Hubbard dimer in GW and beyond

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Autumn School on Correlated Electrons: Simulating Correlations with Computers
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Plan of the lecture

- **Notation**
- **Theoretical Background: the GW approximation and beyond**
  - GW (self-screening and incorrect atomic limit)
  - Corrections to GW (T matrix)
- **The Hubbard dimer**
  - Exact solution
  - GW solution
  - T-matrix solution

Notation

- Zero temperature, equilibrium, BOA, non-relativistic

many-body Hamiltonian

$$\hat{H} = \int d\mathbf{x}\hat{\psi}^\dagger(\mathbf{x})h(\mathbf{r})\hat{\psi}(\mathbf{x}) + \frac{1}{2}\int\int d\mathbf{x}d\mathbf{x}'\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x})v_c(\mathbf{x},\mathbf{x}')$$

- Combined space-spin-time indices

$$(1^+) = (\mathbf{x}_1, t_1^+) \text{ with } t_1^+ = t_1 + \delta\ (\delta \to 0^+)$$

- Implicit integration:

integration over indices not present on the left-hand side of an equation is implicit

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

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$$= -\frac{\nabla^2_{\mathbf{r}}}{2} + v_{ext}(\mathbf{r})$$

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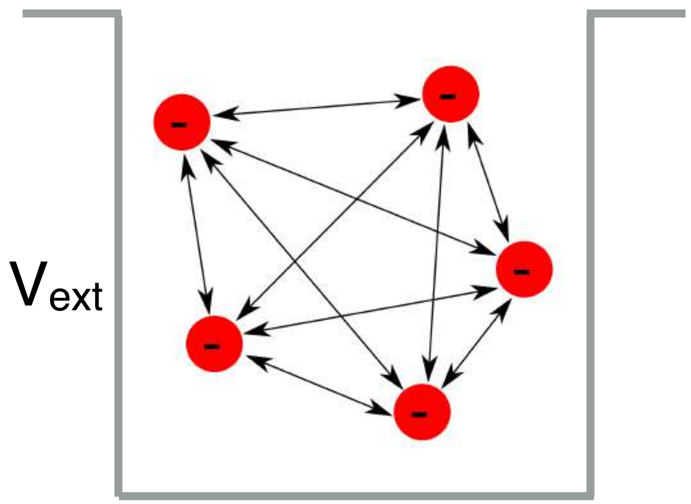
Theoretical Background

- **Wave-function based approaches**

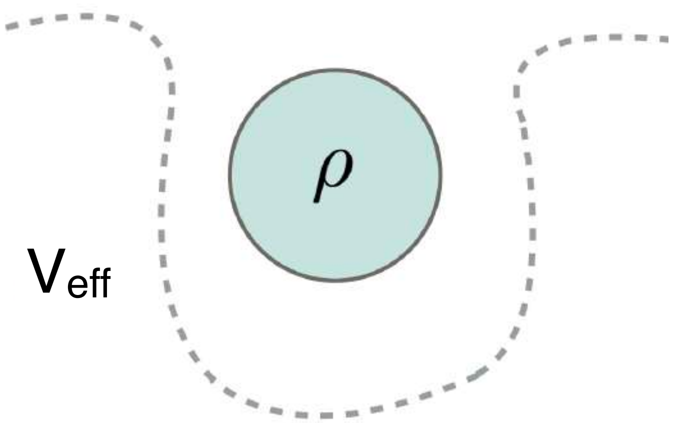
Key quantity: many-body wavefunction



Observable $= \langle \Psi | \hat{O} | \Psi \rangle$

- **Reduced quantity based approaches**

Key quantity: Simpler physical quantity, e.g. the density



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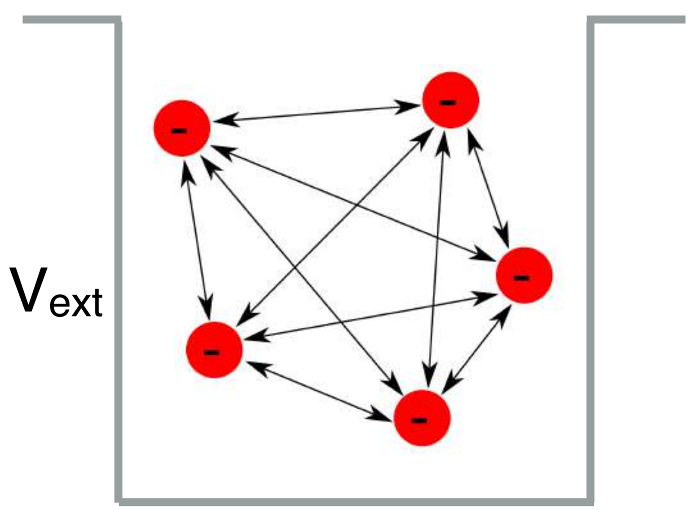

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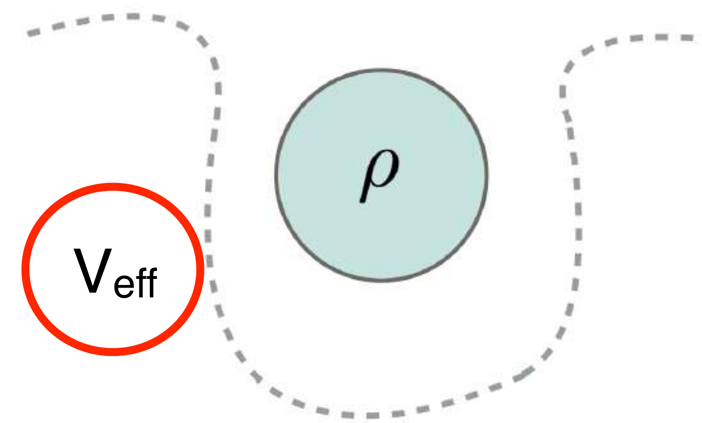

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Observable $= \mathrm{F}[\rho]$

Theoretical Background

Reduced quantities

density	$\rho(\mathbf{r})$	Density Functional Theory
current-density	$\mathbf{j}(\mathbf{r})$	Current-Density Functional Theory
1-body density matrix	$\gamma(\mathbf{r},\mathbf{r}')$	Reduced Density Matrix Functional Theory
1-body Green's function	$G(\mathbf{x},\mathbf{x}';\omega)$	Many-Body Perturbation theory

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Theoretical Background

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Theoretical Background

One-body Green's function

$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+}\left[\sum_m \frac{B_m^A(\mathbf{x},\mathbf{x}')}{\omega-(E_m^{N+1}-E_0^N)+\mathrm{i}\eta} + \sum_n \frac{B_n^R(\mathbf{x},\mathbf{x}')}{\omega-(E_0^N-E_n^{N-1})-\mathrm{i}\eta}\right]$$

Theoretical Background

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ground-state energy of the *N*-electron system

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(ground/excited)-state energies of the ($N\pm 1$)-electron system

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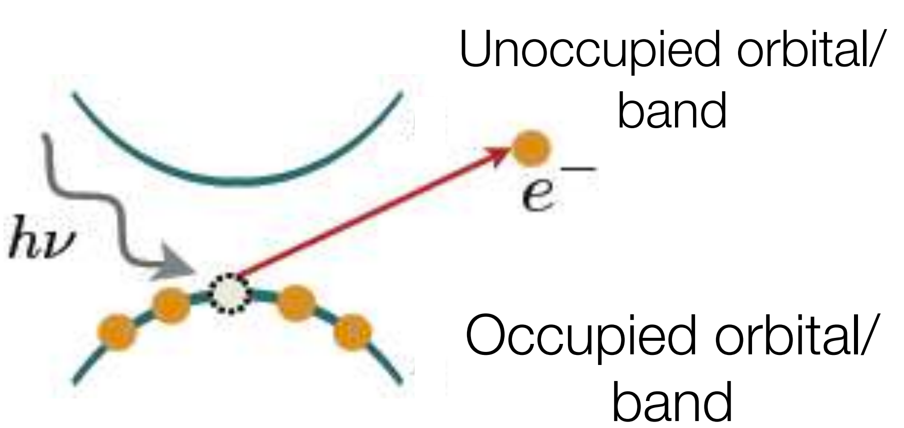

direct photoemission : N ⟶ N-1

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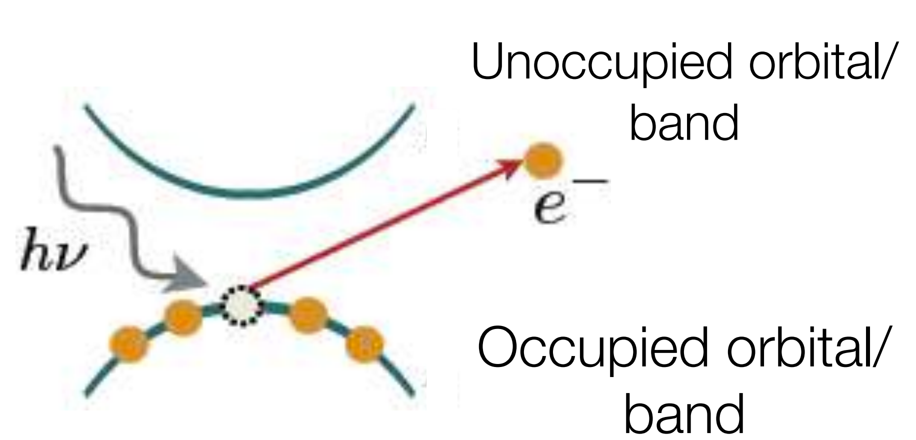

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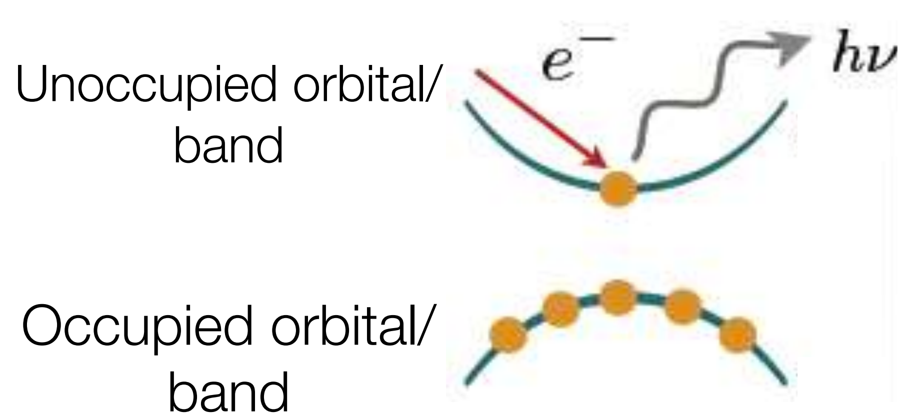

inverse photoemission : N⟶ N+1

Theoretical Background

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ground-state many-body wavefunction of the *N*-electron system

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ground-state many-body wavefunction of the *N*-electron system

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Theoretical Background

- **Spectral function**

$$
\begin{aligned}
A(\mathbf{x},\mathbf{x}';\omega) &= \frac{1}{\pi}\mathrm{sign}(\mu-\omega)\,\mathrm{Im}\,G(\mathbf{x},\mathbf{x}';\omega) \\
&= \sum_m B_m^A(\mathbf{x},\mathbf{x}')\delta(\omega-(E_m^{N+1}-E_0^N))+\sum_n B_m^R(\mathbf{x},\mathbf{x}')\delta(\omega-(E_0^N-E_n^{N-1}))
\end{aligned}
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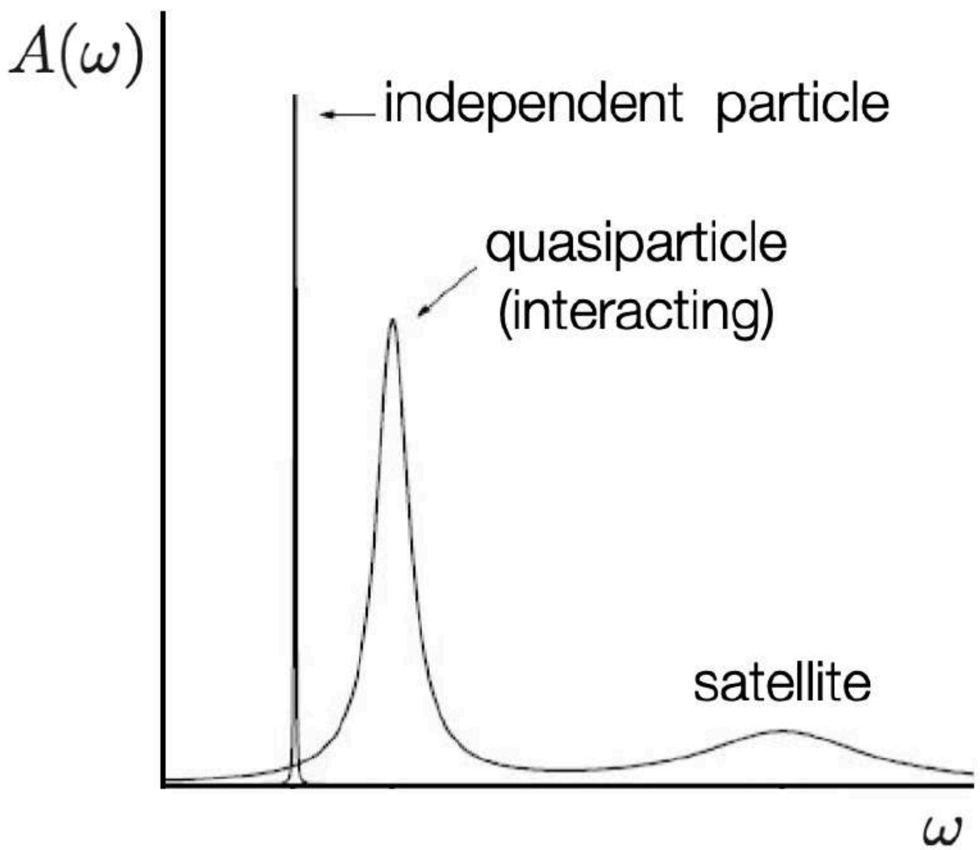

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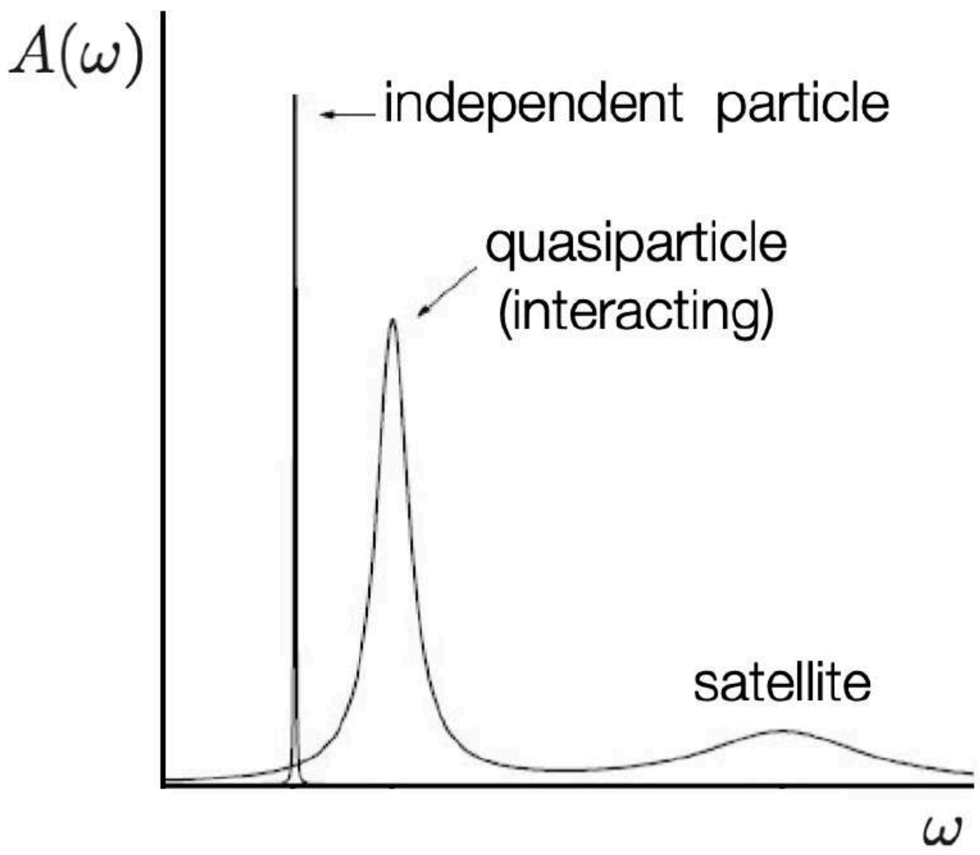
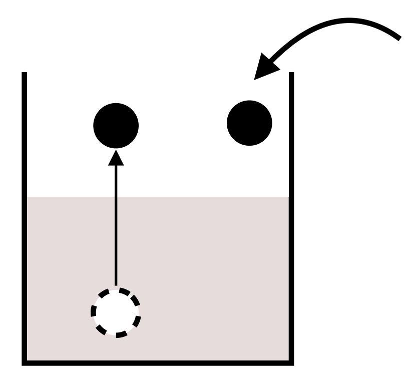
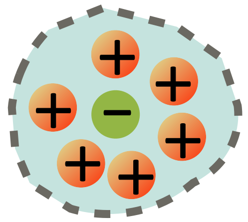
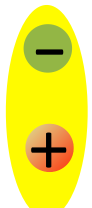






quasiparticles

satellites (e.g., neutral excitations )

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- **Dyson equation**

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self-energy

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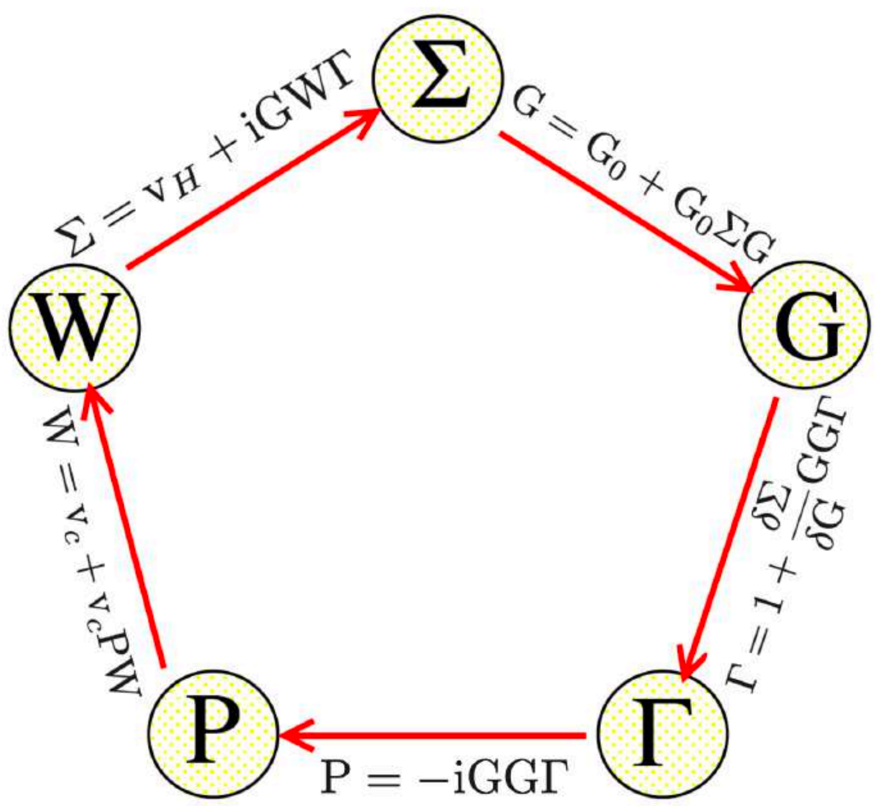
- **Hedin's equations**



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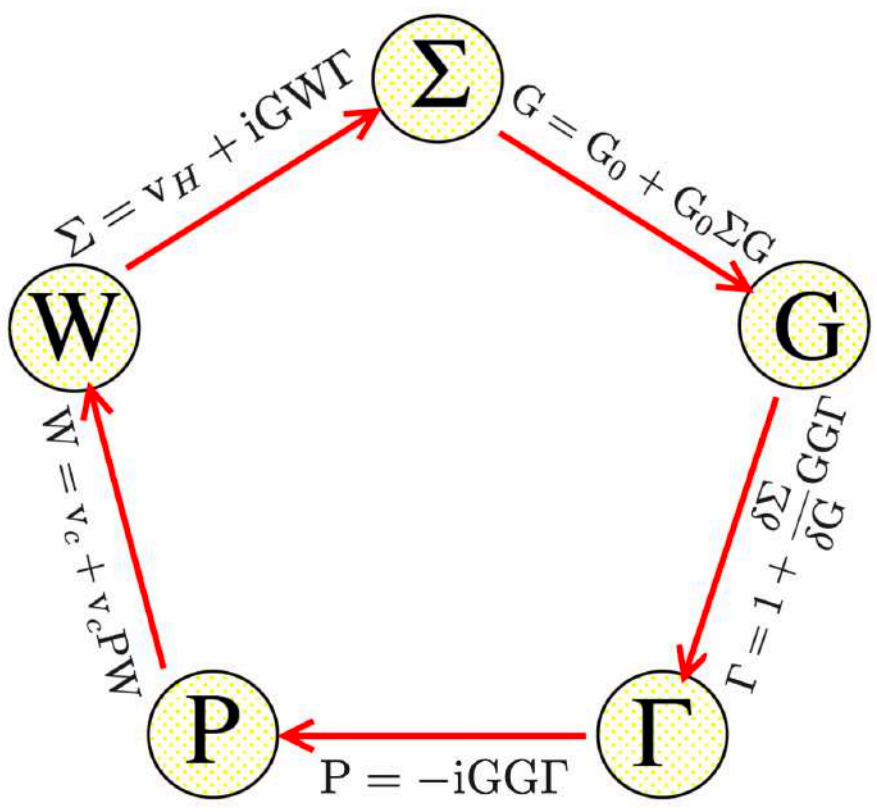

vertex corrections

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

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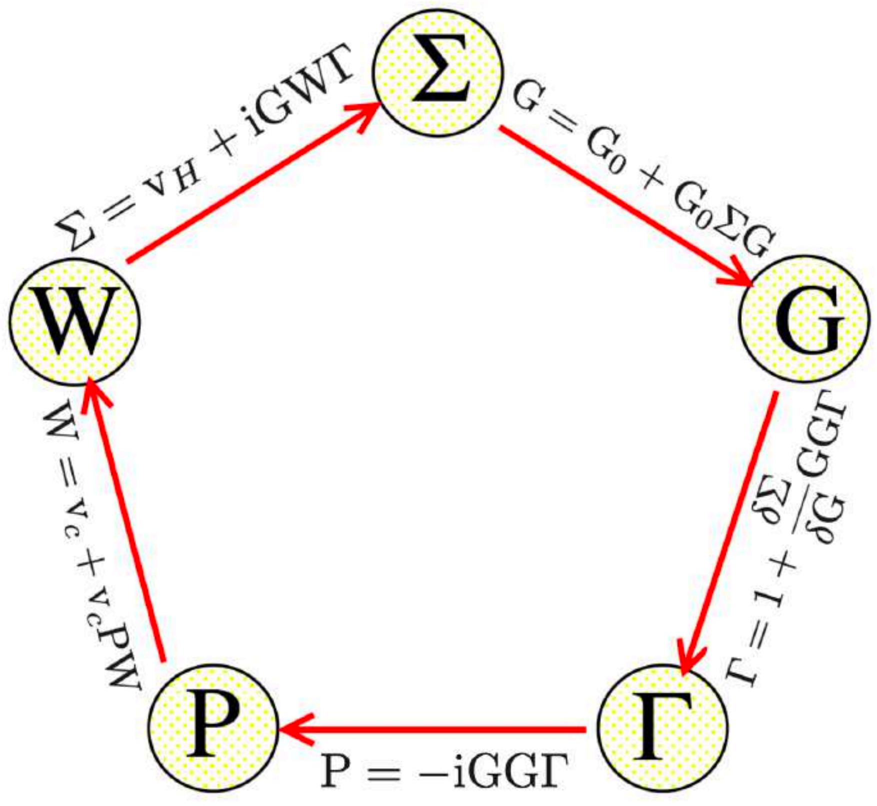

