BEYOND GW: VERTEX CORRECTIONS, MULTIPLE SOLUTIONS, STRONG CORRELATION

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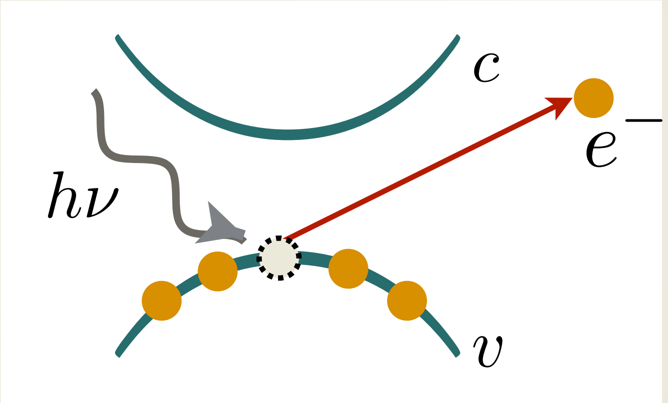
European Theoretical Spectroscopy Facility

an initiative of the Nanoquanta Network of Excellence

Prologue: photoemission spectrum

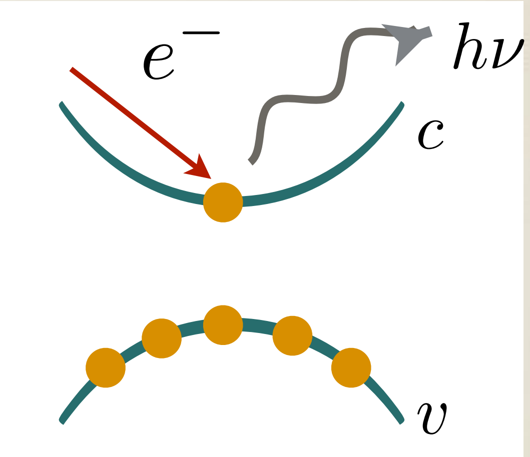
- Direct photoemission



removal energies

$$N \to N-1$$

- Inverse photoemission



addition energies

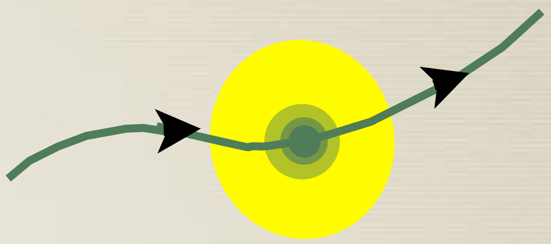
$$N \to N+1$$

Prologue: one-body Green's functions

- Many-body perturbation theory

moving (quasi) particles around

$$G(1,2) \equiv -i\langle\Psi_0|\mathcal{T}\left[\hat{\psi}_H(1)\hat{\psi}^\dagger_H(2)\right]|\Psi_0\rangle$$



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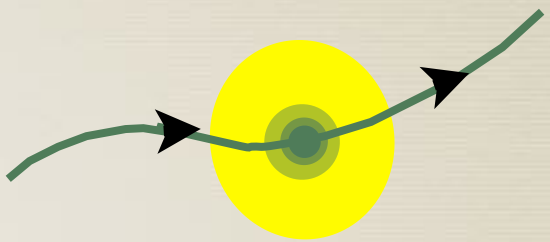

spectral representation

$$G(\mathbf{x}_1,\mathbf{x}_2;\omega) = \lim_{\eta\to 0^+}\left[\sum_k \frac{B^{k,R}(\mathbf{x}_1,\mathbf{x}_2)}{\omega-(E_0^N-E_k^{N-1})-i\eta} + \sum_k \frac{B^{k,A}(\mathbf{x}_1,\mathbf{x}_2)}{\omega-(E_k^{N+1}-E_0^N)+i\eta}\right]$$

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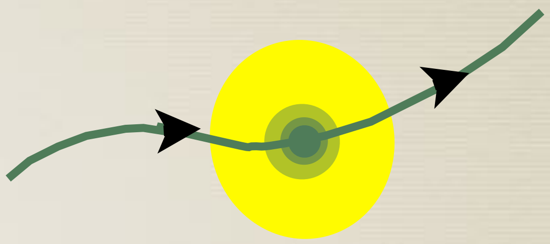

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spectral function $A(\omega) = \frac{1}{\pi}\Im|G(\omega)|$ → photoemission spectrum

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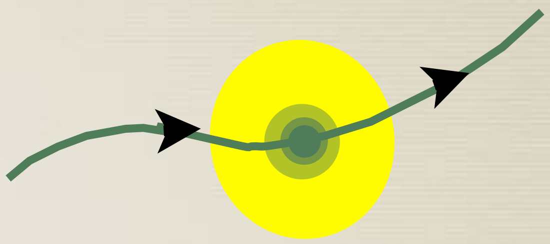

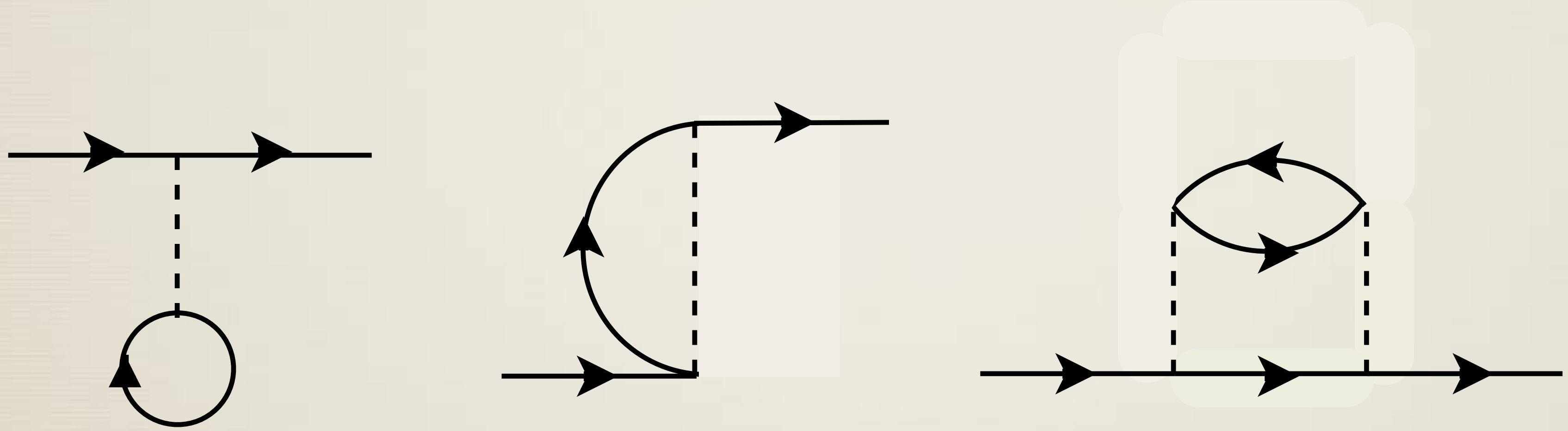

etc etc...

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* Many-body perturbation theory

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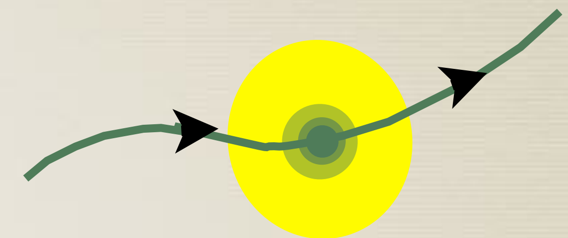

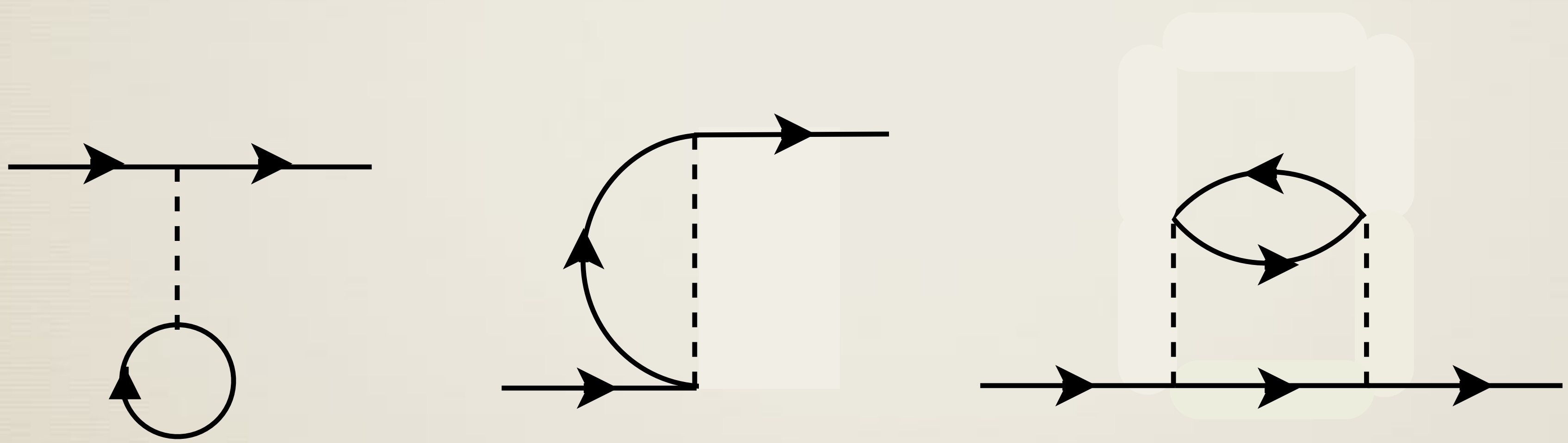

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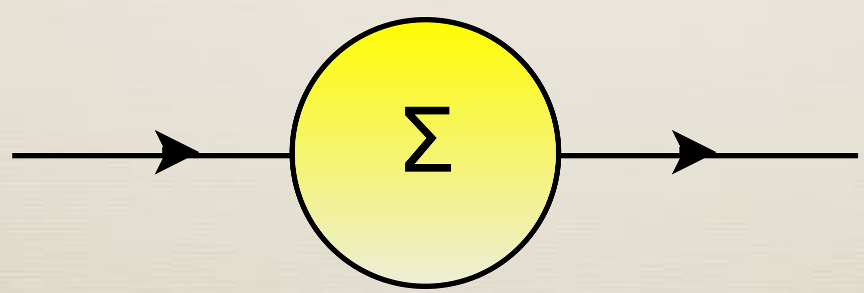
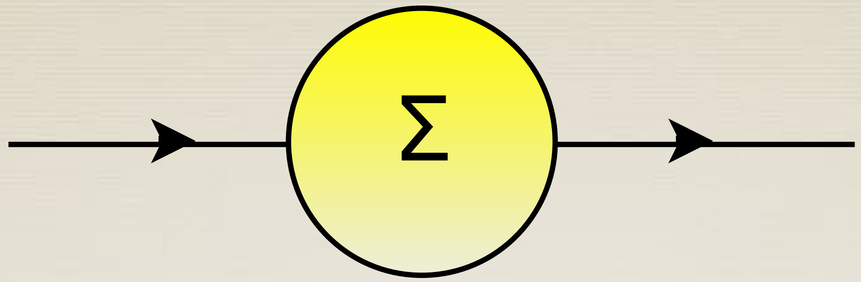


Self-energy

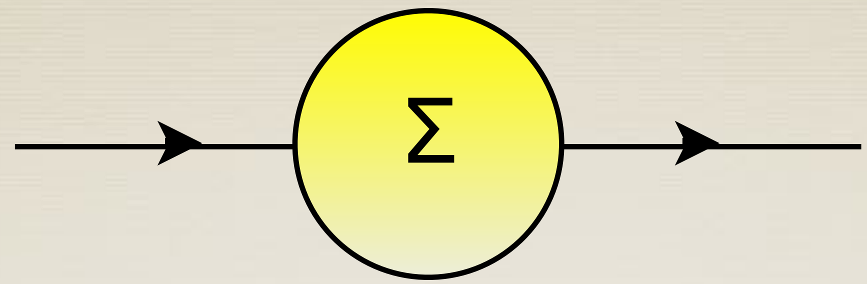
$$G = G_0 + G_0\Sigma G$$

Prologue: self-energy



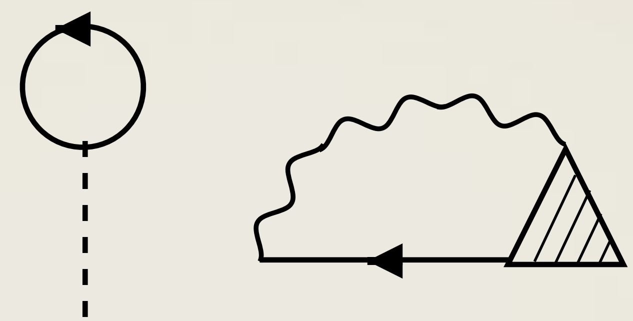
L. Hedin, Phys. Rev. 139, A796 (1965)

Prologue: self-energy



Hedin's eqs

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



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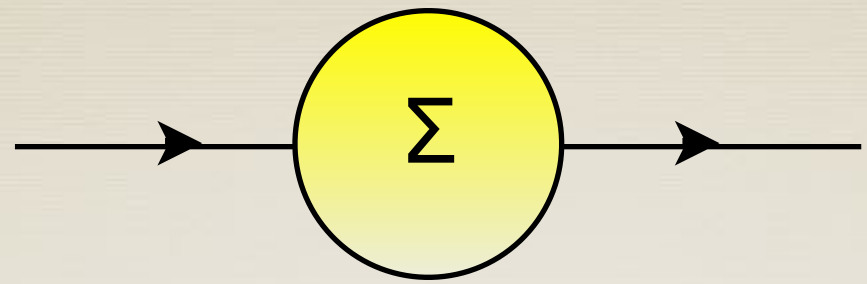

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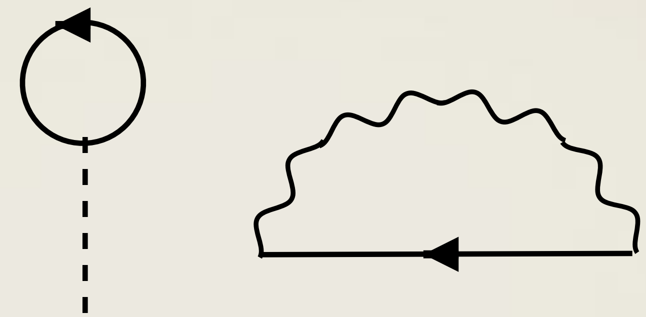

