DFT: INSIGHT FROM MBPT

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Université Paul Sabatier
TOULOUSE III

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The many-body problem

$$\hat{H}\Psi(x_1, ..., x_N) = E\Psi(x_1, ..., x_N) \longrightarrow F[\Psi]$$

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$\Psi \longrightarrow$ Reduced quantities

$\rho(1)$ density

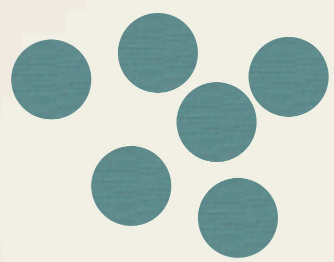
$G(12)$ 1-particle Green's function

DFT & MBPT

* DFT

density $\rho(1)$

Kohn-Sham system



electron-electron interaction $\longrightarrow V_{xc}$

DFT & MBPT

✳DFT

density $\rho(1)$

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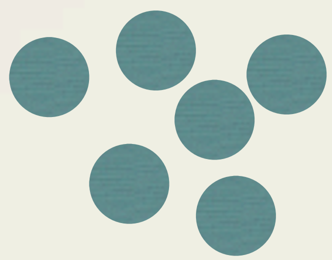

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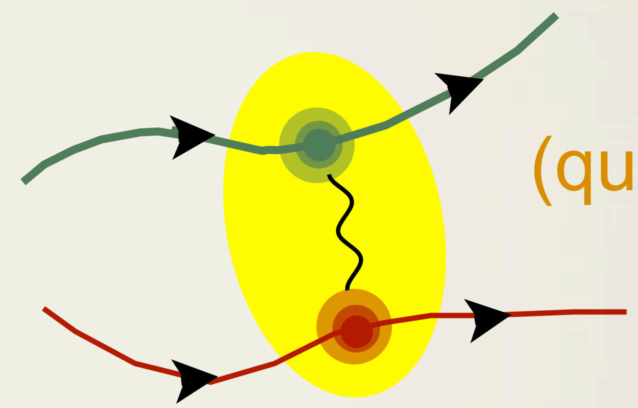
✳MBPT

$G(12)$ 1-particle Green's function



(quasi)particles

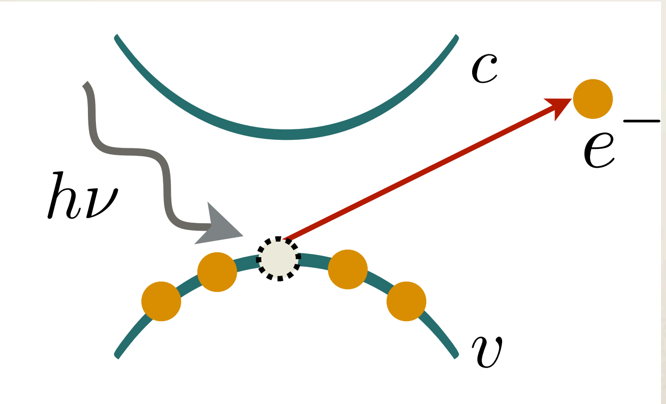
$\Sigma_{xc} \longleftarrow$ electron-electron interaction

One-particle Green's function

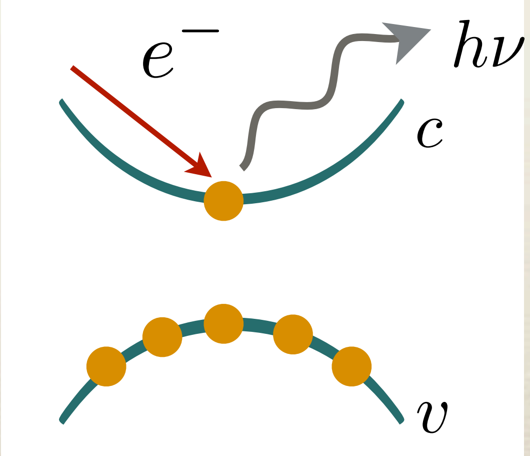
MBPT

$$G(12) = -i\langle\Psi|T\left[\psi(1)\psi^{\dagger}(2)\right]\Psi\rangle$$

- Expectation value of any single particle operator, e.g., $\rho(1) = -iG(11^{+})$
- Total energy $E_0 = -\frac{i}{2}\int dx_1 \lim_{x_2\to x_1}\lim_{t_2\to t_1^{+}}\left[i\frac{\partial}{\partial t_1} + h_0(r_1)\right]G(12)$
- Photoemission spectra $\sim Im[G(\omega)]$



removal energies



addition energies

The Sham-Schlüter equation

$$\rho(1) = -iG_{KS}(11^+) = -iG(11^+)$$

L. J. Sham and M. Schlüter, Phys. Rev. Lett. 51, 1888 (1983);Y. M. Niquet, M. Fuchs, and X. Gonze, J. Chem. Phys. 118, 9504 (2003)

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$$\rho(1) = -iG_{KS}(11^+) = -iG(11^+)$$

- Sham-Schlüter equation

$$\int dr_3 v_{xc}(r_3) \int d\omega e^{i\omega\eta} G_{KS}(r_1 r_3;\omega) G(r_3 r_1;\omega) =$$

$$\int d\omega dr_3 dr_4 e^{i\omega\eta} G_{KS}(r_1 r_3;\omega) \Sigma_{xc}(r_3 r_4;\omega) G(r_4 r_1;\omega)$$

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DFT $\longleftarrow$ MBPT

- Linearized Sham-Schlüter equation (OEP)

$$\int dr_3 v_{xc}(r_3) \chi_{KS}(r_1 r_3;\omega = 0) =$$

$$-\frac{i}{2\pi} \int d\omega dr_3 dr_4 e^{i\omega\eta} G_{KS}(r_1 r_3;\omega) \Sigma_{xc}(r_3 r_4;\omega) G_{KS}(r_4 r_1;\omega)$$

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Outline

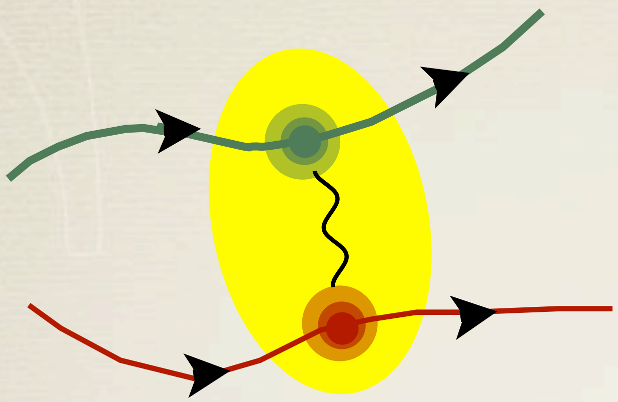
- How to calculate G?
  - Approximations to the self-energy
  - Approximations to the 1-particle Green's function
- Summary

Collaborations

- Lucia Reining
  Ecole Polytechnique, Palaiseau (France)
- Giovanna Lani
  Ecole Polytechnique, Palaiseau (France)
- Matteo Guzzo
  Ecole Polytechnique, Palaiseau (France)
- Friedhelm Bechstedt
  Friedrich-Schiller-Univeritaet, Jena (Germany)

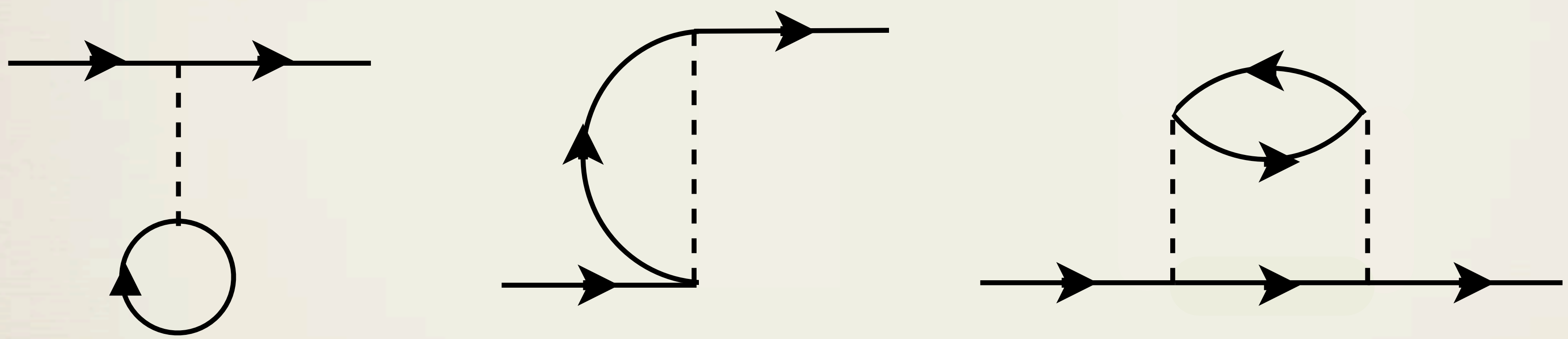
One-particle Green's function

- MBPT



moving (quasi) particles around

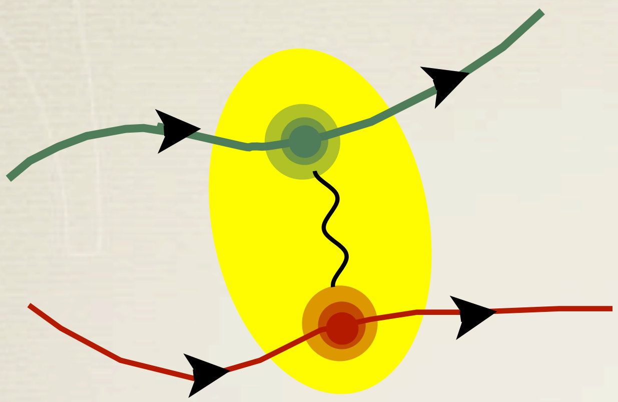
$$G(12) = -i\langle\Psi|T\left[\psi(1)\psi^{\dagger}(2)\right]\Psi\rangle$$



etc etc...

One-particle Green's function

- MBPT



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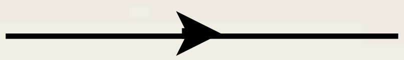
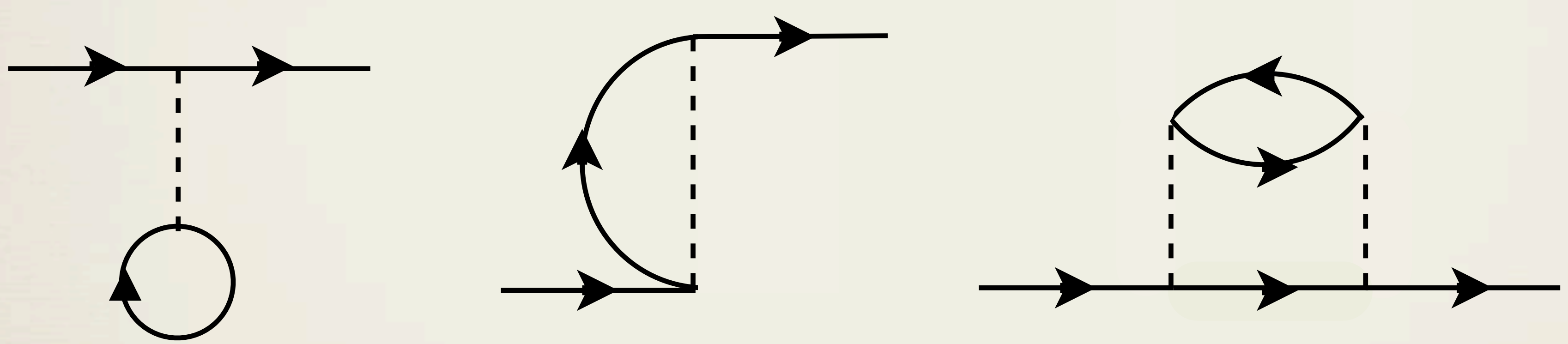
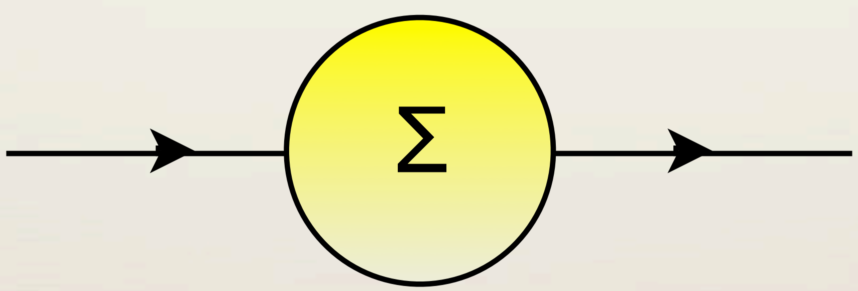




etc etc...