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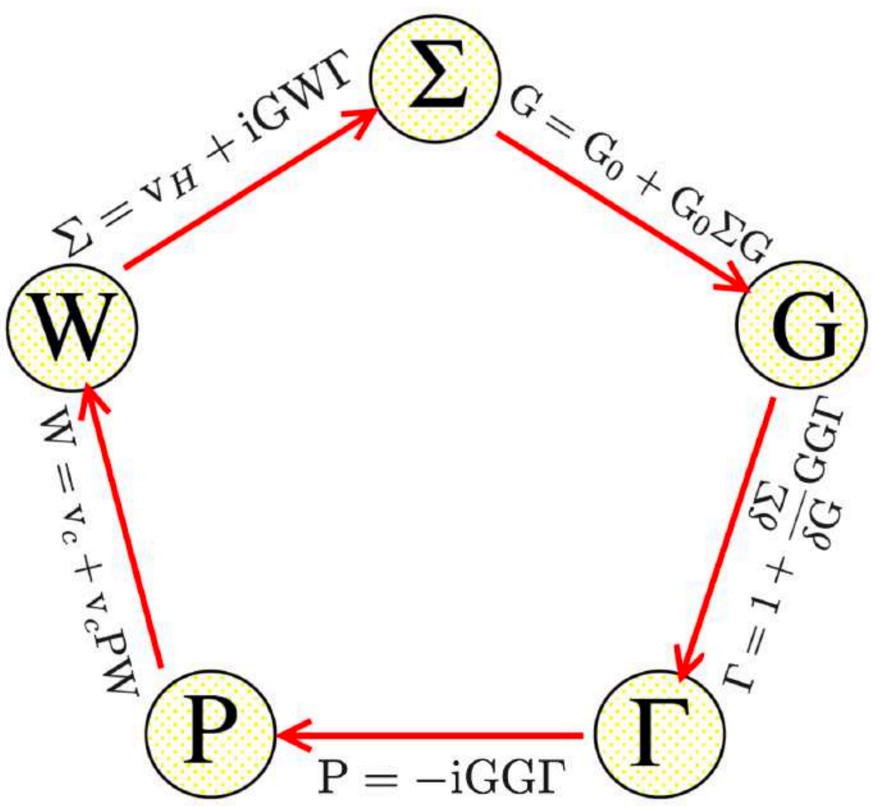

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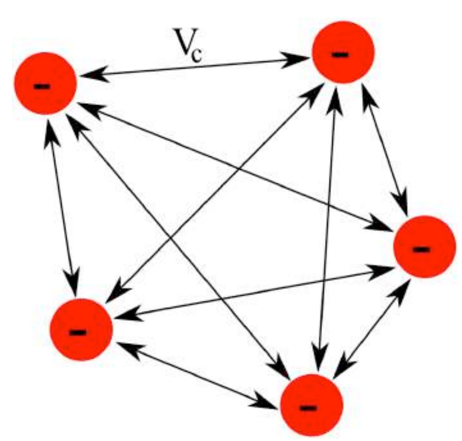

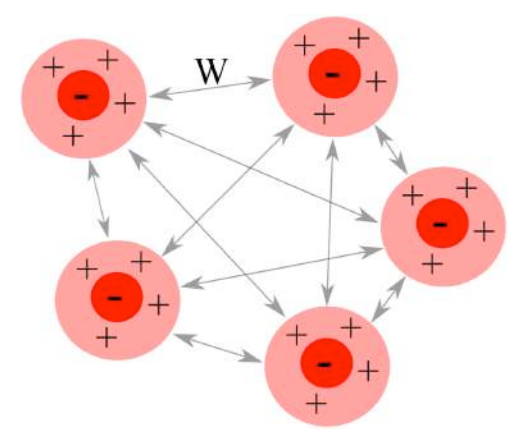

Theoretical Background

- **Dyson equation**

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- **Self-energy**

$$\Sigma(1,1') = v_H(1)\delta(1,1') + \Sigma_x(1,1') + iv_c(1^+,2)G(1,3)\Xi(3,5;1',4)L(4,2;5,2^+)$$

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$$= \frac{\delta\Sigma(31')}{\delta G(45)}$$

$$= \left.\frac{\delta G(45)}{\delta U_{ext}(2)}\right|_{U_{ext}=0}$$

Theoretical Background

- **GW**

$$\Sigma = v_H + \Sigma_x + iv_c G \Xi L$$

screening important $\Rightarrow$ L well-approximated

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

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Theoretical Background

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$$\Sigma \approx v_H + iGW$$ GW

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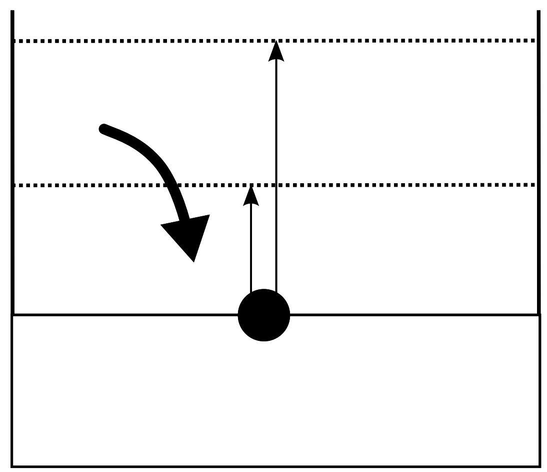
$$\Sigma \approx v_H + iGW$$ GW

dynamically screened
Coulomb potential

$$W = v_c + v_c P W$$

Theoretical Background

GW: self-screening

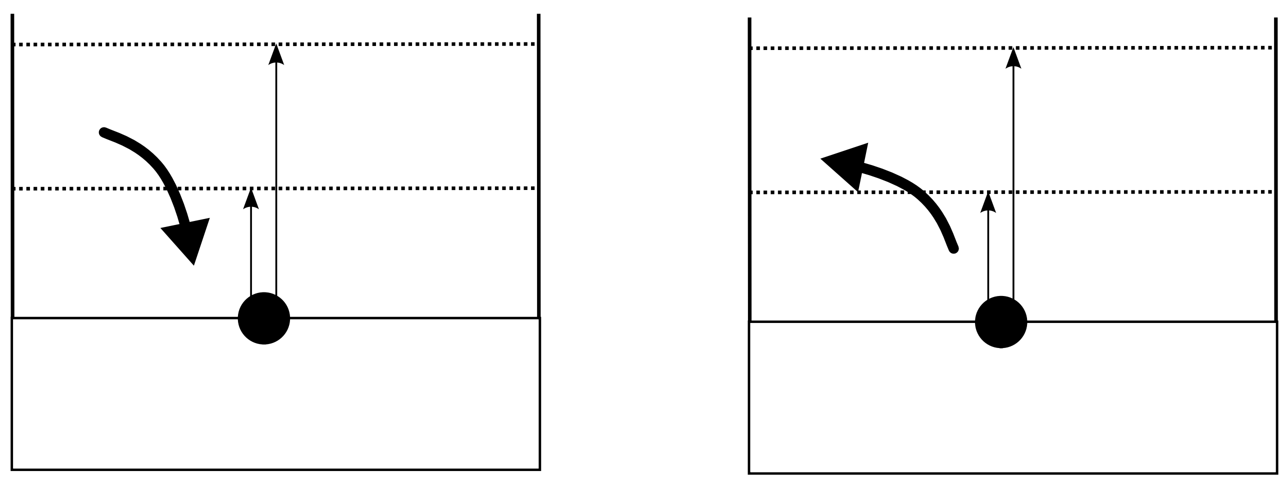


- Exact

addition energy $E_{N+1=1} - E_{N=0} = \epsilon_1^A$

Theoretical Background

GW: self-screening



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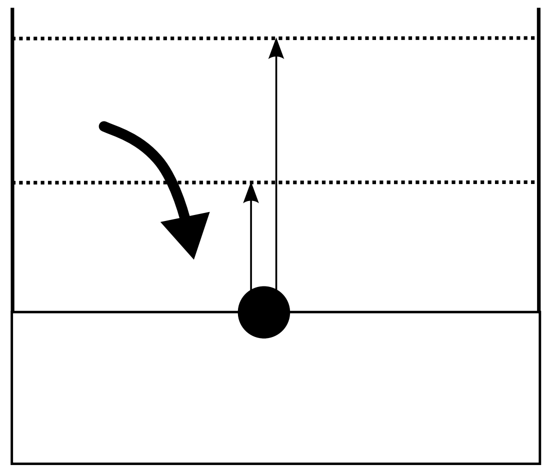
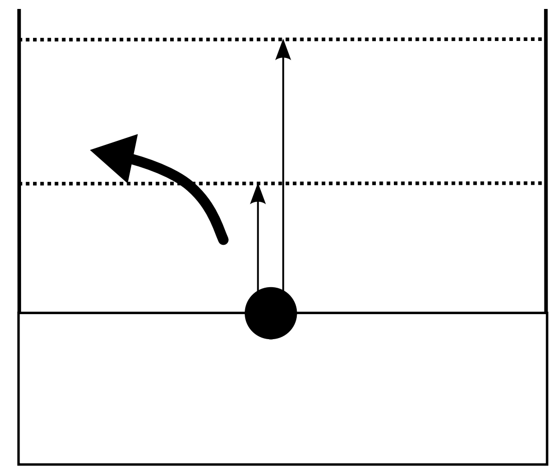
$E_{N=1} - E_{N-1=0} = \epsilon_1^R$ removal energy

Theoretical Background

GW: self-screening

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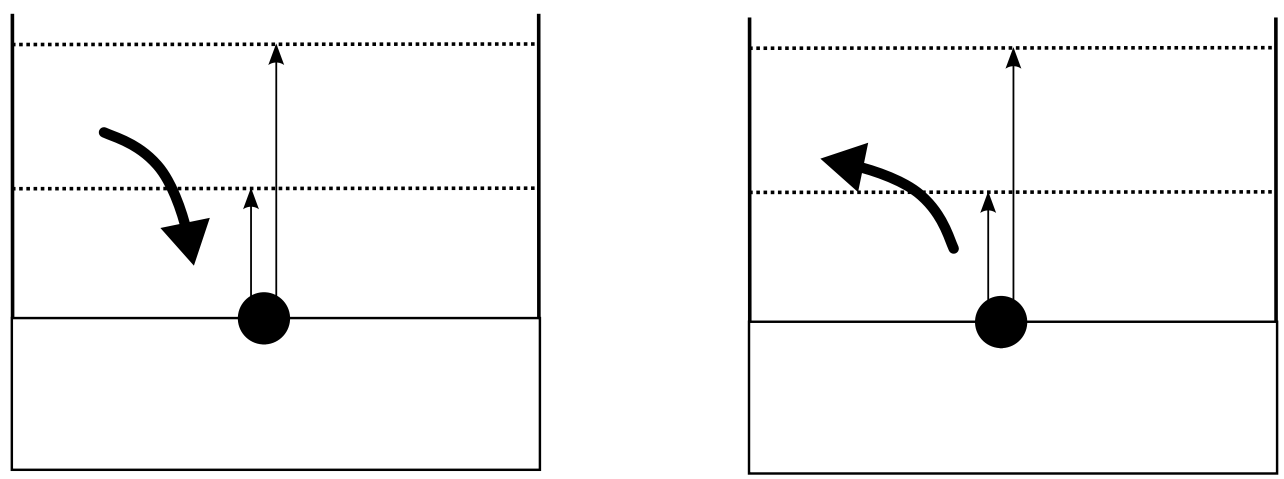

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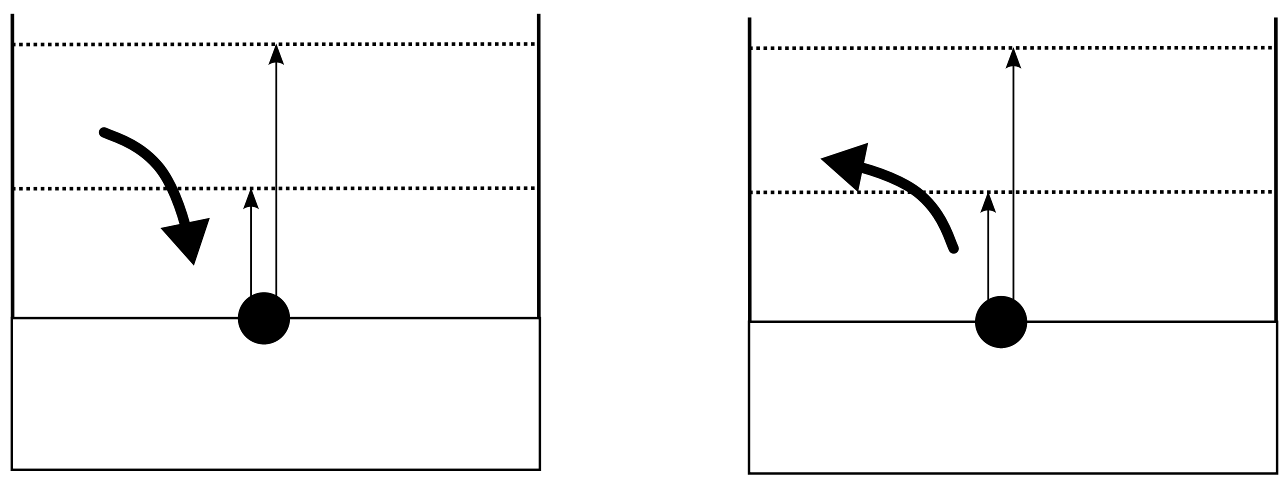
- GW

$$\epsilon_1^{A,GW} = \epsilon_1^A \qquad \epsilon_1^{R,GW} \neq \epsilon_1^R$$

Theoretical Background

GW: self-screening



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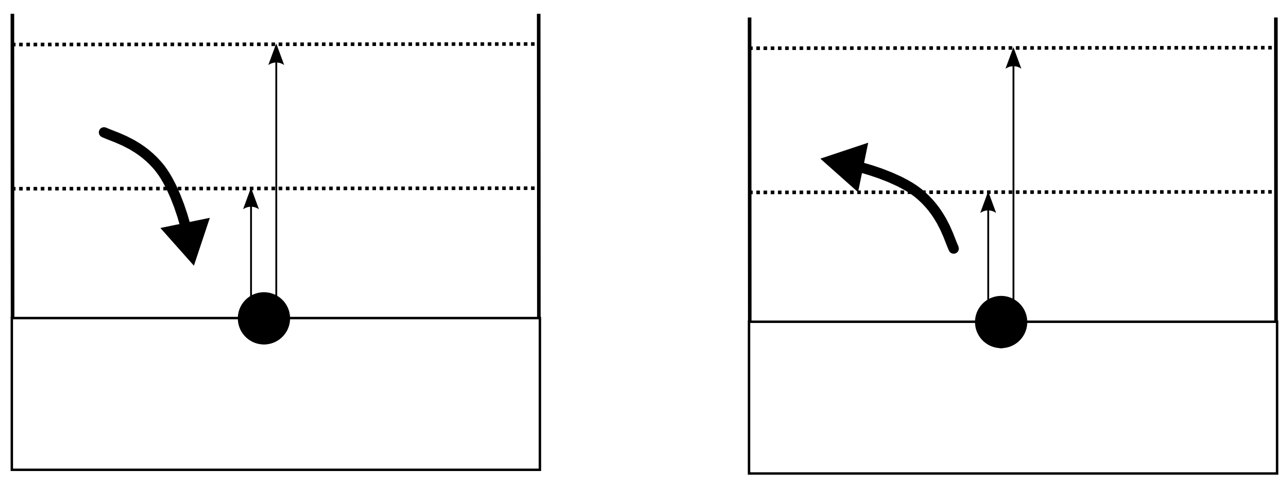
addition energy $E_{N+1=1} - E_{N=0} = \epsilon_1^A$ $=$ $E_{N=1} - E_{N-1=0} = \epsilon_1^R$ removal energy

- GW

$$\epsilon_1^{A,GW} = \epsilon_1^A \quad \neq \quad \epsilon_1^{R,GW} \neq \epsilon_1^R$$

Theoretical Background

GW: self-screening



- Exact

addition energy $E_{N+1=1} - E_{N=0} = \epsilon_1^A$ $=$ $E_{N=1} - E_{N-1=0} = \epsilon_1^R$ removal energy

- GW

$$\epsilon_1^{A,GW} = \epsilon_1^A \neq \epsilon_1^{R,GW} \neq \epsilon_1^R$$

Self-screening: the extracted particle screens itself

(bad treatment of the induced exchange)

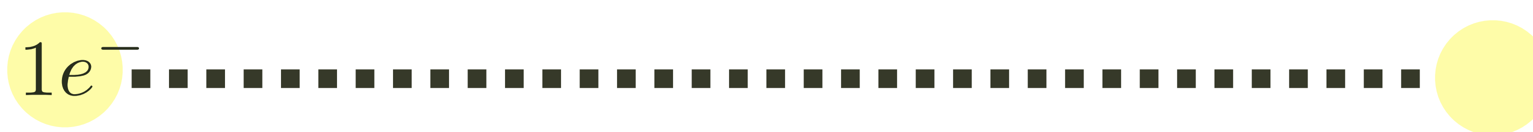
Theoretical Background

- **GW: incorrect atomic limit**

Theoretical Background

- **GW: incorrect atomic limit**
    - Exact

H_2^+



Theoretical Background

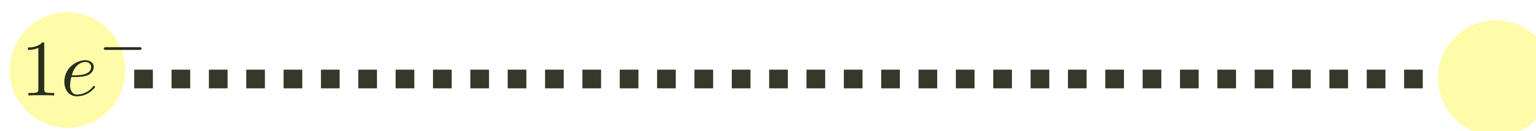
- **GW: incorrect atomic limit**
    - Exact

H_2^+ $1e^-$ $\longrightarrow$ two types of addition energies

Theoretical Background

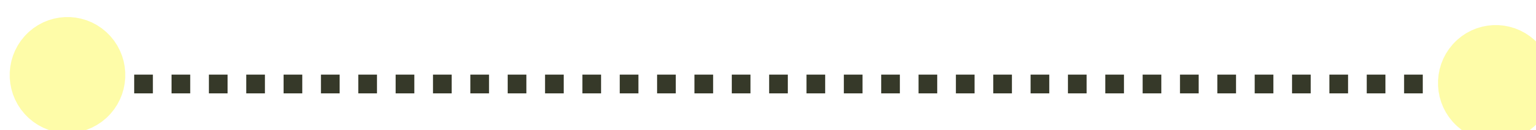
GW: incorrect atomic limit

- Exact

H_2^+ 

$\longrightarrow$ two types of addition energies

- GW

H_2^+ 

Theoretical Background

GW: incorrect atomic limit

- Exact

H_2^+ $1e^-$ .... $\longrightarrow$ two types of addition energies

- GW

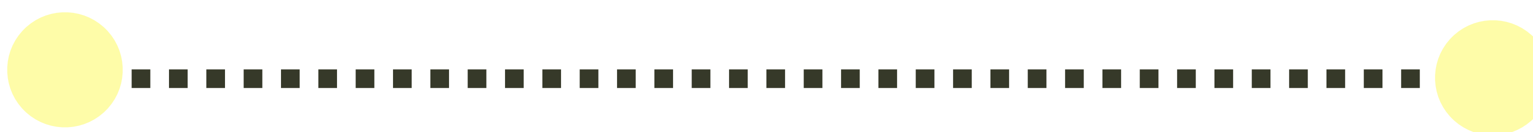
H_2^+ $\frac{1}{2}e^-$ .... $\frac{1}{2}e^-$ $\longrightarrow$ one type of addition energy

Theoretical Background

GW: incorrect atomic limit

- Exact

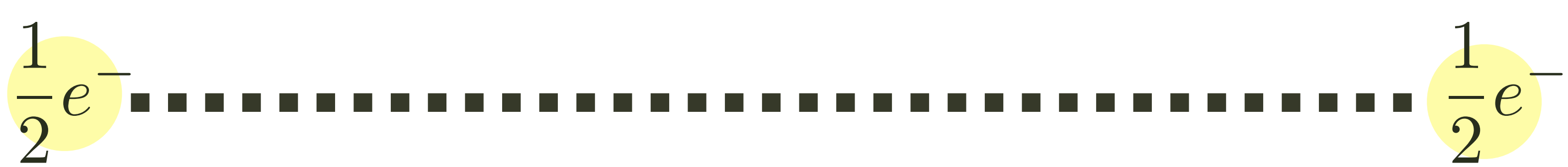
H_2^+



$\longrightarrow$ two types of addition energies

- GW

H_2^+



$\longrightarrow$ one type of addition energy

GW treats the system and its response classically

(bad treatment of correlation)

Theoretical Background

- GW

$$\Sigma = v_H + \Sigma_x + iv_c G \Xi L$$

screening important $\Rightarrow$ L well-approximated

$$\Xi = \frac{\delta(v_H + \cancel{\Sigma}_{xc})}{\delta G} \approx -iv_c$$ rough approximation

$$\Sigma \approx v_H + iGW$$ GW

Beyond GW: keep an approximate Σ_{xc} in Ξ

Theoretical Background

T matrix

$$\Sigma = v_H + \Sigma_x + iv_c G \Xi L$$

quantum nature important

Ξ well-approximated

$$L = \frac{\delta G}{\delta U_{ext}} = -G\frac{\delta G^{-1}}{\delta U_{ext}}G = -G\frac{\delta[G_0^{-1} - U_{ext} - \Sigma]}{\delta U_{ext}}G$$