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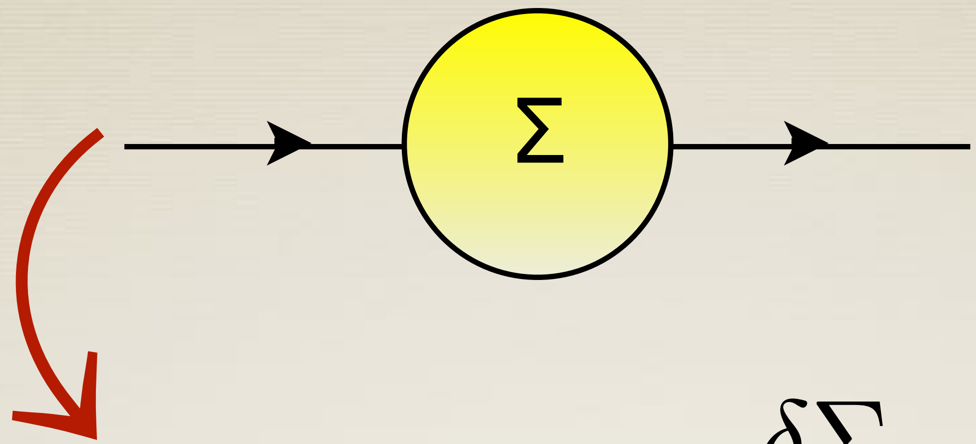
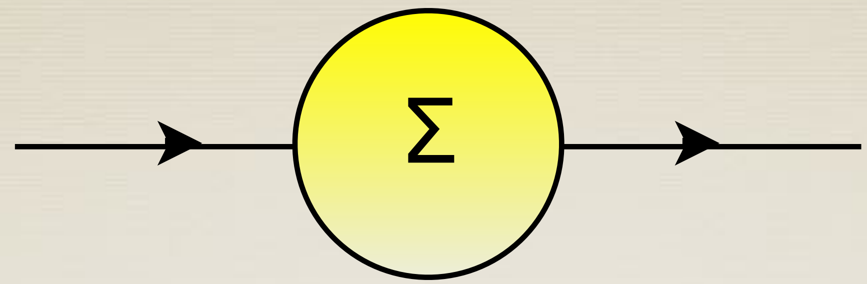


$$\Sigma = v_H + \Sigma_x + i v_c G \underbrace{\frac{\delta\Sigma}{\delta G}}_{\Xi} \underbrace{\left.\frac{\delta G}{\delta U_{ext}}\right|_{U_{ext}=0}}_{L = L_0 + L_0 \Xi L}$$

P. R., F. Bechstedt, and L. Reining, Phys. Rev. B 85, 155131 (2012)

Prologue: self-energy



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GW

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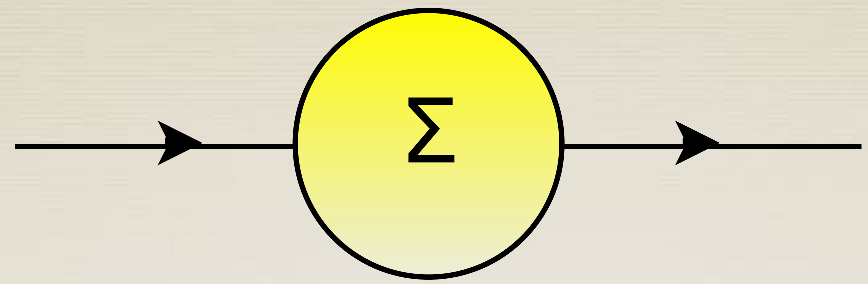

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$$\Xi \approx \frac{\delta v_H}{\delta G} = -i v_c \qquad \approx L_0 + L_0 \frac{\delta v_H}{\delta G} L$$

GW^{RPA}

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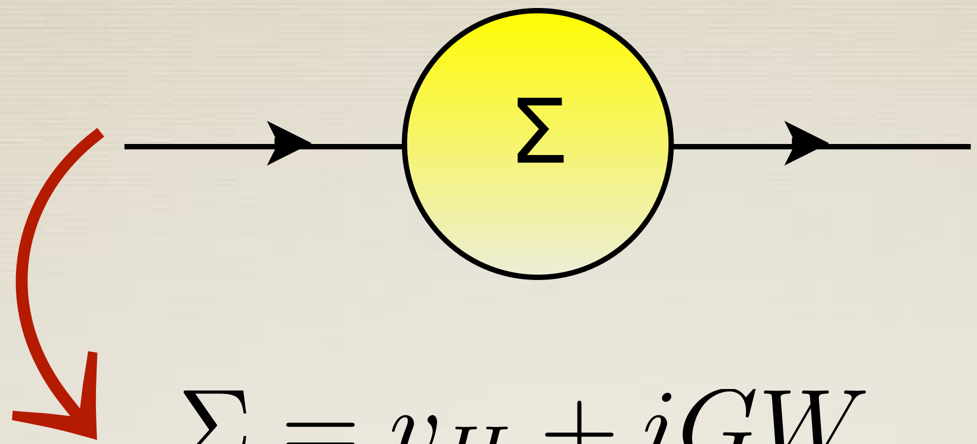

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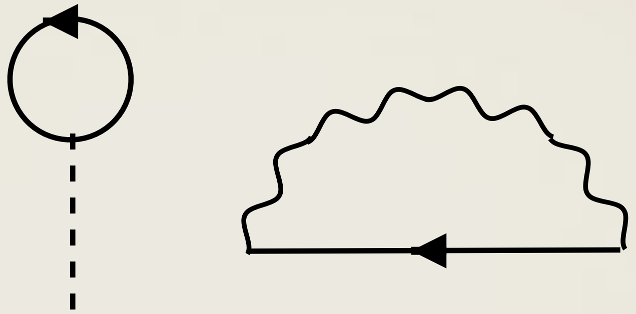

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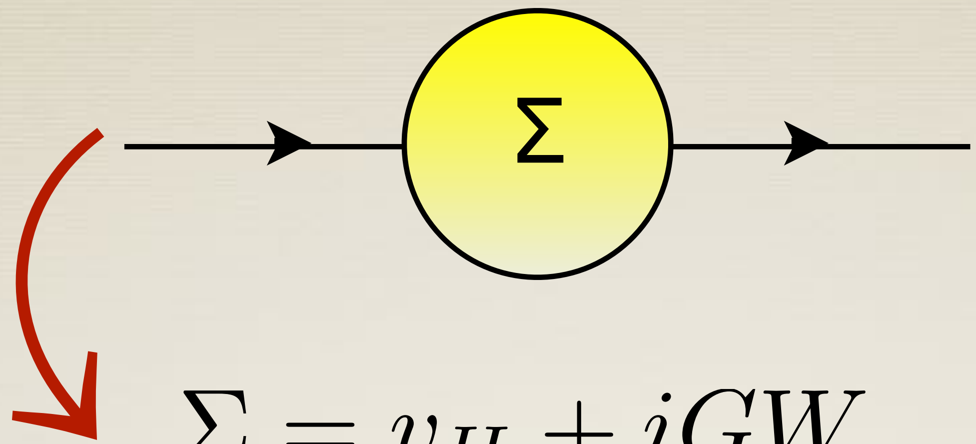

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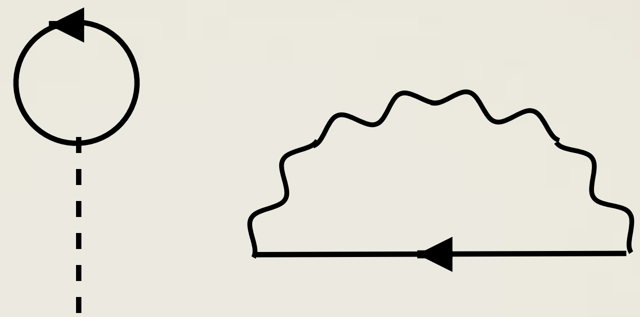
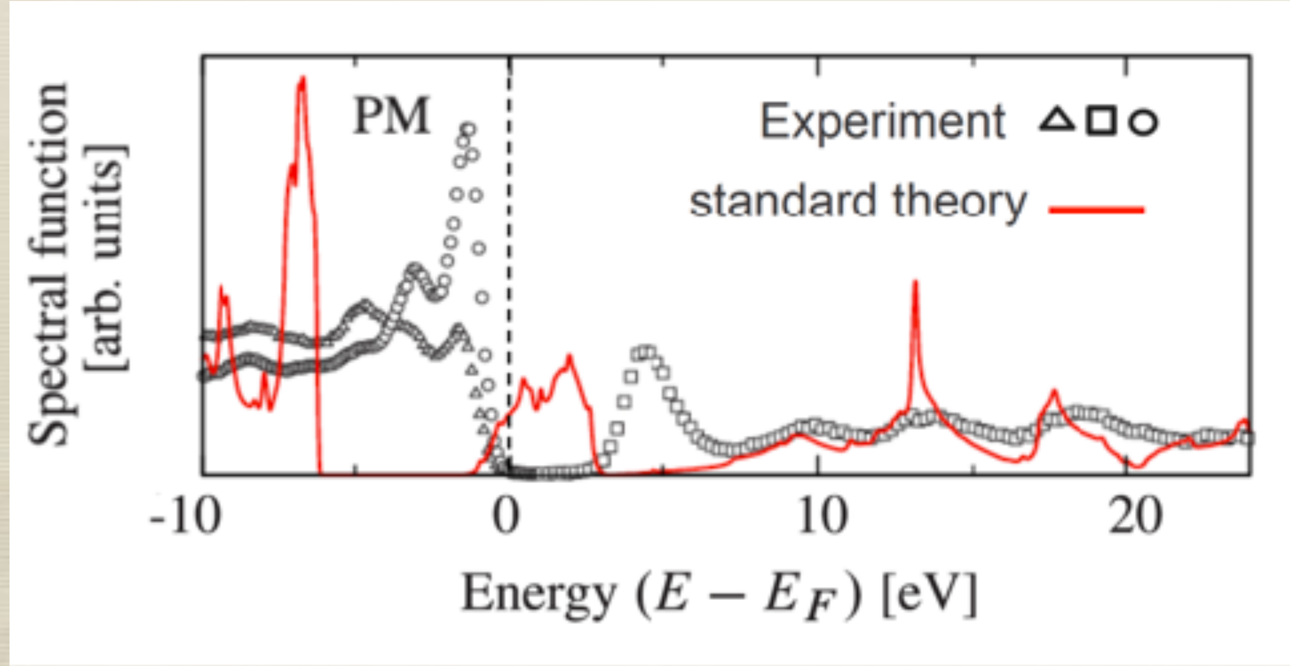


- Strongly correlated systems: paramagnetic (PM) NiO



Exp band gap: 4.3 eV

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

Outline

- Vertex corrections beyond GW
- Multiple solutions
- Self-energyless approach:
  - many-body effective energy theory (MEET)
- Conclusions & Outlooks

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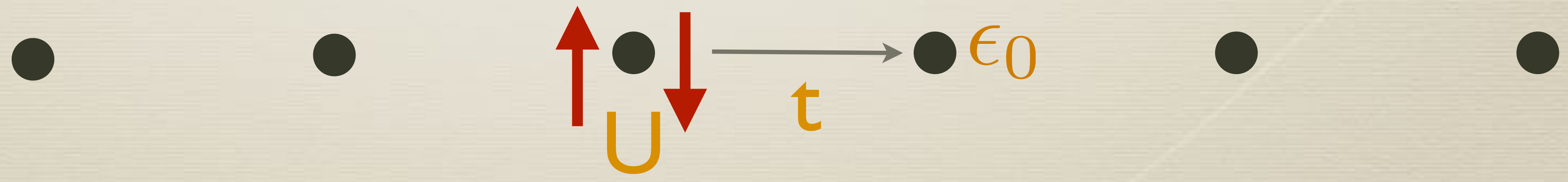
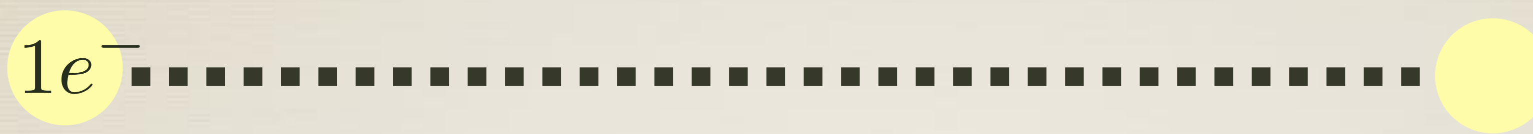
Hubbard model



Vertex corrections: correcting the atomic limit

- **Atomic limit**

H_2^+



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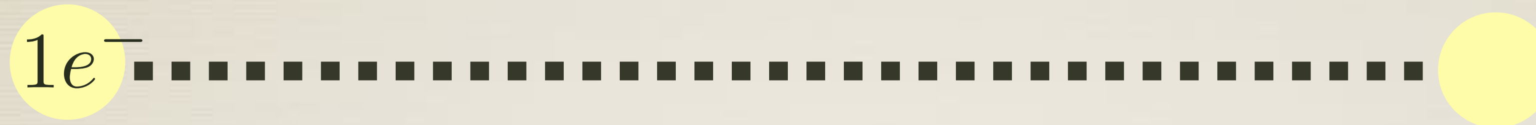

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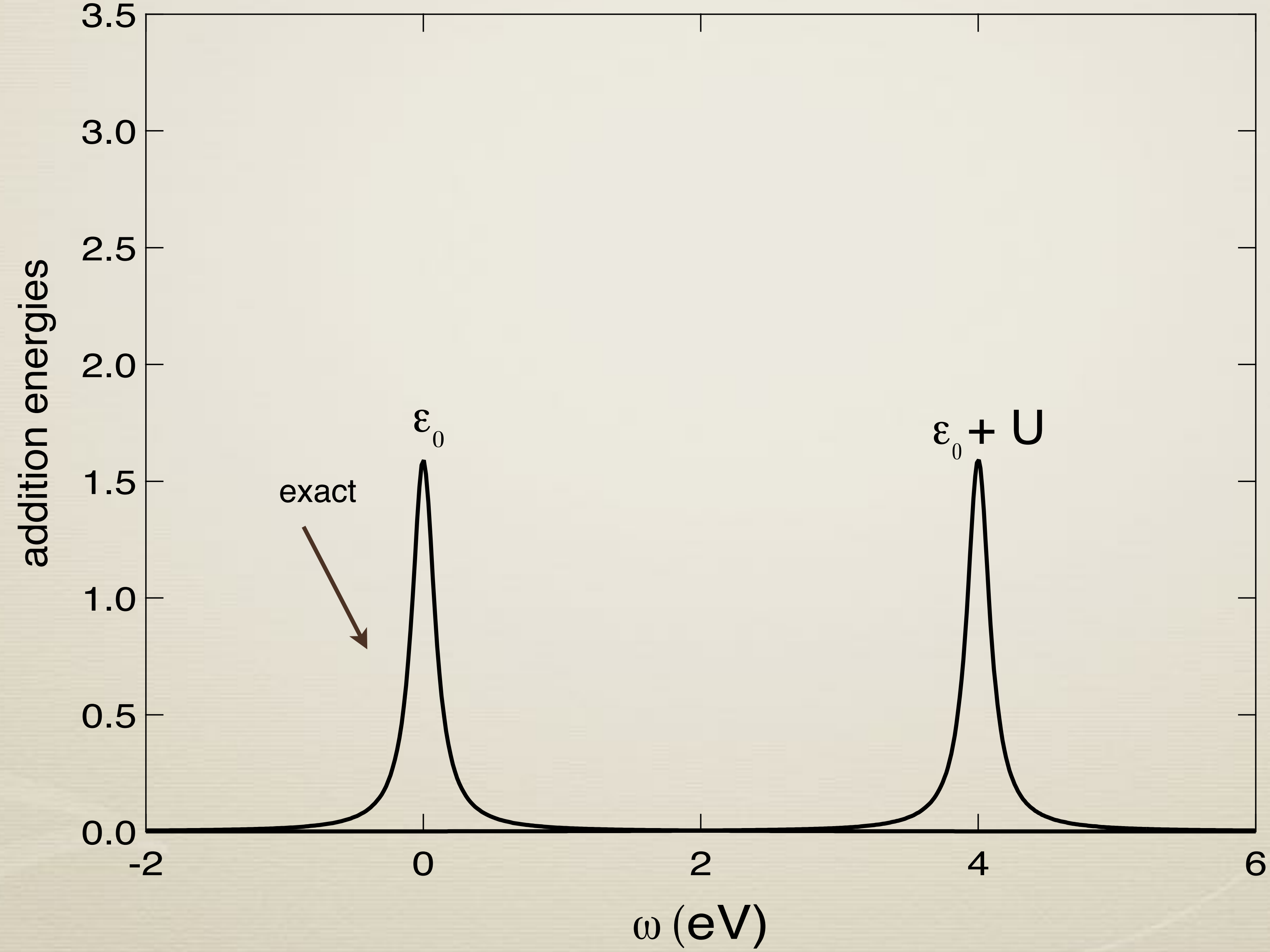
Vertex corrections: correcting the atomic limit

