua Kas**

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