Beyond GW: local and nonlocal vertex corrections

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European
Theoretical
Spectroscopy
Facility
an initiative of the
Nanoquanta
Network of Excellence

KITP, Santa Barbara 2009

Prologue

xc self-energy $$\Sigma_{xc}(12) = iG(14)W(31^+)\Gamma(42;3)$$

vertex $$\Gamma(12;3) = \delta(13)\delta(23) + \frac{\delta\Sigma_{xc}(12)}{\delta\rho(4)}P(43)$$

$$(\delta\Sigma/\delta V) = (\delta\Sigma/\delta\rho)(\delta\rho/\delta V)$$

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$$f_{xc}^{eff}(14) = -iP_0^{-1}(16)G(65)G(76)\frac{\delta\Sigma_{xc}(57)}{\delta\rho(4)}$$

$$\Delta\Gamma(12;3) = \left[\frac{\delta\Sigma_{xc}(12)}{\delta\rho(4)} - \delta(12)f_{xc}^{eff}(14)\right]P(43)$$

F. Bruneval, F. Sottile, V. Olevano, R. Del Sole, and L. Reining, PRL 94, 186402 (2005)

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only the two-point part contributes $P = -iGG\Gamma$ and $E_{xc} = -iG\Sigma_{xc}$ ... what about quasiparticle energies?

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How local and nonlocal parts of Γ correct the self-screening error and the incorrect atomic limit of GW?

F. Bruneval, F. Sottile, V. Olevano, R. Del Sole, and L. Reining, PRL 94, 186402 (2005)

Outline

- *Theory*

  GW: self-screening and incorrect atomic limit

  Vertex corrections

- *Illustration*

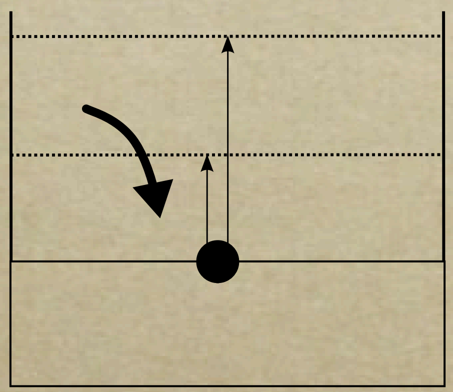
  2-site Hubbard model: $GW\Gamma$ *vs* exact solution

- *Conclusions*

THEORY

Self-screening

- Addition energy



$$E_{N+1=1} - E_{N=0} = \epsilon_1$$

$$\left(-\frac{\nabla^2}{2} + V_0(x_1)\right)\phi_1(x_1) = \epsilon_1\phi_1(x_1)$$ (exact, DFT, HF, GW)

W. Nelson, P. Bokes, P. Rinke, R.W. Godby, PRA 75, 032505 (2007); F. Bruneval, PRL 103, 176403 (2009)

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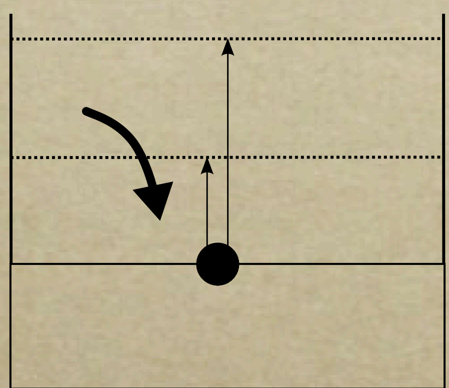

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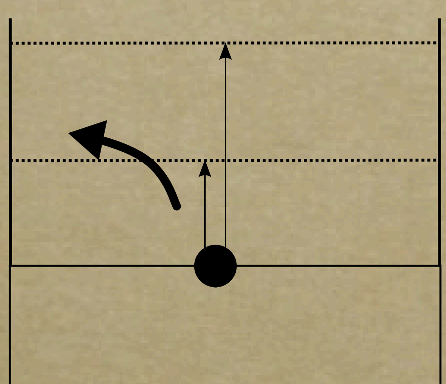

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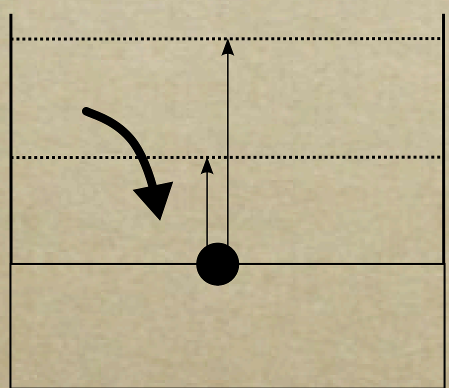

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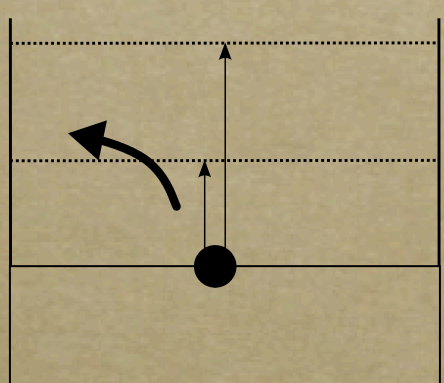

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$$\left(-\frac{\nabla^2}{2} + V_0(x_1) + v_H(x_1\right)\phi_1(x_1) - \int dx_2\left(\phi_1(x_1)\phi_1^*(x_2)W(x_1x_2) + \delta(x_1 - x_2)\frac{1}{2}W_p(x_1x_2)\right)\phi_1(x_2) = \epsilon_1^{GW}\phi_1(x_1) \quad \text{(GW (COHSEX))}$$

W_p: $W - v$

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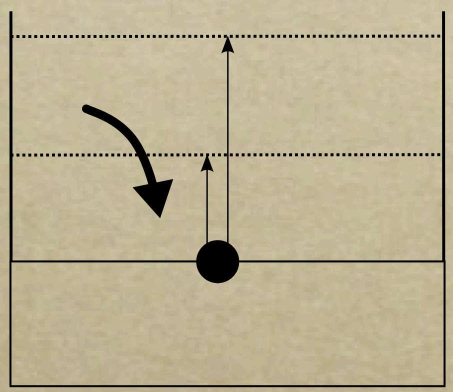

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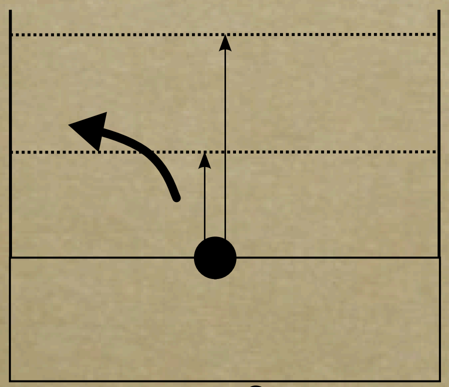