Atomic limit

H_2^+

→ two types of addition energy



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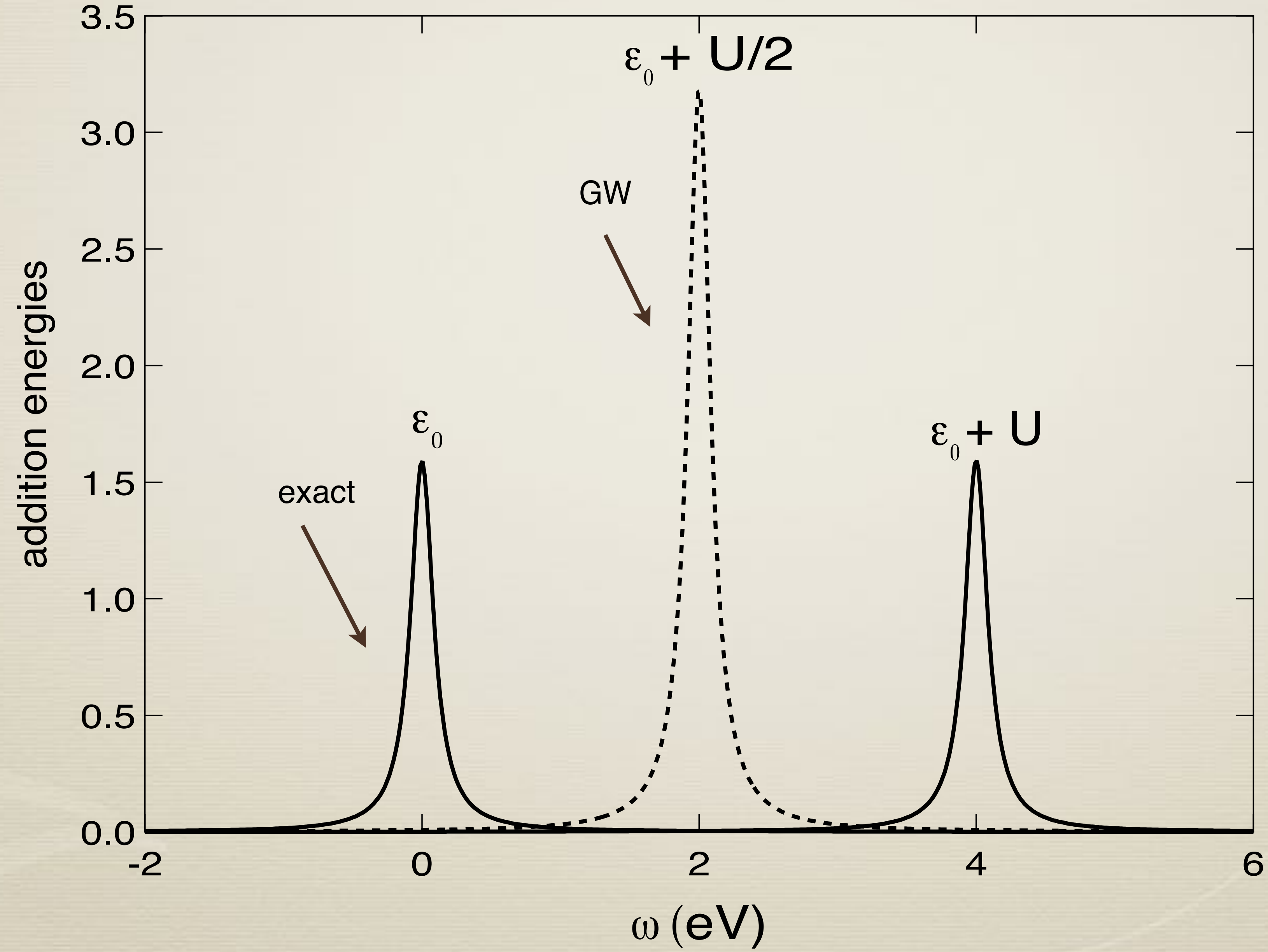
Vertex corrections: correcting the atomic limit

- **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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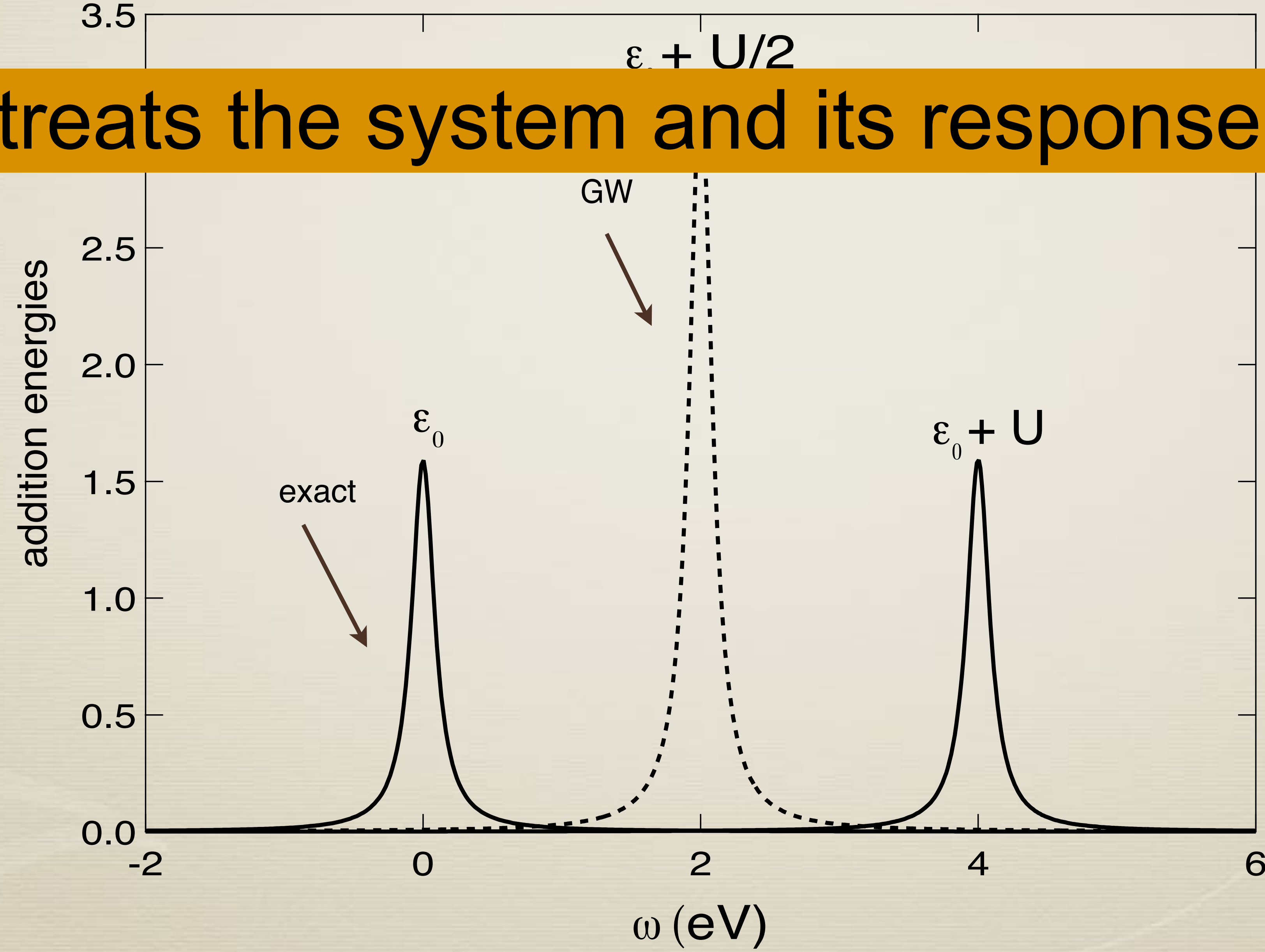

GW treats the system and its response classically

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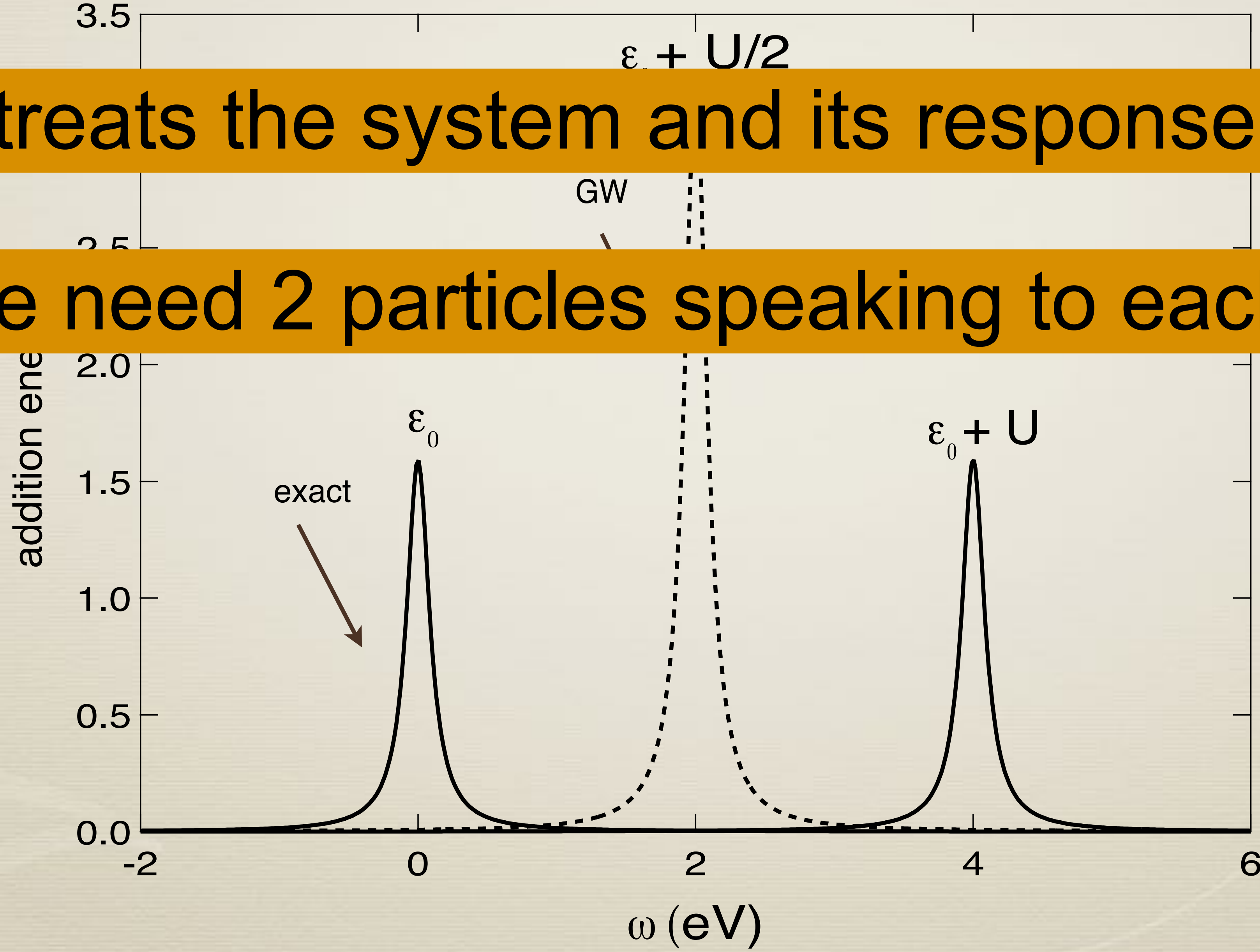

GW treats the system and its response classically

We need 2 particles speaking to each other!

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

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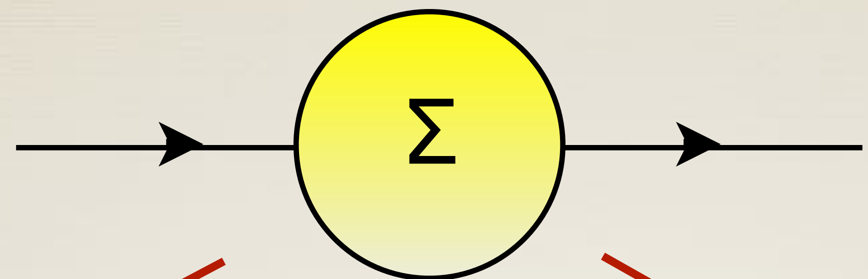
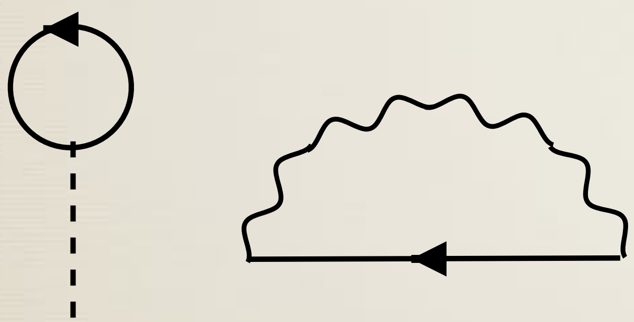