Theoretical Background

- **T matrix**

$$\Sigma = v_H + \Sigma_x + i v_c G \Xi L$$

quantum nature important ⇨ Ξ well-approximated

$$L = \frac{\delta G}{\delta U_{ext}} = -G \frac{\delta G^{-1}}{\delta U_{ext}} G = -G \frac{\delta [G_0^{-1} - U_{ext} - \cancel{\Sigma}]}{\delta U_{ext}} G \approx GG$$

rough approximation

Theoretical Background

- **T matrix**

$$\Sigma = v_H + \Sigma_x + i v_c G \Xi L$$

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rough approximation

Theoretical Background

- **T matrix**

$$\Sigma = v_H + \Sigma_x + iv_c G\Xi L$$

quantum nature important $\Rightarrow$ Ξ well-approximated $\Sigma = iGT \Rightarrow \Xi \approx T$

$$L = \frac{\delta G}{\delta U_{ext}} = -G\frac{\delta G^{-1}}{\delta U_{ext}}G = -G\frac{\delta[G_0^{-1} - U_{ext} - \cancel{\Sigma}]}{\delta U_{ext}}G \approx GG$$

rough approximation

$$\Sigma = iGT$$

$$\approx v_H + \Sigma_x - v_c GGT$$

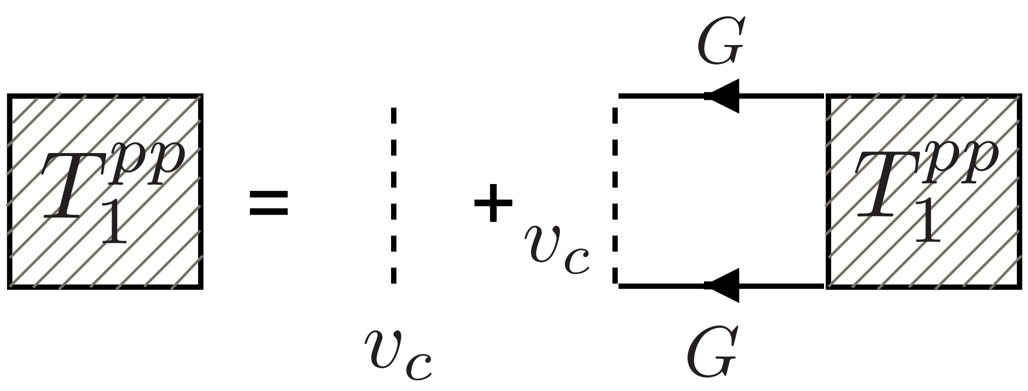
T matrix

Theoretical Background

T matrix

- pp T matrix

$$T^{pp} = \underbrace{T_1^{pp}}_{\text{Hartree-like term}} + \underbrace{T_2^{pp}}_{\text{exchange-like term}}$$



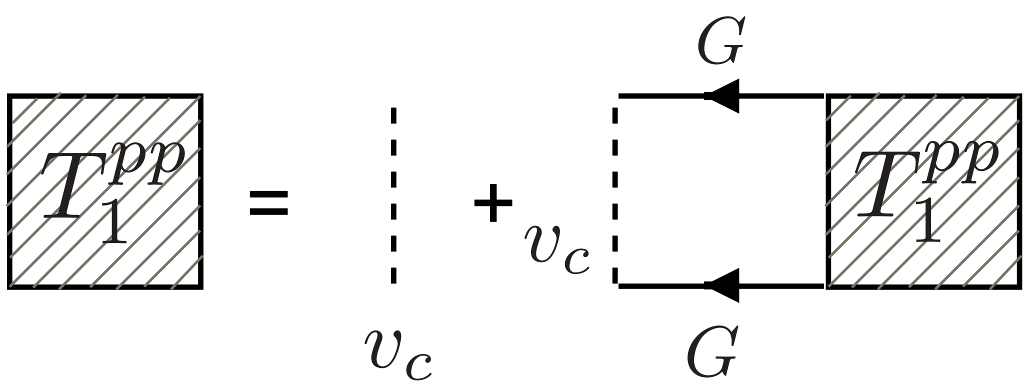
Theoretical Background

T matrix

- pp T matrix

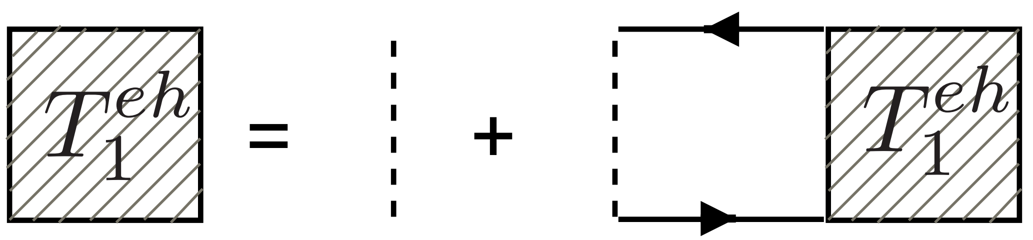
$$T^{pp} = T_1^{pp} + T_2^{pp}$$

Hartree-like term　exchange-like term



- eh T matrix

$$T^{eh} = T_1^{eh} + T_2^{eh}$$



Theoretical Background

- **Physics of GW and T matrix**

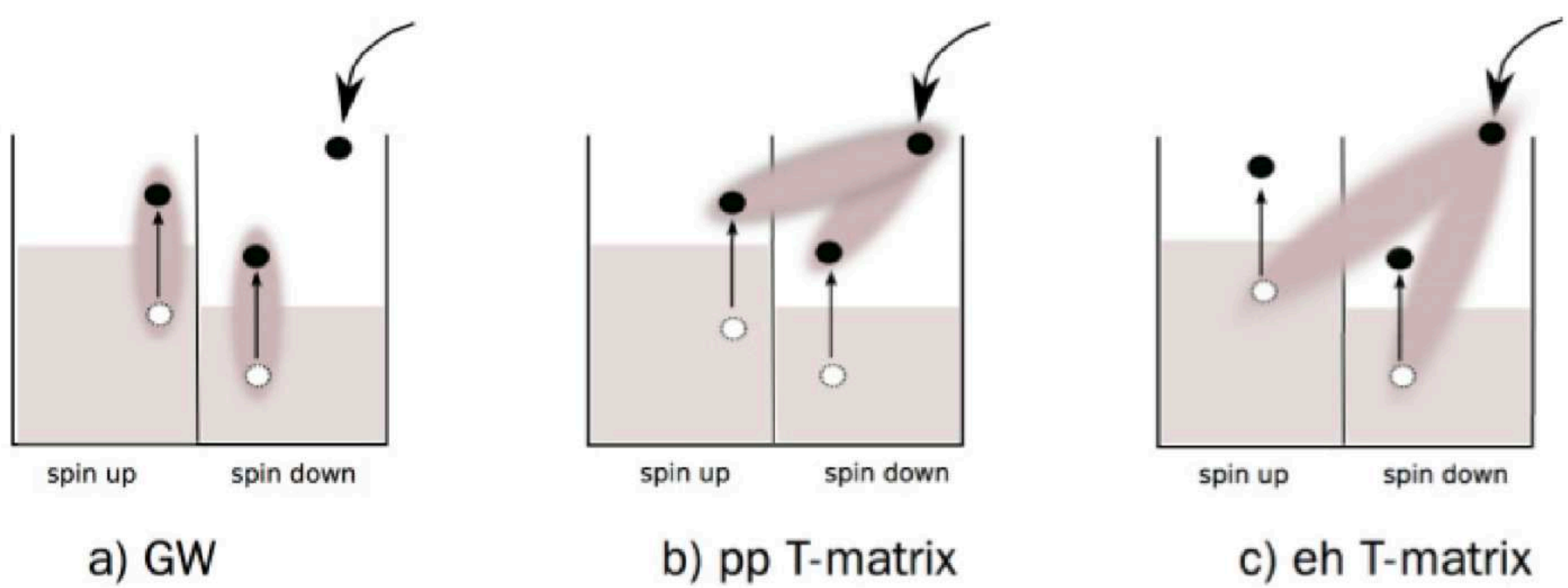
$$\Sigma = v_H + \Sigma_x + i v_c G \Xi L$$

Theoretical Background

- **Physics of GW and T matrix**

$$\Sigma = v_H + \Sigma_x + i v_c G \Xi L$$

3 particles in the game

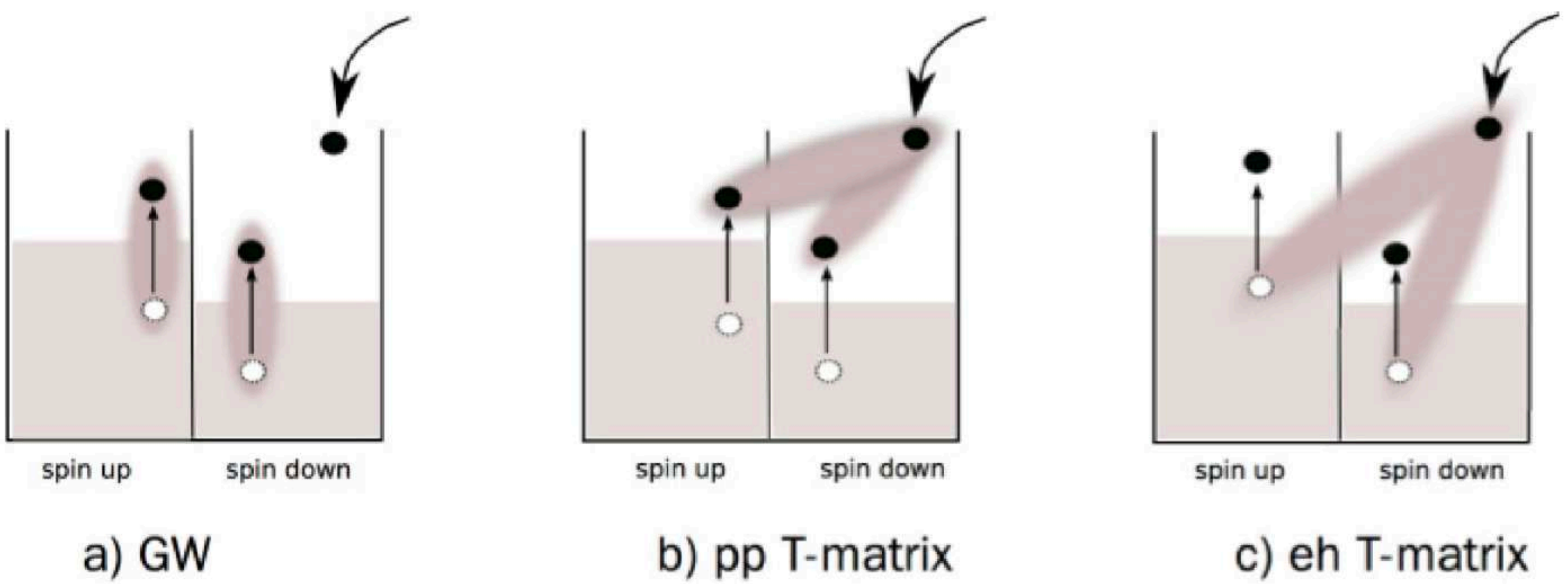


Theoretical Background

- **Physics of GW and T matrix**

$$\Sigma = v_H + \Sigma_x + i v_c G \Xi L$$

3 particles in the game



Let's work with combinations!

Theoretical Background

Screened T matrix

$$\Sigma = v_H + \Sigma_x + i v_c G \Xi L$$

quantum nature important

Ξ well-approximated

$$L = -G \frac{\delta[G_0^{-1} - U_{ext} - \Sigma]}{\delta G} G \approx G \epsilon^{-1} G$$

Theoretical Background

Screened T matrix

$$\Sigma = v_H + \Sigma_x + iv_c G \Xi L$$

quantum nature important

Ξ well-approximated

$$L = -G \frac{\delta[G_0^{-1} - U_{ext} - \Sigma]}{\delta G} G \approx G\epsilon^{-1} G$$

$$\Sigma = iGT_s$$

Theoretical Background

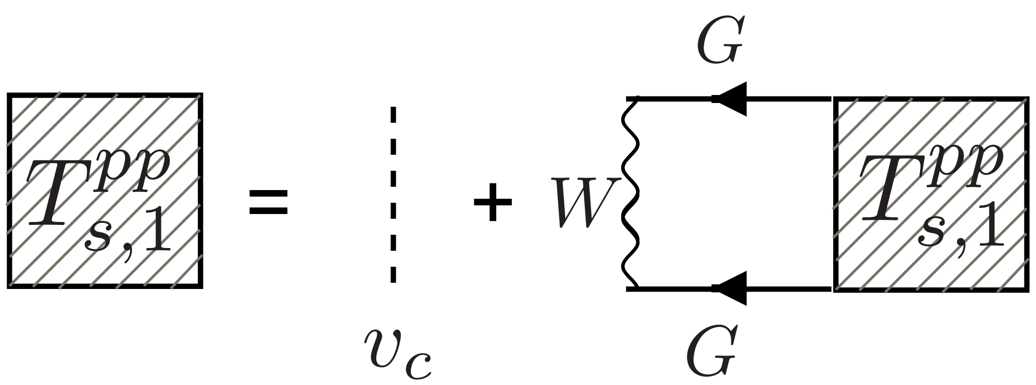
Screened T matrix

- pp screened T matrix

$$T_s^{pp} = T_{s,1}^{pp} + T_{s,2}^{pp}$$

Hartree-like term

exchange-like term

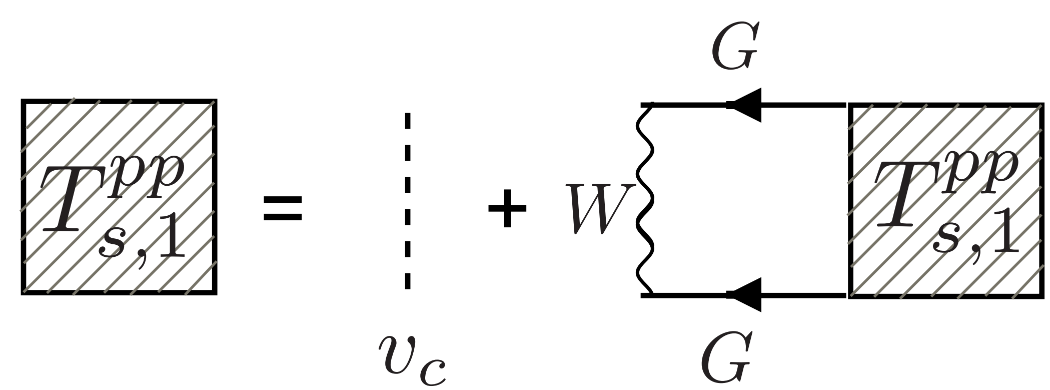


Theoretical Background

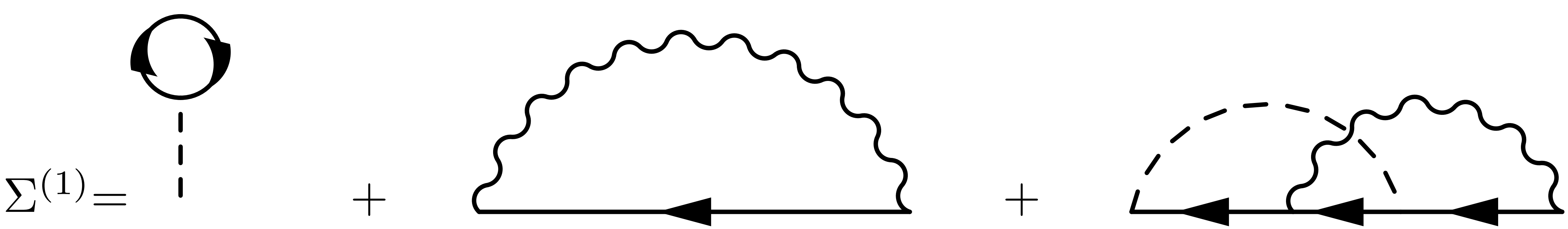
Screened T matrix

- pp screened T matrix

$$T_s^{pp} = \underbrace{T_{s,1}^{pp}}_{\text{Hartree-like term}} + \underbrace{T_{s,2}^{pp}}_{\text{exchange-like term}}$$



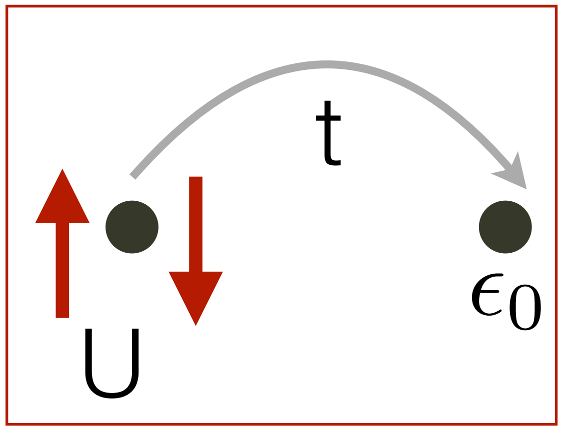
- screened T-matrix self-energy (1st iteration)



Hartree GW SOSEX

The Hubbard dimer

Hamiltonian

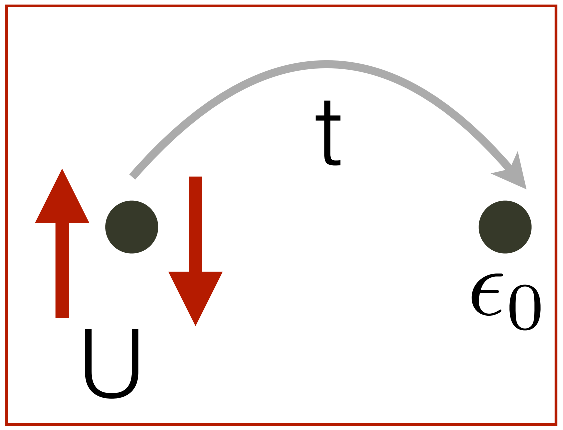


$$H = -t \sum_{\substack{i,j=1,2 \\ i \neq j}} \sum_{\sigma} c^\dagger_{i\sigma} c_{j\sigma} + \frac{U}{2} \sum_{i=1,2} \sum_{\sigma\sigma'} c^\dagger_{i\sigma} c^\dagger_{i\sigma'} c_{i\sigma'} c_{i\sigma} + \epsilon_0 \sum_{\sigma, i=1,2} n_{i\sigma} + V_0$$

N=1 (1/4 filling) and **N=2** (1/2 filling) in the ground state

The Hubbard dimer

Hamiltonian



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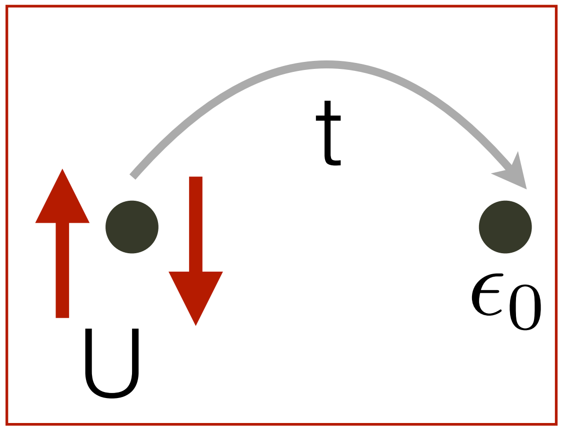
N=1 (1/4 filling) and **N=2** (1/2 filling) in the ground state

weakly and strongly correlated regimes:

- U—> 0 **noninteracting limit**
- U—> ∞ (t—>0) **strongly correlated limit**

The Hubbard dimer

Hamiltonian



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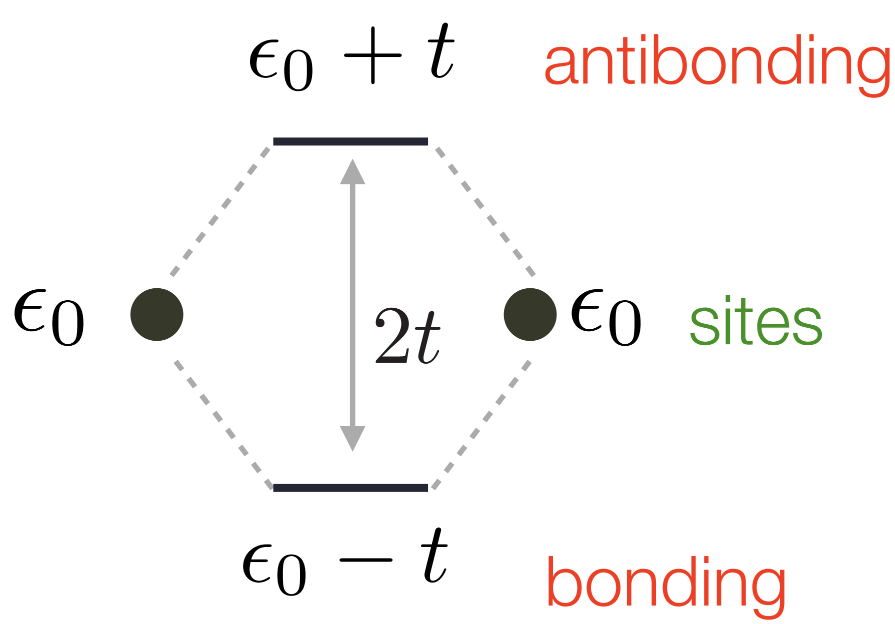
Site vs bonding/antibonding basis

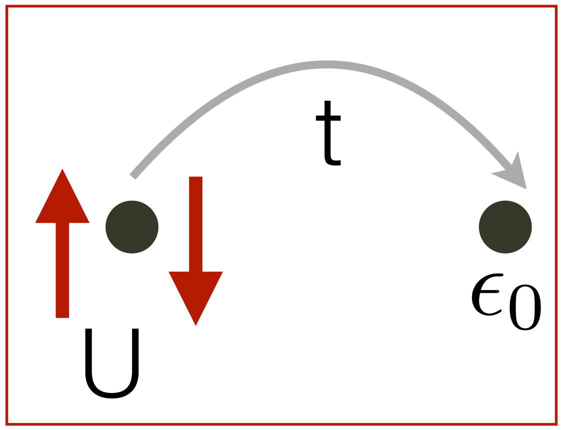


$$\psi_b(\mathbf{x}) = \frac{1}{\sqrt{2}} [\varphi_1(\mathbf{x}) + \varphi_2(\mathbf{x})]$$

$$\psi_a(\mathbf{x}) = \frac{1}{\sqrt{2}} [\varphi_1(\mathbf{x}) - \varphi_2(\mathbf{x})]$$