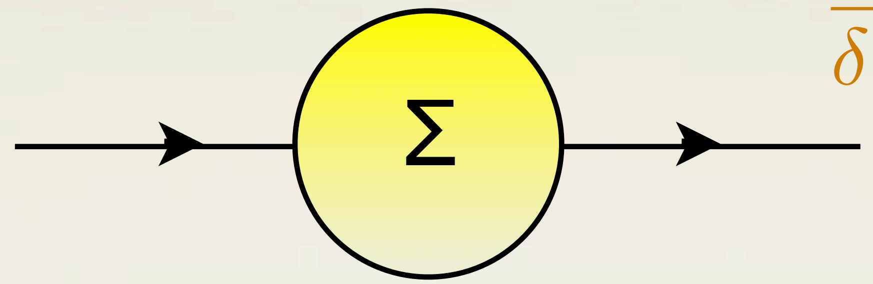
Self-energy

$$G = G_0 + G_0\Sigma G$$

Self-energy

$$\Sigma(12) = v_H(12) + \Sigma_x(12) + iG(13)\Xi(35;26)L(64;54)v(41)$$

$$\frac{\delta \Sigma}{\delta G} \qquad \frac{\delta G}{\delta \varphi}$$



L. Hedin, Phys. Rev. 139, A796 (1965)

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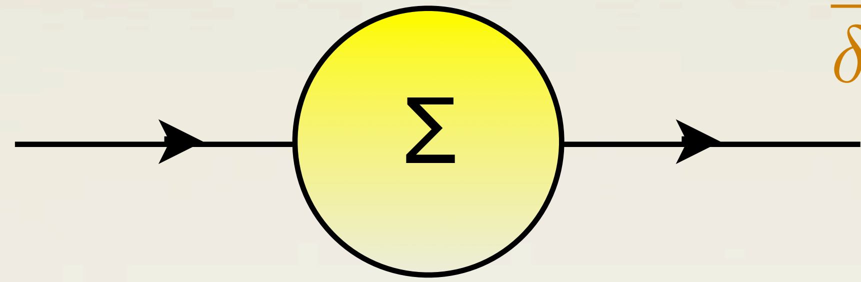
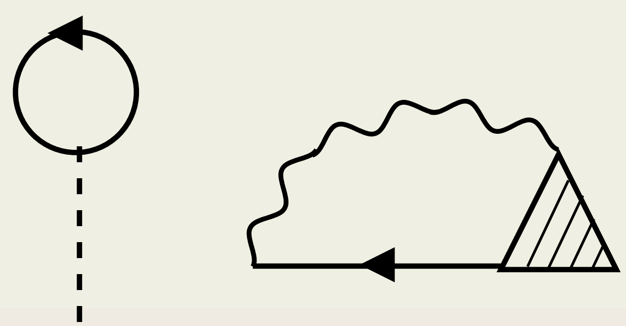
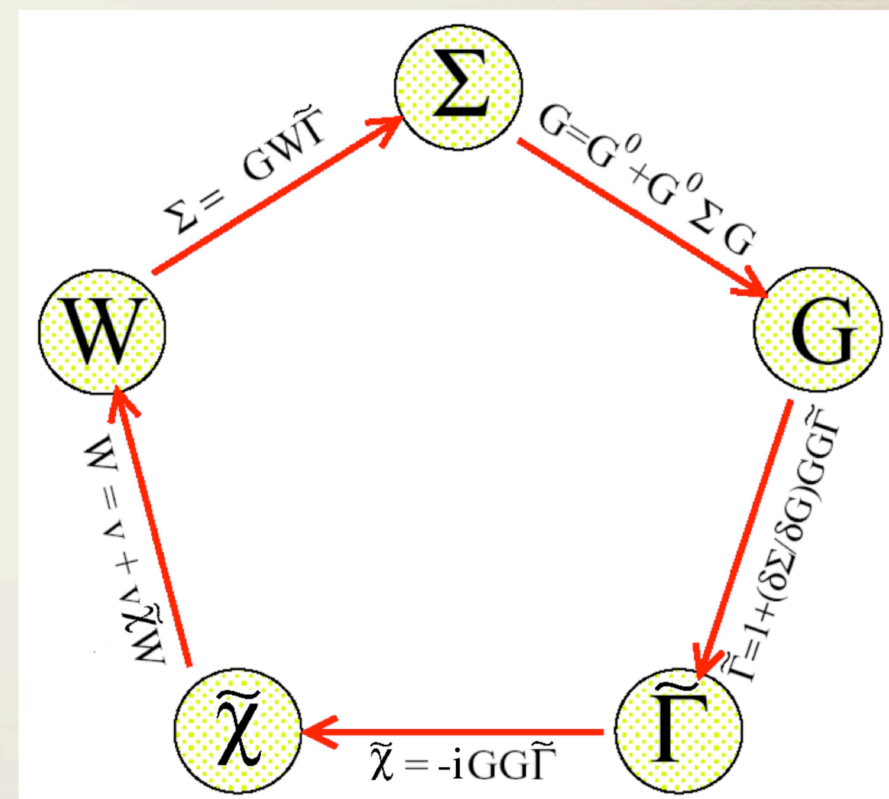


Hedin's eqs

$$\Sigma = v_H + iGW\Gamma$$





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GW Self-energy

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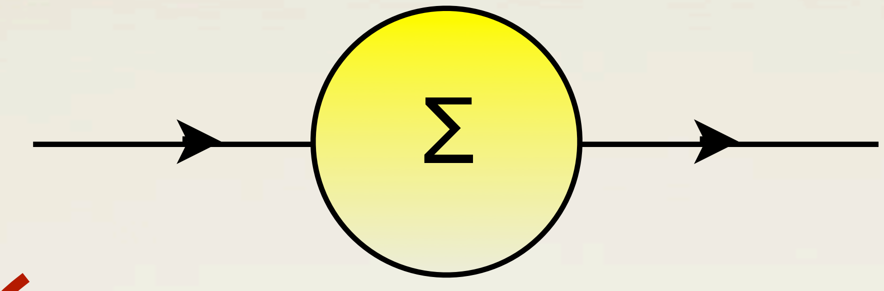

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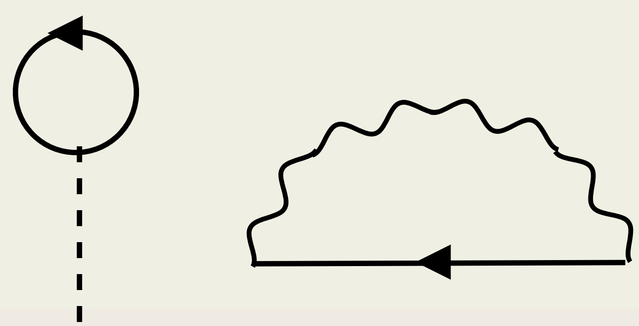

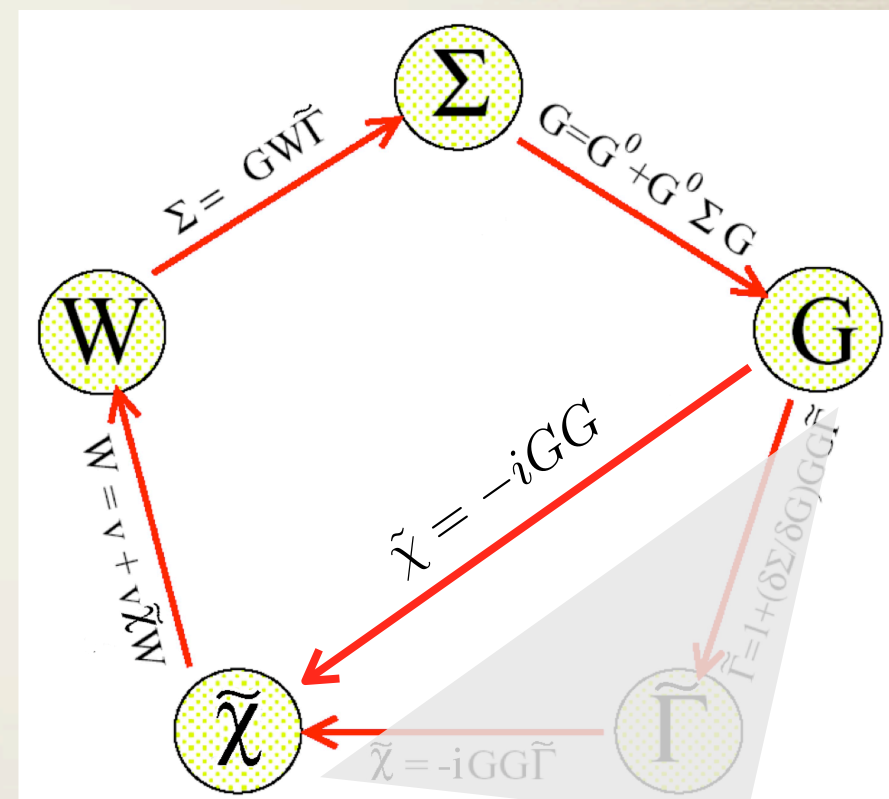

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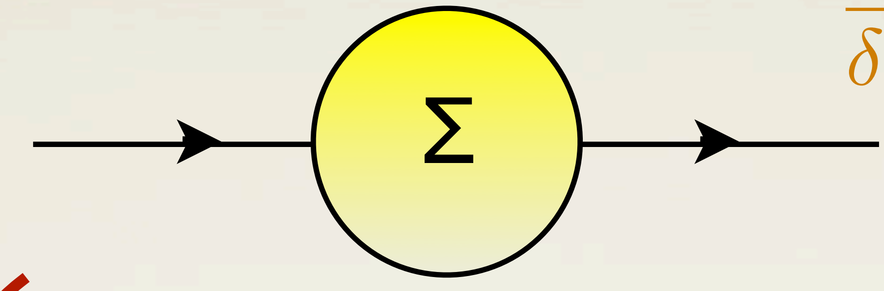
GW Self-energy

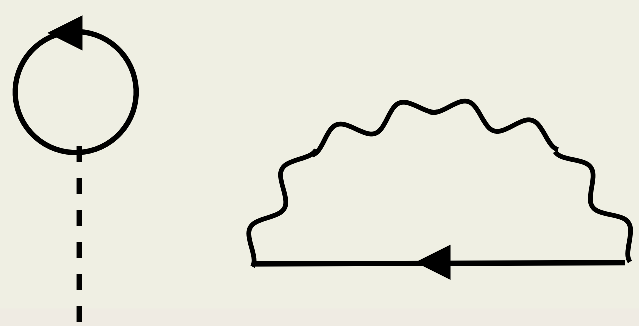
$$\Sigma(12) = v_H(12) + \Sigma_x(12) + iG(13)\Xi(35;26)L(64;54)v(41)$$

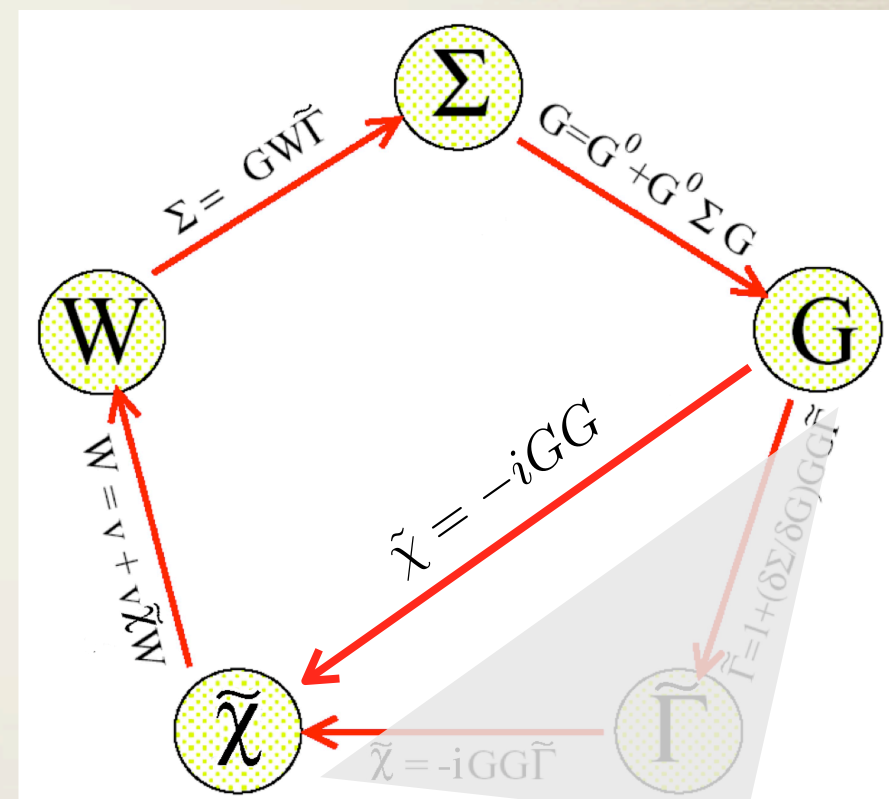
$$\frac{\delta\Sigma}{\delta G} \approx \frac{\delta v_H}{\delta G} \qquad \frac{\delta G}{\delta\varphi} \approx GG$$



Hedin's eqs

$$\Sigma = v_H + iGW$$





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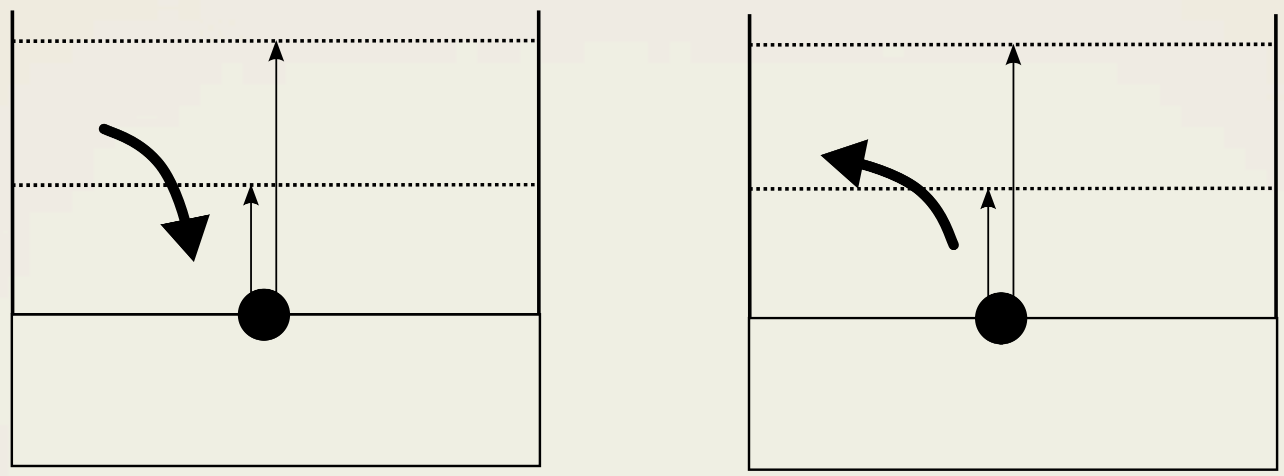
Limits of GW

- **Self-screening** (bad treatment of the induced exchange)



Addition energy $\neq$ Removal energy

$$E_{N+1} - E_N = \epsilon^{add} \neq E_N - E_{N-1} = \epsilon^{rem}$$

Change in the total energy adding and then removing an electron!