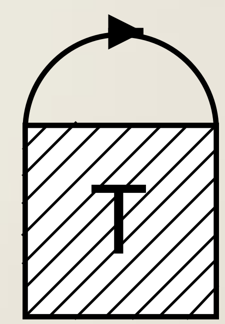
Hedin's eqs

T-matrix

$$\Sigma = v_H + iGW$$



$$\Sigma = GT$$

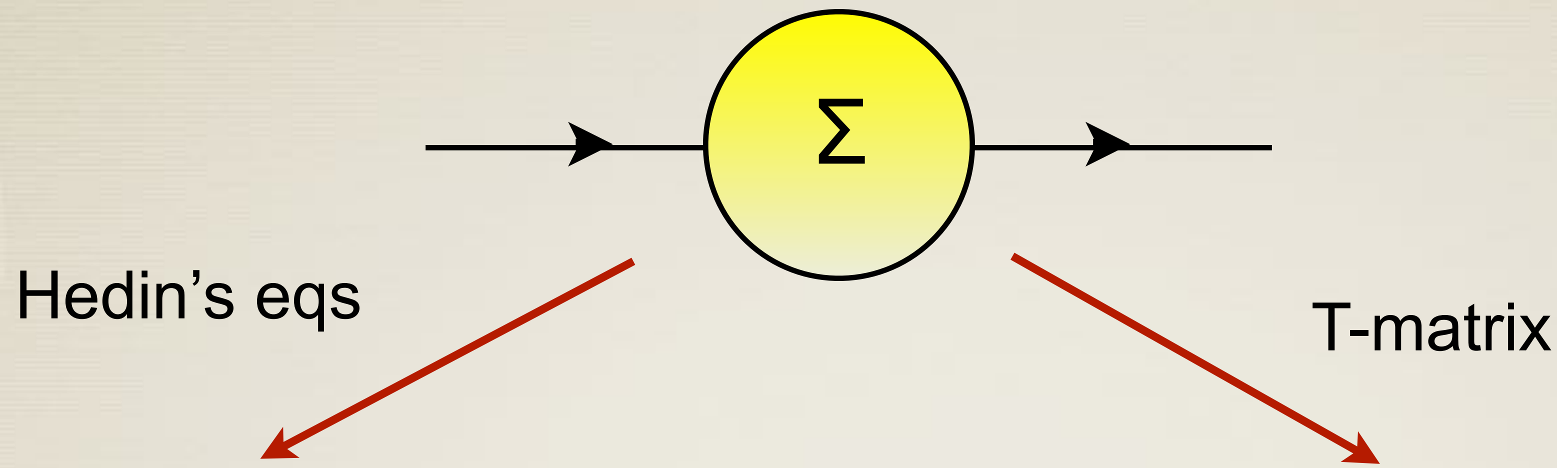


$$T = T_1 + T_2$$

$$T_i = v_c + v_c G G T_i$$

L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics, (W.A. Benjamin Inc., New York), 1964

Vertex corrections: correcting the atomic limit



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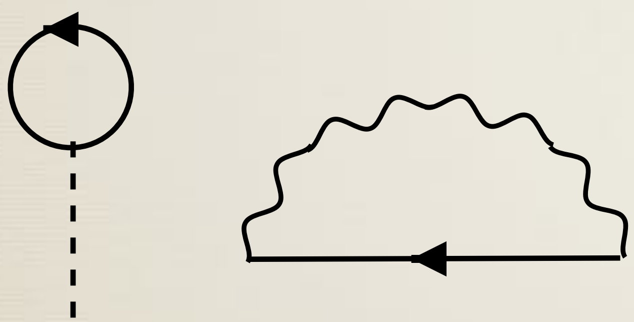

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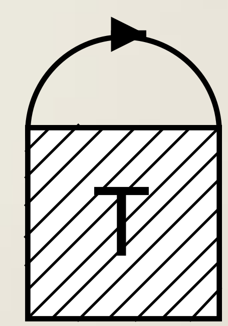

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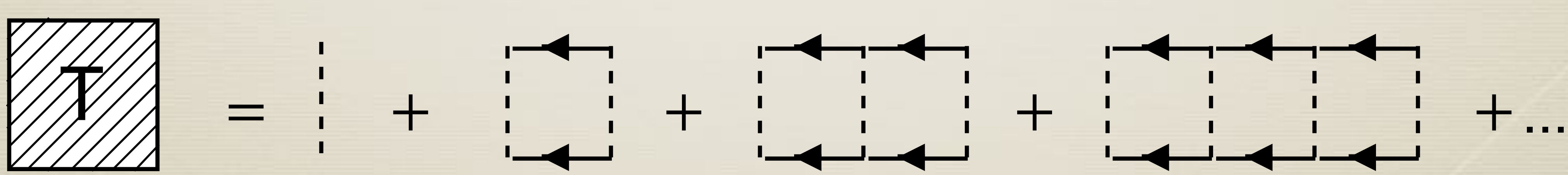

− exchange terms

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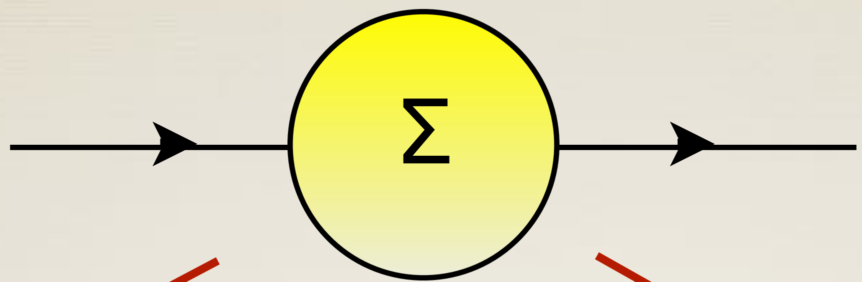


Hedin's eqs

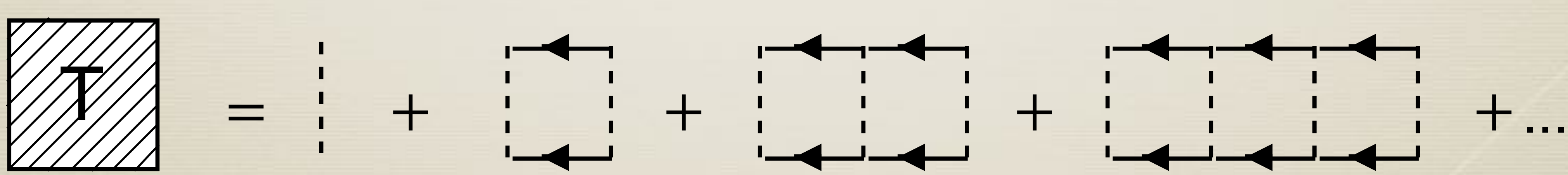
T-matrix

$\Sigma =$

$$\Sigma = v_H + \Sigma_x + i v_c G \underbrace{\frac{\delta \Sigma}{\delta G}}_{\Xi} \underbrace{\frac{\delta G}{\delta U_{ext}}\bigg|_{U_{ext}=0}}_{L}$$

$+ T_2$

$_c G G T_i$



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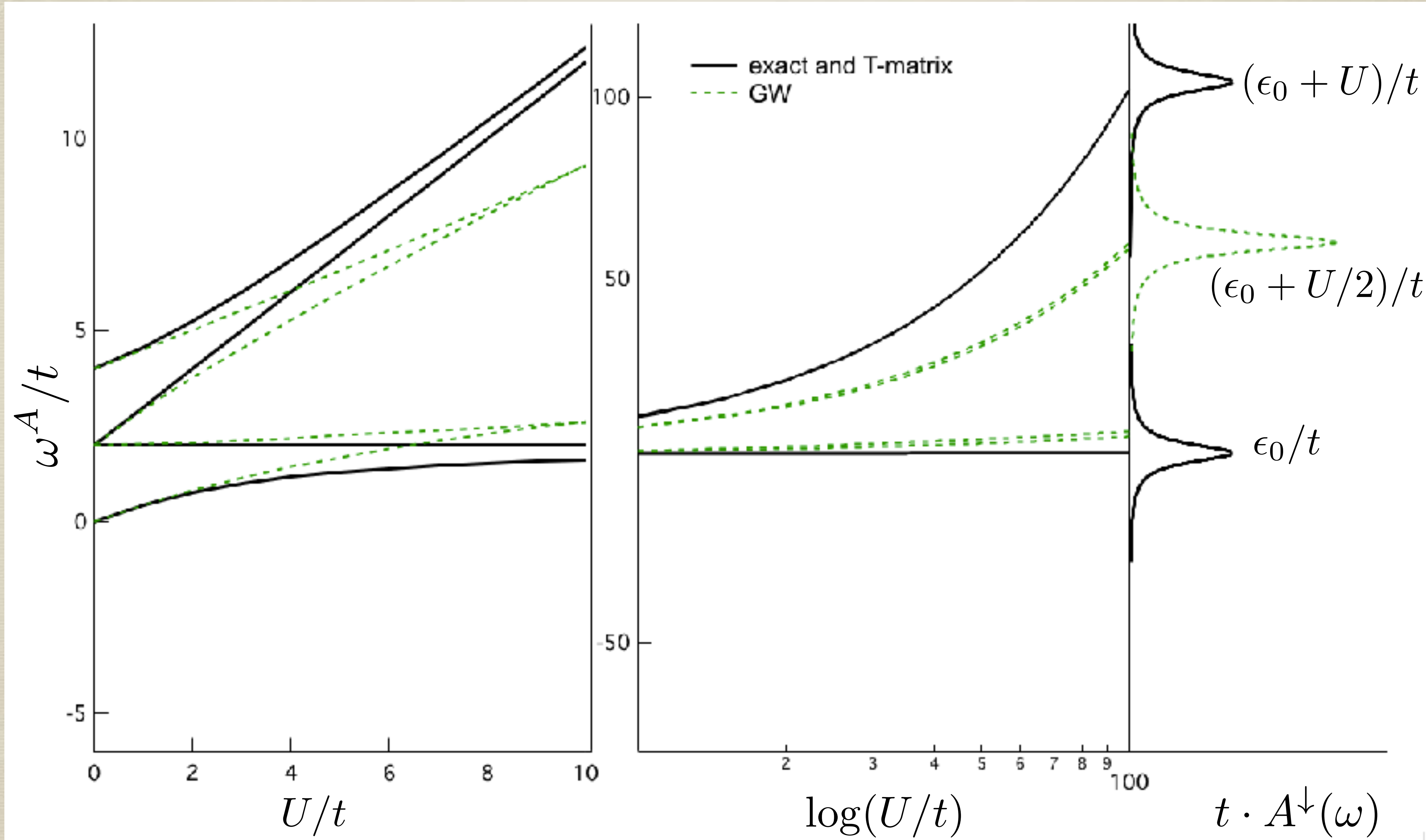
T-matrix approximation: 1 electron

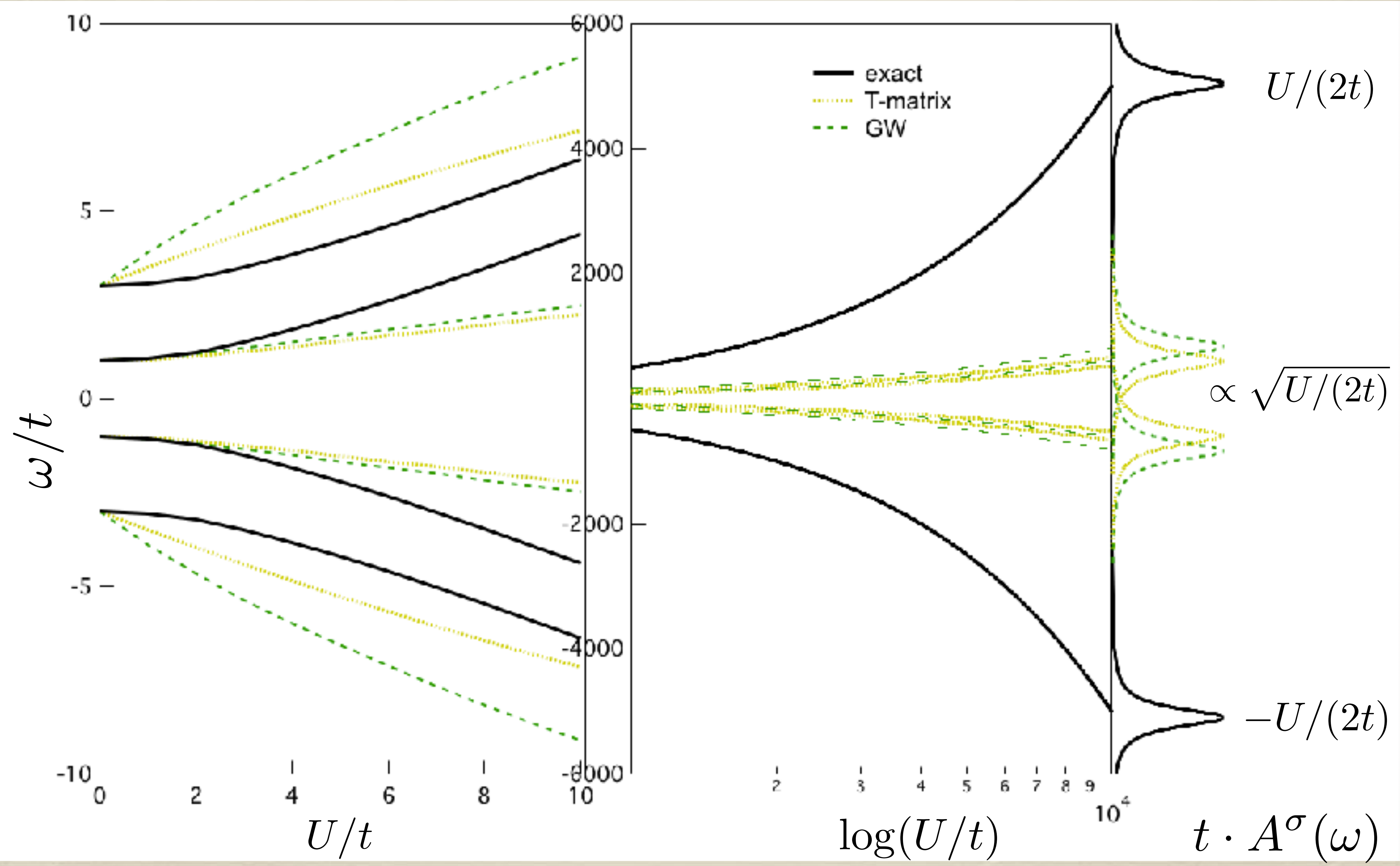
H_2^+



P. R., F. Bechstedt, and L. Reining, Phys. Rev. B 85, 155131 (2012)

T-matrix approximation: 2 electrons

H_2



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Multiple solutions

Dyson equation $$G = G_0 + G_0\Sigma[G]G \xrightarrow[G_0 \to G]{} $$ multiple solutions