The Hubbard dimer

Hamiltonian



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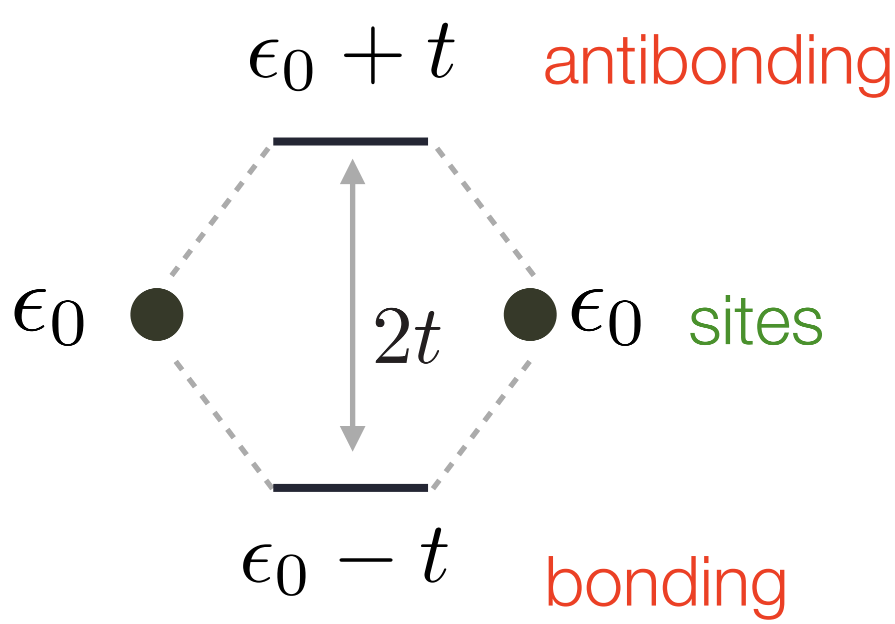
Site vs bonding/antibonding basis



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The Hubbard dimer

1-body Green's function

$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+}\left[\sum_m \frac{\langle\Psi_0^N|\hat{\psi}(\mathbf{x})|\Psi_m^{N+1}\rangle\langle\Psi_m^{N+1}|\hat{\psi}^\dagger(\mathbf{x}')|\Psi_0^N\rangle}{\omega-(E_m^{N+1}-E_0^N)+\mathrm{i}\eta} + \sum_n \frac{\langle\Psi_0^N|\hat{\psi}^\dagger(\mathbf{x}')|\Psi_n^{N-1}\rangle\langle\Psi_n^{N-1}|\hat{\psi}(\mathbf{x})|\Psi_0^N\rangle}{\omega-(E_0^N-E_n^{N-1})-\mathrm{i}\eta}\right]$$

$$\hat{\psi}(\mathbf{x}) = \sum_i \hat{c}_i\varphi_i(\mathbf{x}) \qquad \hat{\psi}^\dagger(\mathbf{x}) = \sum_i \hat{c}_i^\dagger\varphi_i(\mathbf{x})$$ change of basis

$$G(\mathbf{x},\mathbf{x}';\omega) = \sum_{ij} G_{ij}(\omega)\varphi_i(\mathbf{x})\varphi_j^*(\mathbf{x}')$$

$$G_{ij}(\omega) = \lim_{\eta\to 0^+}\left[\sum_m \frac{\langle\Psi_0^N|\hat{c}_i|\Psi_m^{N+1}\rangle\langle\Psi_m^{N+1}|\hat{c}_j^\dagger|\Psi_0^N\rangle}{\omega-(E_m^{N+1}-E_0^N)+\mathrm{i}\eta} + \sum_n \frac{\langle\Psi_0^N|\hat{c}_j^\dagger|\Psi_n^{N-1}\rangle\langle\Psi_n^{N-1}|\hat{c}_i|\Psi_0^N\rangle}{\omega-(E_0^N-E_n^{N-1})-\mathrm{i}\eta}\right]$$

The Hubbard dimer

1-body Green's function

$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+} \left[\sum_m \frac{\langle \Psi_0^N | \hat{\psi}(\mathbf{x}) | \Psi_m^{N+1} \rangle \langle \Psi_m^{N+1} | \hat{\psi}^\dagger(\mathbf{x}') | \Psi_0^N \rangle}{\omega - (E_m^{N+1} - E_0^N) + \mathrm{i}\eta} + \sum_n \frac{\langle \Psi_0^N | \hat{\psi}^\dagger(\mathbf{x}') \big| \Psi_n^{N-1} \rangle \langle \Psi_n^{N-1} | \hat{\psi}(\mathbf{x}) \big| \Psi_0^N \rangle}{\omega - (E_0^N - E_n^{N-1}) - \mathrm{i}\eta} \right]$$

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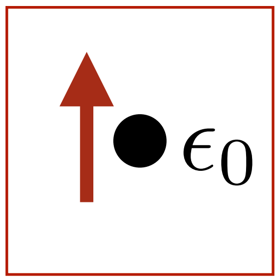
exact solution from eigenvectors and eigenvalues of the N and $(N \pm 1)$ electron systems

The Hubbard monomer: exact solution

- **N=1** (one site)



The Hubbard monomer: exact solution

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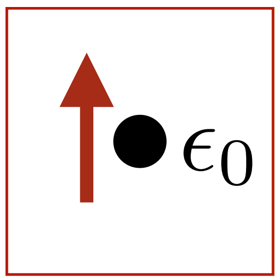

$$G^{\uparrow} = \frac{1}{\omega - \epsilon_0 - \mathrm{i}\eta}$$

removal energy: $\omega = \epsilon_0$

$$G^{\downarrow} = \frac{1}{\omega - \epsilon_0 - U + \mathrm{i}\eta}$$

addition energy: $\omega = \epsilon_0 + U$

The Hubbard monomer: exact solution

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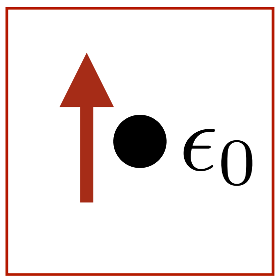
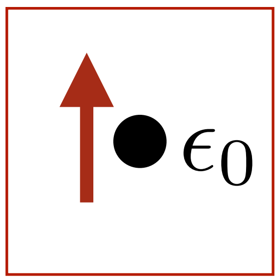


$$G^{\uparrow} = \frac{1}{\omega - \epsilon_0 - \mathrm{i}\eta} = G_0^{\uparrow}$$

$$G^{\downarrow} = \frac{1}{\omega - \epsilon_0 - U + \mathrm{i}\eta} \xrightarrow{U \to 0} \frac{1}{\omega - \epsilon_0 + \mathrm{i}\eta}$$

The Hubbard monomer: exact solution

N=1 (one site)



$$G^{\uparrow} = \frac{1}{\omega - \epsilon_0 - \mathrm{i}\eta} = G_0^{\uparrow}$$

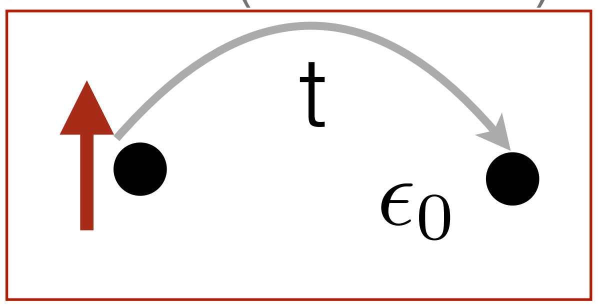
$$G^{\downarrow} = \frac{1}{\omega - \epsilon_0 - U + \mathrm{i}\eta} \xrightarrow{U \to 0} \frac{1}{\omega - \epsilon_0 + \mathrm{i}\eta}$$

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

$$\Sigma(\omega) = \begin{array}{c c} & \begin{array}{cc} \uparrow & \downarrow \end{array} \\ \begin{array}{c} \uparrow \\ \downarrow \end{array} & \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix} \end{array}$$

The Hubbard dimer: exact solution

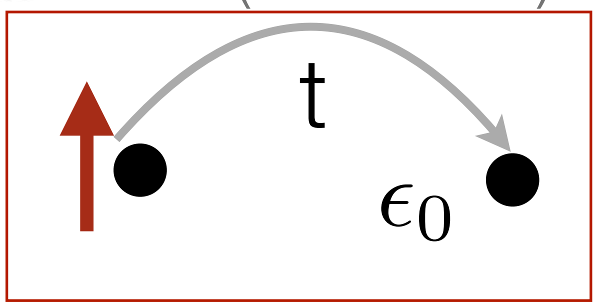
- **N=1** (two sites)



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

The Hubbard dimer: exact solution

- **N=1** (two sites)

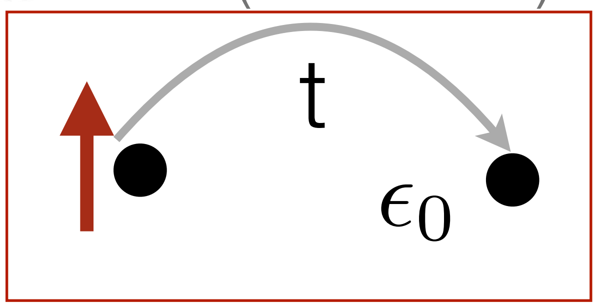


$$|\psi_0^{N=1}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\ 0\rangle + |0\ \uparrow\rangle\right) \qquad E_0 = \epsilon_0 - t$$

$$G(\omega) = \begin{array}{c} \\ \end{array} \begin{array}{cc} \begin{array}{cccc} 1\uparrow & 2\uparrow & 1\downarrow & 2\downarrow \end{array} & \\ \begin{pmatrix} G_{11}^{\uparrow} & G_{12}^{\uparrow} & 0 & 0 \\ G_{21\uparrow}^{\uparrow} & G_{22}^{\uparrow} & 0 & 0 \\ 0 & 0 & G_{11}^{\downarrow} & G_{12}^{\downarrow} \\ 0 & 0 & G_{21}^{\downarrow} & G_{22}^{\downarrow} \end{pmatrix} & \begin{array}{c} 1\uparrow \\ 2\uparrow \\ 1\downarrow \\ 2\downarrow \end{array} \end{array}$$

The Hubbard dimer: exact solution

N=1 (two sites)



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

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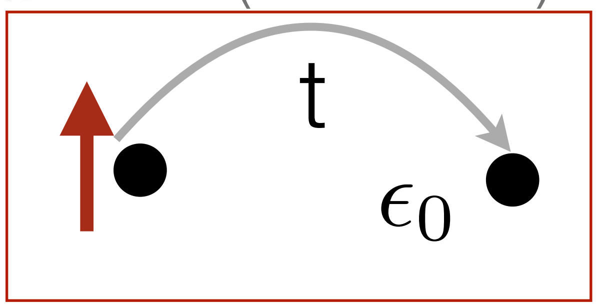
Symmetric in the sites

The Hubbard dimer: exact solution

N=1 (two sites)



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

$$\begin{array}{cc} & \begin{array}{cccc} 1\uparrow & 2\uparrow & 1\downarrow & 2\downarrow \end{array} \\ G(\omega) = & \begin{pmatrix} G_{11}^{\uparrow} & G_{12}^{\uparrow} & 0 & 0 \\ G_{21\uparrow}^{\uparrow} & G_{22}^{\uparrow} & 0 & 0 \\ 0 & 0 & G_{11}^{\downarrow} & G_{12}^{\downarrow} \\ 0 & 0 & G_{21}^{\downarrow} & G_{22}^{\downarrow} \end{pmatrix} \begin{array}{c} 1\uparrow \\ 2\uparrow \\ 1\downarrow \\ 2\downarrow \end{array} \end{array}$$

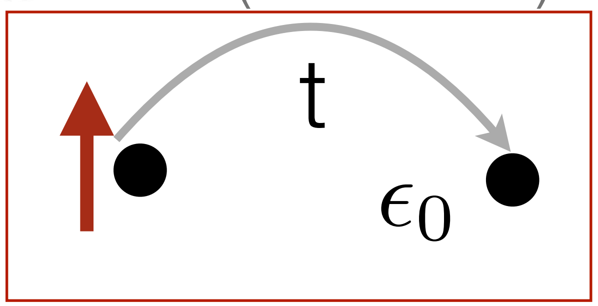
Symmetric in the sites

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

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

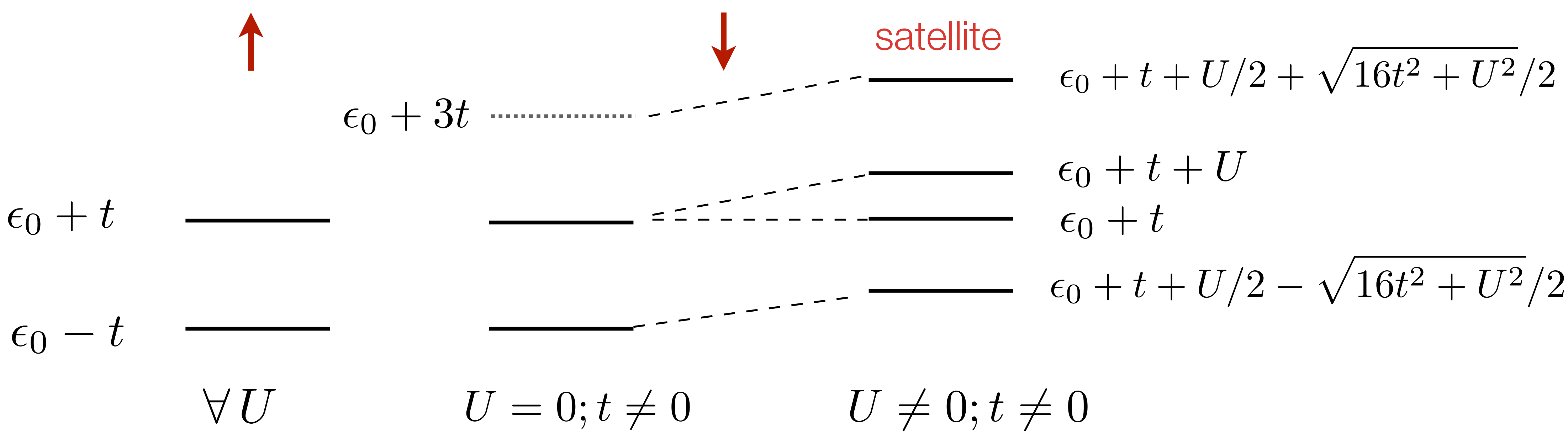
The Hubbard dimer: exact solution

N=1 (two sites)



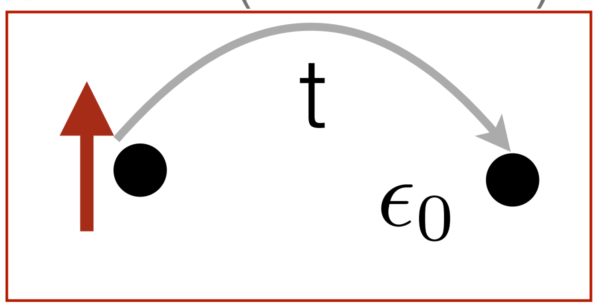
$$|\psi_0^{N=1}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\ 0\rangle + |0\ \uparrow\rangle) \qquad E_0 = \epsilon_0 - t$$

- **Removal/addition energies:** noninteracting limit $U \rightarrow 0$



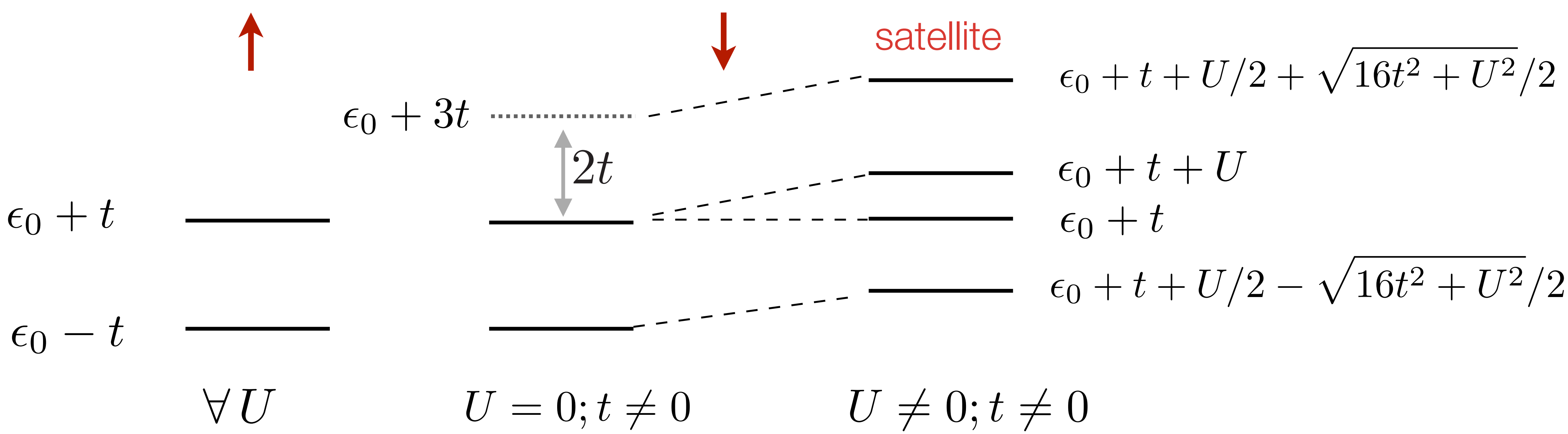
The Hubbard dimer: exact solution

N=1 (two sites)



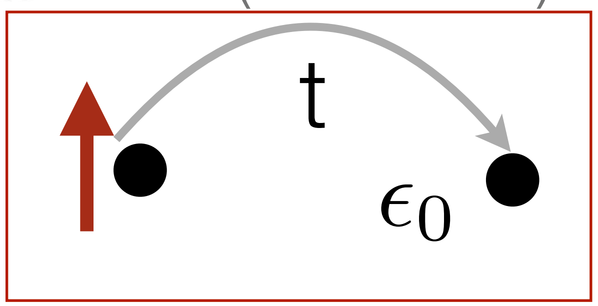
$$|\psi_0^{N=1}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\ 0\rangle + |0\ \uparrow\rangle\right) \qquad E_0 = \epsilon_0 - t$$

- **Removal/addition energies:** noninteracting limit $U \rightarrow 0$



The Hubbard dimer: exact solution

N=1 (two sites)



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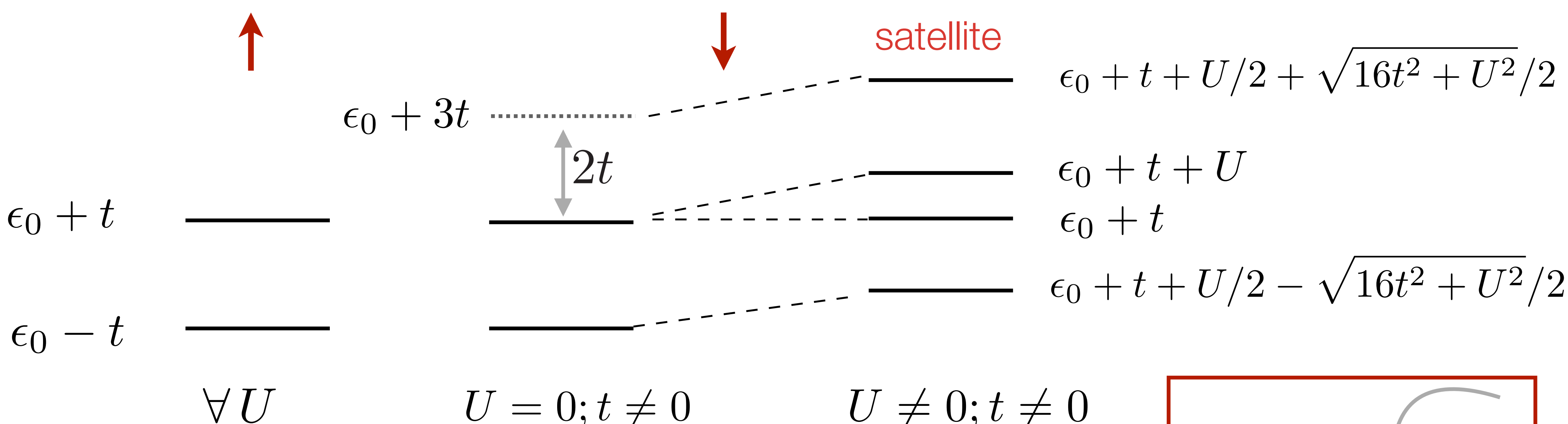

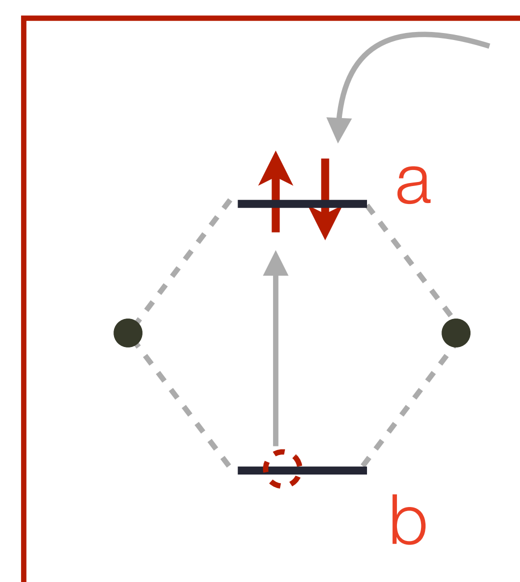

The Hubbard dimer: exact solution

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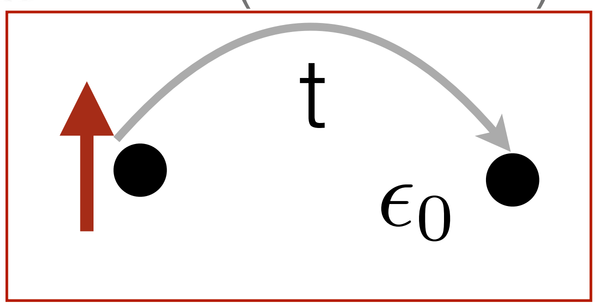

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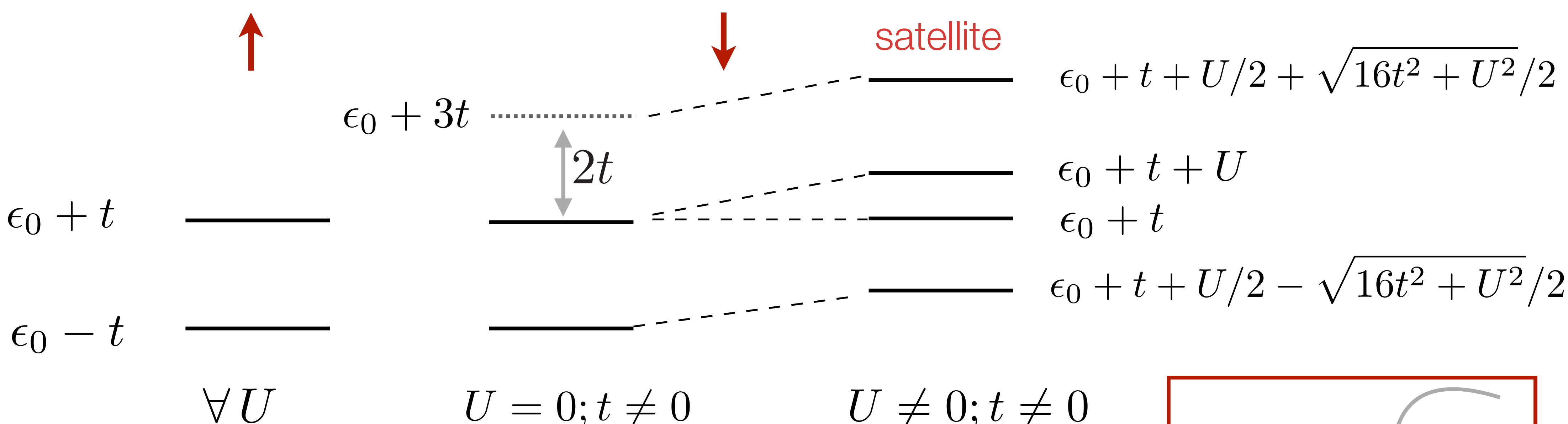