P. Romaniello, S. Guyot, and L. Reining, J. Chem. Phys., 131, 154111 (2009)

Limits of GW

- Incorrect atomic limit (bad treatment of correlation)

H_2^+

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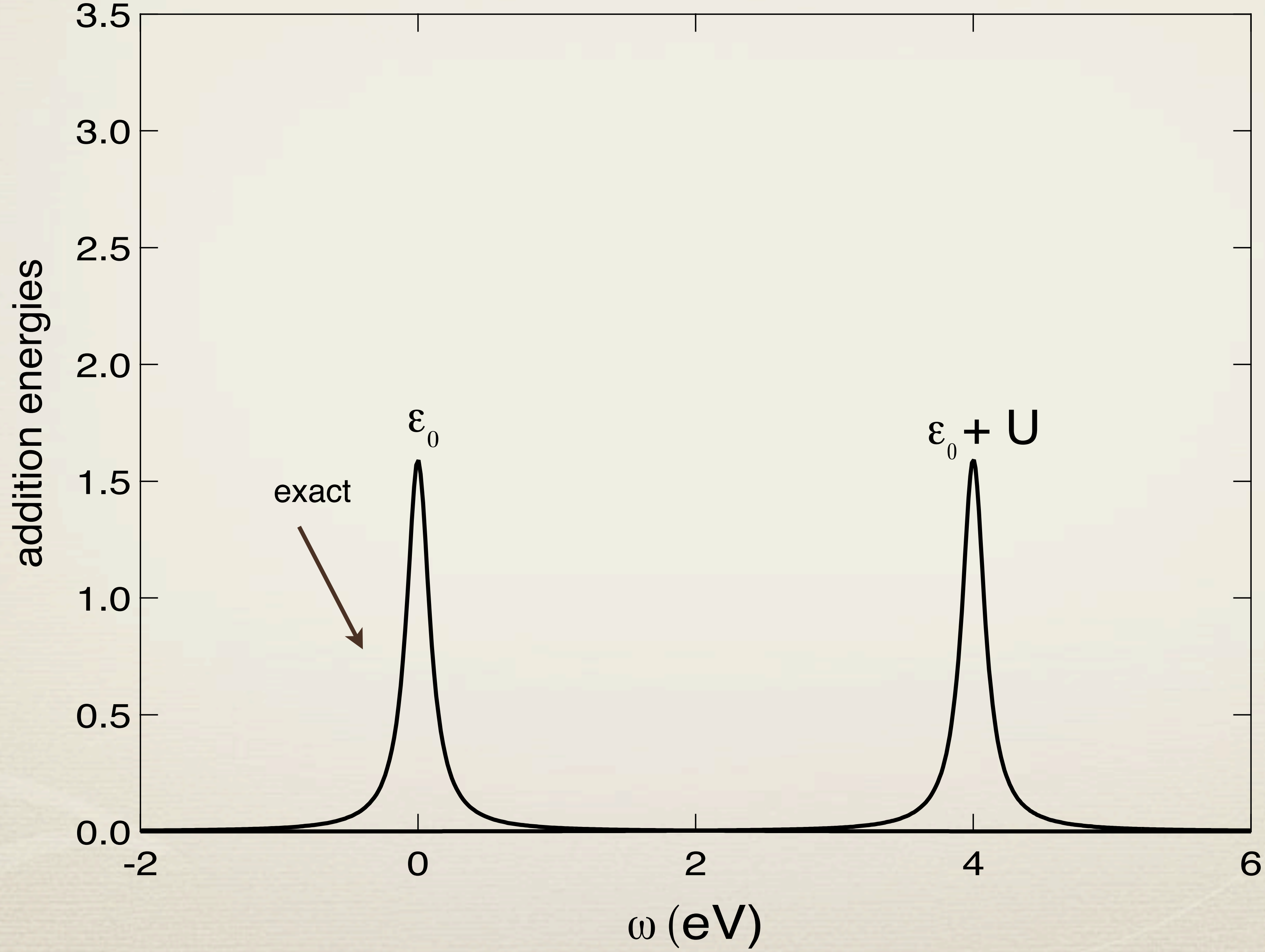
Limits of GW

- **Incorrect atomic limit** (bad treatment of correlation)

H_2^+

→ two types of addition energy



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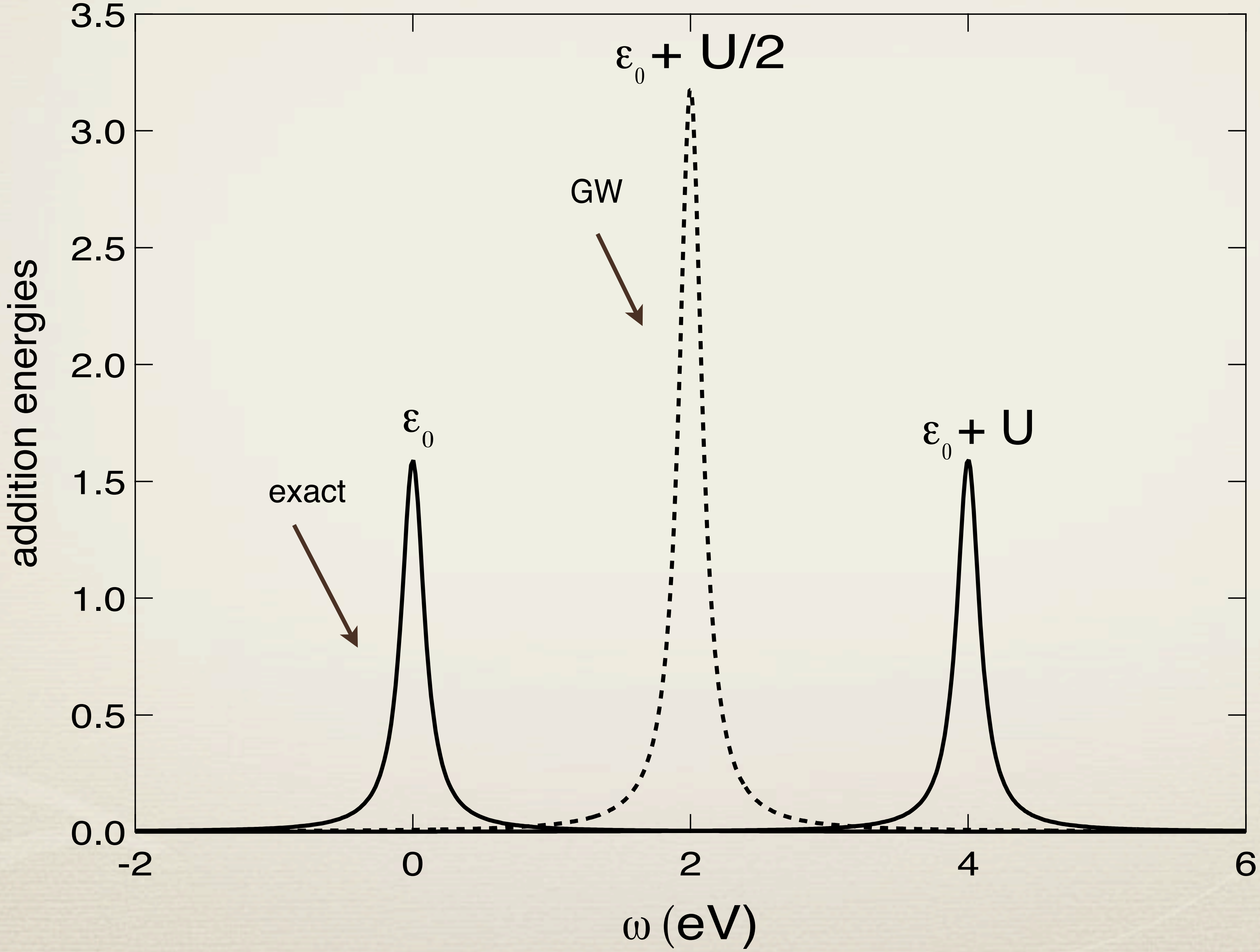
Limits of GW

- **Incorrect atomic limit** (bad treatment of correlation)

H_2^+ $\frac{1}{2}e^-$ .... $\frac{1}{2}e^-$ → one type of addition energy



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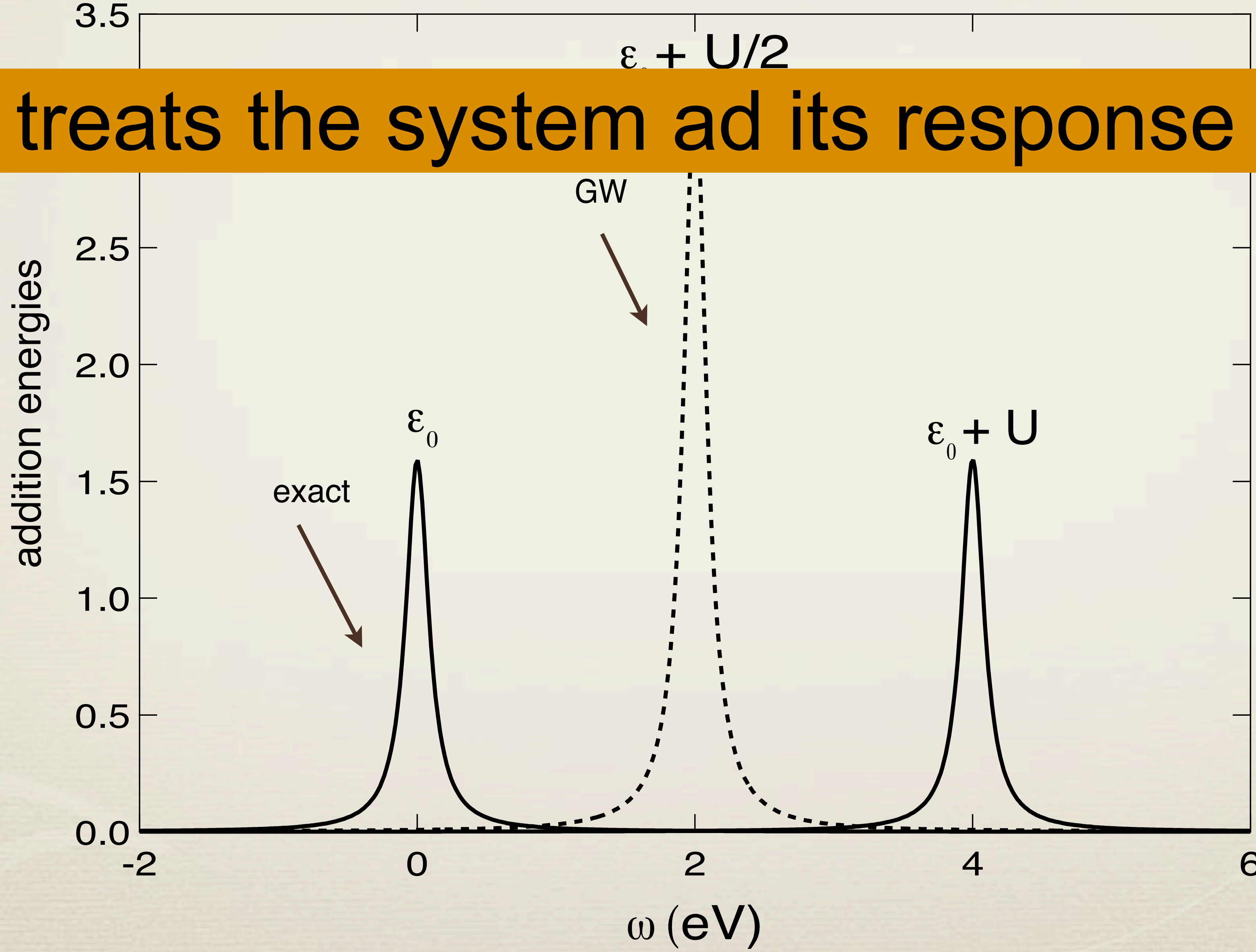
GW treats the system ad its response classically