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W_p: $W - v$

Self-screening: the extracted particle screens itself $\longrightarrow \epsilon_1^{GW} \neq \epsilon_1$

(bad treatment of the induced exchange)

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Atomic limit

N.E. Dahlen, R. van Leeuwen, U. von Barth, PRA 73, 012511 (2006); A. Stan, N.E. Dahlen, R. van Leeuwen, JCP 130, 114105 (2009)

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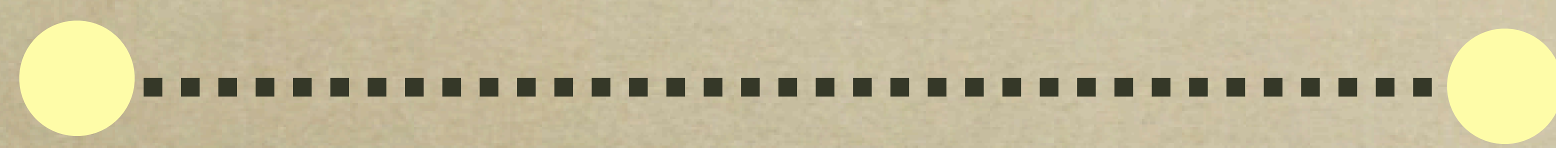

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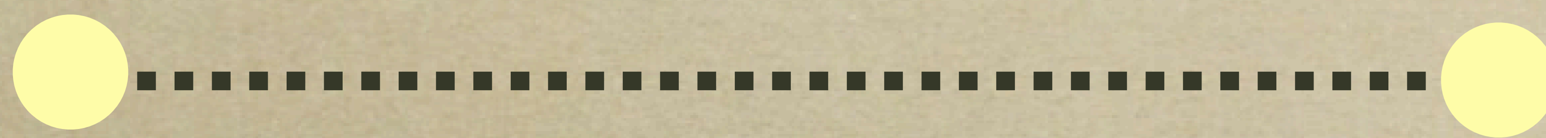

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Atomic limit

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

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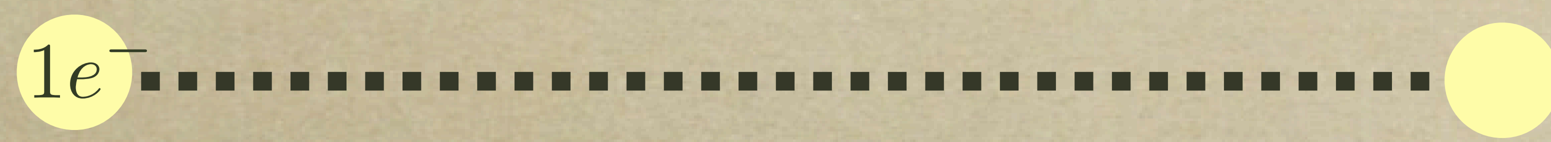

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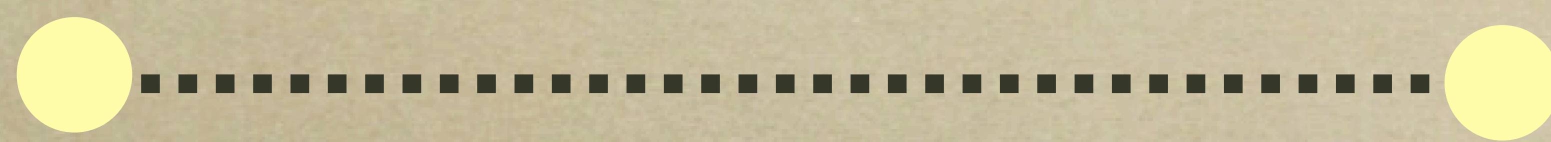
H_2^+  $\longrightarrow$ two types of addition energies

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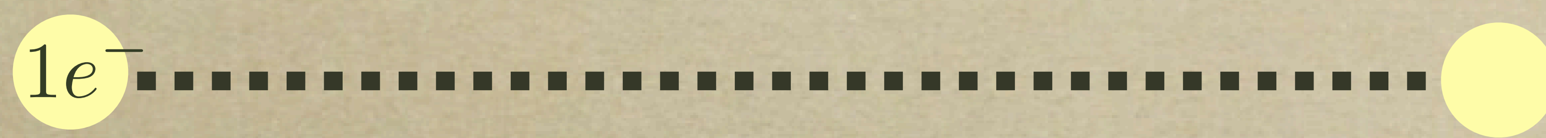

$\longrightarrow$ two types of addition energies

Incorrect atomic limit

(bad treatment of the correlation)

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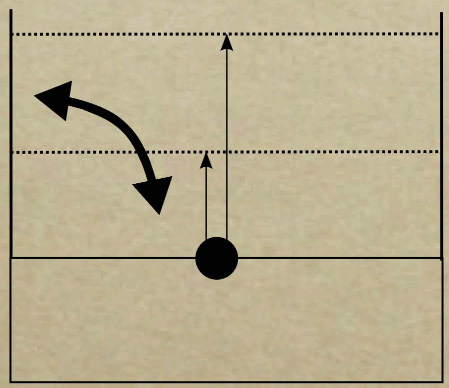
Vertex corrections: $P = -iGG\Gamma$



$$P = -iGG\Gamma \quad \longrightarrow \quad W = v + vPW$$

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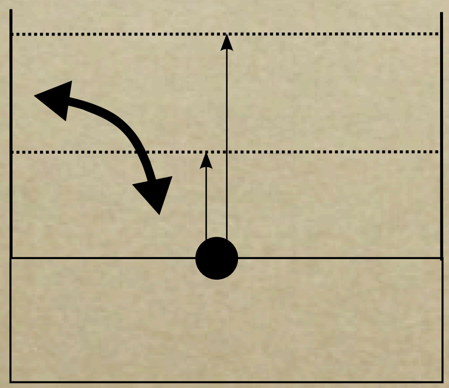

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From TDDFT the exact vertex

$f_{xc} = -v$

$$\chi = \chi_0 + \chi_0(v + f_{xc})\chi = \chi_0 \longrightarrow W = v + v\chi_0 v$$