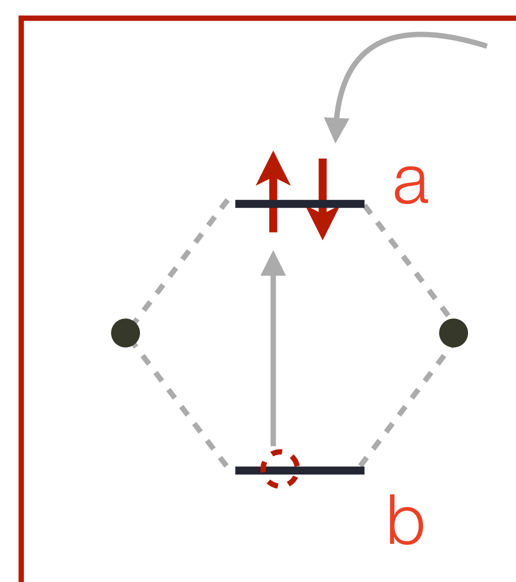

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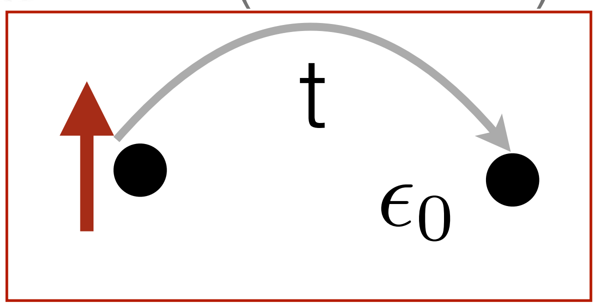
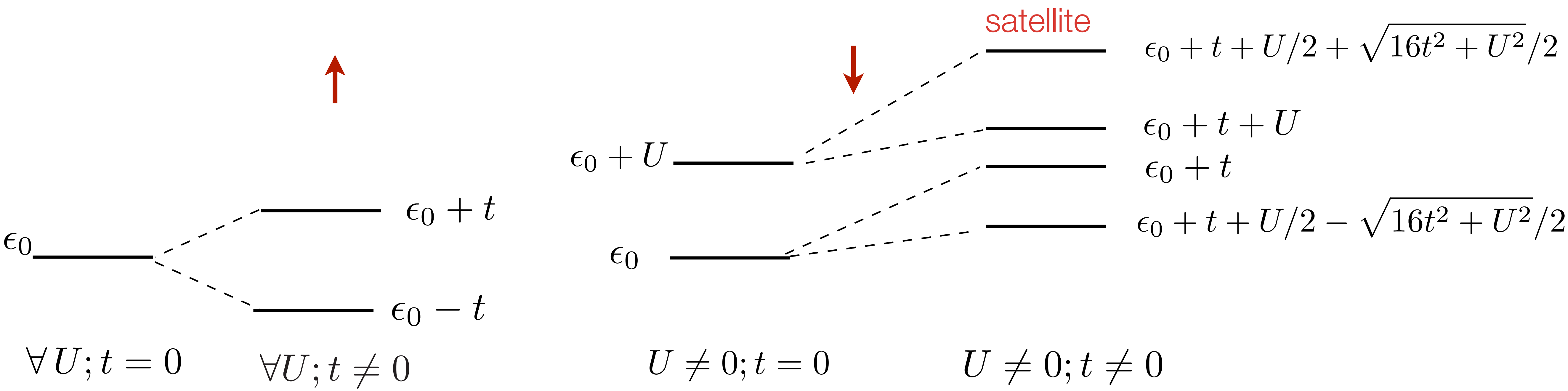
N=1 (two sites)



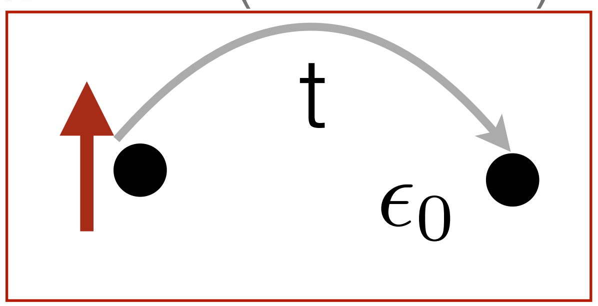
$$|\psi_0^{N=1}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\ 0\rangle + |0\ \uparrow\rangle) \qquad E_0 = \epsilon_0 - t$$

- **Removal/addition energies:** atomic limit $t \longrightarrow 0$



The Hubbard dimer: exact solution

N=1 (two sites)



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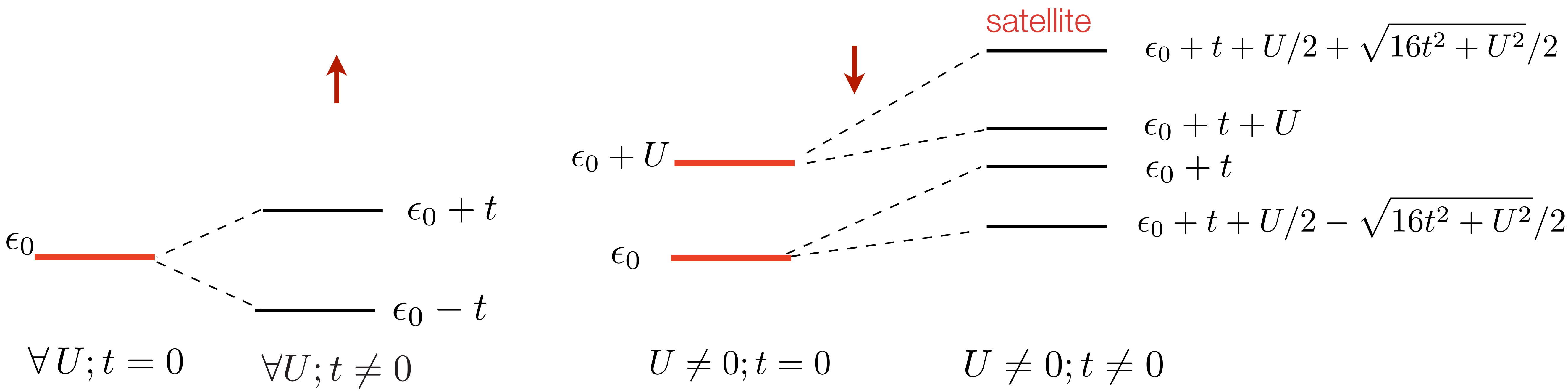
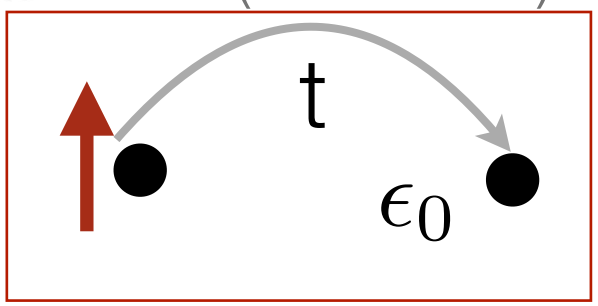


The Hubbard dimer: exact solution

N=1 (two sites)



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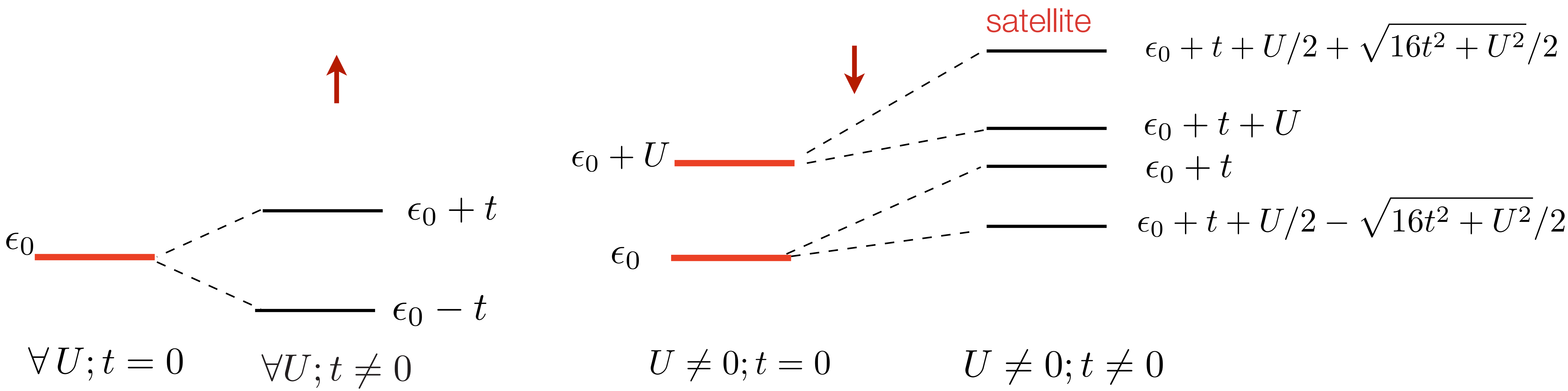
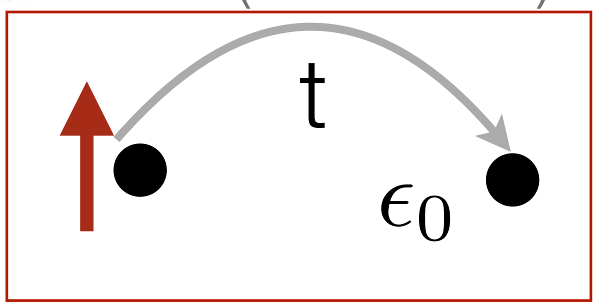


removal/addition energies of an empty atom and an atom with one electron

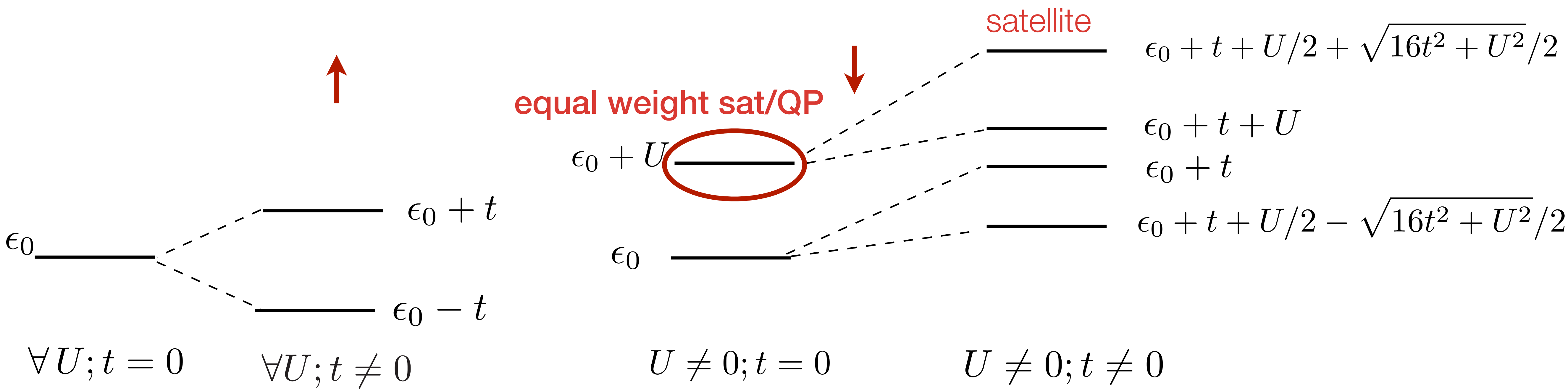
The Hubbard dimer: exact solution

N=1 (two sites)



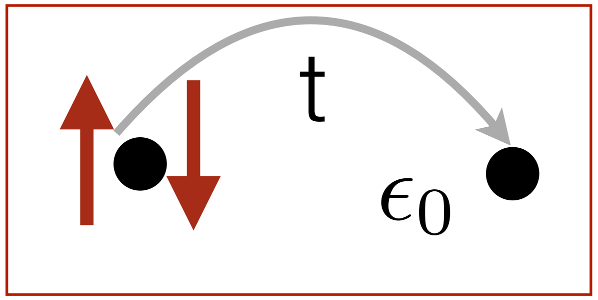
$$|\psi_0^{N=1}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\ 0\rangle + |0\ \uparrow\rangle\right) \qquad E_0 = \epsilon_0 - t$$

- **Removal/addition energies:** atomic limit $t \longrightarrow 0$



The Hubbard dimer: exact solution

- **N=2**

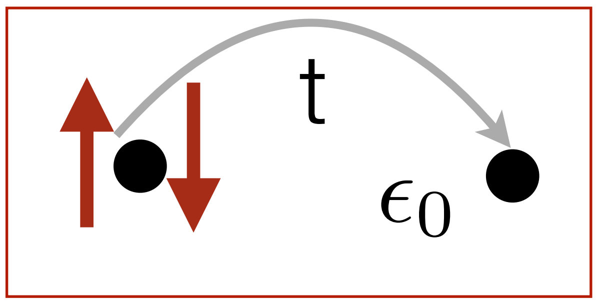


$$G(\omega) = \begin{pmatrix} G^{\uparrow}_{11} & G^{\uparrow}_{12} & 0 & 0 \\ G^{\uparrow}_{21\uparrow} & G^{\uparrow}_{22} & 0 & 0 \\ 0 & 0 & G^{\downarrow}_{11} & G^{\downarrow}_{12} \\ 0 & 0 & G^{\downarrow}_{21} & G^{\downarrow}_{22} \end{pmatrix}$$

Symmetric in the sites and in the spin

The Hubbard dimer: exact solution

N=2



$$G(\omega) = \begin{pmatrix} G^{\uparrow}_{11} & G^{\uparrow}_{12} & 0 & 0 \\ G^{\uparrow}_{21\uparrow} & G^{\uparrow}_{22} & 0 & 0 \\ 0 & 0 & G^{\downarrow}_{11} & G^{\downarrow}_{12} \\ 0 & 0 & G^{\downarrow}_{21} & G^{\downarrow}_{22} \end{pmatrix}$$

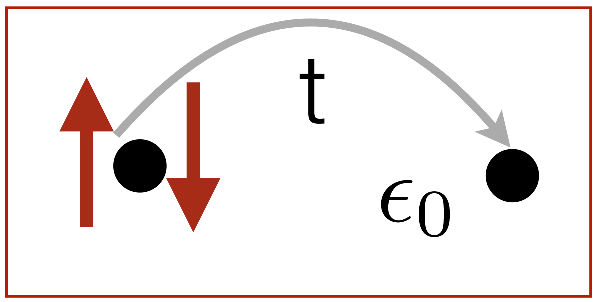
Symmetric in the sites and in the spin

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

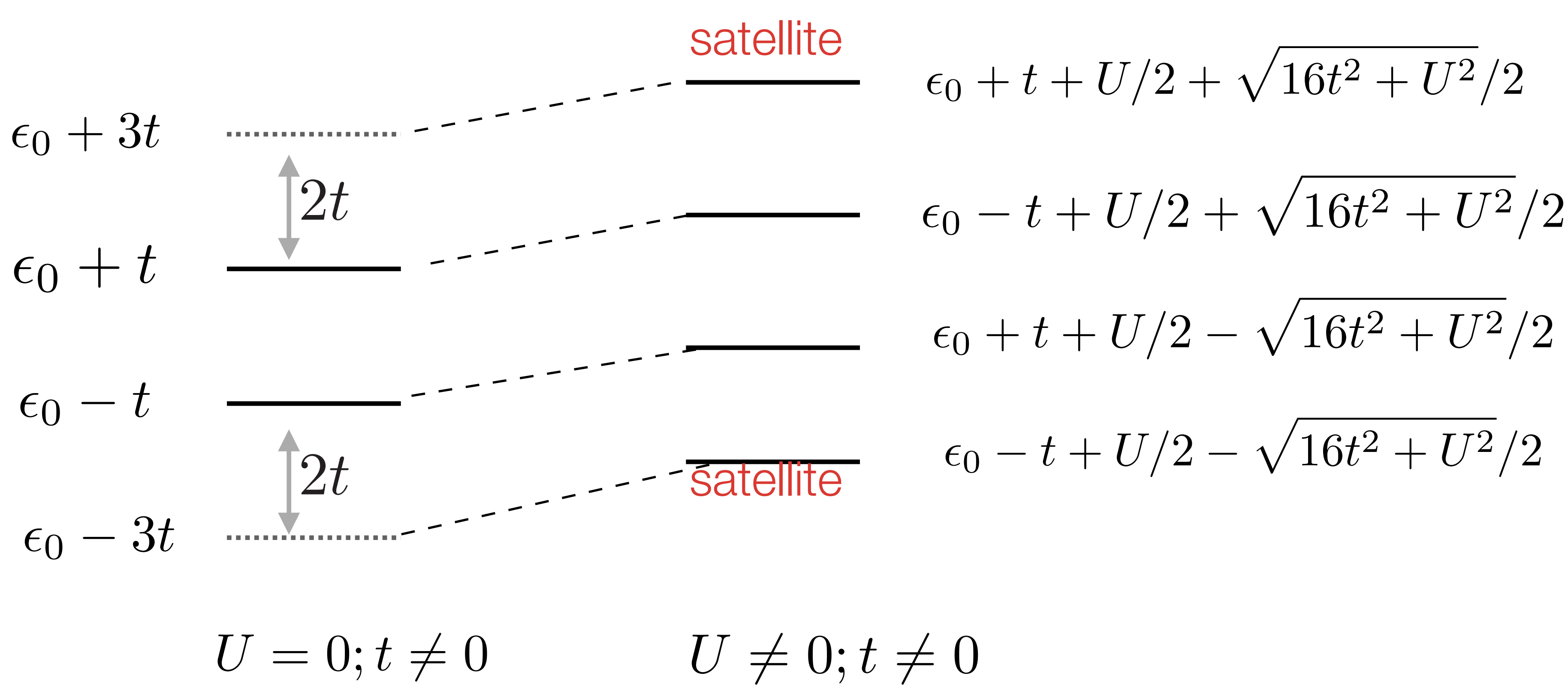
$$\Sigma(\omega) = \begin{pmatrix} \Sigma^{\uparrow}_{11} & \Sigma^{\uparrow}_{12} & 0 & 0 \\ \Sigma^{\uparrow}_{12} & \Sigma^{\uparrow}_{11} & 0 & 0 \\ 0 & 0 & \Sigma^{\downarrow}_{11} & \Sigma^{\downarrow}_{12} \\ 0 & 0 & \Sigma^{\downarrow}_{12} & \Sigma^{\downarrow}_{11} \end{pmatrix}$$