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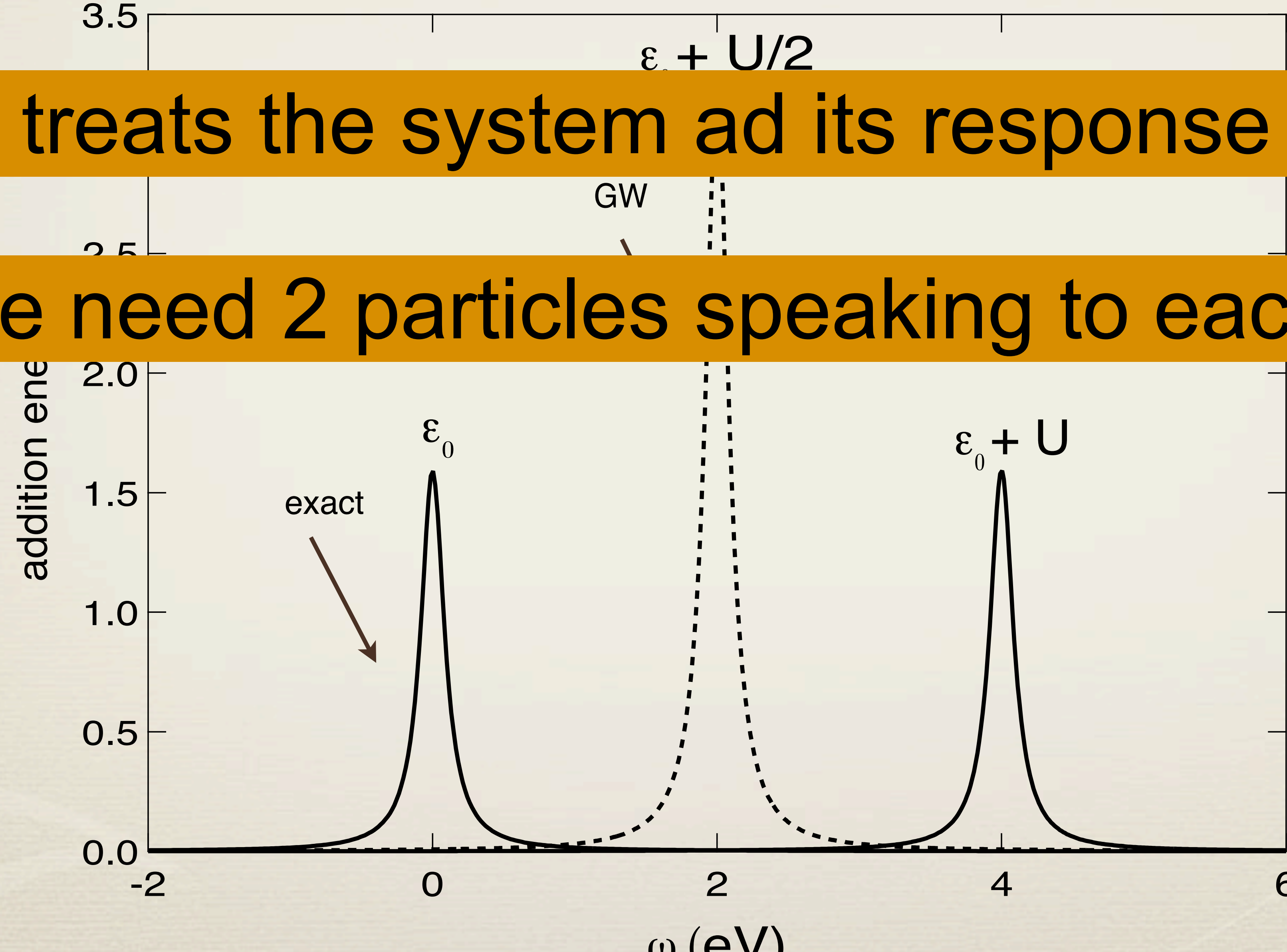
Limits of GW

- **Incorrect atomic limit** (bad treatment of correlation)

H_2^+ $\frac{1}{2}e^-$ ▪▪▪▪▪▪▪▪▪ $\frac{1}{2}e^-$ → one type of addition energy

GW treats the system ad its response classically

We need 2 particles speaking to each other!



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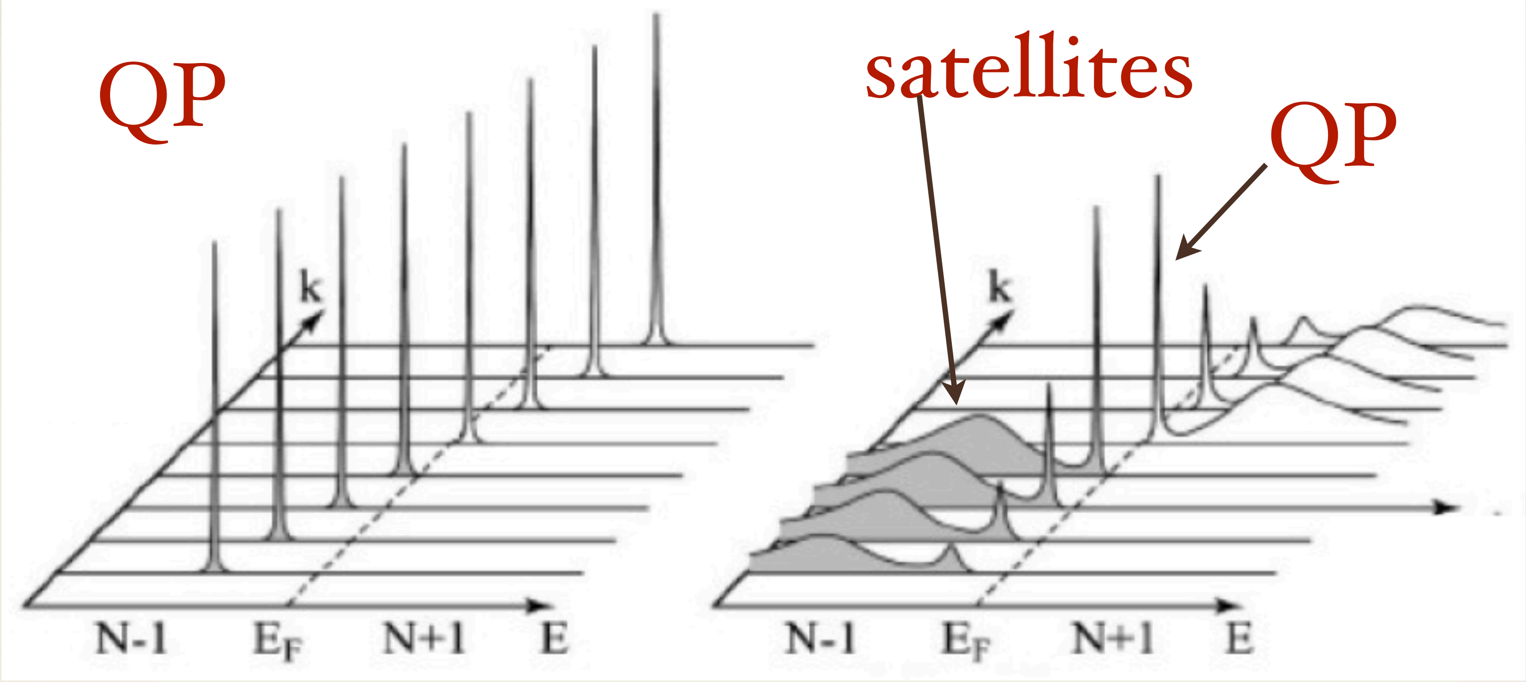
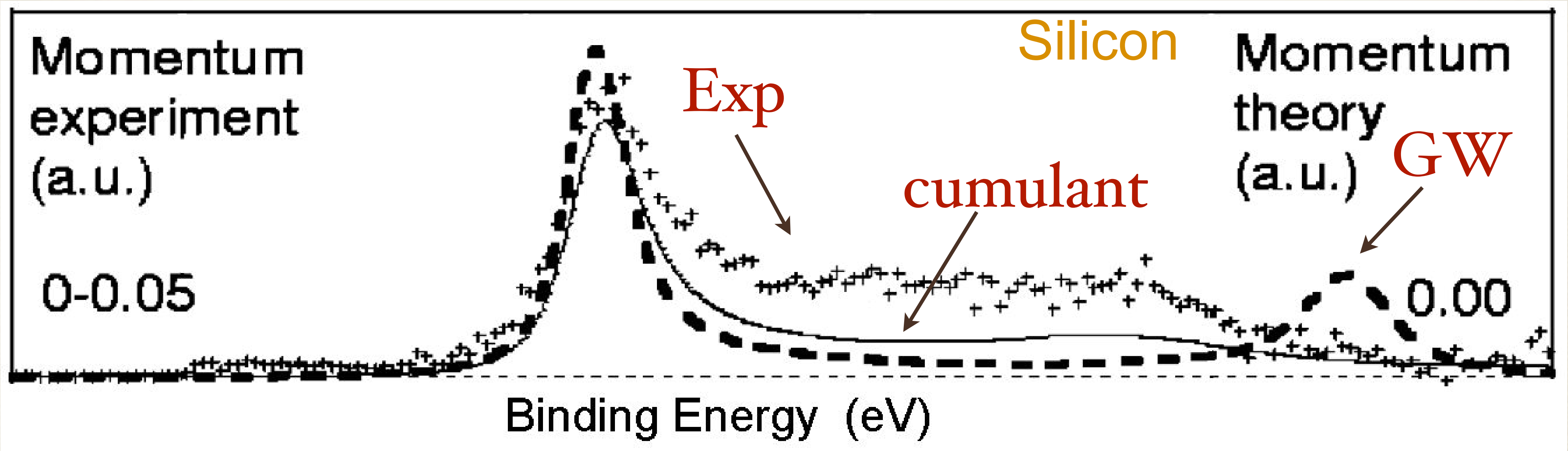
Limits of GW

* No multiple satellites (limits of thinking in terms of only one W)



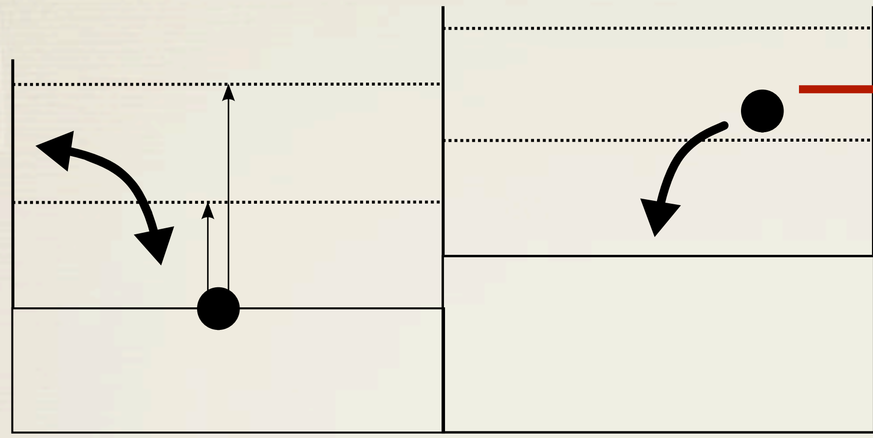
Damascelli et al. RMP 75, 473 (2003)



A. S. Kheifets et al. Phys. Rev. B 68, 233205 (2005)

Beyond GW

Vertex corrections from simple models



feels only induced Hartree
(different spatial distribution/opposite spin)

$$\Gamma = \begin{cases} \delta + f_{xc}P & for\ \ valence \\ \delta & for\ \ conduction \end{cases}$$

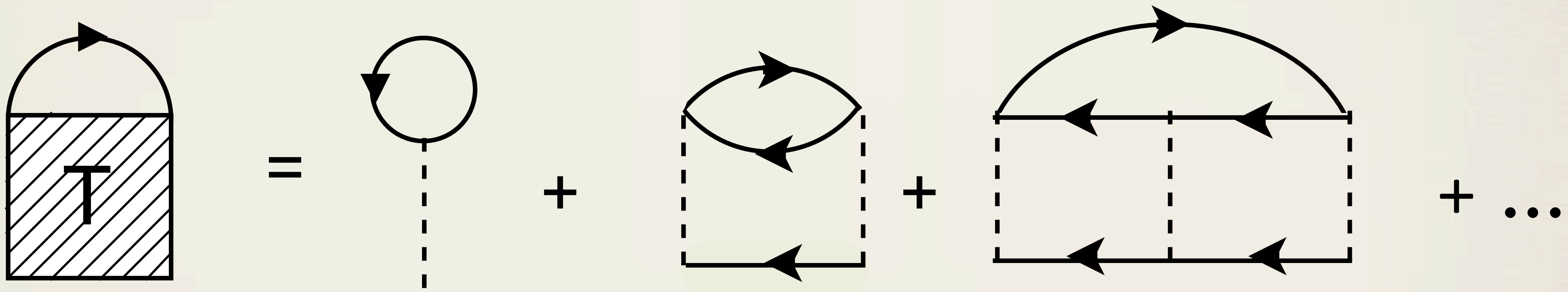
Self-screening free

P. Romaniello, S. Guyot, and L. Reining, J. Chem. Phys., 131, 154111 (2009)

Beyond GW

- Vertex corrections from other formulations: T-matrix

$$\Sigma(11') = G(42)T(12;1'4)$$



+ exchange terms

P. Romaniello, F. Bechstedt, and L. Reining, in preparation

Link GWΓ ↔ T-matrix

$$\Sigma(12) = v_H(12) + \Sigma_x(12) + iG(13)\Xi(35;26)L(64;54)v(41)$$

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$$L = \frac{\delta G}{\delta \varphi} = -G\frac{\delta G^{-1}}{\delta \varphi}G$$

$$\Xi = \frac{\delta(v_H + \Sigma_{xc})}{\delta G}$$

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quantum nature $\Xi = \frac{\delta(v_H + \cancel{\Sigma}_{xc})}{\delta G}$

(*) $\Sigma = v_H + iGW$ GW

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(*) $$\Sigma = v_H + iGW$$ GW