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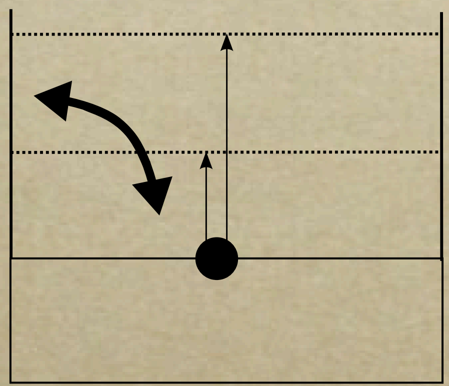

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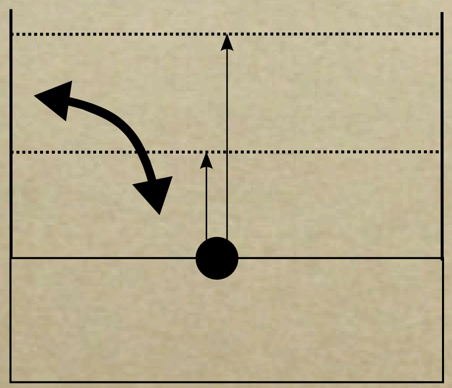
Exact vertex in P does not correct self-screening

Vertex corrections: $\Sigma_{xc} = iGW\Gamma$

- Valence state



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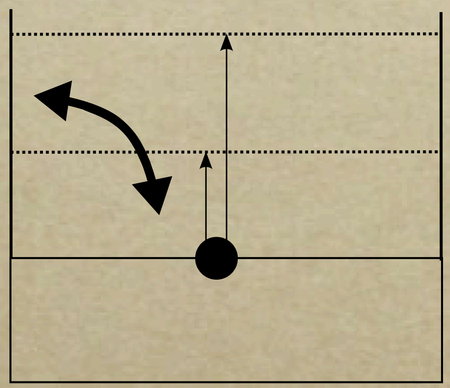

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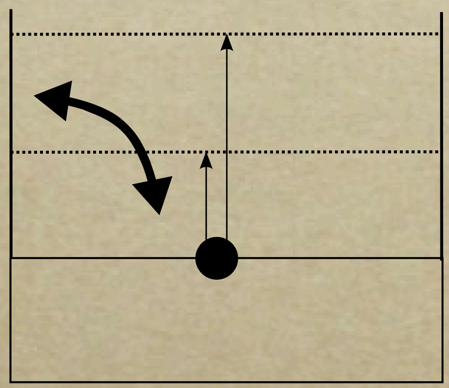

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$$\Gamma(12;3) = \delta(13)\delta(23) + \frac{\delta\Sigma_{xc}(12)}{\delta\rho(4)}P(43) \approx \delta(13)\delta(23) + \frac{\delta v_{xc}(1)\delta(12)}{\delta\rho(4)}P(43)$$

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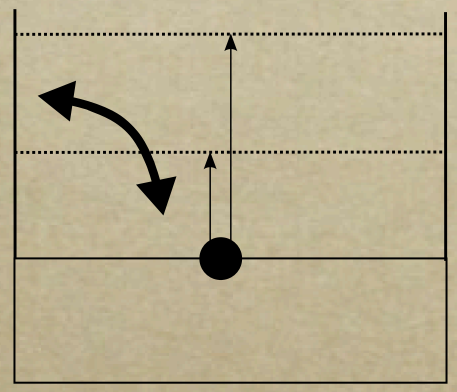

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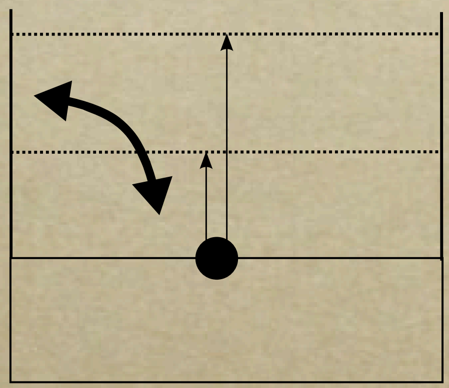

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A two-point vertex is sufficient to remove the self-screening

It is built from the total f_{xc} and not only from the excitonic part $f_{xc}^{eff} = f_{xc} - f_{xc}^{QP}$

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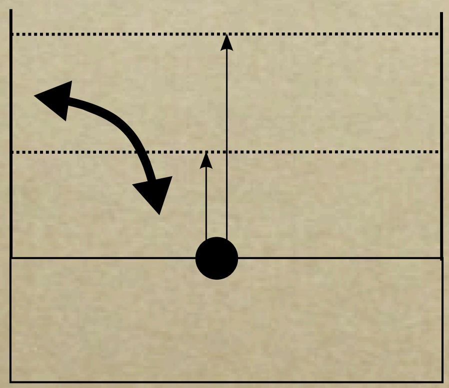

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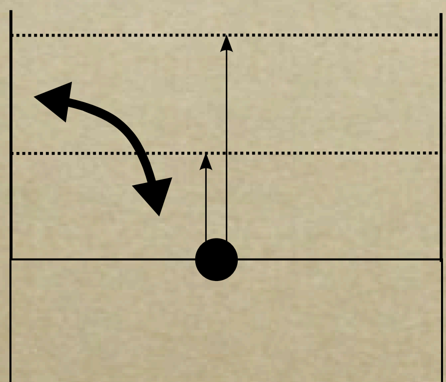

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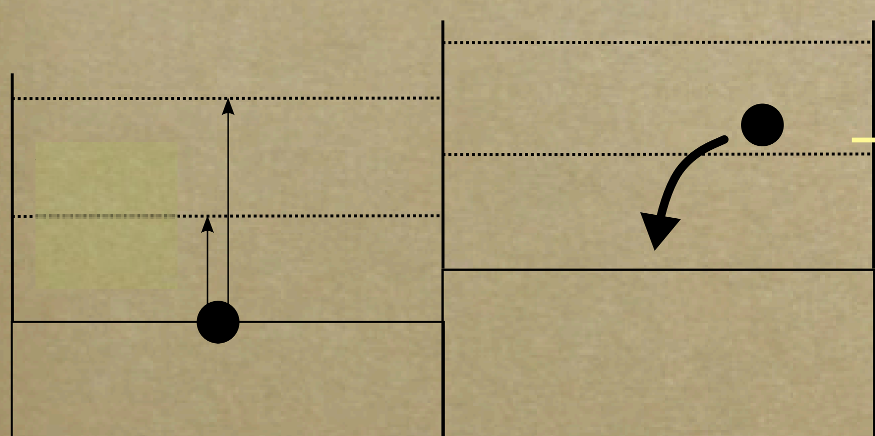
- Conduction state