Map $G_0 \to G$ ● $y_0 \to y$

* Dyson equation

exact self-energy $\tilde{s}[y_0, u] = -\frac{1}{2} u y_0$ → $y = y_0 + y_0 \tilde{s}[y_0, u] y$

self-energy as functional of y → $y = y_0 + y_0 s[y, u] y$

A. Stan, P. Romaniello, S. Rigamonti, L. Reining, J.A. Berger, New J. Phys. 17, 093045 (2015)

Map $G_0 \to G$ ● $y_0 \to y$

✳ Dyson equation

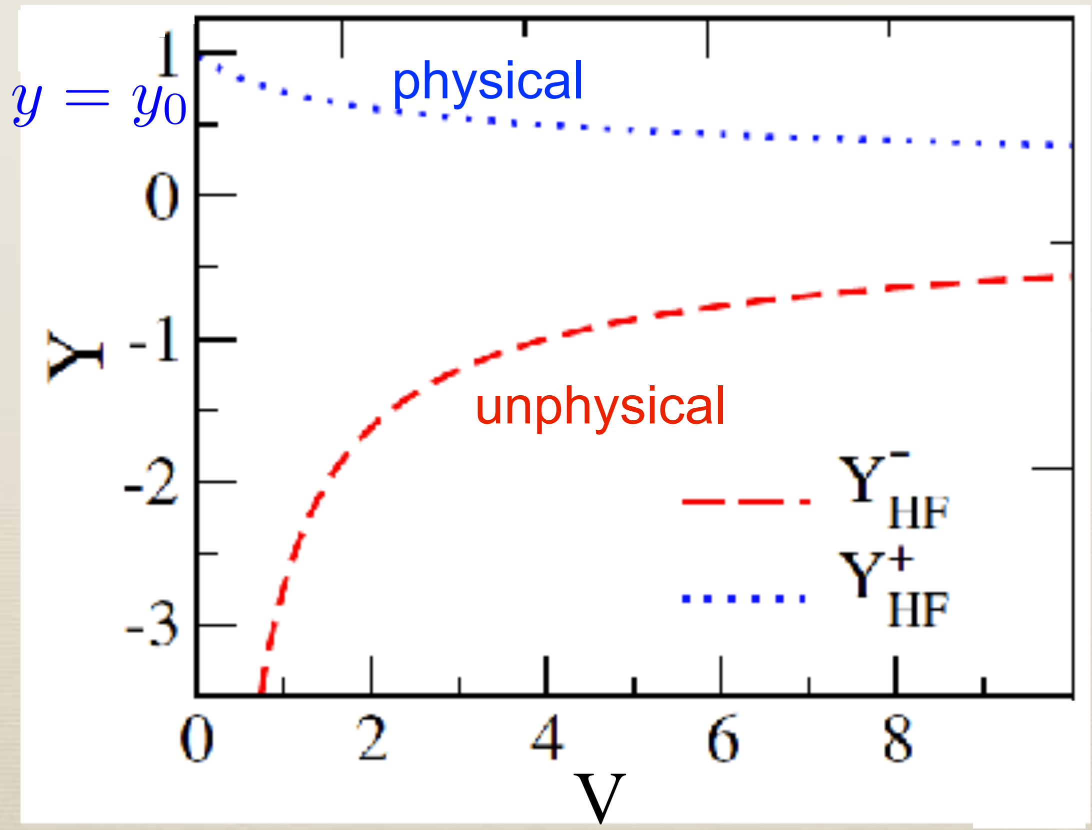
exact self-energy $\tilde{s}[y_0, u] = -\frac{1}{2} u y_0$ → $y = y_0 + y_0 \tilde{s}[y_0, u] y$

self-energy as functional of y → $y = y_0 + y_0 s[y, u] y$

✳ HF self-energy $s^{HF}[y, u] = -\frac{1}{2} u y$

$$y = y_0 + y_0 s^{HF}[y, u] y \;\longrightarrow\; Y^{\pm}_{\text{HF}} = \frac{1}{V}\left[-1 \pm \sqrt{1 + 2V}\right] \quad (Y = y/y_0,\ V = u y_0^2)$$

2 solutions



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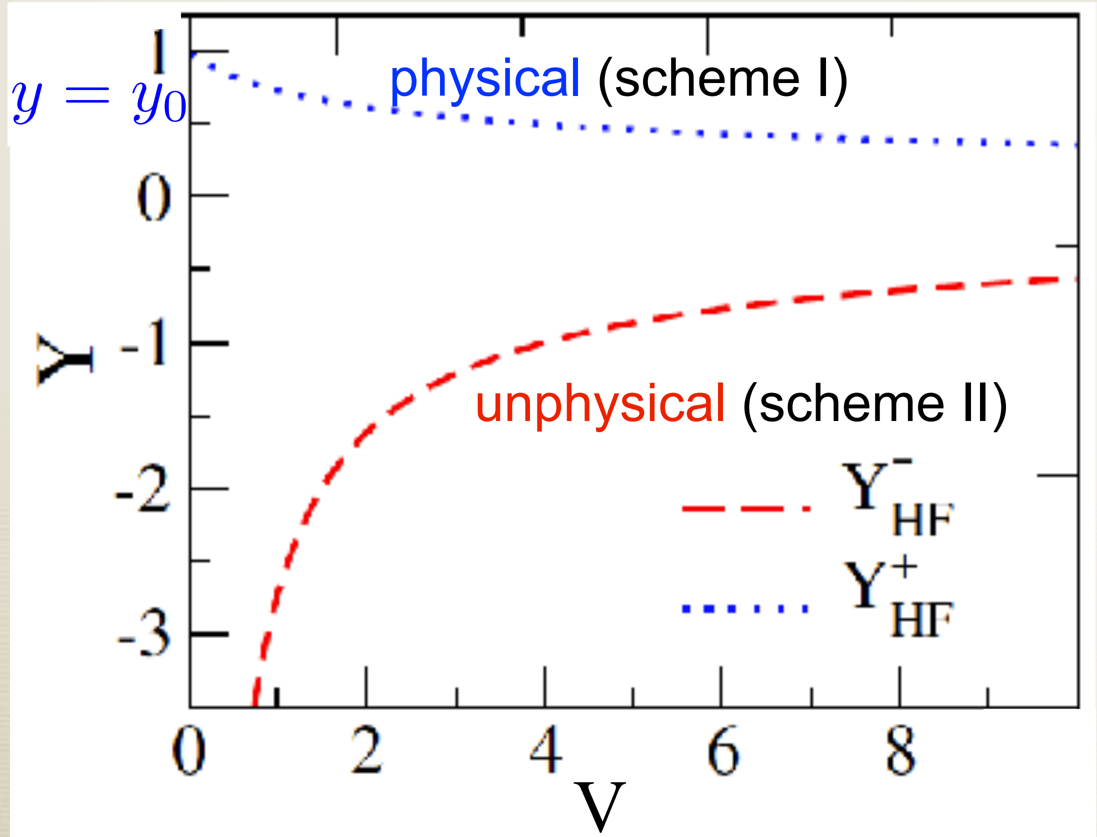
Map $G_0 \to G$ $y_0 \to y$

* Iterative schemes

$$y = y_0 + y_0 s^{HF}[y,u]y$$

scheme I $y^{(n+1)} = \frac{y_0}{1 - y_0 s^{HF}[y^{(n)},u]}$

scheme II $s^{HF}[y^{(n+1)},u] = \frac{1}{y_0} - \frac{1}{y^{(n)}}$



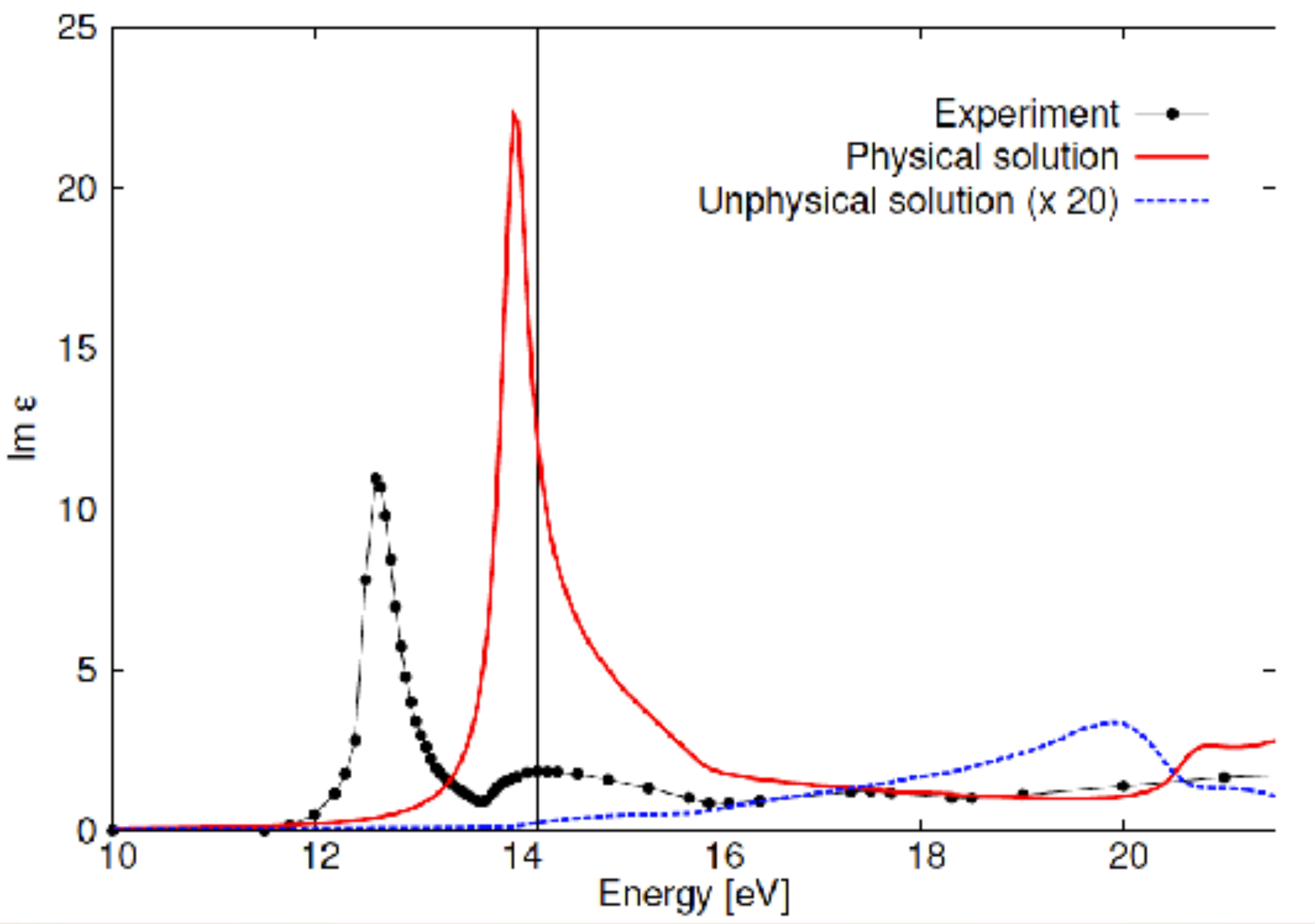
N.B.

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

A. Stan, P. Romaniello, S. Rigamonti, L. Reining, J.A. Berger, New J. Phys. 17, 093045 (2015)

From one point to real life

* Absorption spectrum of LiF



$$\epsilon(\omega) = 1/[1 + v_c \chi(\omega)]$$

$$\chi(\omega) = \chi_0(\omega) + \chi_0(\omega) f_{Hxc}[\chi]\chi(\omega)$$

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

Sharma et. al. PRL (2011)

A. Stan, P. Romaniello, S. Rigamonti, L. Reining, J.A. Berger, New J. Phys. 17, 093045 (2015)

Limits of using a self-energy?

Limits of using a self-energy?

Is there any alternative approach?

G from a many-body effective energy theory

- Spectral representation of G

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

S. Di Sabatino, J.A. Berger, L. Reining, and P. R., Phys. Rev. B 94, 155141 (2016)

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

$$B_{ij}^{k,R} = \langle \Psi_0 | \hat{c}_j^\dagger | \Psi_k^{N-1} \rangle \langle \Psi_k^{N-1} | \hat{c}_i | \Psi_0 \rangle$$

$$B_{ij}^{k,A} = \langle \Psi_0 | \hat{c}_i | \Psi_k^{N+1} \rangle \langle \Psi_k^{N+1} | \hat{c}_j^\dagger | \Psi_0 \rangle$$

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G from a many-body effective energy theory

* Spectral representation of G

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

$i = j$, basis of natural orbitals $\gamma(\mathbf{x}, \mathbf{x}') = \sum_i n_i \phi_i(\mathbf{x}) \phi_i^*(\mathbf{x}')$

$$\sum_k B_{ii}^{k,R} = n_i \qquad \sum_k B_{ii}^{k,A} = 1 - n_i$$

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G from a many-body effective energy theory

- Removal part of G

$$G^R_{ii}(\omega) = \sum_k \frac{B^{k,R}_{ii}}{\omega - \epsilon^R_k}$$

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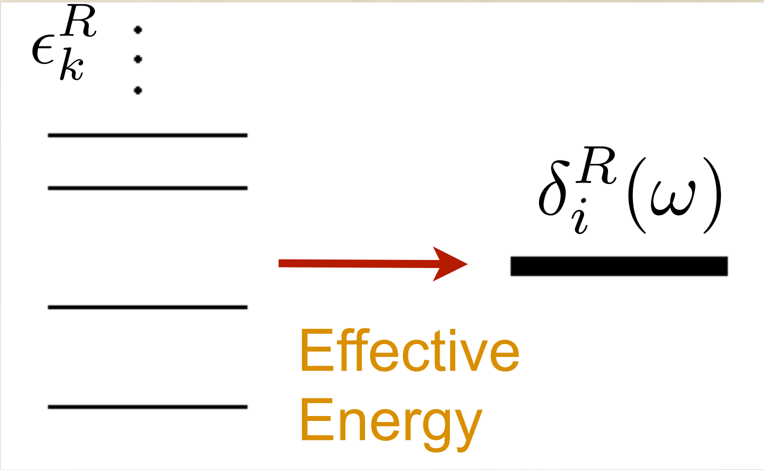
G from a many-body effective energy theory

* Removal part of G

$$G_{ii}^{R}(\omega) = \sum_k \frac{B_{ii}^{k,R}}{\omega - \epsilon_k^R} = \frac{\sum_k B_{ii}^{k,R}}{\omega - \delta_i^R(\omega)}$$



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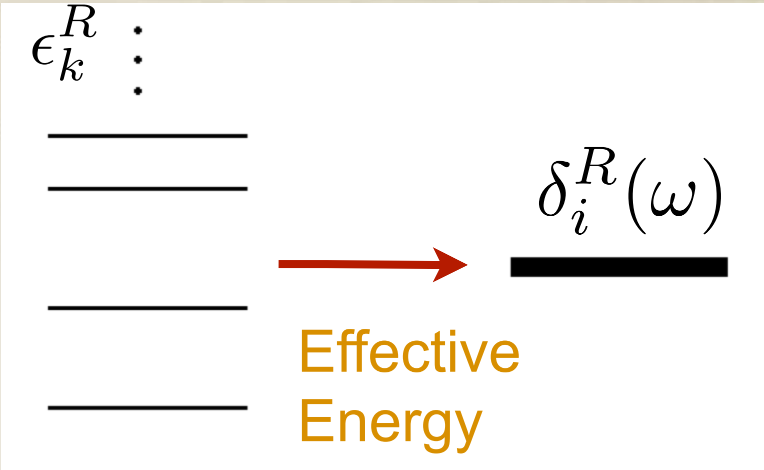
G from a many-body effective energy theory

✳ Removal part of G

$$G_{ii}^{R}(\omega) = \sum_k \frac{B_{ii}^{k,R}}{\omega - \epsilon_k^R} = \frac{\sum_k B_{ii}^{k,R}}{\omega - \delta_i^R(\omega)} = \frac{n_i}{\omega - \delta_i^R(\omega)}$$



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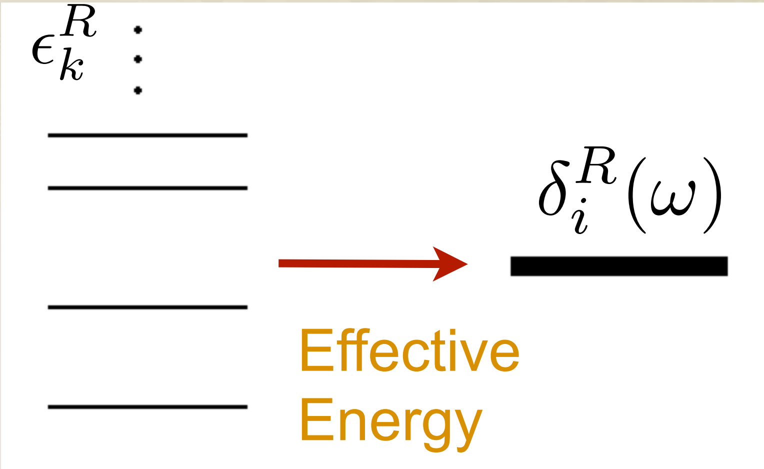
G from a many-body effective energy theory