(**) $$\Sigma = GT$$ T-matrix

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(*) $\Sigma = v_H + iGW$ GW

(**) $\Sigma = GT$ T-matrix

Vertex corrections from the T-matrix

$$\Gamma = 1 - Pv + TGG$$

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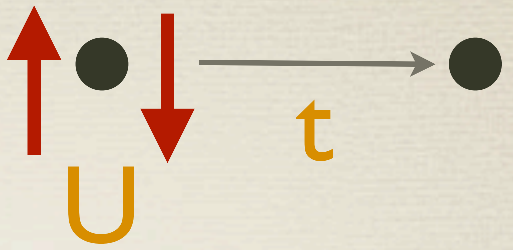
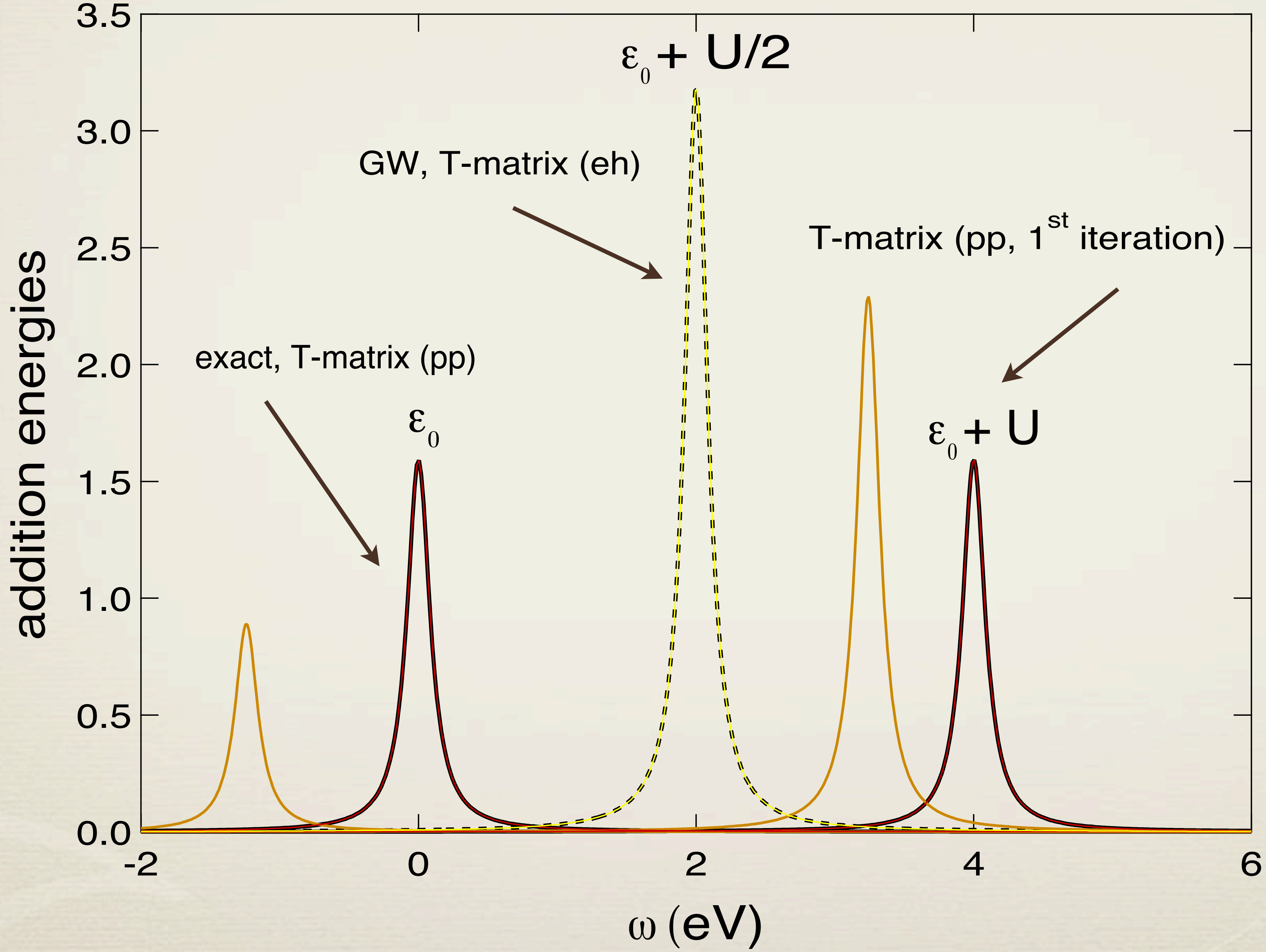
Hubbard molecule 1/4 filling: atomic limit

- 1e⁻ $|\Psi_0\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\ 0\rangle + |0\ \uparrow\rangle\right]$





P. Romaniello, F. Bechstedt, and L. Reining, in preparation

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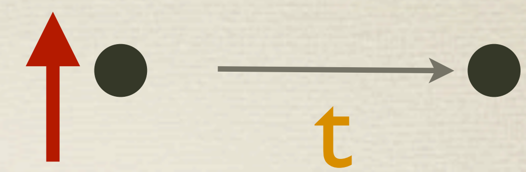

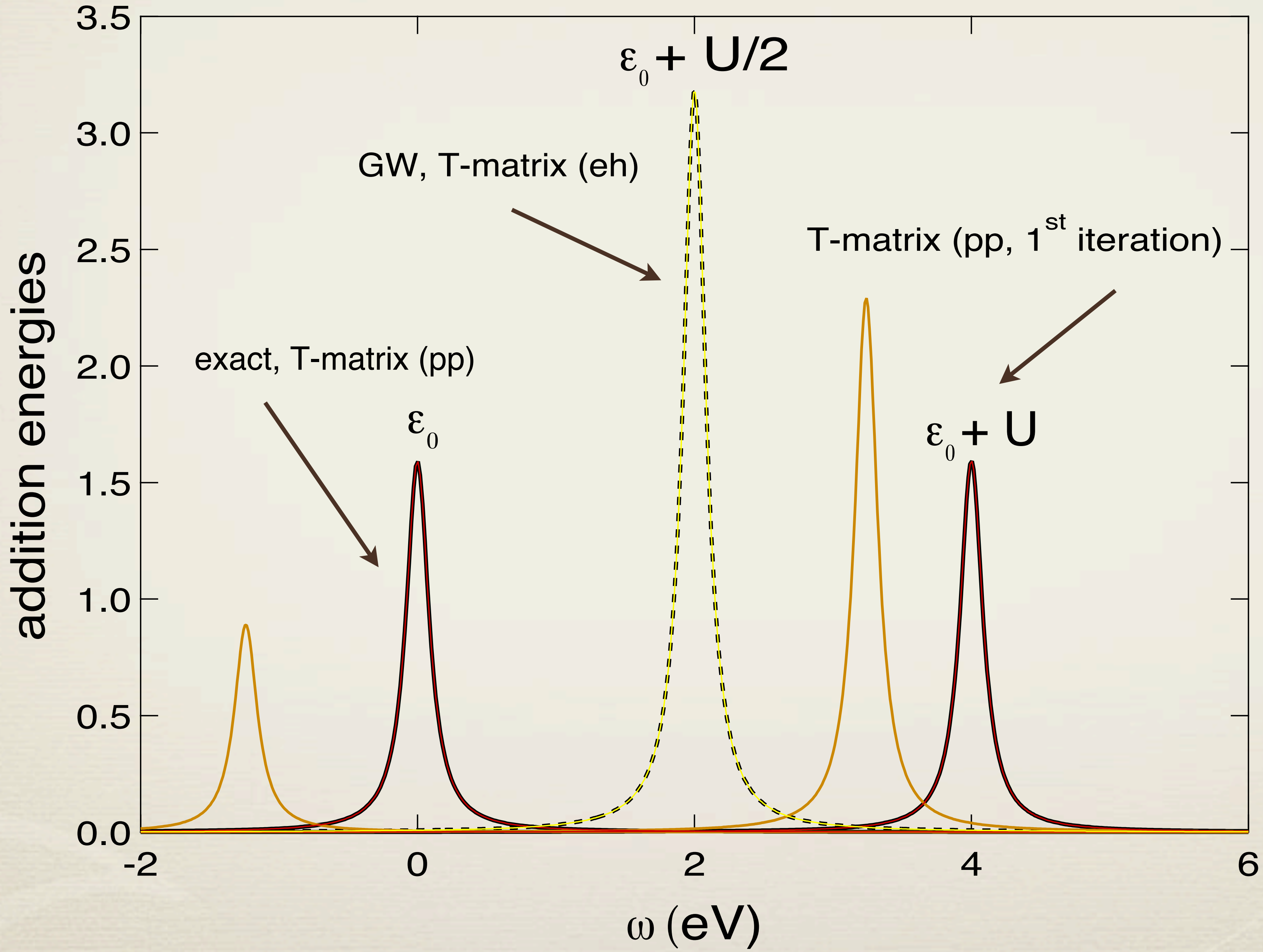

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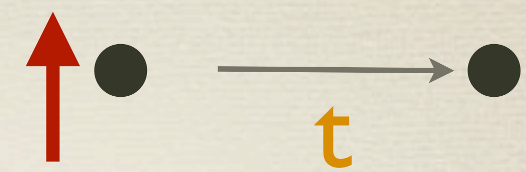