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

$$\Gamma(23) = \delta(23)$$

Vertex corrections: $\Sigma_{xc} = iGW\Gamma$

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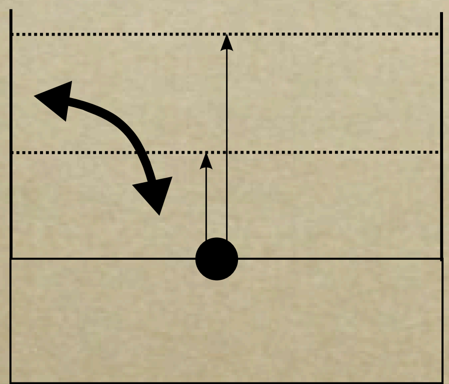

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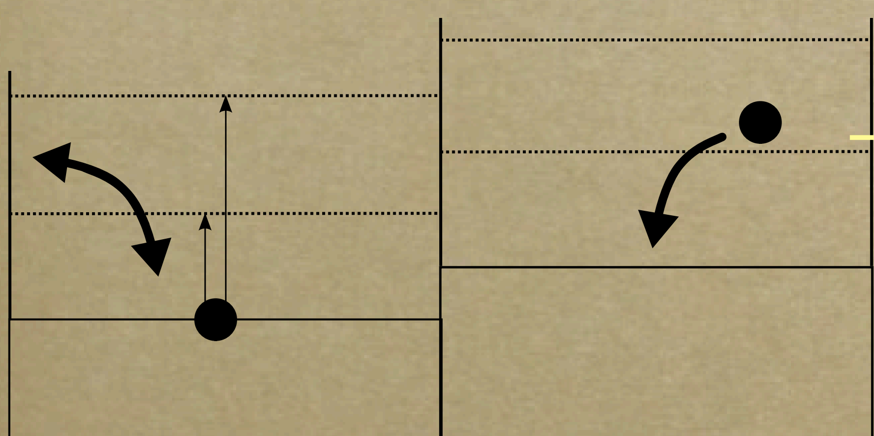

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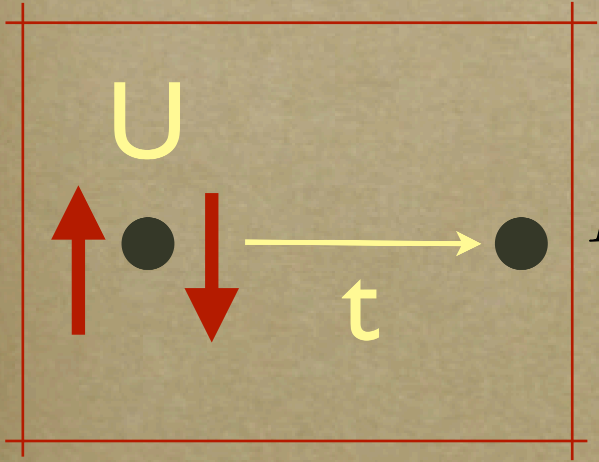
$$\Gamma(23) = \delta(23)$$

nonlocal vertex $\Gamma = \begin{cases} \delta + f_{xc}P & for\ valence \quad\ \ \rightarrow W^{TC-TE} \\ \delta & for\ conduction \rightarrow W^{TC-TC} \end{cases}$

ILLUSTRATION



$$H = -t \sum_{\substack{i,j=1,2 \\ i \neq j}} \sum_{\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{U}{2} \sum_{i=1,2} \sum_{\sigma\sigma'} c^{\dagger}_{i\sigma} c^{\dagger}_{i\sigma'} c_{i\sigma'} c_{i\sigma} + \epsilon_0 \sum_{\sigma,i=1,2} n_{i\sigma} + V_0$$

C. Verdozzi, R.W. Godby, S. Holloway, PRL 74, 2327 (1995);J. M. Tomczak, Ph.D. thesis, Ecole Polytechnique, France (2007).

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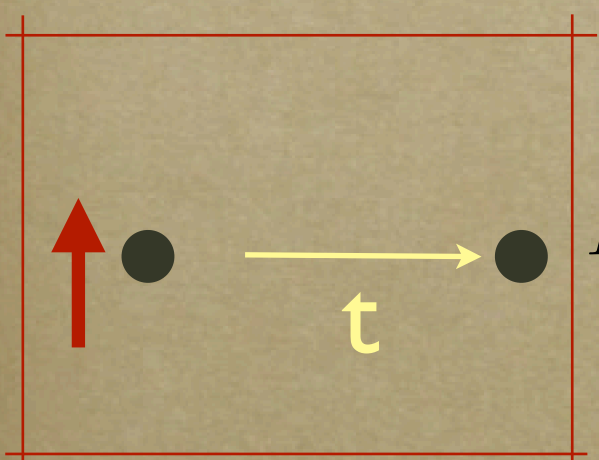

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$$|\psi_0^{N=1}\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\ 0\rangle + |0\ \uparrow\rangle \right) \qquad E_0 = \epsilon_0 - t$$

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Hubbard model: exact solution

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- One-particle Green's function

$$G_{ij\uparrow}(\omega) = \frac{(-1)^{(i-j)}}{2}\left[\frac{1}{\omega-(\epsilon_0+t)+i\eta}+\frac{(-1)^{(i-j)}}{\omega-(\epsilon_0-t)-i\eta}\right]$$

1 removal energy
5 addition energies

$$G_{ij\downarrow}(\omega) = \frac{(-1)^{(i-j)}}{4}\left[\frac{1}{\omega-(\epsilon_0+t)+i\eta}+\frac{1}{\omega-(\epsilon_0+t+U)+i\eta}\right]$$

$$+\frac{1}{2}\left[\frac{\frac{1}{a^2}(1+\frac{4t}{(c-U)})^2}{\omega-(\epsilon_0+t-(c-U)/2)+i\eta}+\frac{\frac{1}{b^2}(1-\frac{4t}{(c+U)})^2}{\omega-(\epsilon_0+t+(c+U)/2)+i\eta}\right]$$

Hubbard model: exact solution

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5 addition energies

$$G_{ij\downarrow}(\omega) = \frac{(-1)^{(i-j)}}{4}\left[\frac{1}{\omega-(\epsilon_0+t)+i\eta} + \frac{1}{\omega-(\epsilon_0+t+U)+i\eta}\right]$$

$$+\frac{1}{2}\left[\frac{\frac{1}{a^2}(1+\frac{4t}{(c-U)})^2}{\omega-(\epsilon_0+t-(c-U)/2)+i\eta} + \frac{\frac{1}{b^2}(1-\frac{4t}{(c+U)})^2}{\omega-(\epsilon_0+t+(c+U)/2)+i\eta}\right]$$