✳ Removal part of G

$$G^R_{ii}(\omega) = \sum_k \frac{B^{k,R}_{ii}}{\omega - \epsilon^R_k} = \frac{\sum_k B^{k,R}_{ii}}{\omega - \delta^R_i(\omega)} = \frac{n_i}{\omega - \delta^R_i(\omega)}$$



$$\delta^R_i(\omega) = \frac{1}{G^R_{ii}(\omega)} \sum_k \frac{\langle\Psi_0|\hat{c}^\dagger_i|\Psi^{N-1}_k\rangle\langle\Psi^{N-1}_k|\hat{c}_i|\Psi_0\rangle}{\omega - \epsilon^R_k}\epsilon^R_k$$

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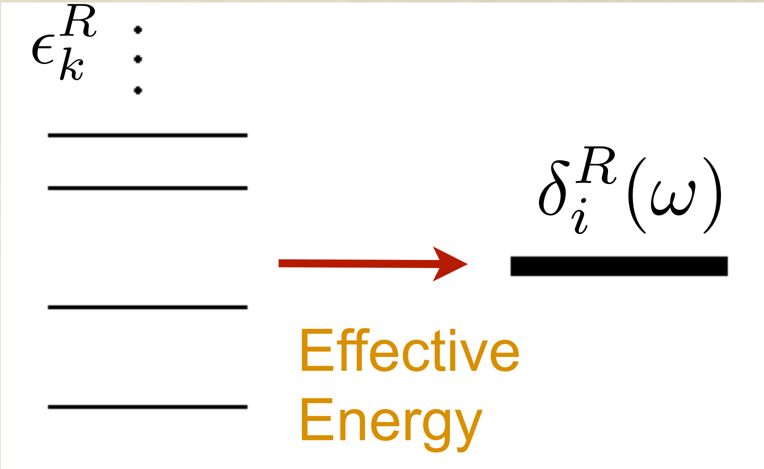
G from a many-body effective energy theory

- Removal part of G

$$G^R_{ii}(\omega) = \sum_k \frac{B^{k,R}_{ii}}{\omega - \epsilon^R_k} = \frac{\sum_k B^{k,R}_{ii}}{\omega - \delta^R_i(\omega)} = \frac{n_i}{\omega - \delta^R_i(\omega)}$$



$$\delta^R_i(\omega) = \frac{1}{G^R_{ii}(\omega)} \sum_k \frac{\langle \Psi_0 | \hat{c}^\dagger_i | \Psi^{N-1}_k \rangle \langle \Psi^{N-1}_k | [\hat{c}_i, \hat{H}] | \Psi_0 \rangle}{\omega - \epsilon^R_k}$$

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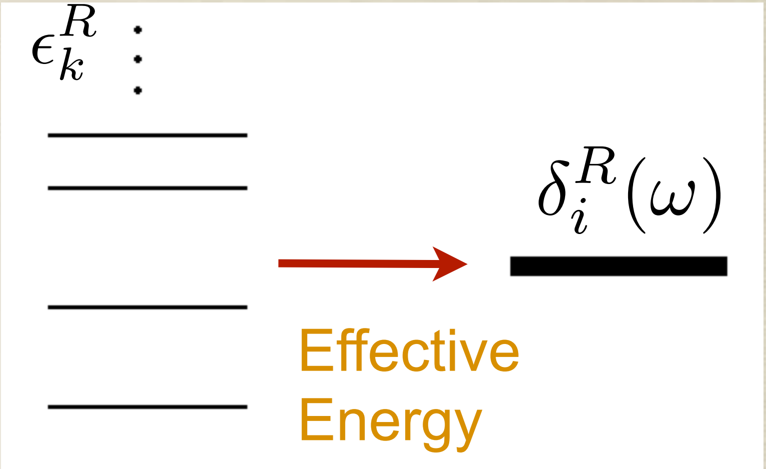
G from a many-body effective energy theory

✳ Removal part of G

$$G^R_{ii}(\omega) = \sum_k \frac{B^{k,R}_{ii}}{\omega - \epsilon^R_k} = \frac{\sum_k B^{k,R}_{ii}}{\omega - \delta^R_i(\omega)} = \frac{n_i}{\omega - \delta^R_i(\omega)}$$



$$\delta^R_i(\omega) = \frac{1}{G^R_{ii}(\omega)} \sum_k \frac{\langle \Psi_0 | \hat{c}^\dagger_i | \Psi^{N-1}_k \rangle \langle \Psi^{N-1}_k | [\hat{c}_i, \hat{H}] | \Psi_0 \rangle}{\omega - \epsilon^R_k} = \frac{\tilde{G}^R_{ii}(\omega)}{G^R_{ii}(\omega)}$$

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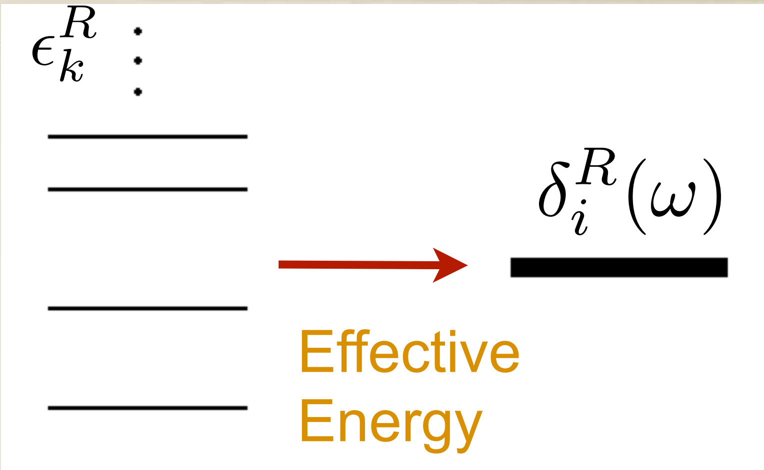
G from a many-body effective energy theory

* Removal part of G

$$G_{ii}^R(\omega) = \sum_k \frac{B_{ii}^{k,R}}{\omega - \epsilon_k^R} = \frac{\sum_k B_{ii}^{k,R}}{\omega - \delta_i^R(\omega)} = \frac{n_i}{\omega - \delta_i^R(\omega)}$$



$$\delta_i^R(\omega) = \frac{1}{G_{ii}^R(\omega)} \sum_k \frac{\langle \Psi_0 | \hat{c}_i^\dagger | \Psi_k^{N-1} \rangle \langle \Psi_k^{N-1} | [\hat{c}_i, \hat{H}] | \Psi_0 \rangle}{\omega - \epsilon_k^R} = \frac{\tilde{G}_{ii}^R(\omega)}{G_{ii}^R(\omega)}$$

$$= \frac{\tilde{n}_i^R}{n_i} \frac{\omega - \frac{\tilde{G}_{ii}^R(\omega)}{G_{ii}^R(\omega)}}{\omega - \frac{\tilde{\tilde{G}}_{ii}^R(\omega)}{\tilde{G}_{ii}^R(\omega)}}$$

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G from a many-body effective energy theory

* Approximations to the removal effective energy $\delta_i^R(\omega)$

$$\delta_i^{R,(1)} = \frac{\tilde{n}_i^R}{n_i}$$

$$\delta_i^{R,(2)}(\omega) = \frac{\tilde{n}_i^R}{n_i} \frac{\omega - \frac{\tilde{n}_i^R}{n_i}}{\omega - \frac{\tilde{\tilde{n}}_i^R}{\tilde{n}_i^R}}$$

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G from a many-body effective energy theory

* Approximations to the removal effective energy $\delta_i^R(\omega)$

$$\delta_i^{R,(1)} = \frac{\tilde{n}_i^R}{n_i}$$

$$\delta_i^{R,(2)}(\omega) = \frac{\tilde{n}_i^R}{n_i} \frac{\omega - \frac{\tilde{n}_i^R}{n_i}}{\omega - \frac{\tilde{\tilde{n}}_i^R}{\tilde{n}_i^R}}$$

$\delta_i^{R,(n)}$ in terms of reduced density matrices

$$\tilde{n}_i^R = \langle \Psi_0 | \hat{c}_i^\dagger [\hat{c}_i, \hat{H}] | \Psi_0 \rangle = h_{ii} n_i + \sum_{jkl} V_{ijkl} \Gamma^{(2)}_{klji}$$

$$\tilde{\tilde{n}}_i^R = \langle \Psi_0 | [\hat{H}, \hat{c}_i^\dagger][\hat{c}_i, \hat{H}] | \Psi_0 \rangle = h_{ii}^2 n_i + h_{ii} \sum_{jkl} \left(V_{ijkl} \Gamma^{(2)}_{klji} + V_{jkil} \Gamma^{(2)}_{ilkj} \right)$$

$$+ \sum_{jklk'l'} V_{jkil} V_{ilk'l'} \Gamma^{(2)}_{k'l'kj} + \sum_{jklj'k'l'} V_{jkil} V_{ij'k'l'} \Gamma^{(3)}_{k'l'lj'kj}$$

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G from a many-body effective energy theory

* Approximations to $\delta_i^R(\omega)$ and $\delta_i^A(\omega)$

$$\delta_i^{R,(1)} = \frac{\tilde{n}_i^R}{n_i} \qquad \delta_i^{A,(1)} = \frac{\tilde{n}_i^A}{1-n_i}$$

$$\delta_i^{R,(2)}(\omega) = \frac{\tilde{n}_i^R}{n_i}\frac{\omega - \frac{\tilde{n}_i^R}{n_i}}{\omega - \frac{\tilde{\tilde{n}}_i^R}{\tilde{n}_i^R}} \qquad \delta_i^{A,(2)}(\omega) = \frac{\tilde{n}_i^A}{1-n_i}\frac{\omega - \frac{\tilde{n}_i^A}{1-n_i}}{\omega - \frac{\tilde{\tilde{n}}_i^A}{\tilde{n}_i^A}}$$

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G from a many-body effective energy theory

✳ Approximations to $\delta_i^R(\omega)$ and $\delta_i^A(\omega)$

$$\delta_i^{R,(1)} = \frac{\tilde{n}_i^R}{n_i} \qquad \delta_i^{A,(1)} = \frac{\tilde{n}_i^A}{1-n_i}$$

$$\delta_i^{R,(2)}(\omega) = \frac{\tilde{n}_i^R}{n_i}\frac{\omega - \frac{\tilde{n}_i^R}{n_i}}{\omega - \frac{\tilde{\tilde{n}}_i^R}{\tilde{n}_i^R}} \qquad \delta_i^{A,(2)}(\omega) = \frac{\tilde{n}_i^A}{1-n_i}\frac{\omega - \frac{\tilde{n}_i^A}{1-n_i}}{\omega - \frac{\tilde{\tilde{n}}_i^A}{\tilde{n}_i^A}}$$

✳ Spectral function

$$A_{ii}(\omega) = n_i\delta(\omega - \delta_i^R(\omega)) + (1-n_i)\delta(\omega - \delta_i^A(\omega))$$

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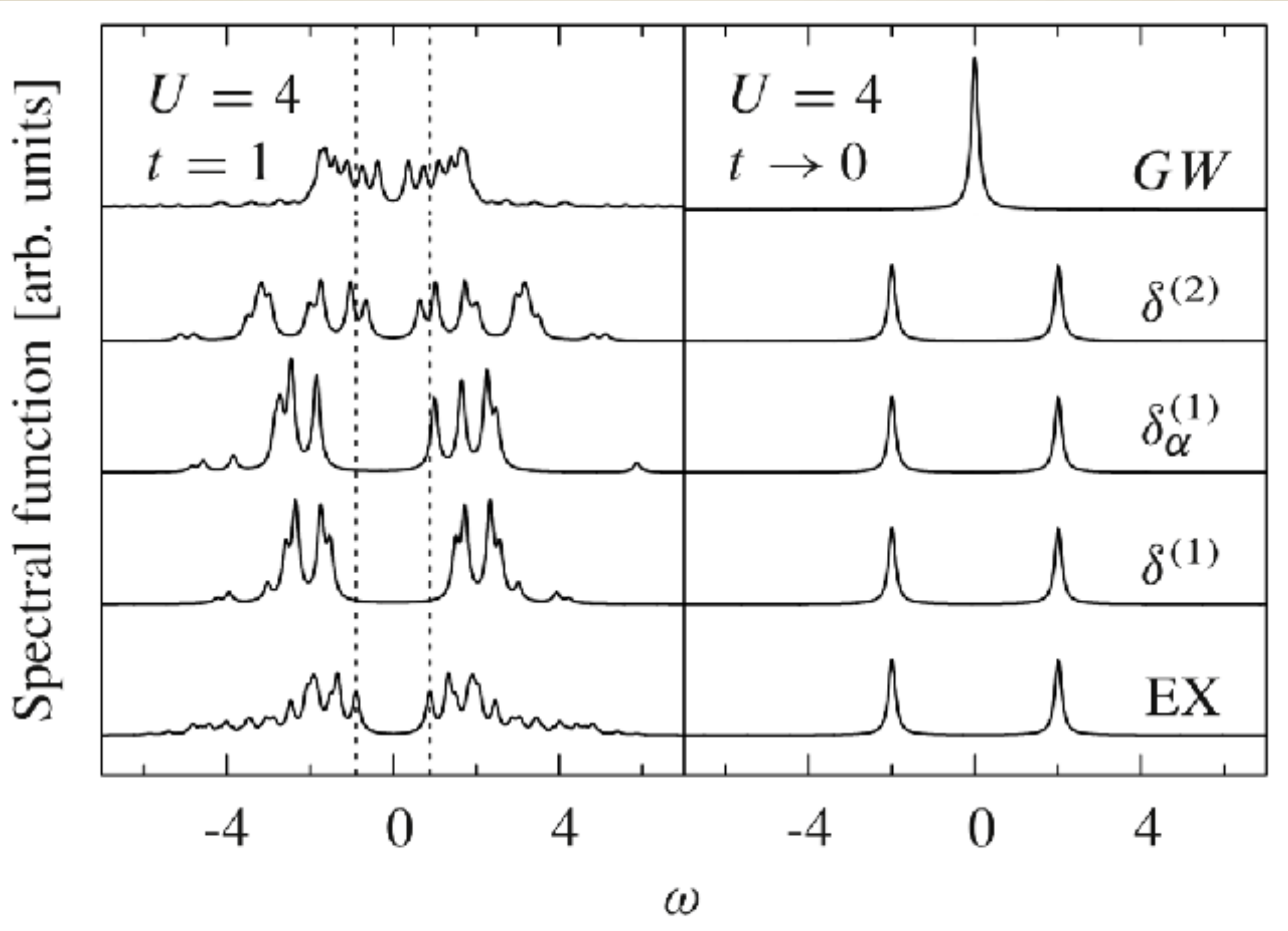
G from a many-body effective energy theory