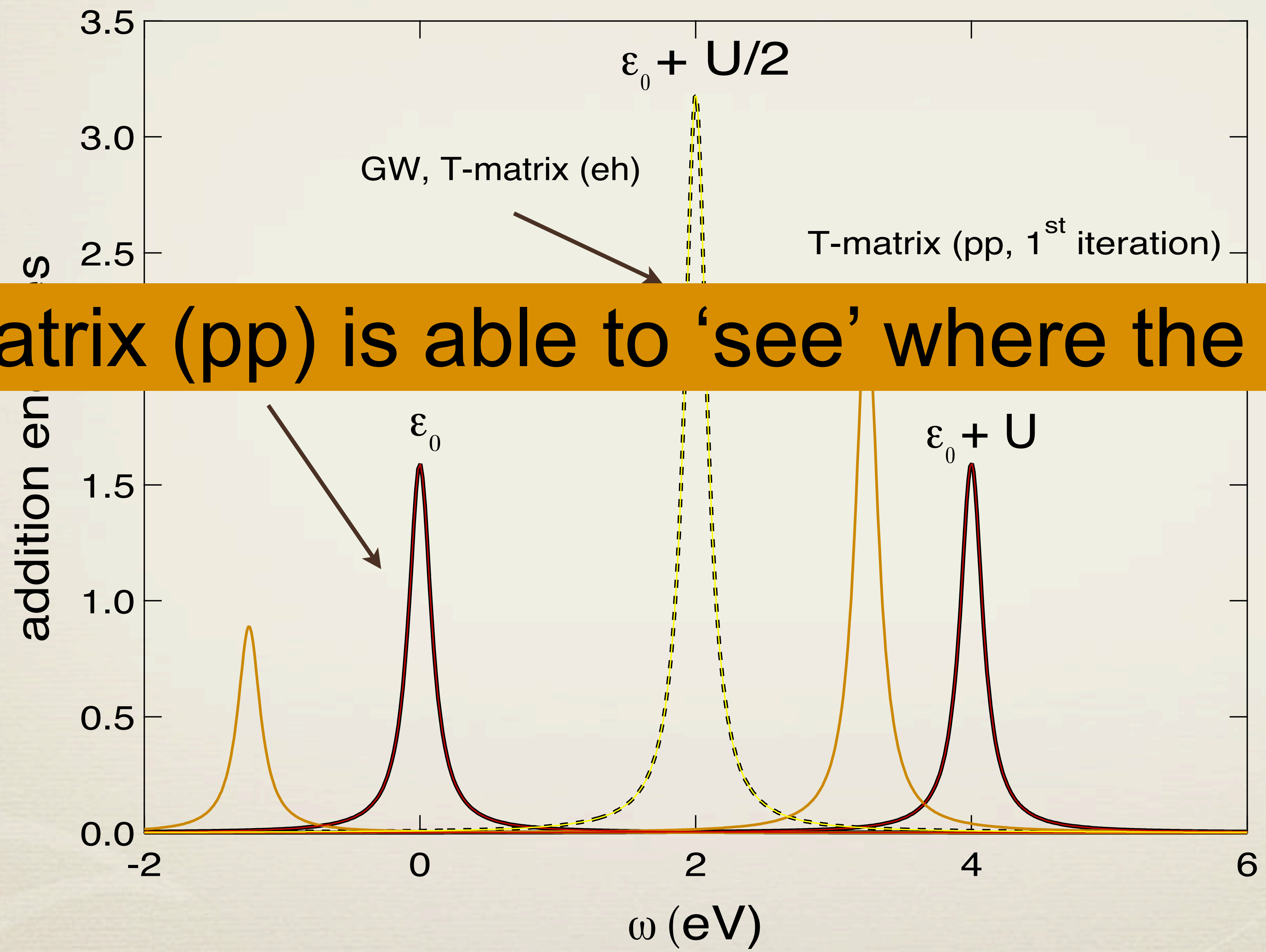

T-matrix (pp) is able to 'see' where the electron is

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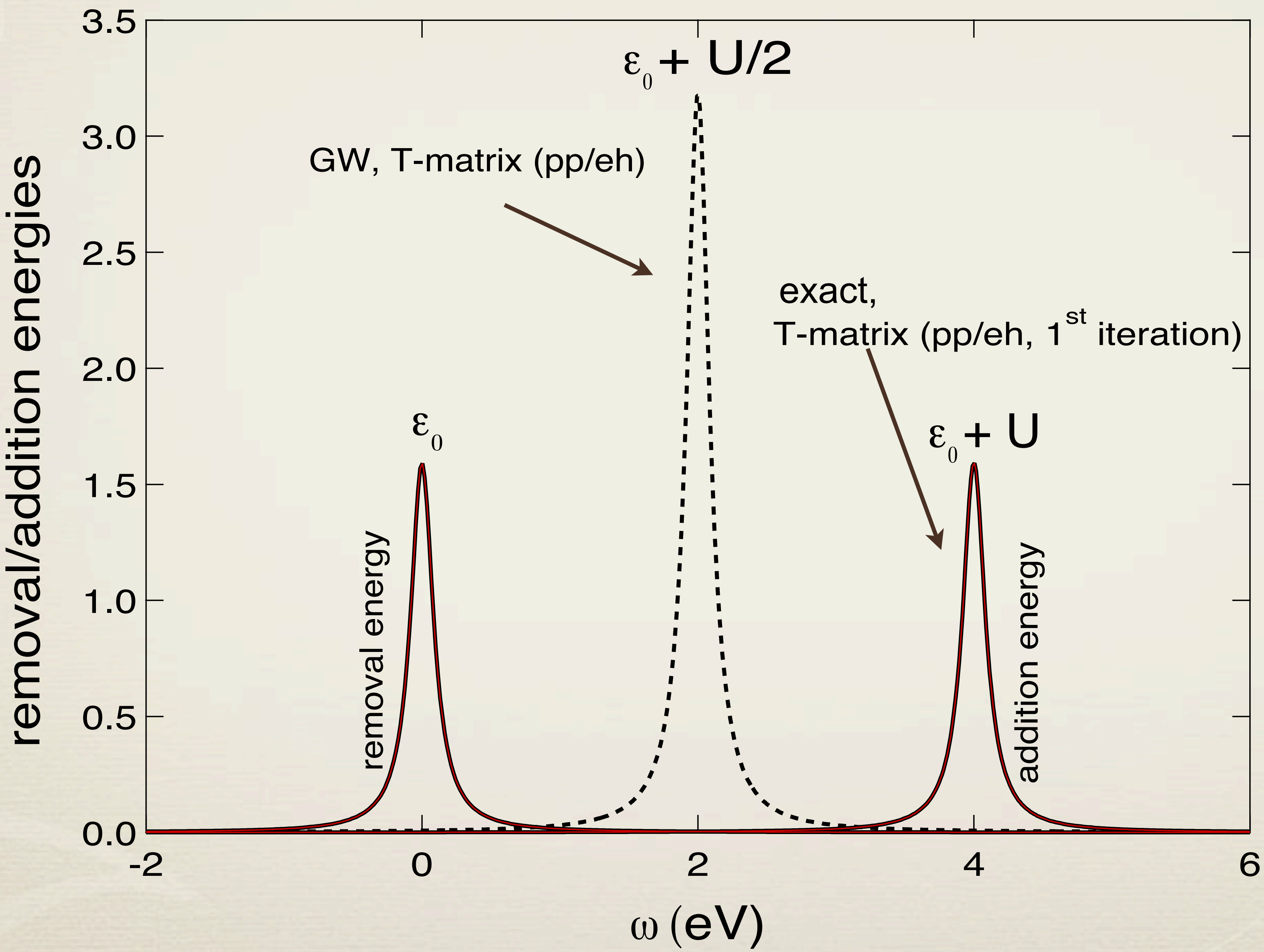
Hubbard molecule 1/2 filling: atomic limit

- 2e$^-$ $|\Psi_0\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right]$



P. Romaniello, F. Bechstedt, and L. Reining, in preparation

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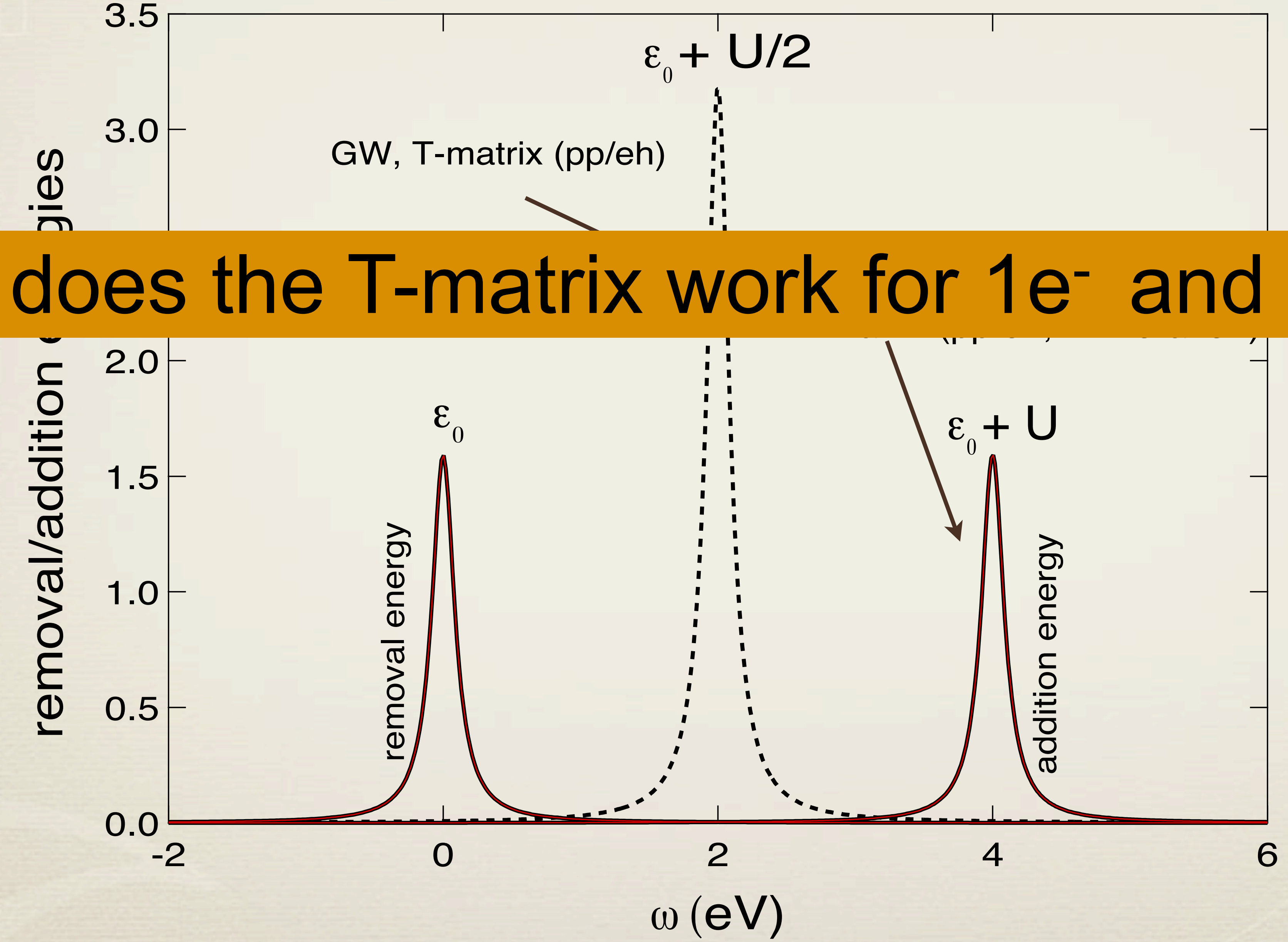

Why does the T-matrix work for 1e$^-$ and not for 2 e$^-$?

P. Romaniello, F. Bechstedt, and L. Reining, in preparation

Limits of thinking in terms of self-energy?

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Is there any alternative approach?

One-particle GF without self-energy

- One-particle Green's function

$$G(12) = -i\langle N|T[\psi(1)\psi^\dagger(2)]|N\rangle$$

eq. of motion for G

$$G(12) = G_0(12) + iG_0(13)v(3^+4)G_2(34;24^+)$$

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- 1st order nonlinear coupled functional differential eqs

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Unfortunately there exist no practical techniques for solving such functional differential equations exactly.

LP Kadanoff and G Baym -Quantum Statistical Mechanics NY (1962) p. 44

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Giovanna Lani, PhD

Solving the functional problem

* Linearization: $V_H[\varphi] \approx -iv\, G[\varphi]|_{\varphi=0} - iv\, \left.\frac{\delta G[\varphi]}{\delta \varphi}\right|_{\varphi=0} \varphi + \ldots$

$$G(12;[\bar{\varphi}]) = G_H^0(12) + G_H^0(13)\bar{\varphi}(3)G(32;[\bar{\varphi}]) + iG_H^0(13)W(3^+5)\frac{\delta G(32;[\bar{\varphi}])}{\delta \bar{\varphi}(5)}$$

G. Lani, P. Romaniello, and L. Reining, in preparation

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$$\frac{\delta G}{\delta \bar{\varphi}} \approx GG \longrightarrow GW$$

G. Lani, P. Romaniello, and L. Reining, in preparation

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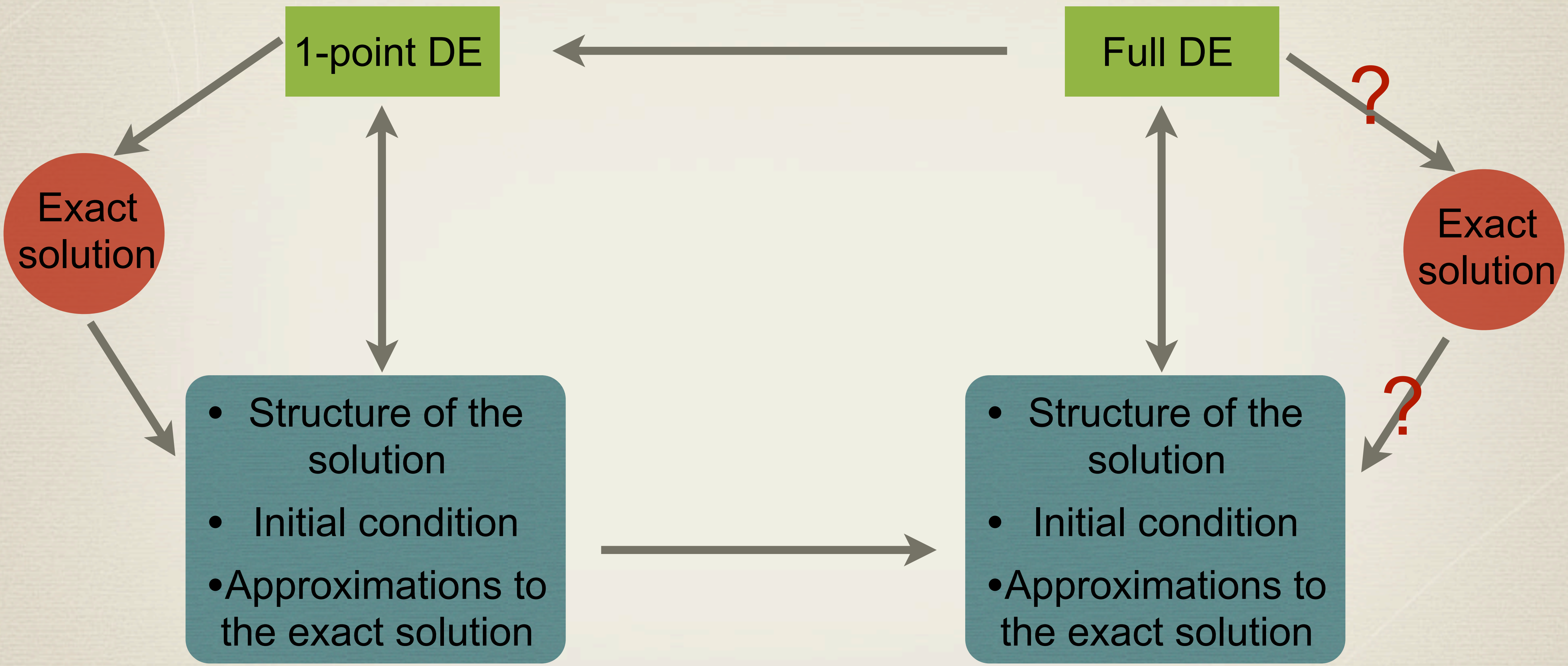
- One-point model: 1 space, 1 spin, 1 time

$$y(x) = y_0 + y_0 x y(x) - u y_0 \frac{d\, y(x)}{dx}$$

G. Lani, P. Romaniello, and L. Reining, in preparation

Solving the functional problem:
the strategy



G. Lani, P. Romaniello, and L. Reining, in preparation

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- Structure of the solution: $y(x) = A(x) \cdot I(x)$

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small u expansion

$$y(x=0)|_{u \to 0} \approx \sqrt{\frac{\pi}{2u}} e^{\frac{1}{2 y_0^2 u}} \left(1 + C(u, y_0)\right) + \left(y_0 - u y_0^3 + 3u^2 y_0^5 - 15 u^3 y_0^7 + \ldots\right)$$

$$y(x=0)|_{u=0} = y_0 \quad \Rightarrow \quad C(u, y_0) = -1$$

G. Lani, P. Romaniello, and L. Reining, in preparation

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The initial condition $y(x_\beta) = y_\beta$ translates in $y(x=0)|_{u=0} = y_0$

G. Lani, P. Romaniello, and L. Reining, in preparation

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An iterative approach takes into account the initial condition

$$y(x=0)|_{u=0} = y_0 \Rightarrow C(u, y_0) = -1$$

The initial condition $y(x_\beta) = y_\beta$ translates in $y(x=0)|_{u=0} = y_0$

G. Lani, P. Romaniello, and L. Reining, in preparation

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$$y(x) = y_0 + y_0 x y(x) - u y_0 \frac{d\,y(x)}{dx} \quad \Rightarrow \quad y(x) = -\sqrt{\frac{\pi}{2u}} e^{\frac{1}{2uy_0^2}} \left(erf\left[\sqrt{\frac{1}{2uy_0^2}}\right] - 1 \right)$$

- New approximations: the continued fraction $erf[z] = 1 - \frac{e^{z^2}}{\sqrt{\pi}} \frac{1}{z + \frac{1/2}{z + \frac{1}{z + \frac{3/2}{z + \dots}}}}$

Approximation to the exact solution

$$y(x=0) = \frac{y_0}{1 + \frac{uy_0^2}{1 + \frac{2uy_0^2}{1 + \frac{3uy_0^2}{1 + \dots}}}}$$

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Manipulation of the DE to get the approximation to the exact solution

$$\begin{aligned}
\frac{dy(x)}{dx} &= y_0 y(x) + y_0 x \frac{dy(x)}{dx} - u y_0 \frac{d^2 y(x)}{dx^2} \\
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\frac{d^3 y(x)}{dx^3} &= 3y_0 \frac{d^2 y(x)}{dx^2} + y_0 x \frac{d^3 y(x)}{dx^3} - u y_0 \frac{d^4 y(x)}{dx^4} \\
&\dots
\end{aligned}$$

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\end{aligned}$$

...