- Self-energy $\Sigma(\omega) = G_0^{-1}(\omega) - G^{-1}(\omega)$

$$\Sigma(\omega) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \Sigma_{11\downarrow} & \Sigma_{12\downarrow} \\ 0 & 0 & \Sigma_{12\downarrow} & \Sigma_{11\downarrow} \end{pmatrix}$$

Hubbard model: exact solution

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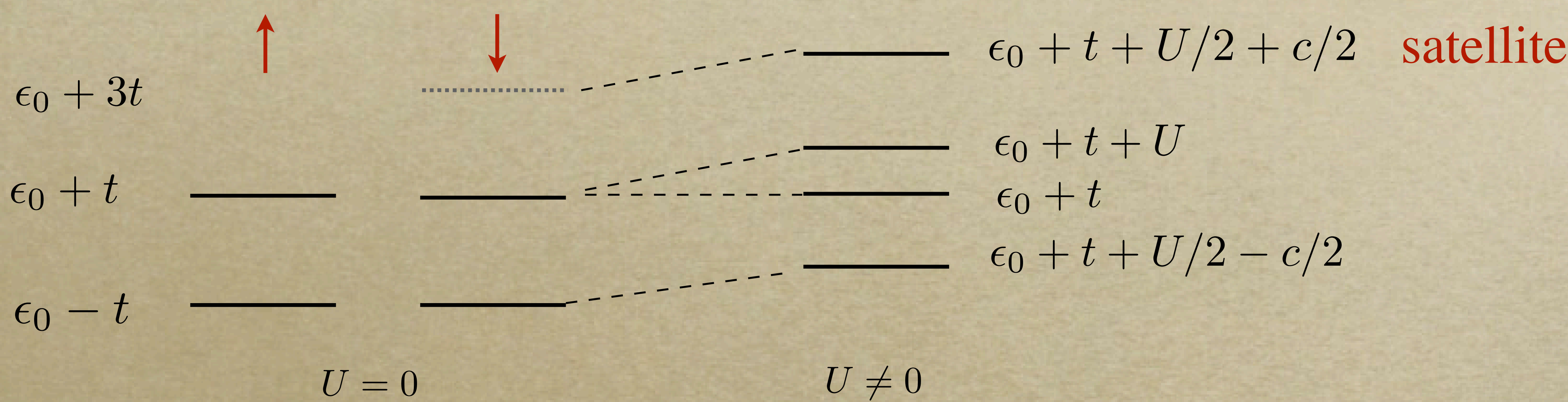
- Noninteracting limit $U \to 0$

$$G_{ij\uparrow}^{U=0}(\omega) = G_{ij\uparrow}(\omega) \qquad G_{ij\downarrow}^{U=0}(\omega) = \frac{(-1)^{(i-j)}}{2}\left[\frac{1}{\omega-(\epsilon_0+t)+i\eta} + \frac{(-1)^{(i-j)}}{\omega-(\epsilon_0-t)+i\eta}\right]$$

Hubbard model: exact solution

- Noninteracting limit $U \to 0$

$$G_{ij\uparrow}^{U=0}(\omega) = G_{ij\uparrow}(\omega) \qquad G_{ij\downarrow}^{U=0}(\omega) = \frac{(-1)^{(i-j)}}{2}\left[\frac{1}{\omega-(\epsilon_0+t)+i\eta} + \frac{(-1)^{(i-j)}}{\omega-(\epsilon_0-t)+i\eta}\right]$$



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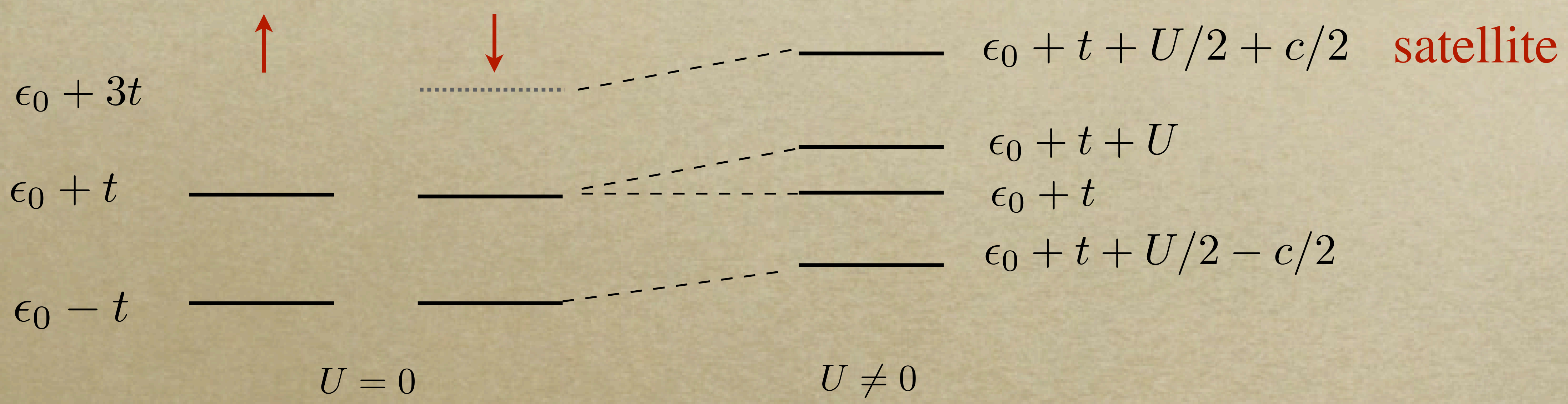

- Atomic limit $t \longrightarrow 0$

$$G^{t=0}_{ij\uparrow}(\omega) = \frac{(-1)^{(i-j)}}{2}\left[\frac{1}{\omega - \epsilon_0 + i\eta} + \frac{(-1)^{(i-j)}}{\omega - \epsilon_0 - i\eta}\right]$$

removal/addition energies of two isolated atoms

$$G^{t=0}_{ii\downarrow}(\omega) = \frac{1}{2}\left[\frac{1}{\omega - \epsilon_0 + i\eta} + \frac{1}{\omega - (\epsilon_0 + U) + i\eta}\right]$$

$$\Sigma_{ij\downarrow}(\omega) = \delta_{ij}\frac{U}{2}\left[1 + \frac{U}{2(\omega - \epsilon_0) - U + i\eta}\right]$$