The Hubbard dimer: exact solution

N=2

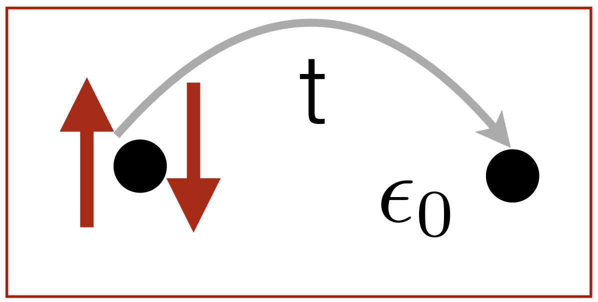


- **Removal/addition energies:** noninteracting limit $U \longrightarrow 0$

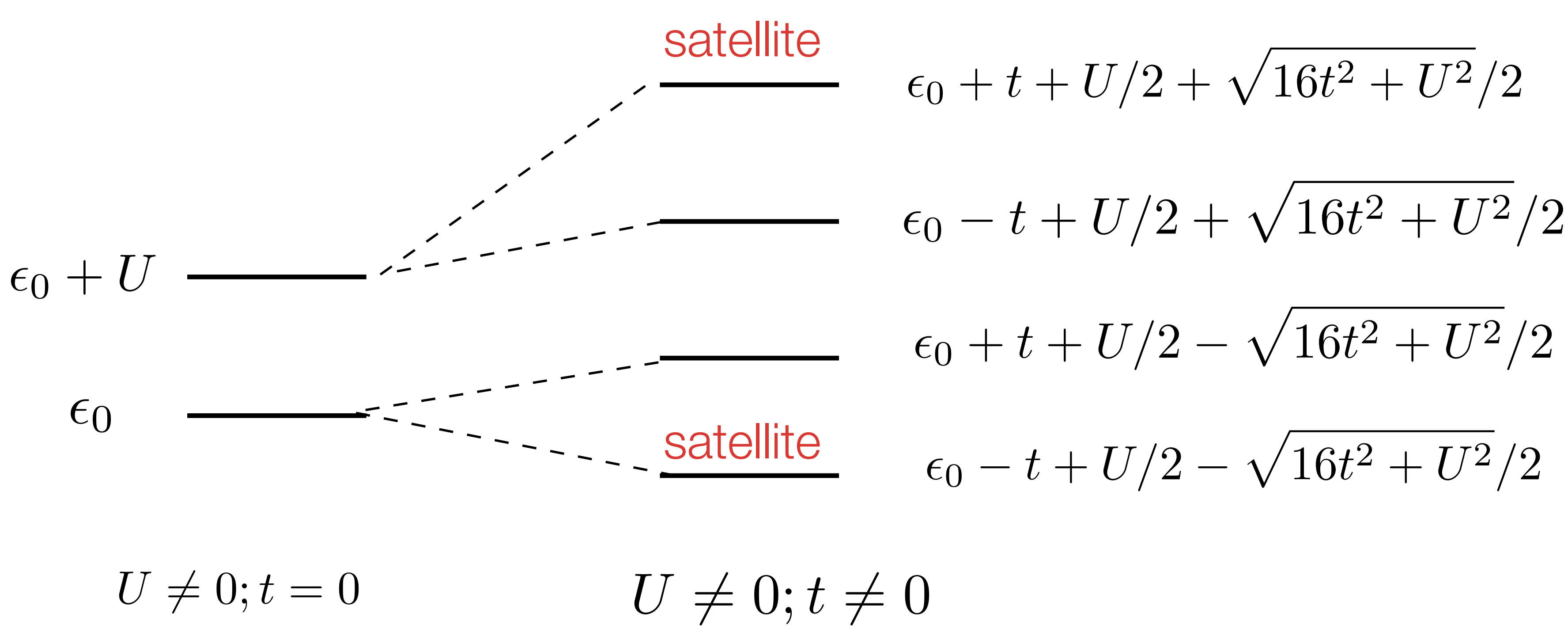


The Hubbard dimer: exact solution

N=2

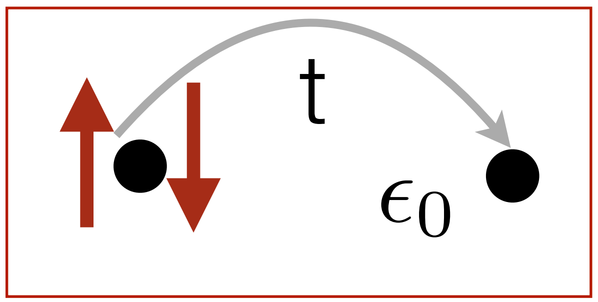


- **Removal/addition energies:** atomic limit $t \longrightarrow 0$

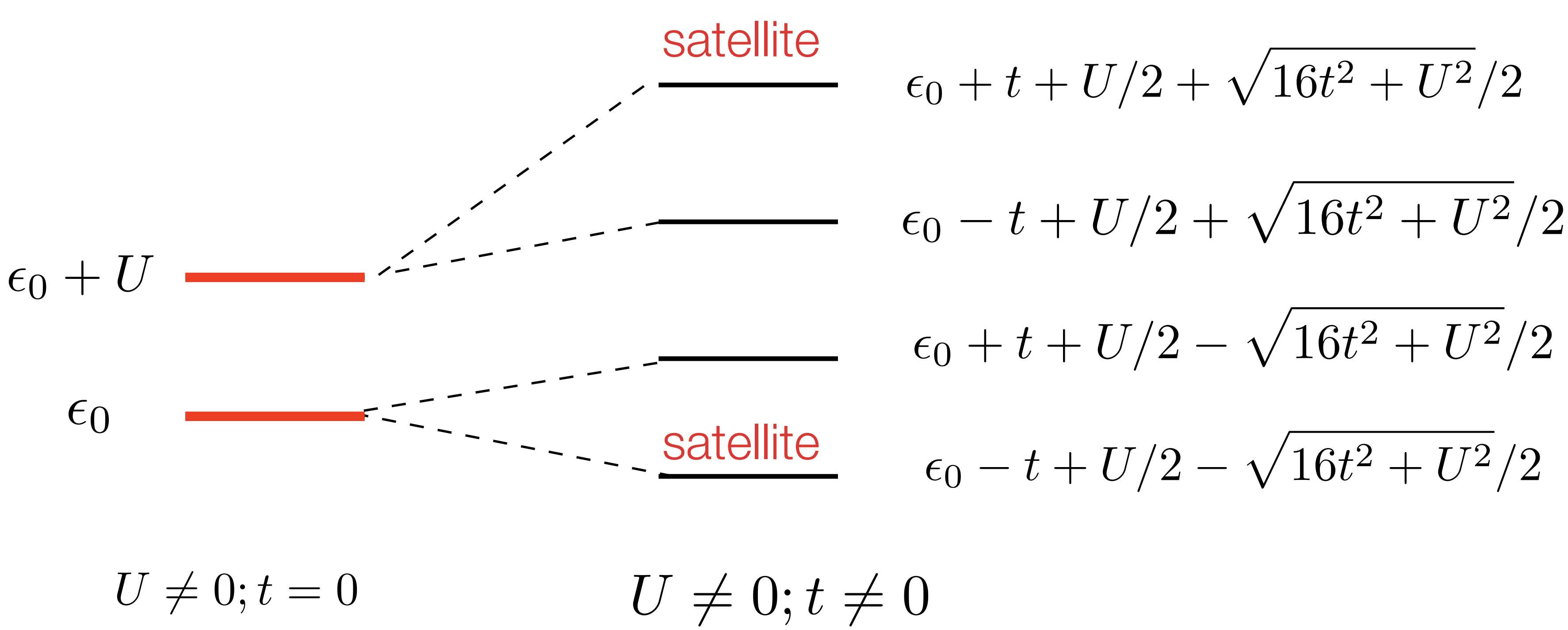


The Hubbard dimer: exact solution

N=2



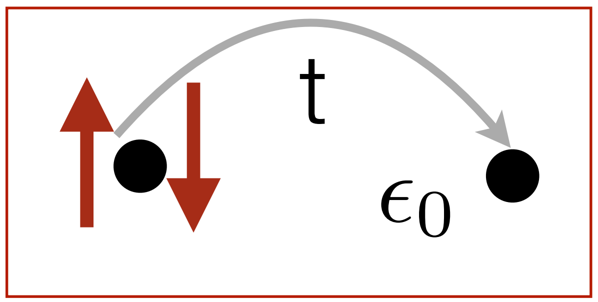
- **Removal/addition energies: atomic limit** $t \rightarrow 0$



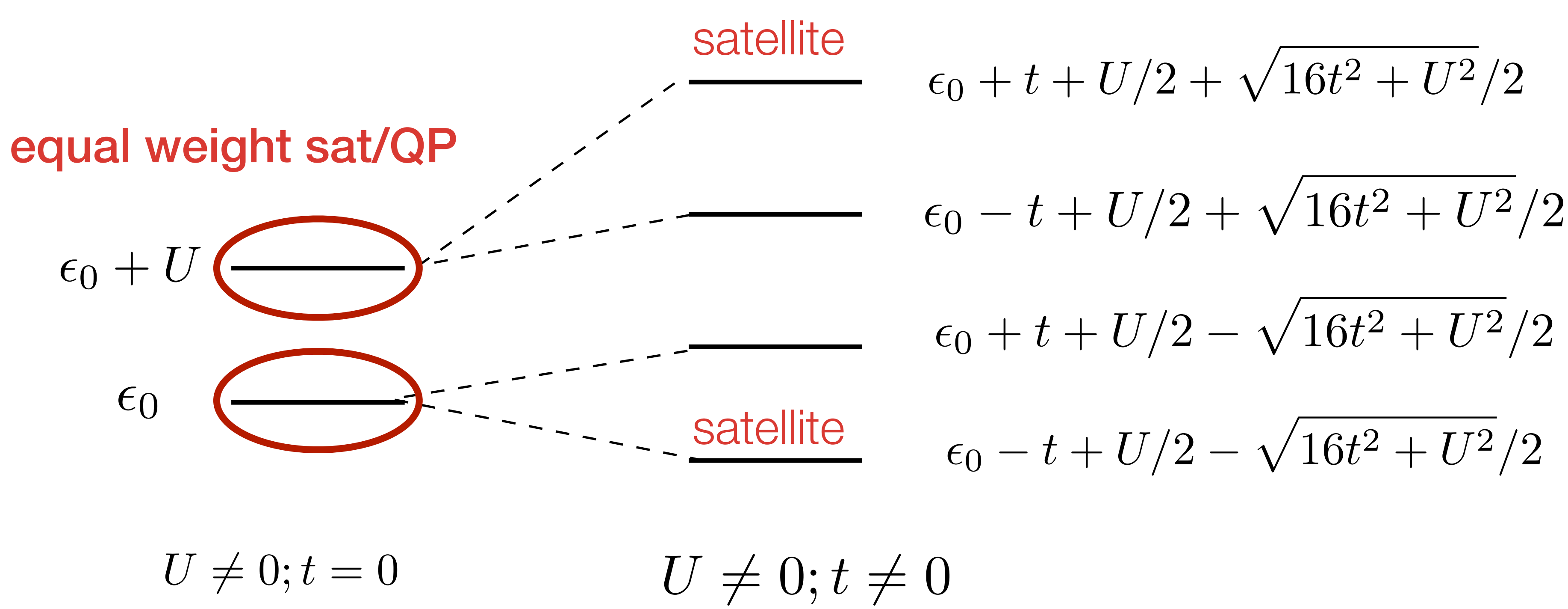
removal/addition energies of one isolated atom with one electron

The Hubbard dimer: exact solution

N=2



- **Removal/addition energies: atomic limit** $t \rightarrow 0$



The Hubbard dimer: GW solution

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

One-shot GW
(G_0 as starting point)

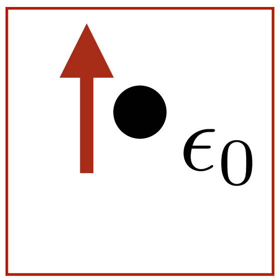
$$\Sigma = v_H + iG_0W_0$$

$$W_0 = [1 + \underbrace{iv_cG_0G_0}_{-v_cP}]^{-1}v_c$$

$$v_H = -iv_cG_0$$

The Hubbard monomer: GW solution

N=1

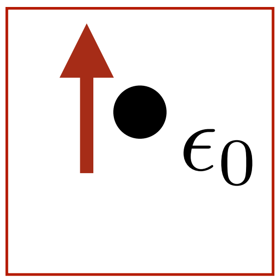


$$P = 0 \Rightarrow W = U$$ exchange

$$\Sigma(\omega) = \begin{array}{c c} & \begin{array}{cc} \uparrow & \downarrow \end{array} \\ \begin{array}{c} \uparrow \\ \downarrow \end{array} & \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix} \end{array}$$

The Hubbard monomer: GW solution

N=1



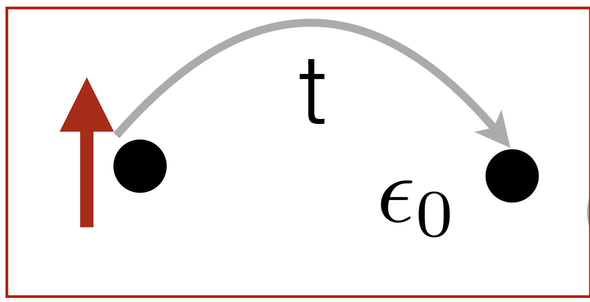
$$P = 0 \Rightarrow W = U$$ exchange

$$\Sigma(\omega) = \begin{array}{c c} & \begin{array}{cc} \uparrow & \downarrow \end{array} \\ \begin{array}{c} \uparrow \\ \downarrow \end{array} & \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix} \end{array}$$

GW is exact for two isolated sites

The Hubbard dimer: GW solution

N=1

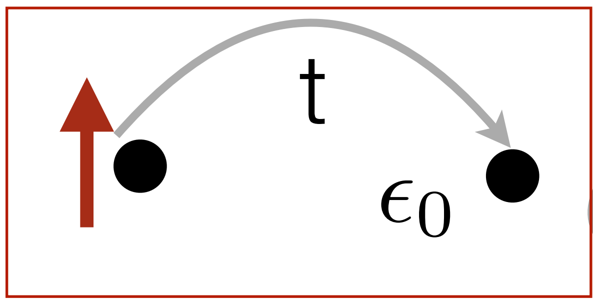


$P \neq 0 \Rightarrow W \neq U \neq$ exchange (for $t \neq 0$)

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

The Hubbard dimer: GW solution

N=1

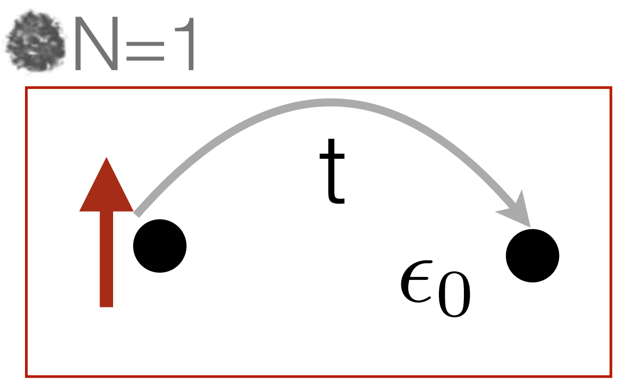


$P \neq 0$ ⇨ $W \neq U$ $\neq$ exchange (for $t \neq 0$)

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

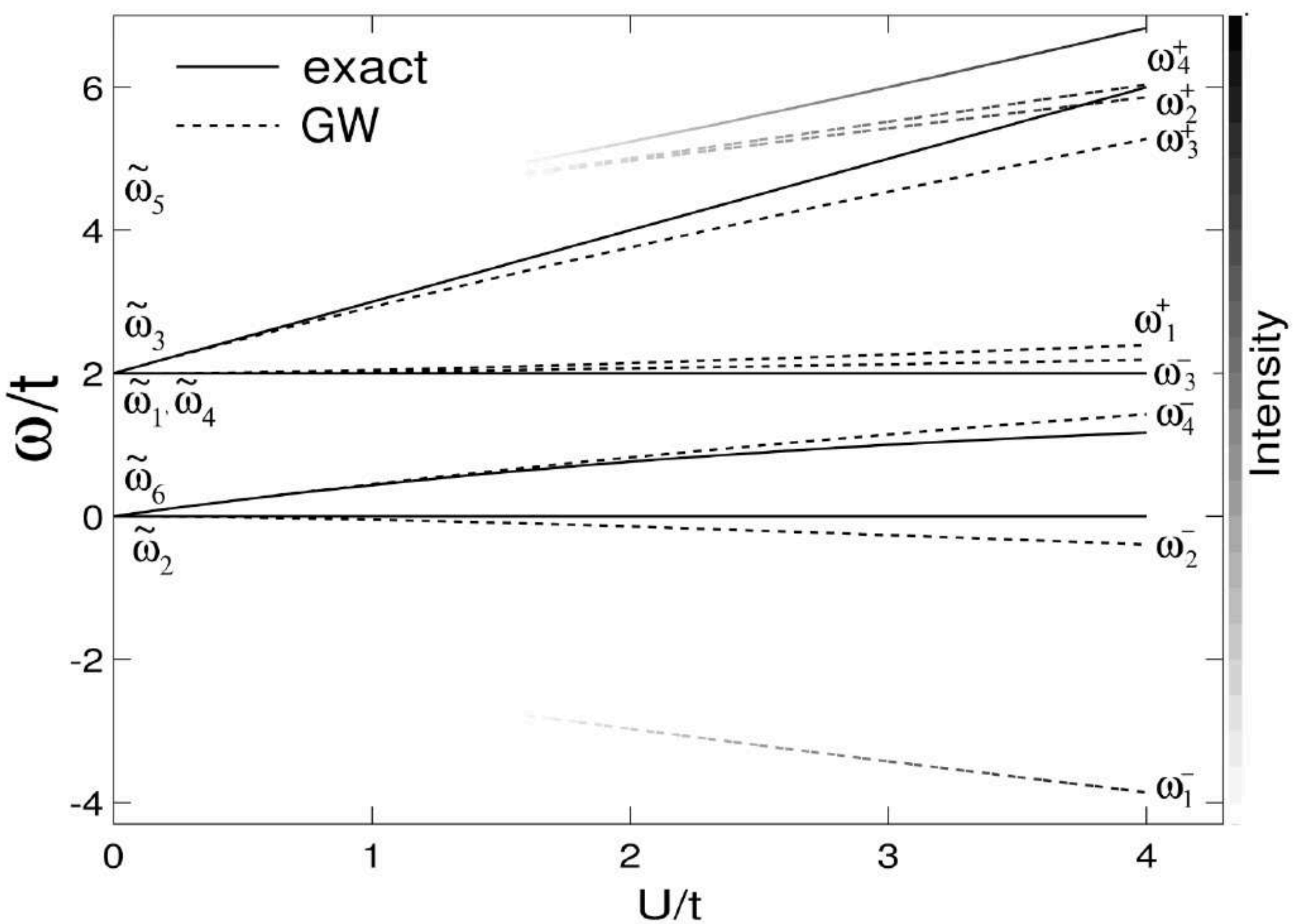
sign of self-screening

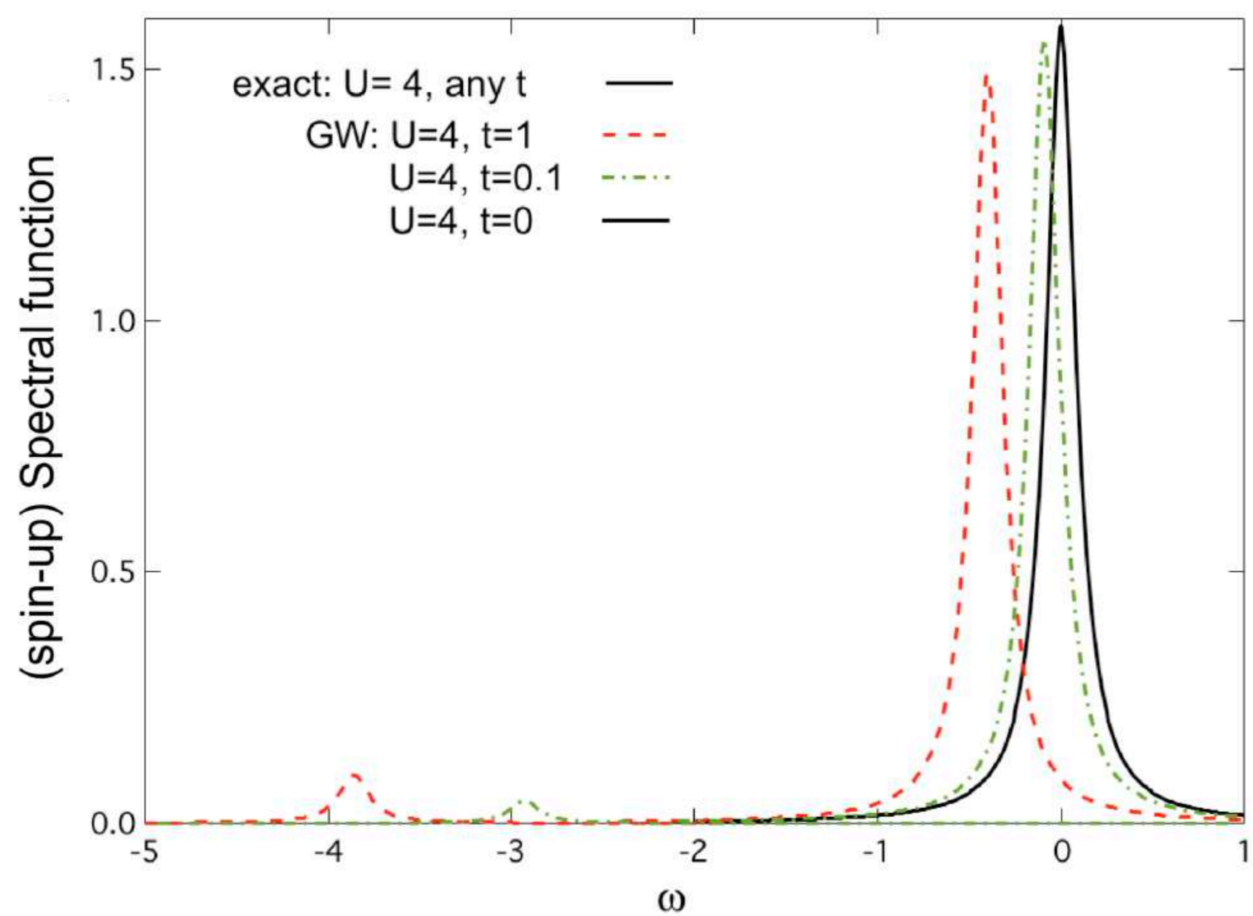
The Hubbard dimer: GW solution



$P \neq 0$ ⇨ $W \neq U$ $\neq$ exchange (for $t \neq 0$)

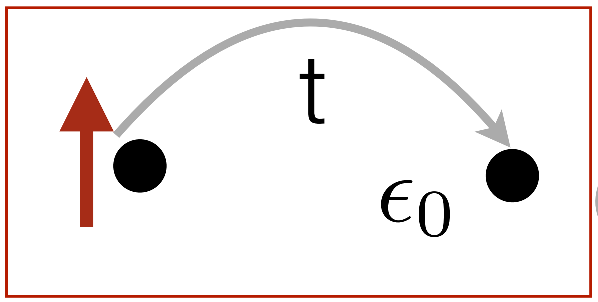
- **Removal/addition energies:** self-screening





The Hubbard dimer: GW solution

N=1



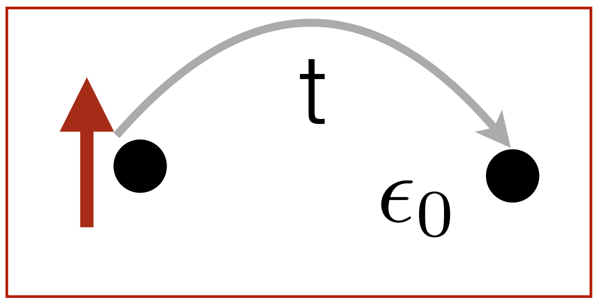
$P \to 0 \implies W \to U$ = exchange (for $t \to 0$)

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

no self-screening at $t \to 0$

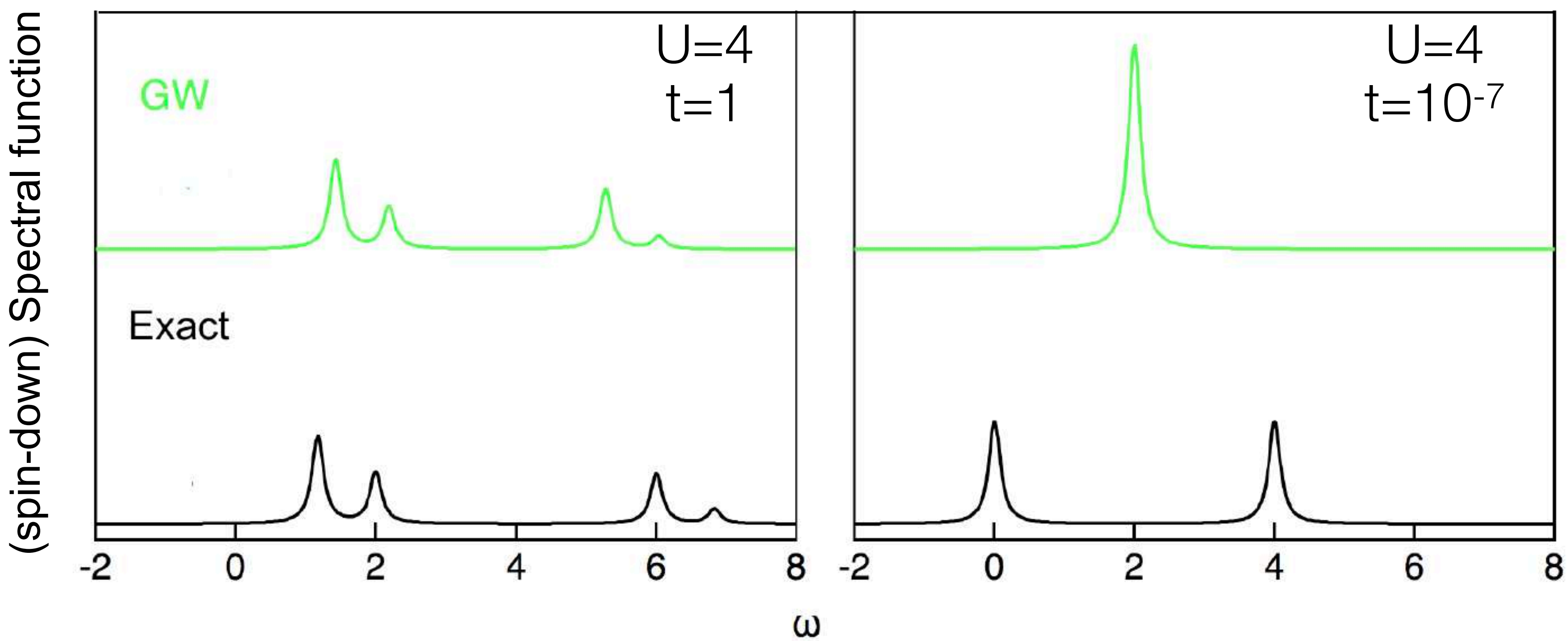
The Hubbard dimer: GW solution

N=1



$P \to 0 \Rightarrow W \to U$ = exchange (for $t \to 0$)