- 12 sites at 1/2 filling



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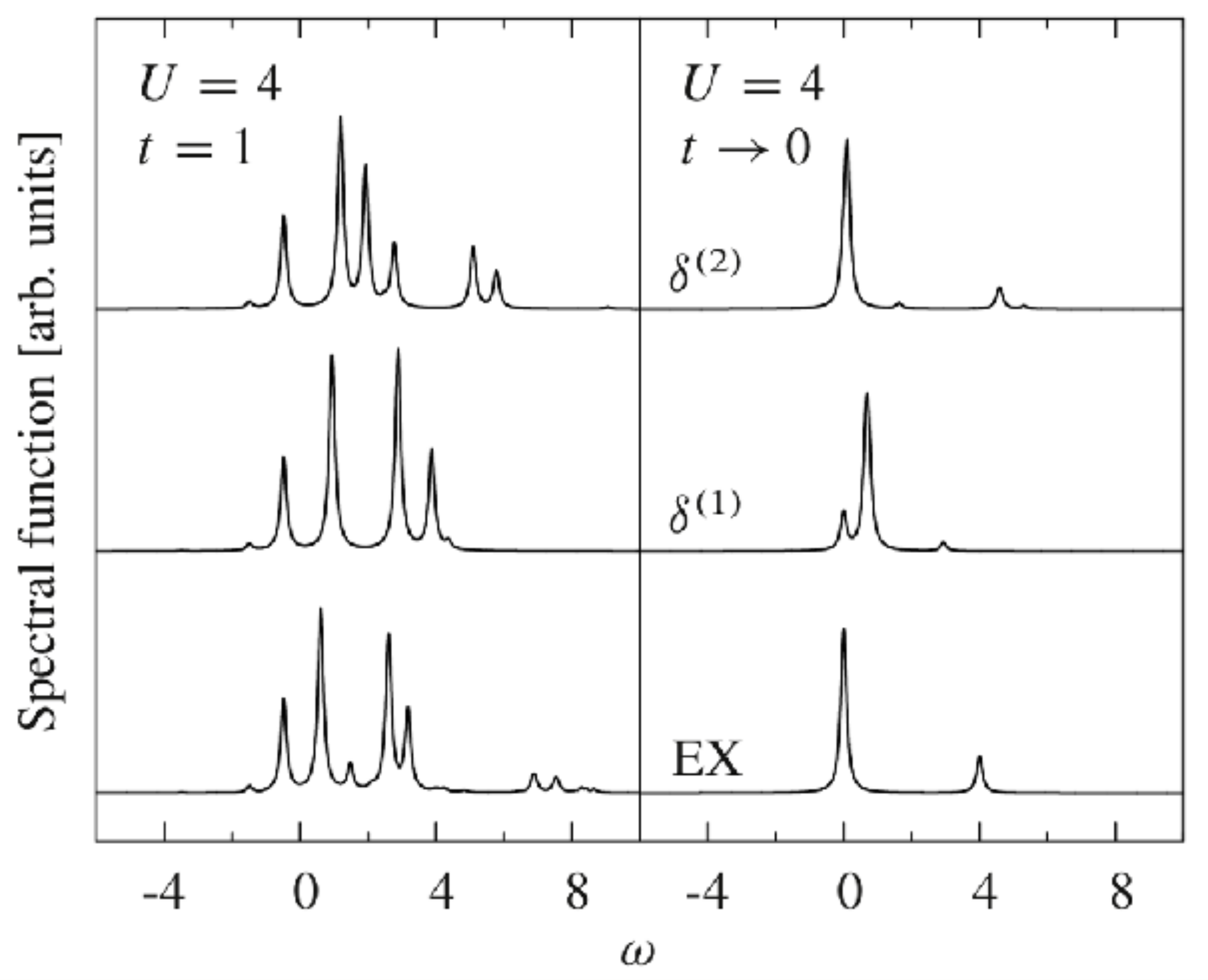
G from a many-body effective energy theory

- 6 sites at 1/6 filling



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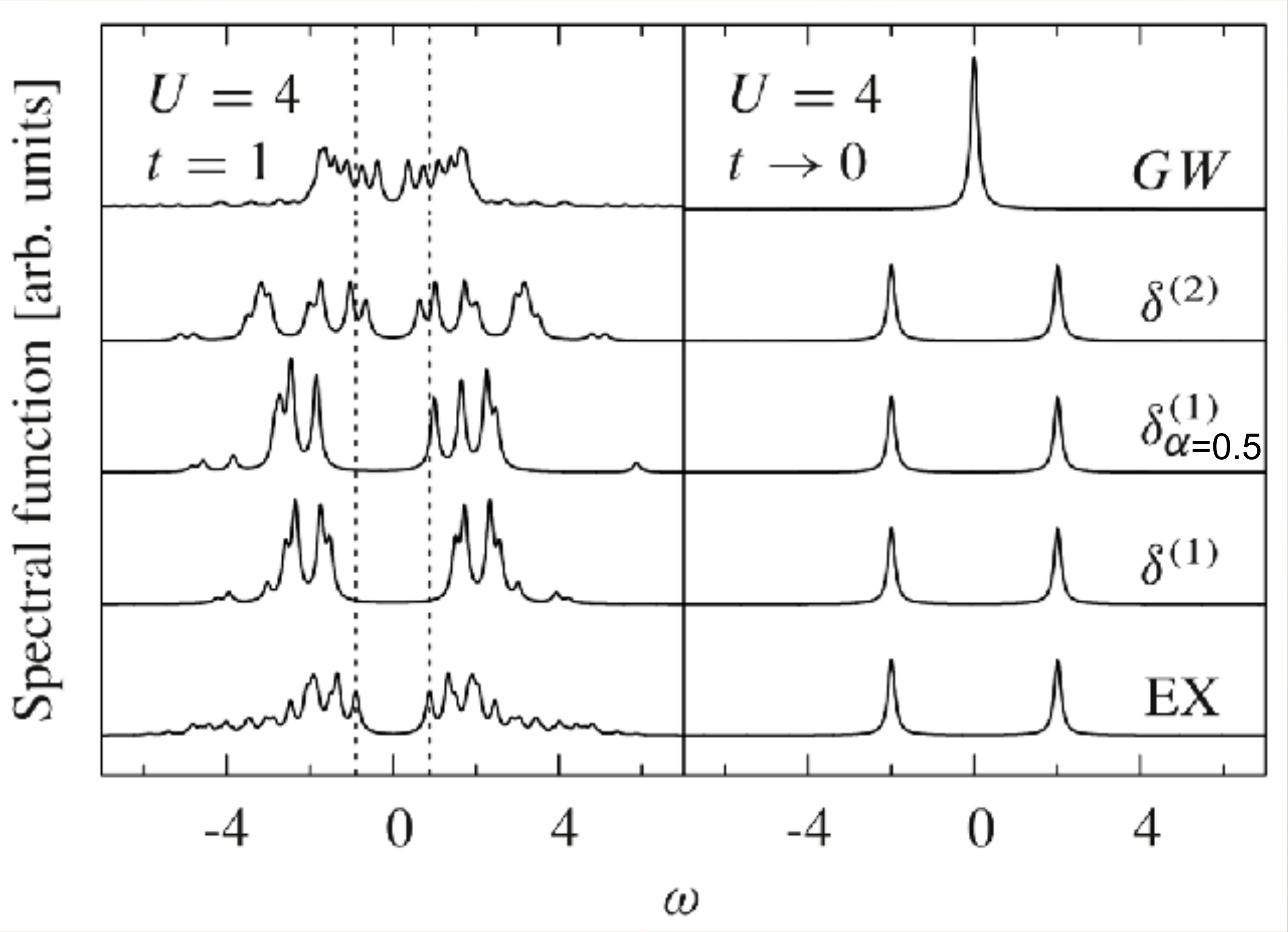
G from a many-body effective energy theory

- 12 sites at 1/2 filling



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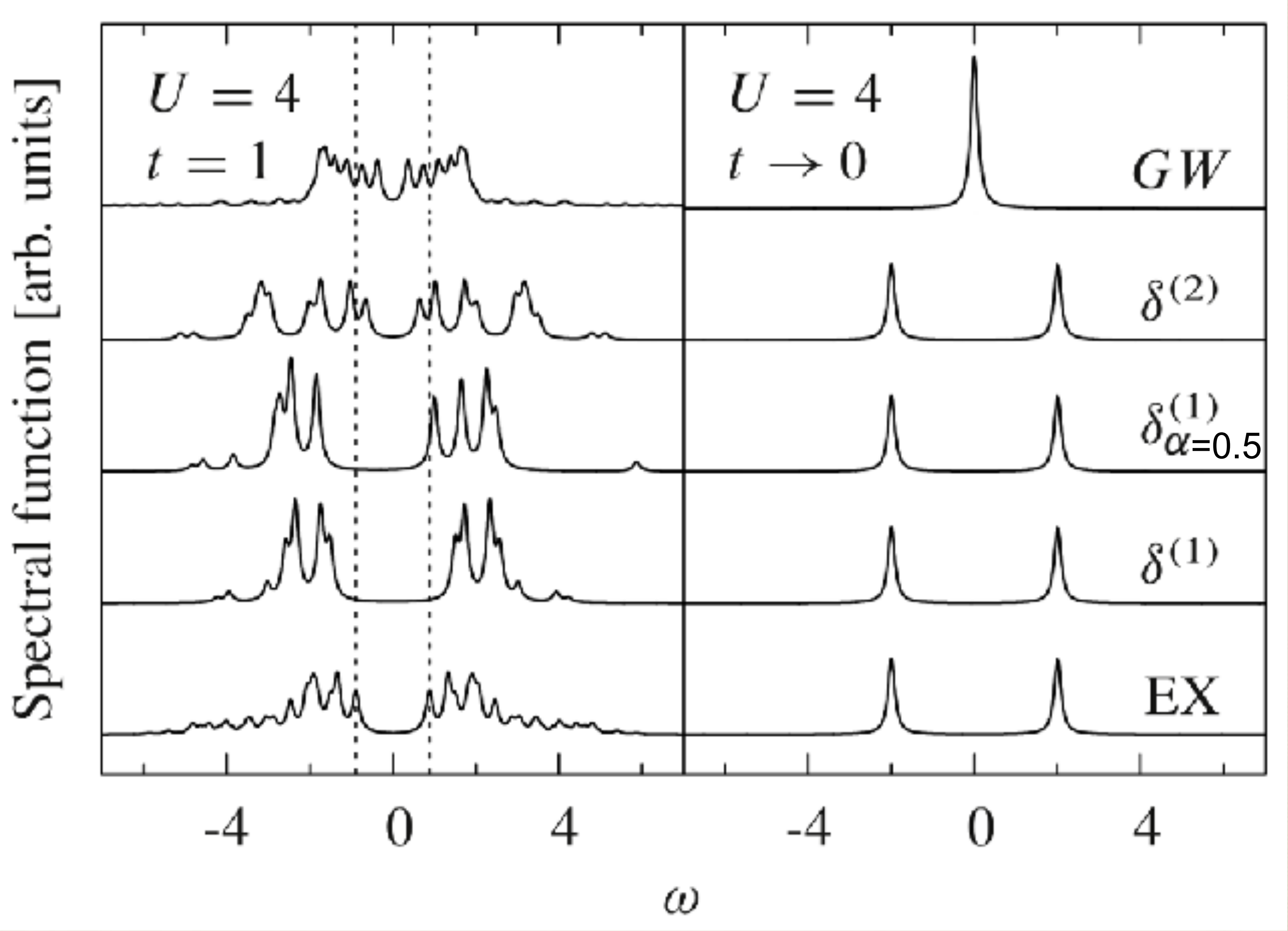
G from a many-body effective energy theory

- 12 sites at 1/2 filling



$$\Gamma^{(2)}_{\alpha} = \gamma\gamma - \gamma^{\alpha}\gamma^{\alpha}, \quad (0.5 \leq \alpha \leq 1)$$

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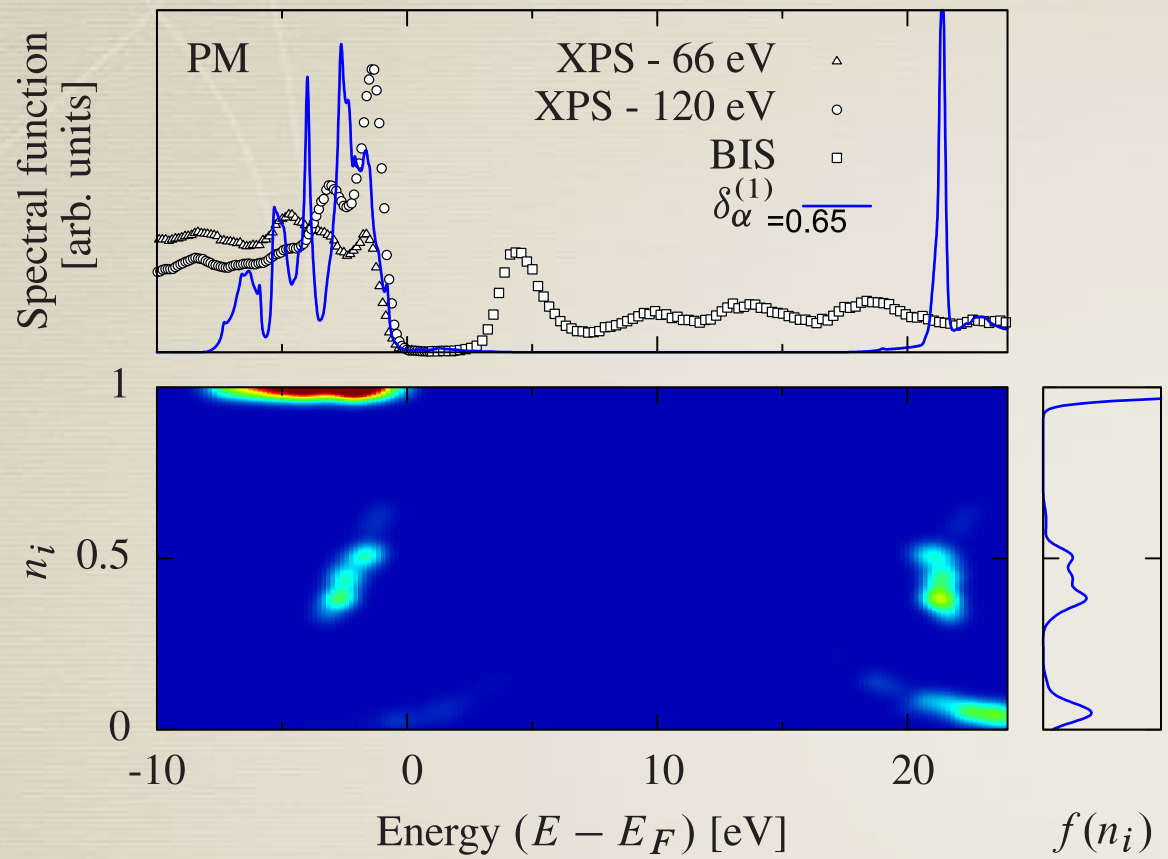
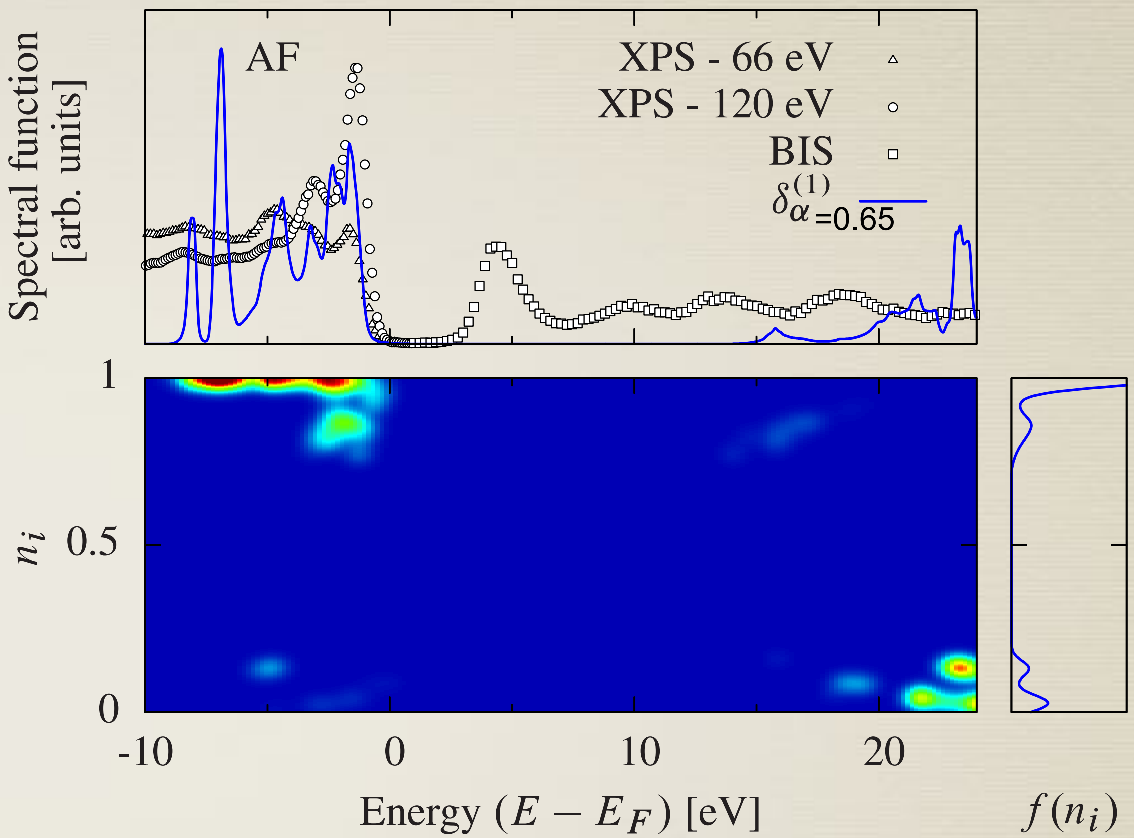
G from a many-body effective energy theory