Hubbard model: GW solution

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- Self-energy $\Sigma(\omega) = v_H + \frac{i}{2\pi}\int d\omega' G(\omega+\omega')W(\omega')e^{i\omega'\eta}$ (G_0, W^{RPA})

$$\Sigma(\omega) = \begin{pmatrix} \Sigma_{11\uparrow} & \Sigma_{12\uparrow} & 0 & 0 \\ \Sigma_{12\uparrow} & \Sigma_{11\uparrow} & 0 & 0 \\ 0 & 0 & \Sigma_{11\downarrow} & \Sigma_{12\downarrow} \\ 0 & 0 & \Sigma_{12\downarrow} & \Sigma_{22\downarrow} \end{pmatrix}$$

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- One-particle Green's function $\quad G^{GW}(\omega) = \left[G_0^{-1}(\omega) - \Sigma(\omega)\right]^{-1}$

2 removal energy
6 addition energies

$$G^{GW}_{ij\uparrow}(\omega) = (-1)^{(i-j)}\left[\frac{\left(\frac{1}{4}+\frac{2t+h}{4A}\right)}{\omega-\omega_1+i\eta} + \frac{\left(\frac{1}{4}-\frac{2t+h}{4A}\right)}{\omega-\omega_2-i\eta}\right] + \frac{\left(\frac{1}{4}-\frac{2t+h}{4A}\right)}{\omega-\omega_3+i\eta} + \frac{\left(\frac{1}{4}+\frac{2t+h}{4A}\right)}{\omega-\omega_4-i\eta}$$

$$G^{GW}_{ij\downarrow}(\omega) = (-1)^{(i-j)}\left[\frac{\left(\frac{1}{4}+\frac{2t-h+U/2}{4B}\right)}{\omega-\omega_5+i\eta} + \frac{\left(\frac{1}{4}-\frac{2t-h+U/2}{4B}\right)}{\omega-\omega_6+i\eta}\right] + \frac{\left(\frac{1}{4}-\frac{2t+h-U/2}{4C}\right)}{\omega-\omega_7+i\eta} + \frac{\left(\frac{1}{4}+\frac{2t+h-U/2}{4C}\right)}{\omega-\omega_8+i\eta}$$

Hubbard model: GW solution

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- Noninteracting limit $U \to 0$

  $G^{GW}_{U=0} \quad \to$ exact solution

1 physical pole+ extra poles $\to \epsilon_0 \pm 3t$ with zero intensity $\to$ satellites

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- Atomic limit $t \rightarrow 0$

$G^{GW}_{ij\uparrow,t=0} \rightarrow$ exact solution

self-screening not detected in $t \rightarrow 0$

$$G^{GW}_{ii\downarrow,t=0}(\omega) = \frac{1}{\omega - (\epsilon_0 + \frac{U}{2}) + i\eta}$$

only one pole ($\epsilon_0 + U/2$) *vs* two in the exact solution ($\epsilon_0, \epsilon_0 + U$)

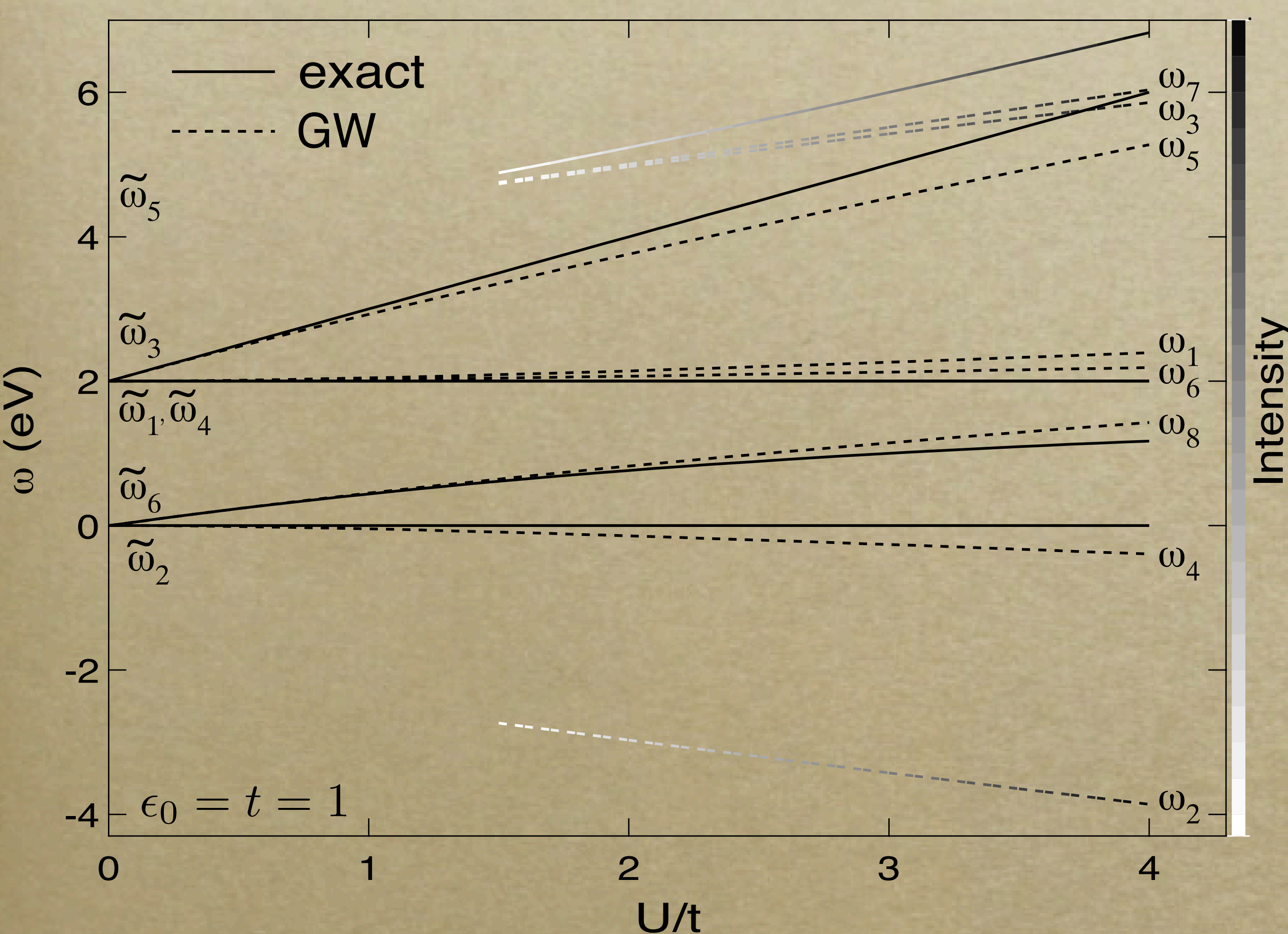
$$\Sigma_{ij\downarrow}(\omega = 0) = \frac{U}{2}\delta_{ij}$$