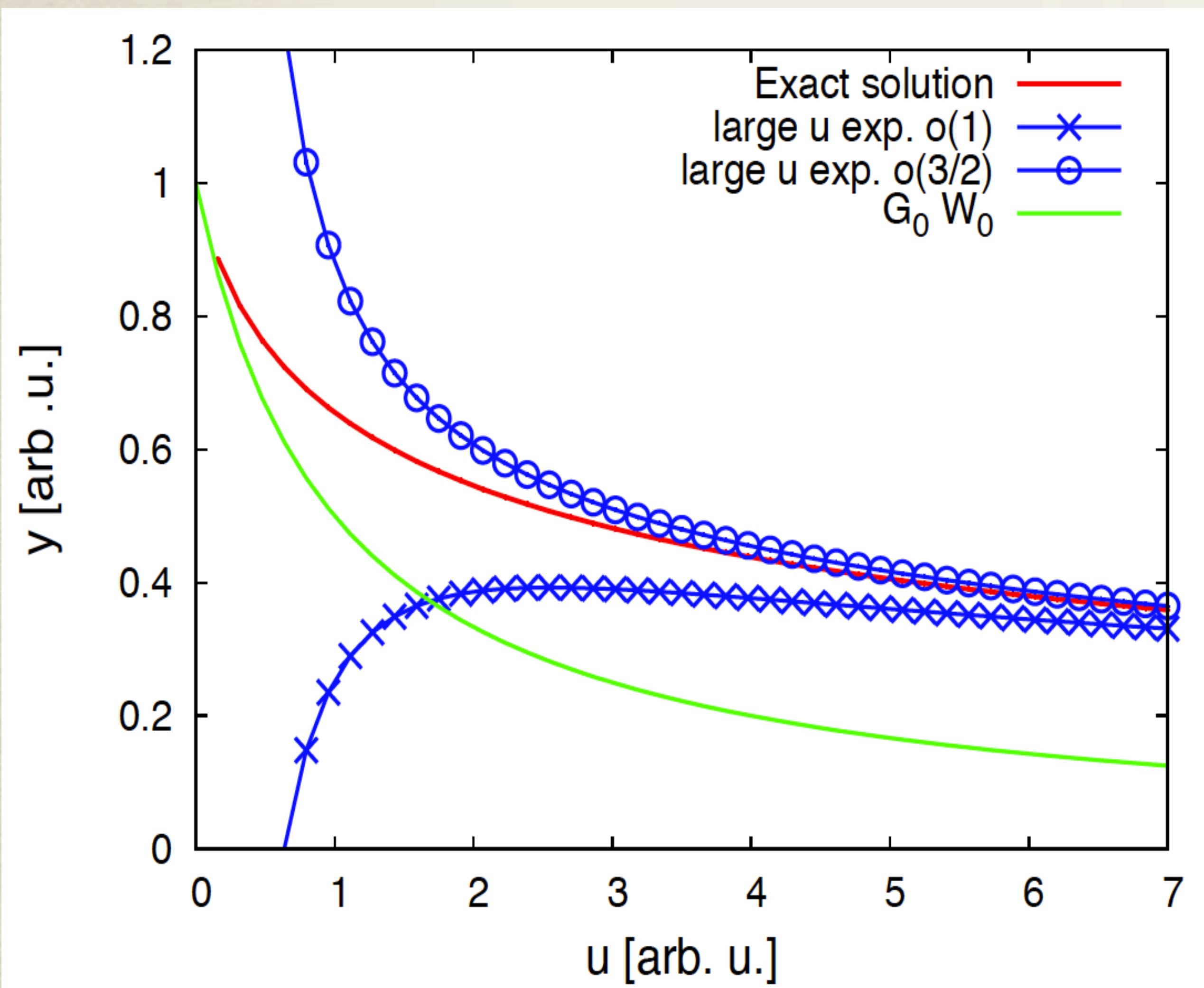
Solving backward

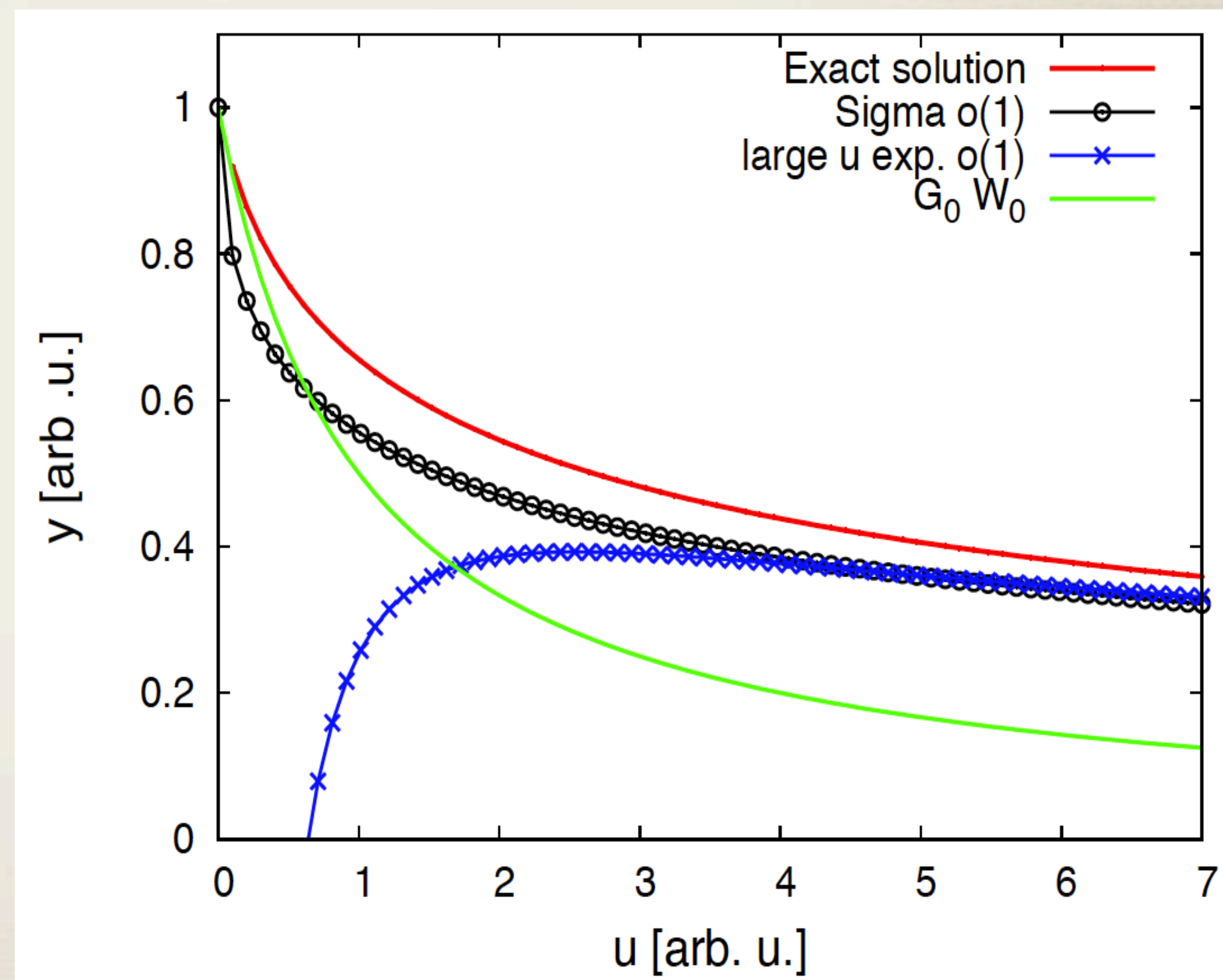
G. Lani, P. Romaniello, and L. Reining, in preparation

1-point model

$$y(x) = y_0 + y_0 x y(x) - u y_0 \frac{d\,y(x)}{dx} \quad \Rightarrow \quad y(x) = -\sqrt{\frac{\pi}{2u}}\, e^{\frac{1}{2uy_0^2}} \left(erf\left[\sqrt{\frac{1}{2uy_0^2}}\right] - 1 \right)$$

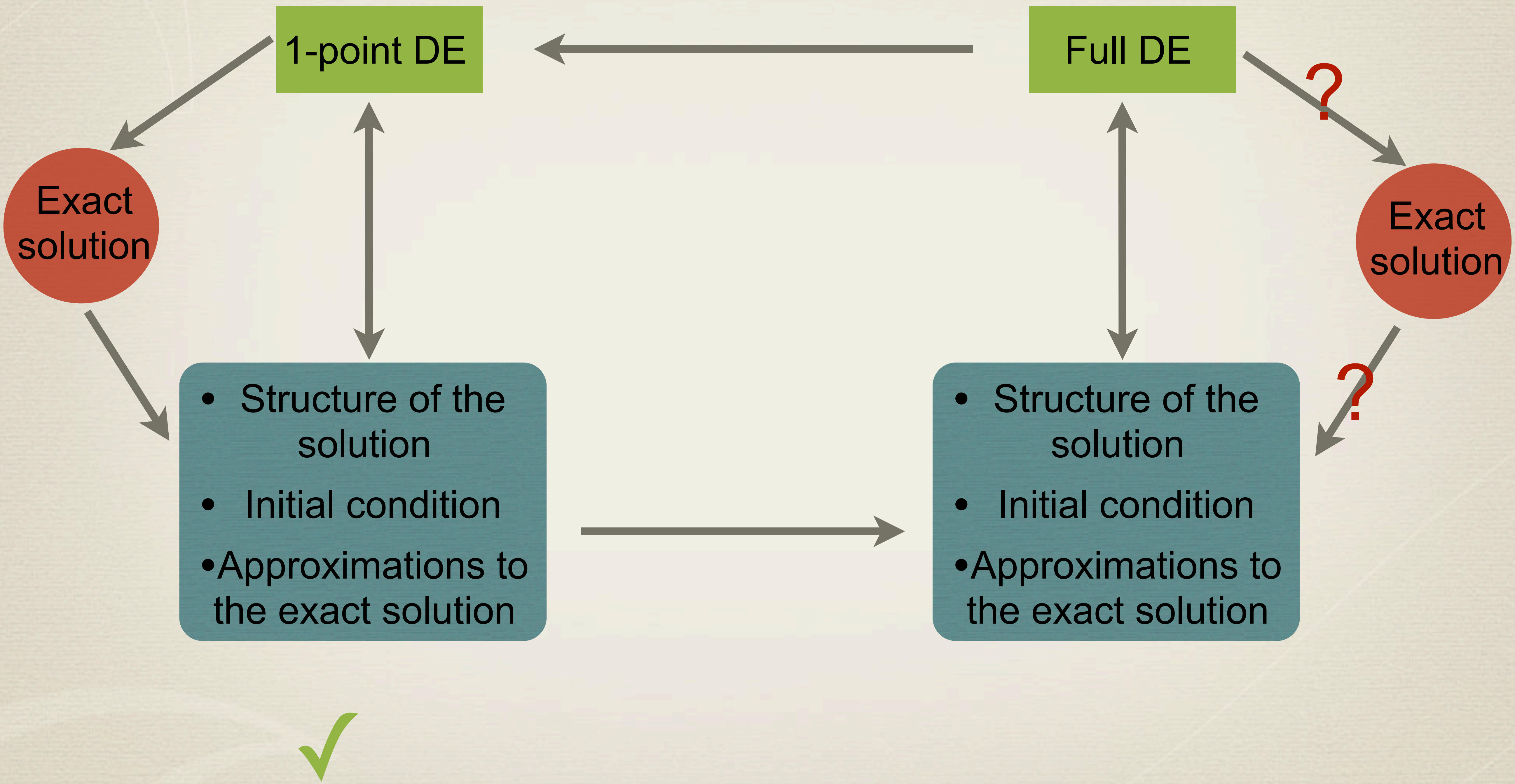
- New approximations: large u expansion of exp, erf, and Dyson