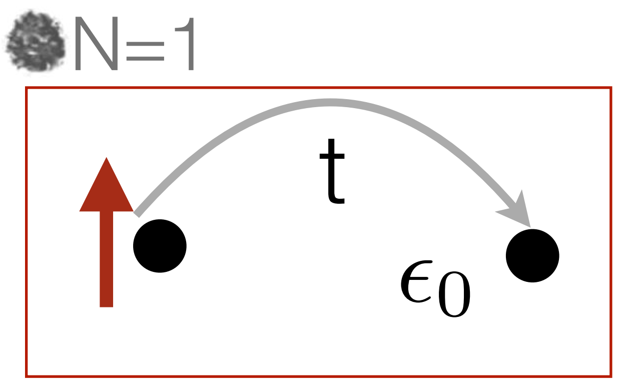
- **Spectral function:** atomic limit $t \to 0$



no gap in GW

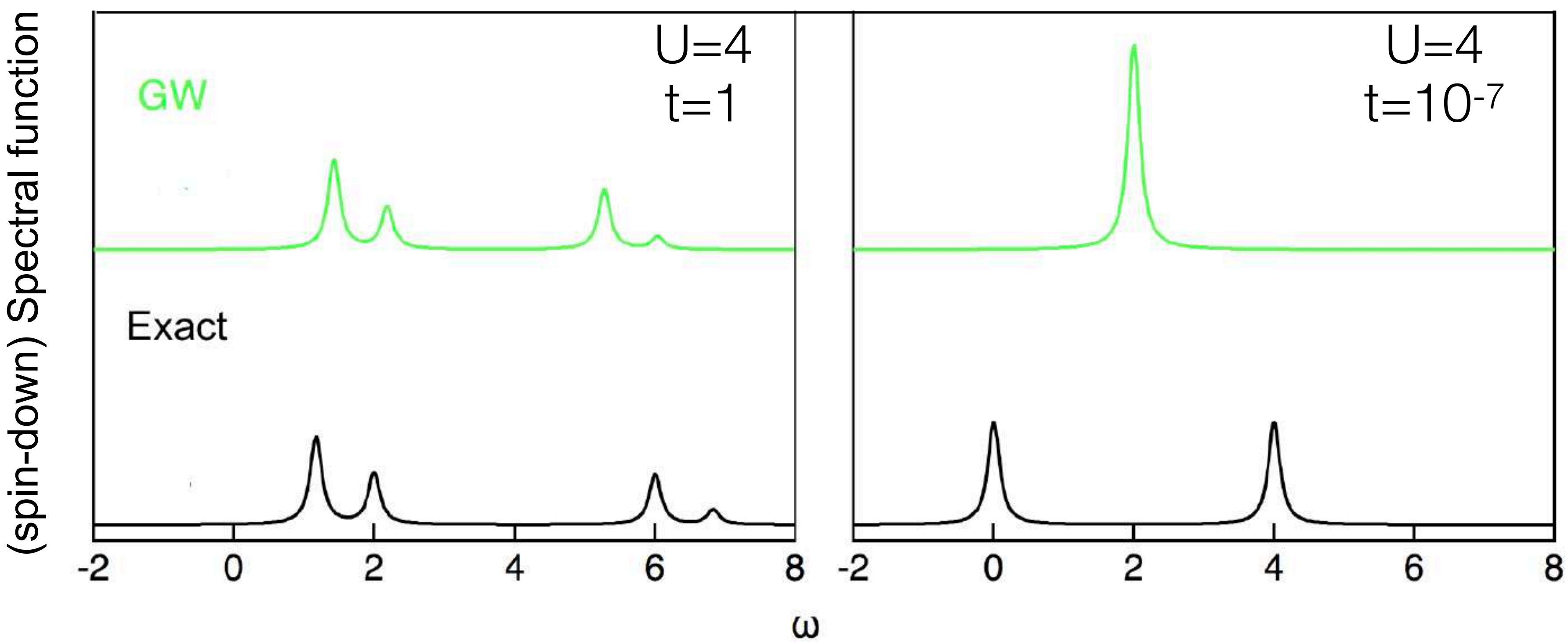
(1/2 e⁻ on each site)

The Hubbard dimer: GW solution



$P \to 0$ ⇨ $W \to U$ = exchange (for $t \to 0$)

- **Spectral function:** atomic limit $t \to 0$

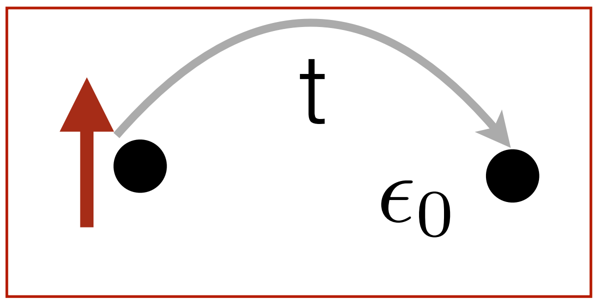


no gap in GW
(1/2 e$^-$ on each site)

$$\Sigma_{ij}^{\downarrow,GW}(\omega) = \delta_{ij}\frac{U}{2} \qquad \text{vs} \qquad \Sigma_{ij}^{\downarrow,exact}(\omega) = \delta_{ij}\frac{U}{2}\left[1 + \frac{U}{2(\omega-\epsilon_0) - U + i\eta}\right]$$

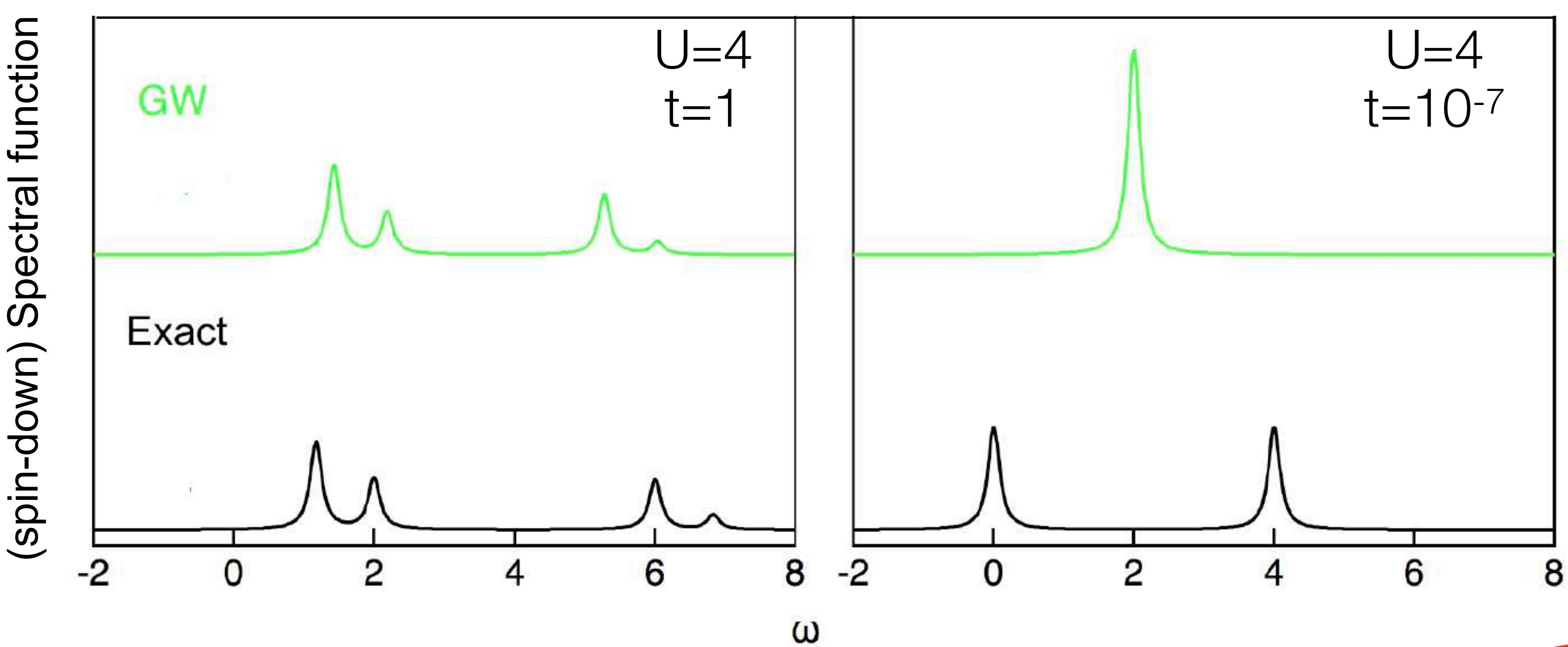
The Hubbard dimer: GW solution

N=1



$P \to 0$ ⇨ $W \to U$ = exchange (for $t \to 0$)

- **Spectral function:** atomic limit $t \to 0$



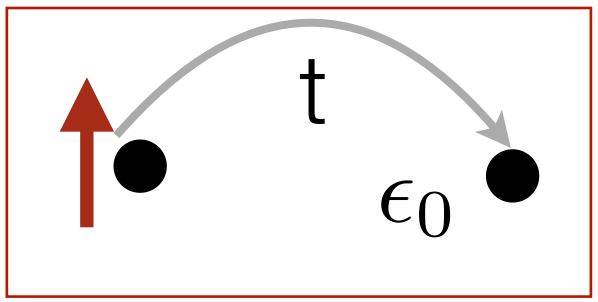
no gap in GW

(1/2 e^- on each site)

$$\Sigma_{ij}^{\downarrow,GW}(\omega) = \delta_{ij}\frac{U}{2} \quad \text{vs} \quad \Sigma_{ij}^{\downarrow,exact}(\omega) = \delta_{ij}\frac{U}{2}\left[1 + \frac{U}{2(\omega-\epsilon_0) - U + i\eta}\right]$$

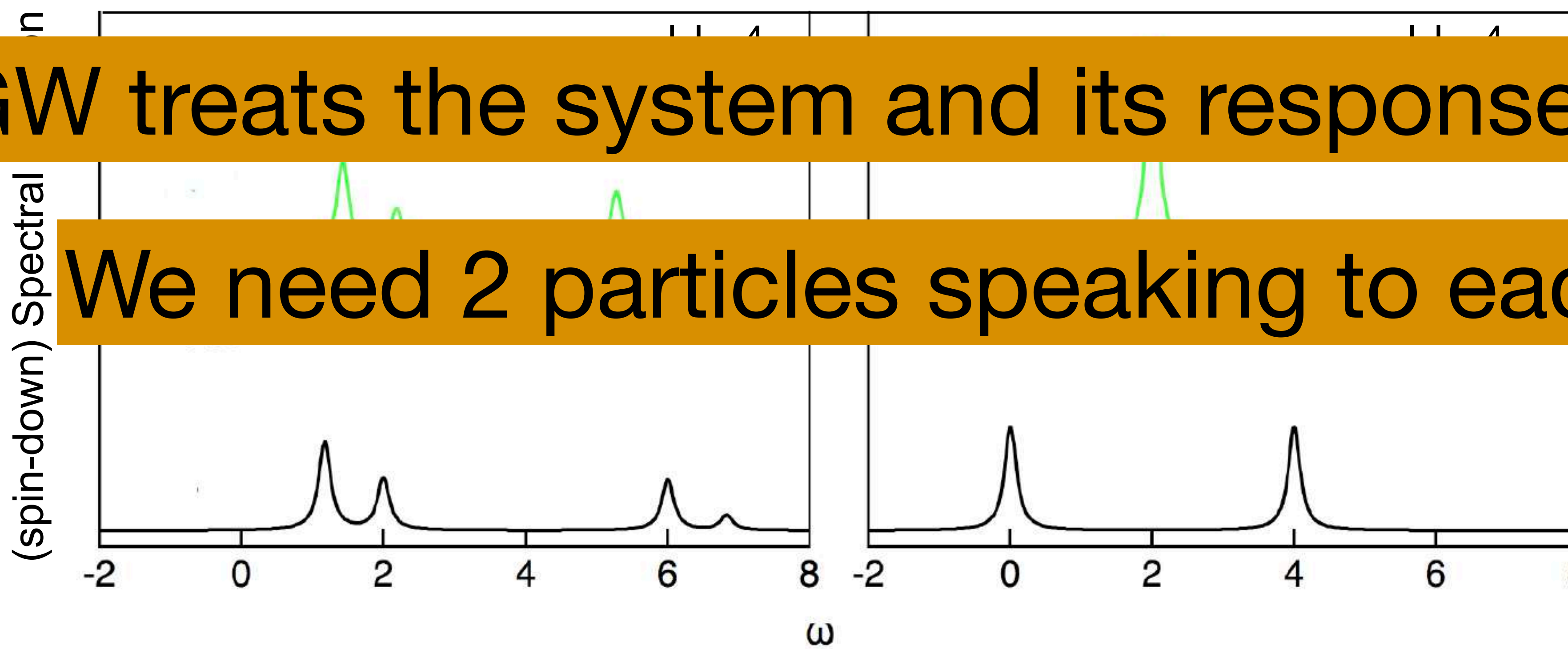
The Hubbard dimer: GW solution

N=1



$P \to 0$ ⇨ $W \to U$ = exchange (for $t \to 0$)

- **Spectral function:** atomic limit $t \to 0$



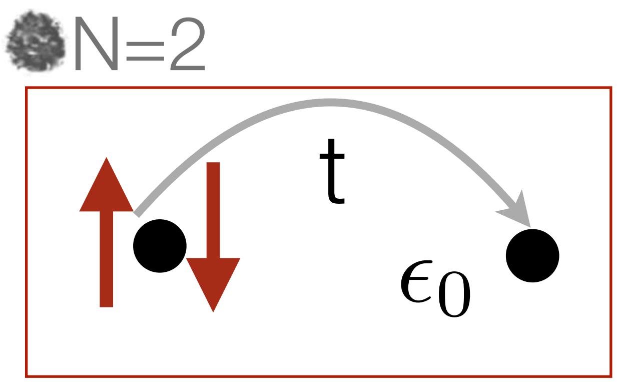
(1/2 e$^-$ on each site)

GW treats the system and its response classically

We need 2 particles speaking to each other!

$$\Sigma_{ij}^{\downarrow,GW}(\omega) = \delta_{ij}\frac{U}{2} \quad \text{vs} \quad \Sigma_{ij}^{\downarrow,exact}(\omega) = \delta_{ij}\frac{U}{2}\left[1 + \frac{U}{2(\omega-\epsilon_0) - U + i\eta}\right]$$

The Hubbard dimer: GW solution



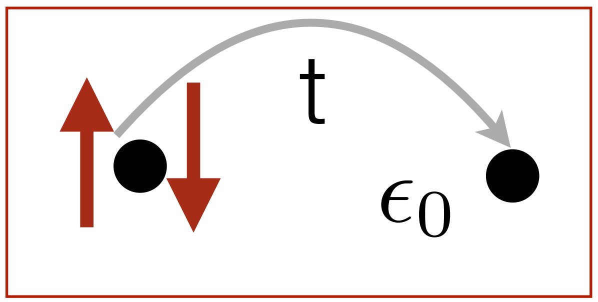
$P \neq 0 \Rightarrow W \neq U$ $\neq$ exchange (for $t \neq 0$)

$P \to 0 \Rightarrow W \to U$ = exchange (for $t \to 0$)

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

The Hubbard dimer: GW solution

N=2



$P \neq 0 \Rightarrow W \neq U$ $\neq$ exchange (for $t \neq 0$)

$P \to 0 \Rightarrow W \to U$ = exchange (for $t \to 0$)

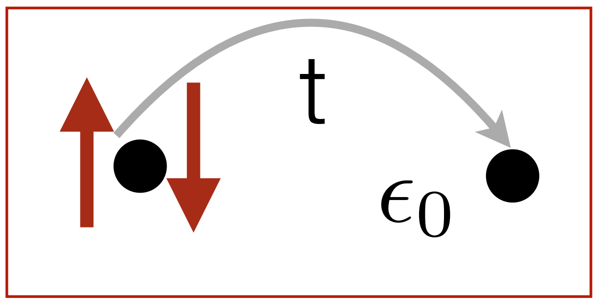
- **Effect of self-screening**

EA 1e-   IP 2e-

$$U = 0$$

The Hubbard dimer: GW solution

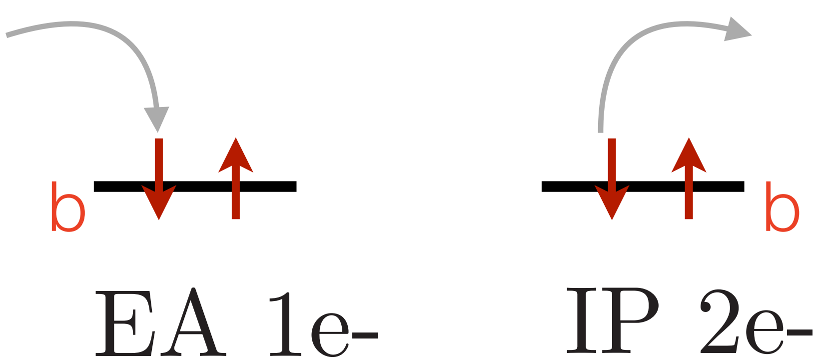
N=2



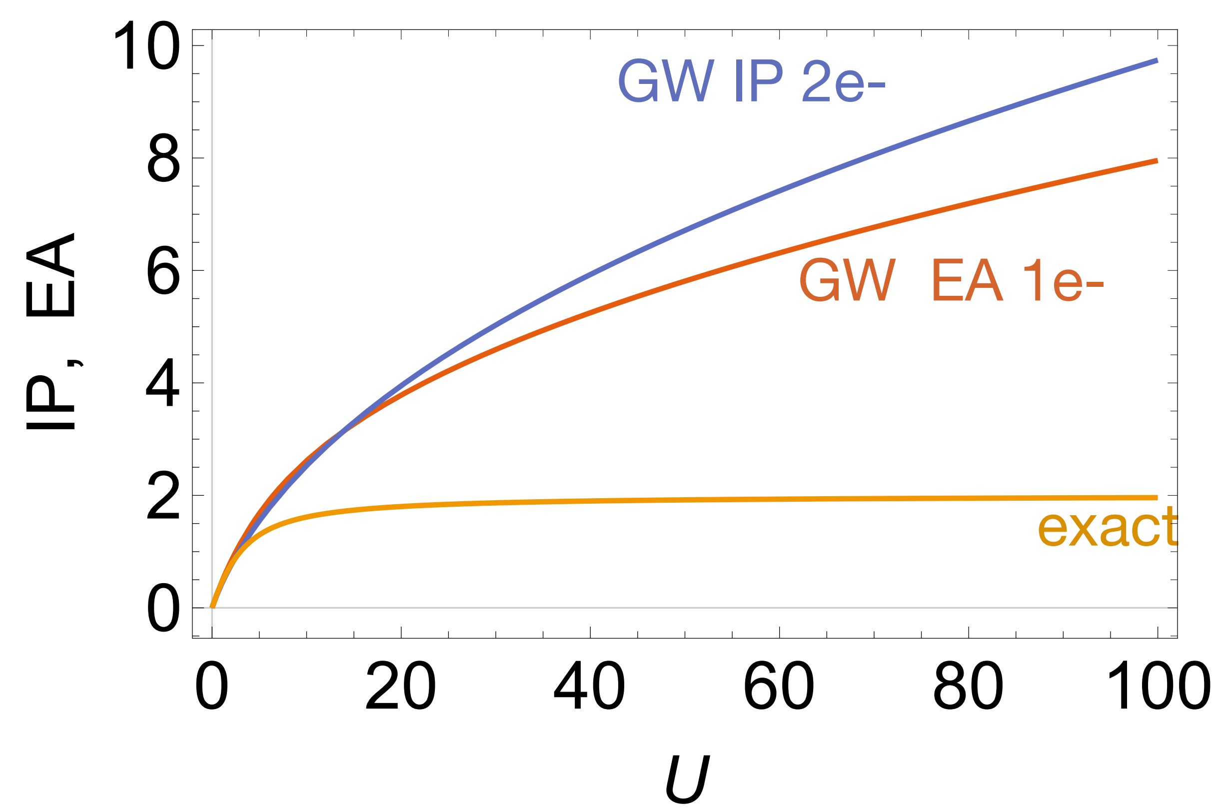
$P \neq 0 \Rightarrow W \neq U \quad \neq$ exchange (for $t \neq 0$)

$P \to 0 \Rightarrow W \to U \quad =$ exchange (for $t \to 0$)

- **Effect of self-screening**

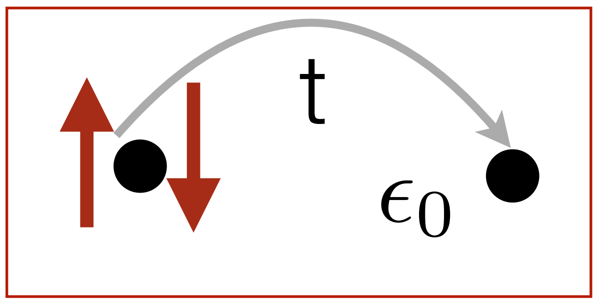


$U = 0$



The Hubbard dimer: GW solution

N=2



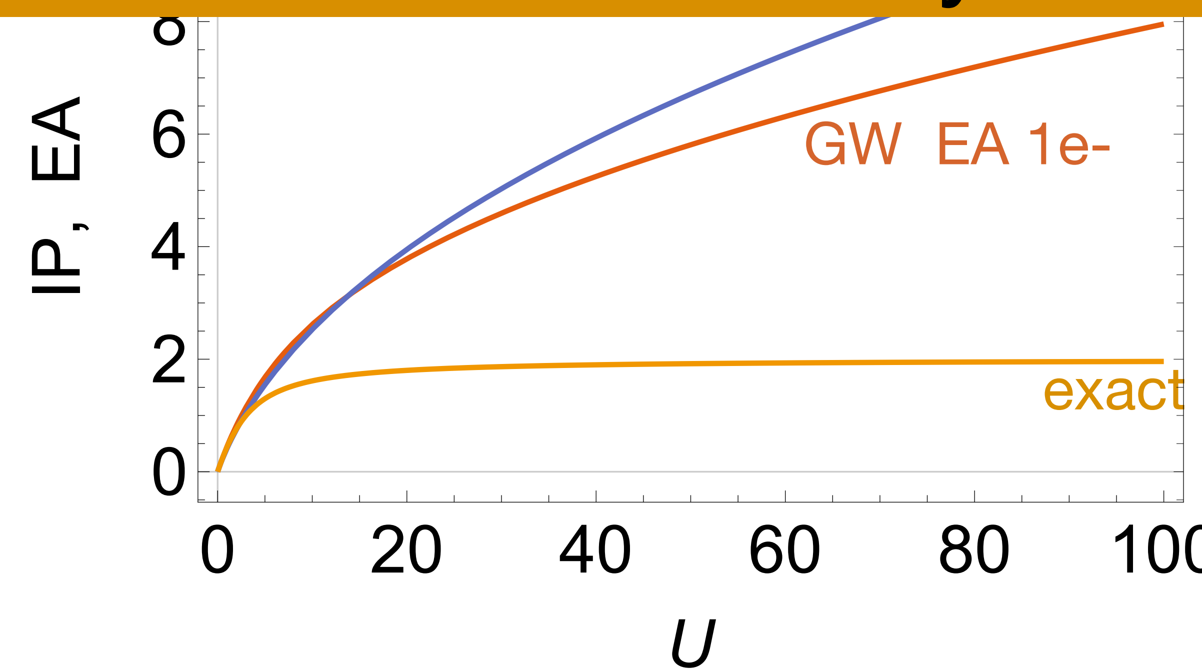
$P \neq 0 \Rightarrow W \neq U$ $\neq$ exchange (for $t \neq 0$)