static (only Hartree potential) *vs* frequency-dependent exact solution

Hubbard model: GW *vs* exact

- Self-screening

exact GW



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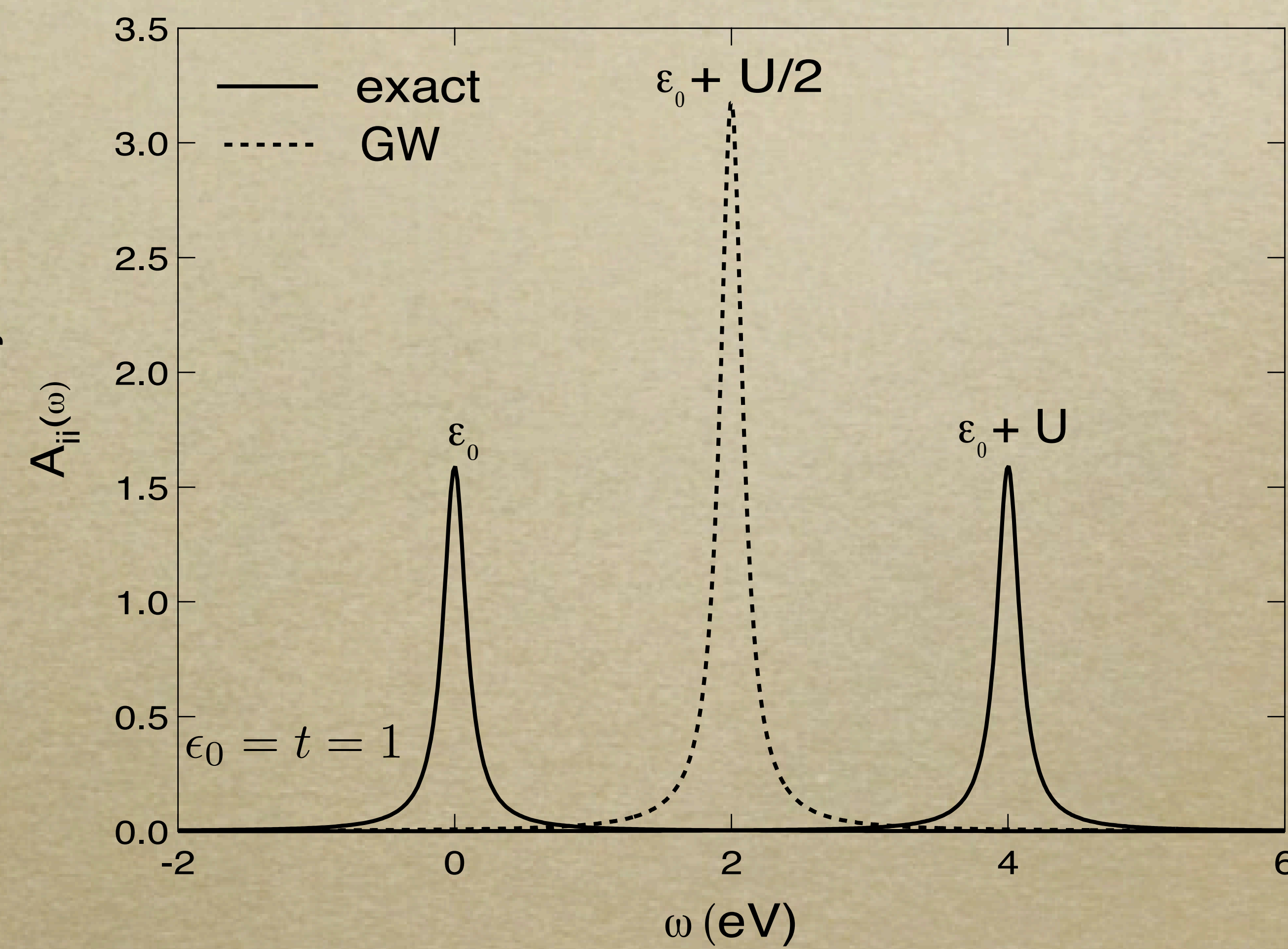

Hubbard model: GW *vs* exact

- Self-screening
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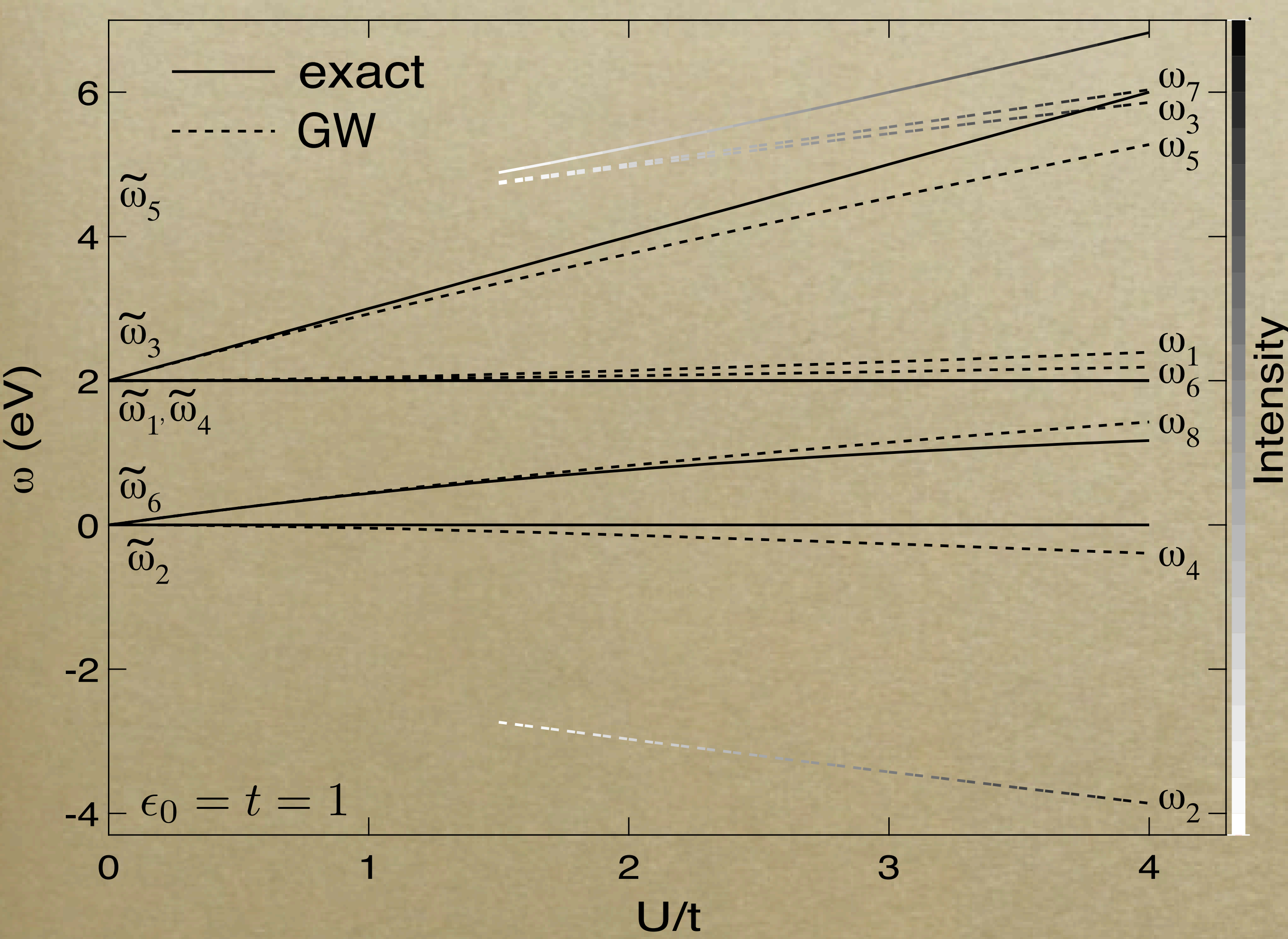