G. Lani, P. Romaniello, and L. Reining, in preparation

Solving the functional problem:
the strategy



Solving the functional problem:
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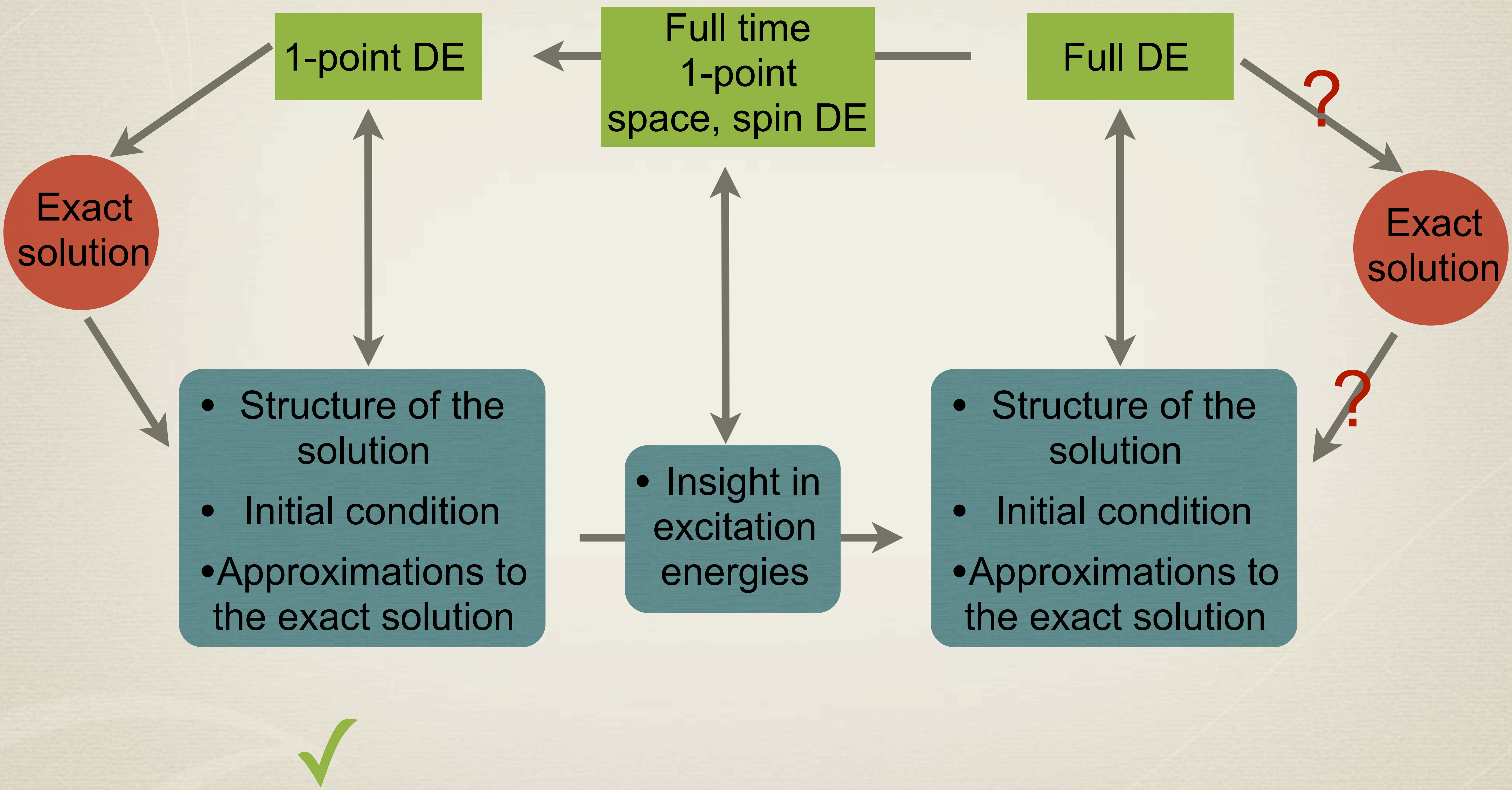

Towards the full solution

* Full time, 1-point in space and spin DE (G, G_H, W diagonal in some basis)

$$G(t_1t_2;[\bar{\varphi}]) = G_{\bar{\varphi}}(t_1t_2;[\bar{\varphi}]) + iG_{\bar{\varphi}}(t_1t_3;[\bar{\varphi}])W(t_3^+t_5)\frac{\delta G(t_3t_2;[\bar{\varphi}]}{\delta\bar{\varphi}(t_5)}$$

M. Guzzo et al. in preparation; F. Aryasetiawan, L. Hedin, and K. Karlsson, Physical Review Letters, 77, 2268 (1996)

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One level approximation (hole part only)

$$G(t_1t_2) = \Theta(t_1 - t_2)e^{-i\epsilon(t_1-t_2)}e^{i\int_{t_2}^{t_1} dt'\bar{\varphi}(t')}e^{-i\int_{t_2}^{t_1} dt'\int_{t'}^{t_2} dt''W(t't'')}$$

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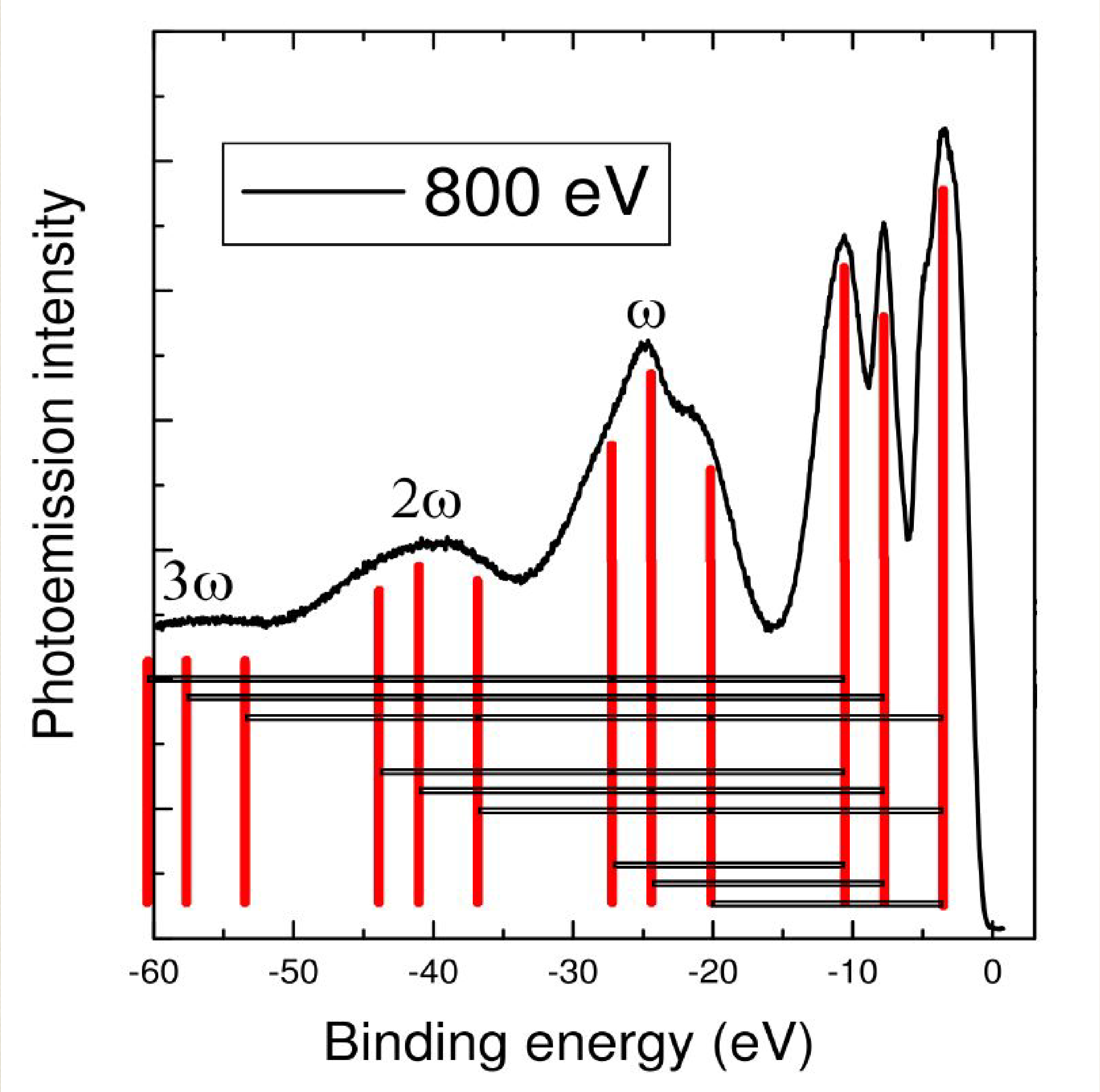
$$\Downarrow \; \bar{\varphi} \to 0$$

Cumulant

M. Guzzo et al. in preparation; F. Aryasetiawan, L. Hedin, and K. Karlsson, Physical Review Letters, 77, 2268 (1996)

Cumulant

- Plasmonic replicas in bulk Si



F. Sirotti, Synchrotron Soleil, France

Matteo Guzzo, PhD

M. Guzzo et al. in preparation

Towards the full solution

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Cumulant

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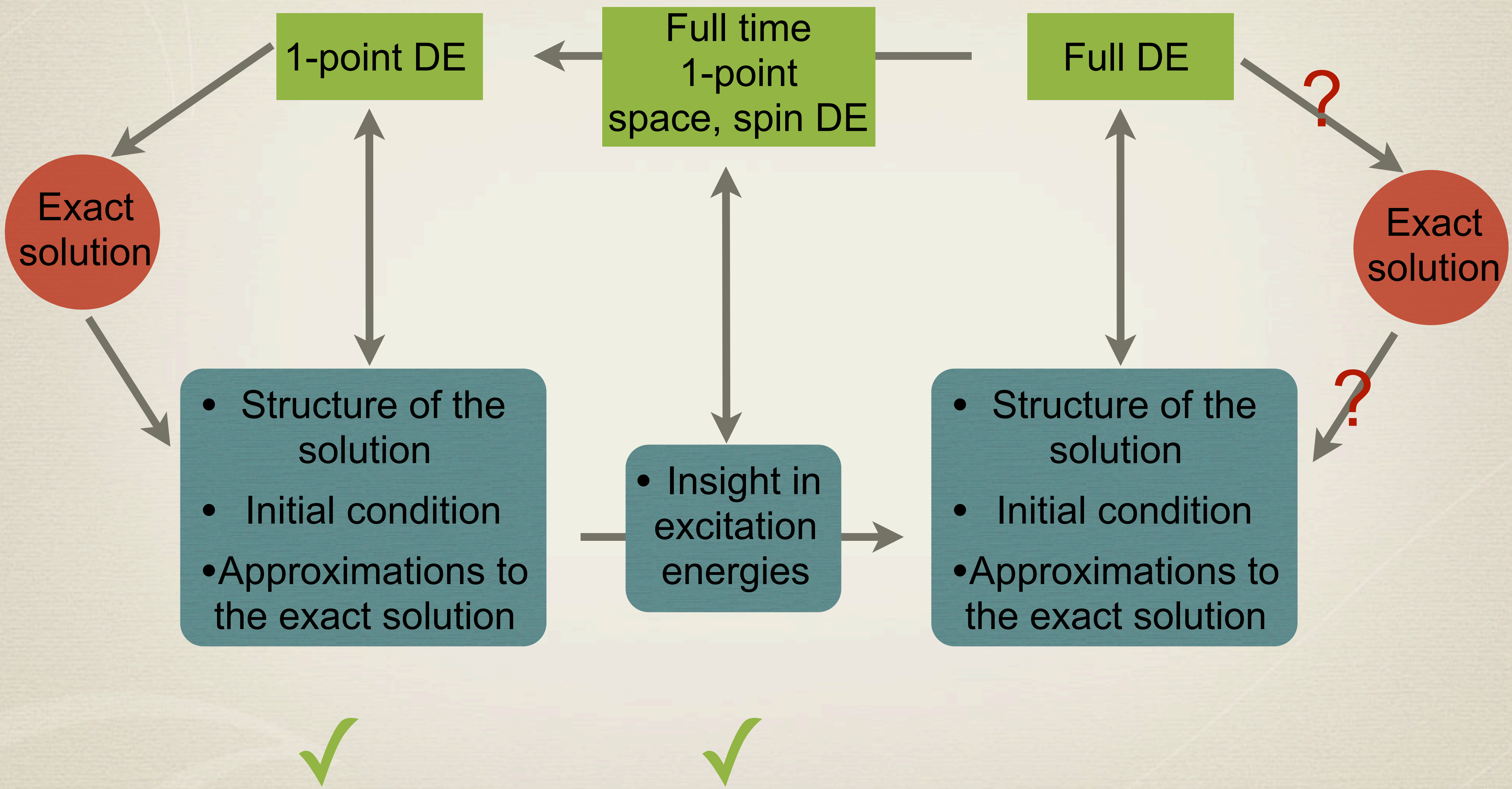
$$\Downarrow \; \bar{\varphi}\to 0$$

Cumulant

Vertex corrections

Guide in the full solution of the functional problem

Solving the functional problem:
the strategy



Ongoing research

our ansatz
(similar to 1-point)

$$G(12;[\bar{\varphi}]) = f[\bar{\varphi}]a(15;[\bar{\varphi}])I(52;[\bar{\varphi}])$$

$$f[\bar{\varphi}] = e^{\frac{i}{2}W^{-1}(65)\bar{\varphi}(5)\bar{\varphi}(6)}$$

$$a(35;[\bar{\varphi}]) = j(35)e^{-i\frac{j(85)}{j(75)}W^{-1}(67)G_0^{-1}(78)\bar{\varphi}(6)}$$

$$\boxed{\delta(52) = -iW(54)f[\bar{\varphi}]a(56;[\bar{\varphi}])\frac{\delta I(62;[\bar{\varphi}])}{\delta\bar{\varphi}(4)}}$$

- This equation has too many solutions! (our ansatz is not well-defined)
- How do we find the right solution?
- What is our initial condition?