- NiO





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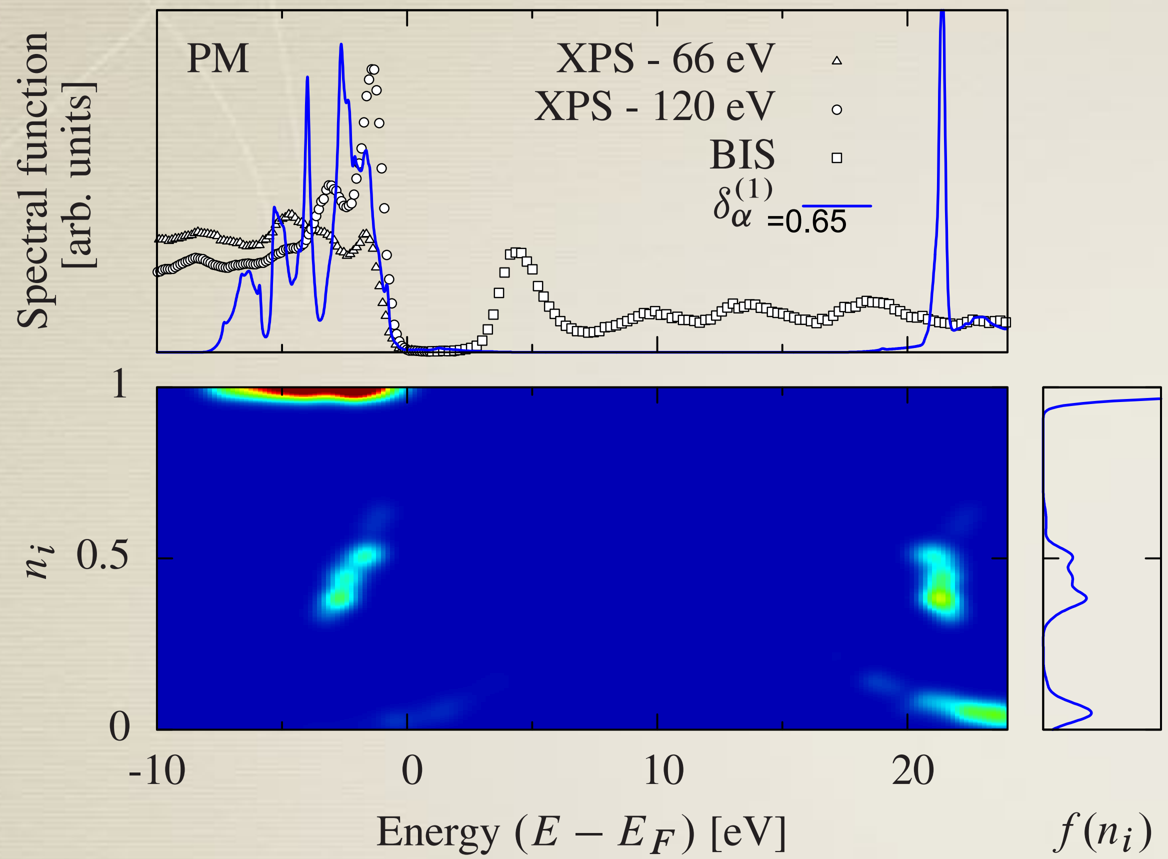
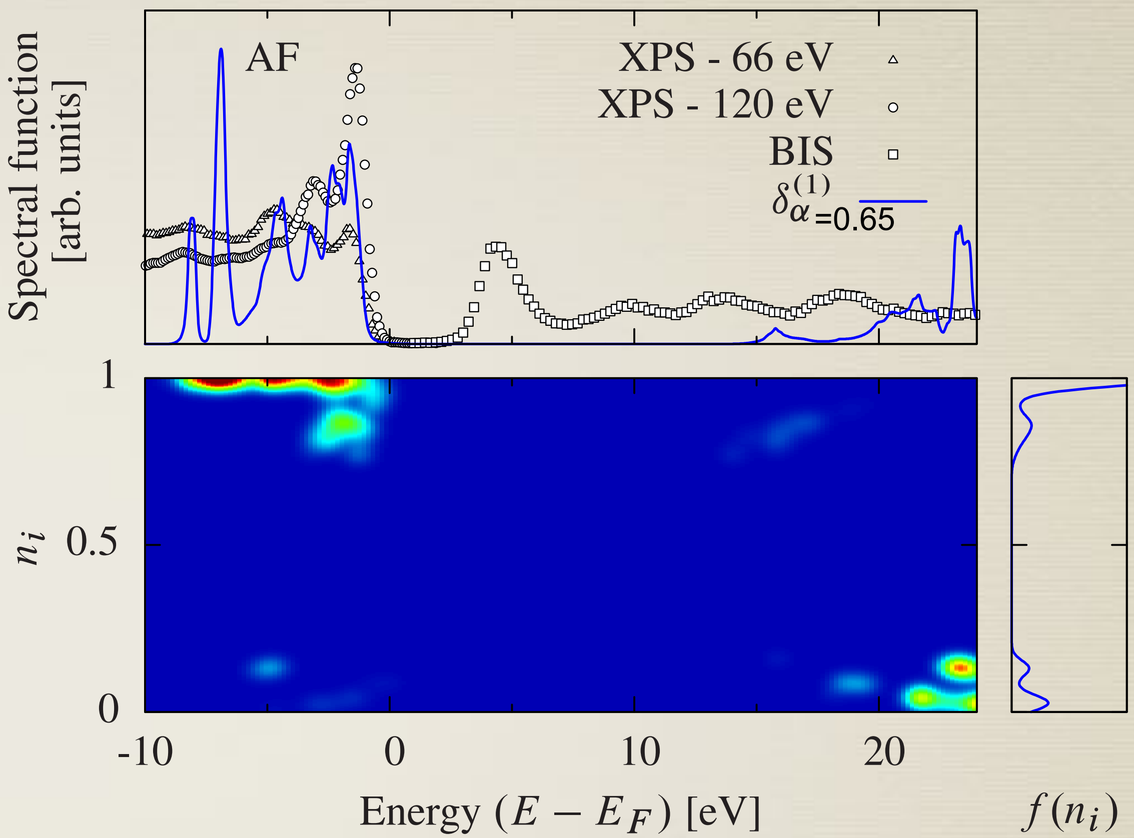
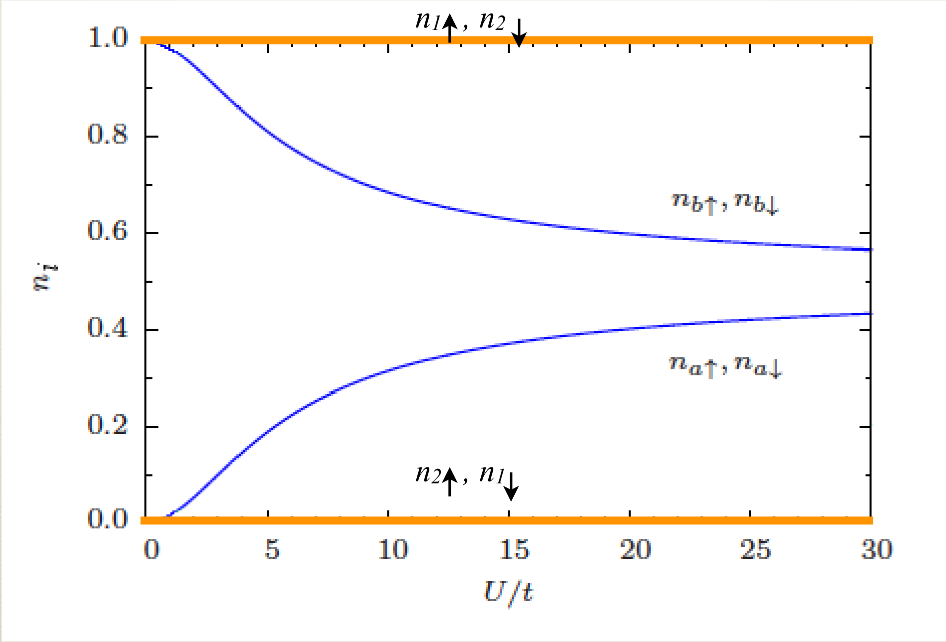
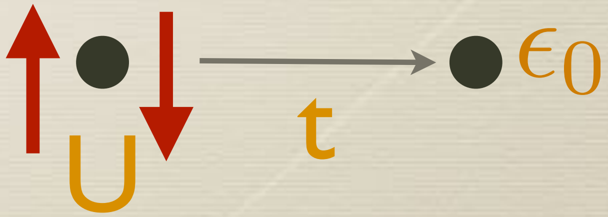
G from a many-body effective energy theory

* NiO









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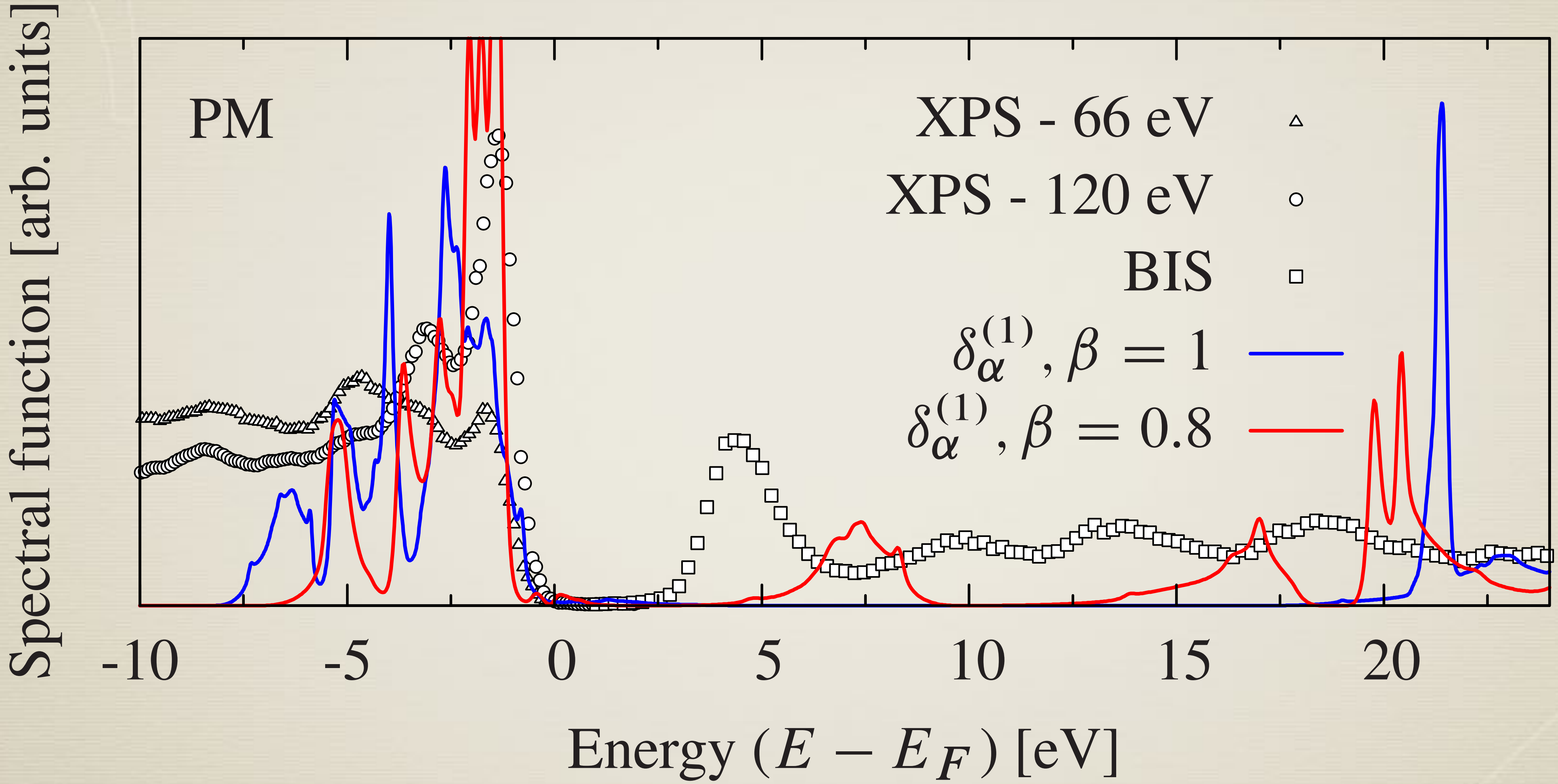
G from a many-body effective energy theory

- PM NiO



$$\delta_i^{R,(1)} = h_{ii} + \sum_j V_{ijij} n_j + \frac{\beta_i}{n_i} \sum_{jkl} V_{ijkl} \Gamma^{(2)}_{\mathrm{xc},klji} \qquad (0 \leq \beta_i \leq 1)$$

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Conclusions & Outlooks

- GW fails in the atomic limit
- Inclusion of vertex corrections too complicated
- Problem of multiple solutions worsen with vertex corrections
- Spectral function from a many-body effective energy theory promising
  - Simple approximations give accurate spectra in model systems at weak and strong correlation (without symmetry breaking)
  - $\delta^{(1)}$ (1- and 2-body reduced density matrices) produces a qualitative correct spectra for the AF and PM phases
  - How to go beyond $\delta^{(1)}$?

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