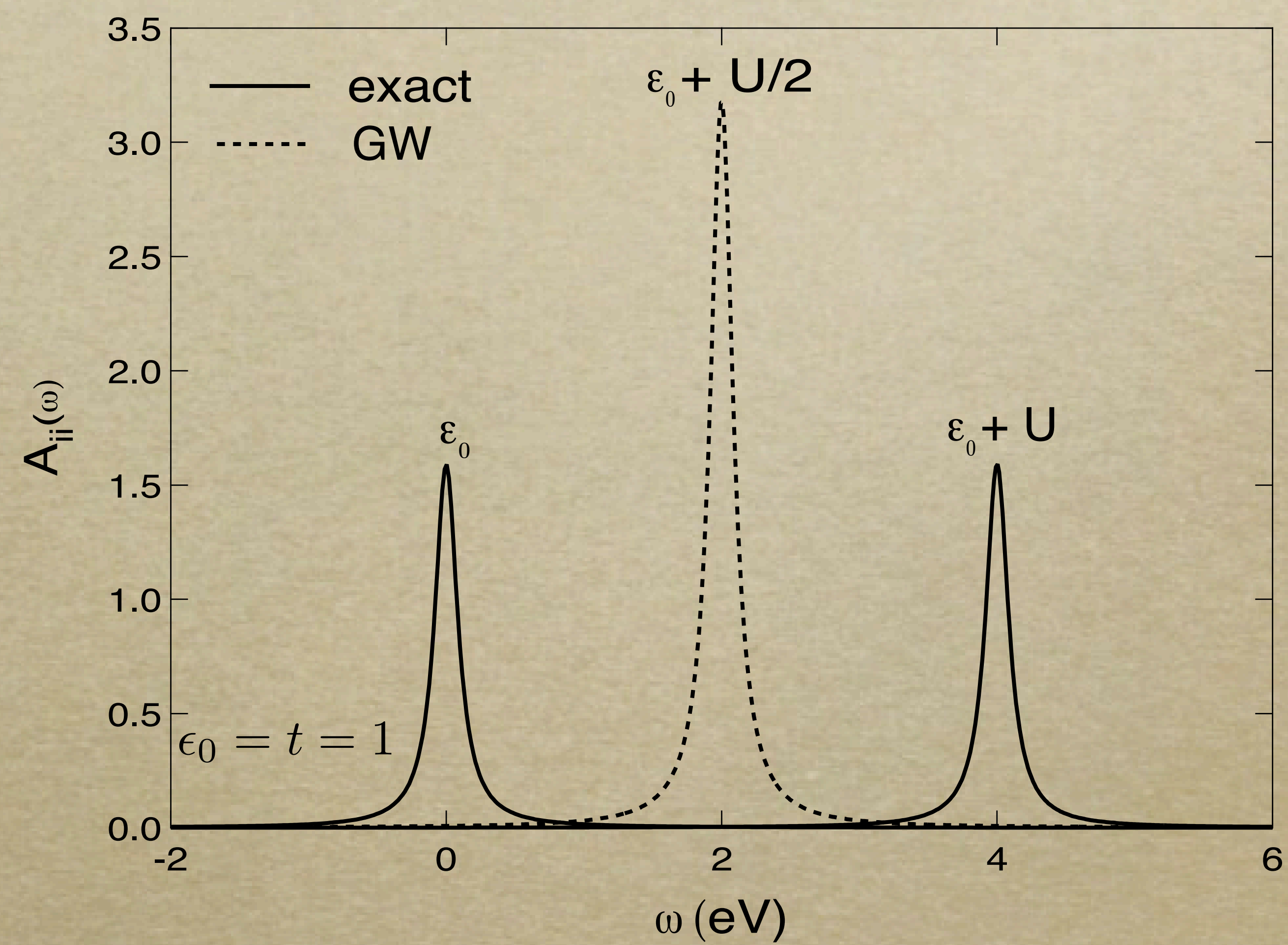

J. M. Tomczak, Ph.D. thesis, Ecole Polytechnique, France (2007)

Hubbard model: vertex corrections

Hubbard model: vertex corrections

- Vertex corrections in P

$W = v + v\chi_0 v \longrightarrow W_{ij}(\omega) = U\delta_{ij} + (-1)^{(i-j)}\frac{U^2 t}{\omega^2 - (2t)^2}$ only shifts poles of Σ

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No self-screening anymore!

Still incorrect atomic limit!

Conclusions

- GW suffers of a self-screening error (bad description of induced exchange) and an incorrect atomic limit (bad description of correlation)
- An approximate vertex $\Gamma = \begin{cases} \delta + f_{xc}P & for\ \ valence \\ \delta & for\ \ conduction \end{cases}$

  can correct the self-screening...but not the incorrect atomic limit
- The approximate vertex (for valence) is built from TDDFT with the total f_{xc} and not only with the excitonic part $f_{xc}^{eff} = f_{xc} - f_{xc}^{QP}$

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P. Romaniello, S. Guyot, and L. Reining, JCP, 131, 154111 (2009)