$P \to 0 \Rightarrow W \to U$ = exchange (for $t \to 0$)

- **Effect of self-screening**

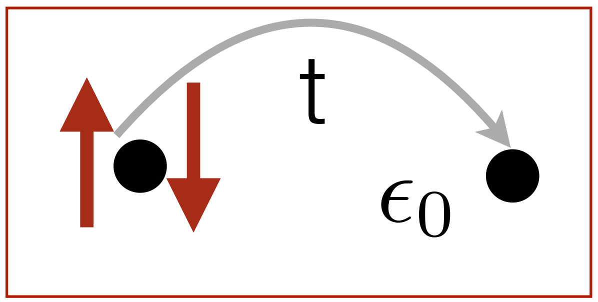
Addition and removal of the same e⁻ is non-symmetric

$U = 0$



The Hubbard dimer: GW solution

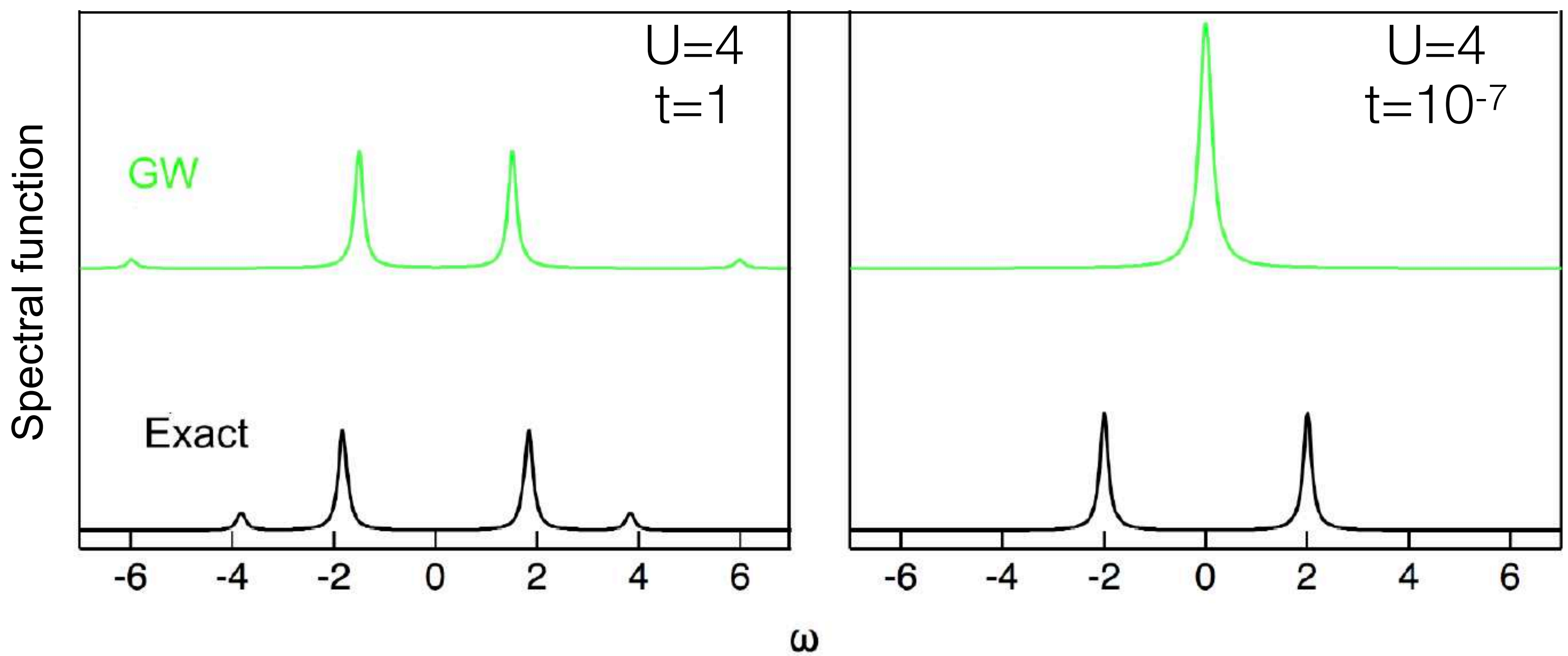
N=2



$P \neq 0 \Rightarrow W \neq U$ $\neq$ exchange (for $t \neq 0$)

$P \to 0 \Rightarrow W \to U$ = exchange (for $t \to 0$)

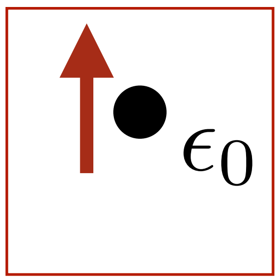
- **Spectral function**



no gap in GW! (1/2 ↑e⁻ and 1/2 ↓e⁻ on each site**)**

The Hubbard monomer: T-matrix solution

N=1

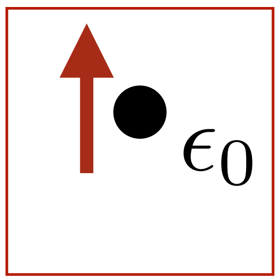


$$L^{pp/eh} = 0 \Rightarrow T^{pp/eh} = U$$ Hartree-Fock

$$\Sigma(\omega) = \begin{array}{c c} & \begin{array}{cc} \uparrow & \downarrow \end{array} \\ \begin{array}{c} \uparrow \\ \downarrow \end{array} & \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix} \end{array}$$

The Hubbard monomer: T-matrix solution

N=1



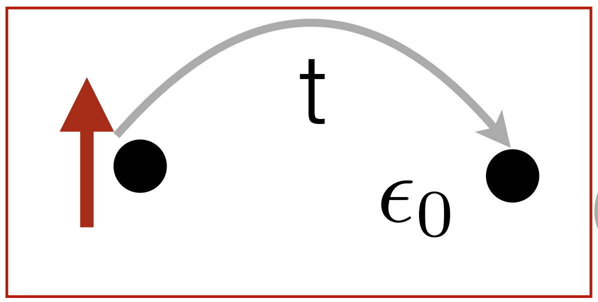
$$L^{pp/eh} = 0 \Rightarrow T^{pp/eh} = U$$ Hartree-Fock

$$\Sigma(\omega) = \begin{array}{c c} & \begin{array}{cc} \uparrow & \downarrow \end{array} \\ \begin{array}{c} \uparrow \\ \downarrow \end{array} & \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix} \end{array}$$

T matrix is exact for two isolated sites

The Hubbard dimer: T-matrix solution

N=1

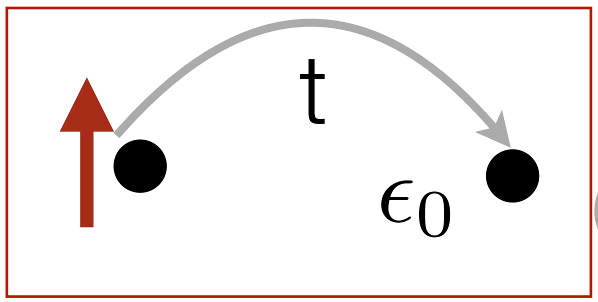


$L^{pp/eh} \neq 0 \Rightarrow T^{pp/eh} \neq$ HF (for any t)

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

The Hubbard dimer: T-matrix solution

N=1



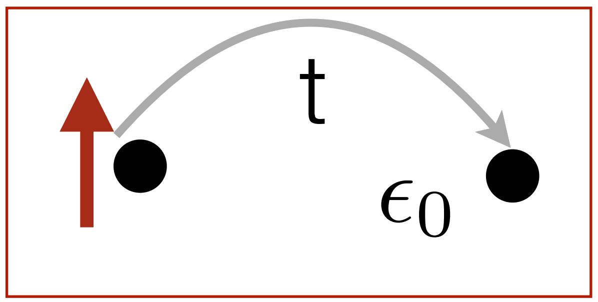
$$L^{pp/eh} \neq 0 \Longrightarrow T^{pp/eh} \neq \text{HF} \quad \text{(for any } t\text{)}$$

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

no self-screening

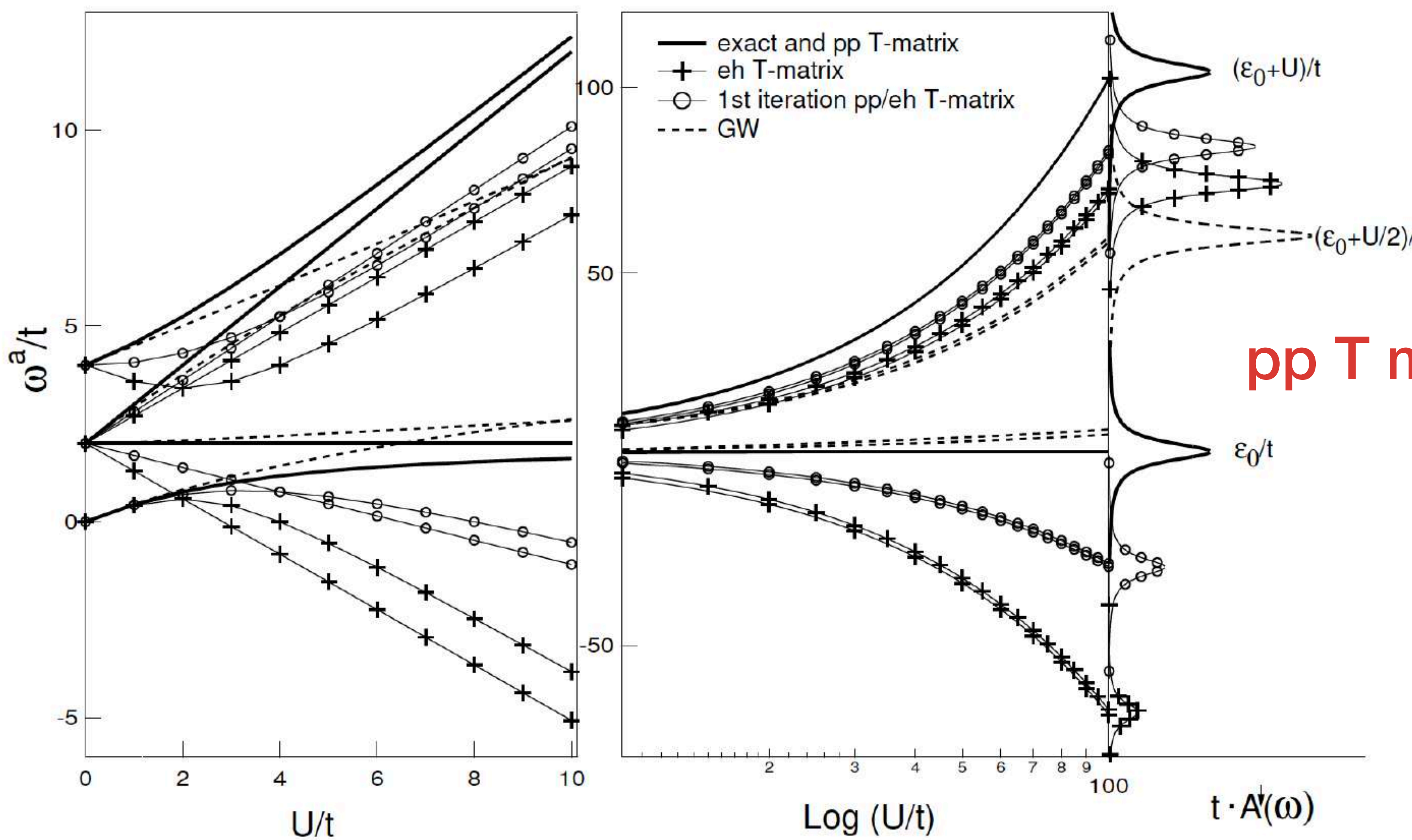
The Hubbard dimer: T-matrix solution

N=1



$$L^{pp/eh} \neq 0 \Longrightarrow T^{pp/eh} \neq \text{HF} \quad (\text{for any } t)$$

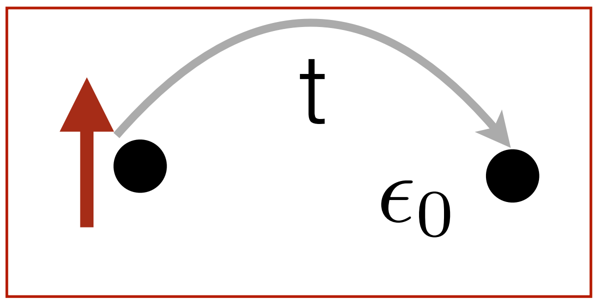
- **Removal/addition energies**



pp T matrix is exact

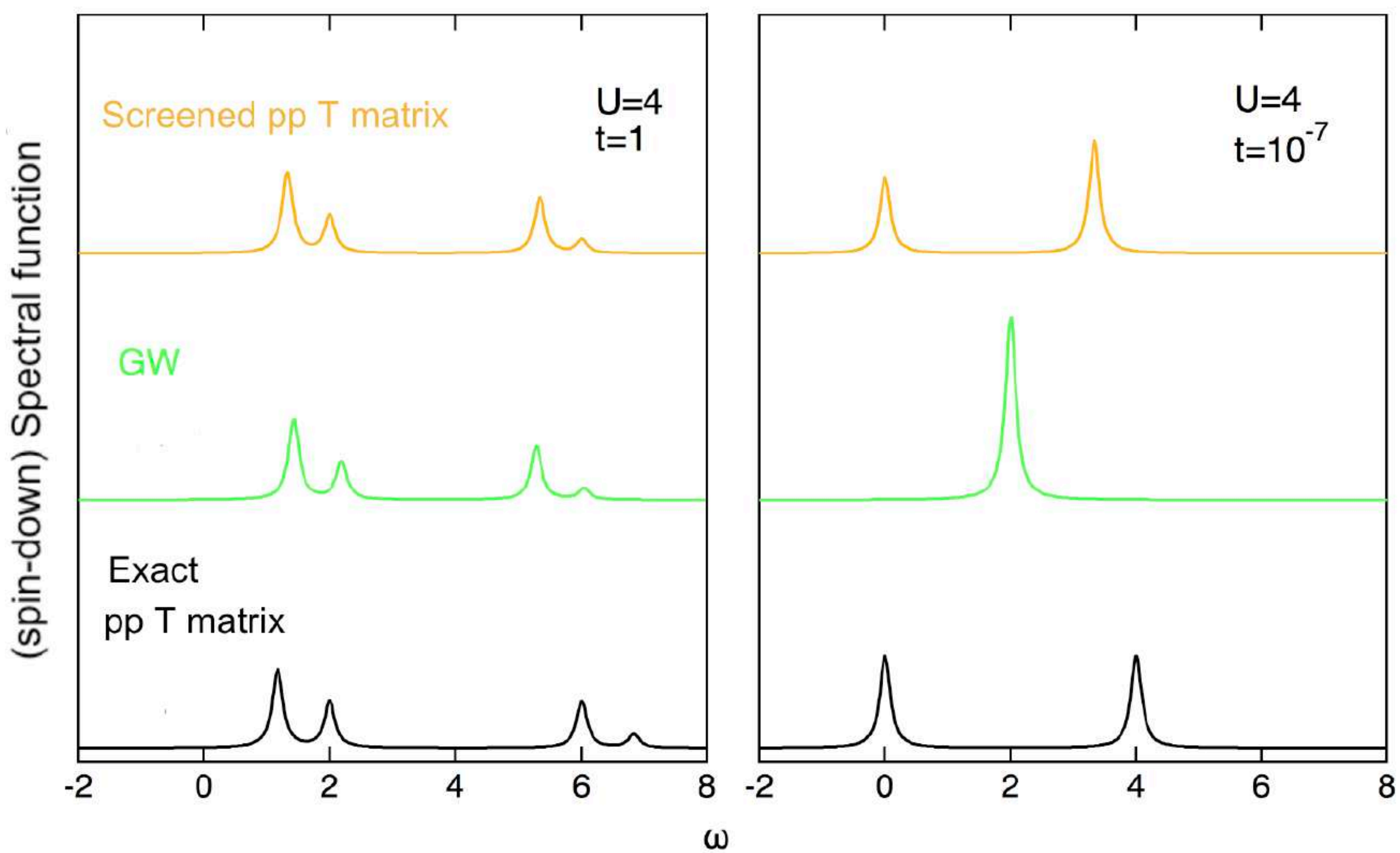
The Hubbard dimer: T-matrix solution

N=1



$$L^{pp/eh} \neq 0 \Rightarrow T^{pp/eh} \neq \text{HF} \text{ (for any } t\text{)}$$

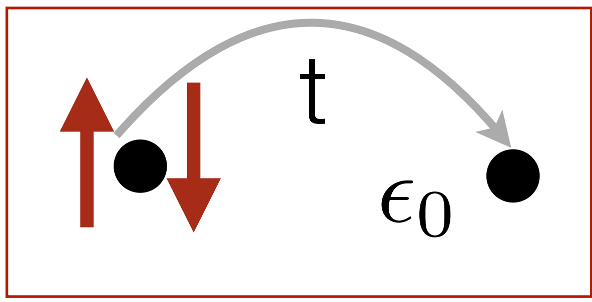
- **Spectral function**



screening corrupts the pp T exact result (but results remain good)

The Hubbard dimer: T-matrix solution

N=2



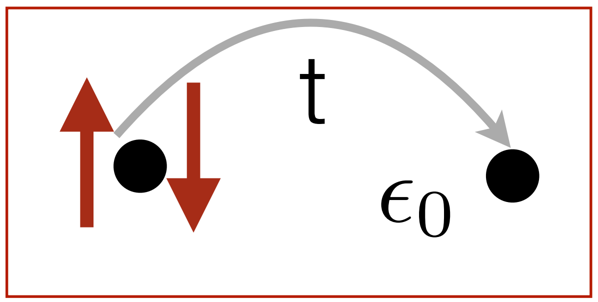
$L^{pp/eh} \neq 0 \Rightarrow T^{pp/eh} \neq$ HF (for $t \neq 0$)

$L^{pp/eh} = 0 \Rightarrow T^{pp/eh} =$ HF (for $t \to 0$)

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

The Hubbard dimer: T-matrix solution

N=2

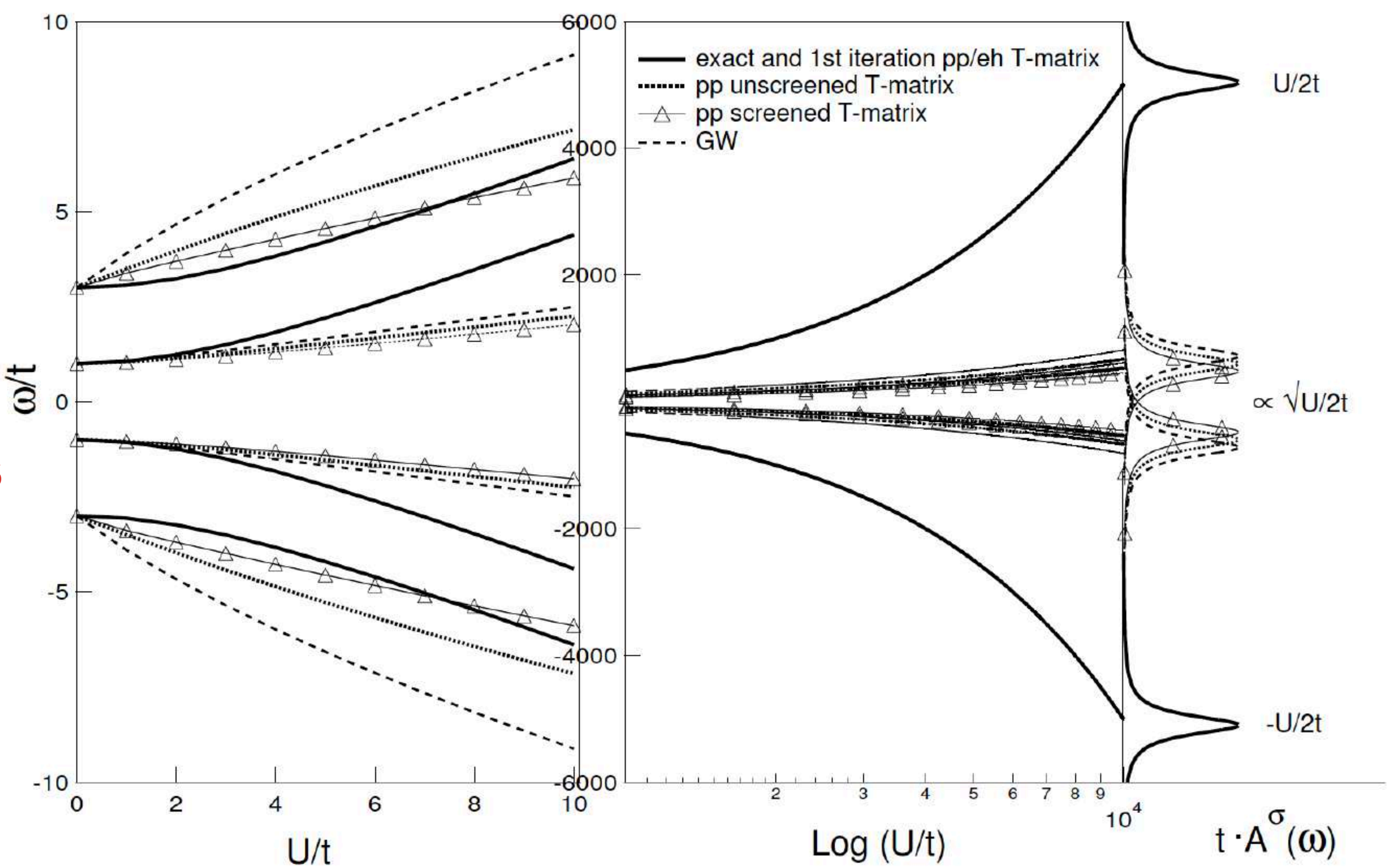


$$L^{pp/eh} \neq 0 \Rightarrow T^{pp/eh} \neq \text{HF} \quad (\text{for } t \neq 0)$$

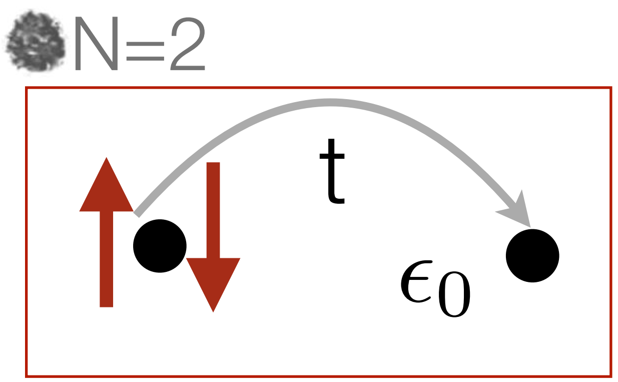
$$L^{pp/eh} = 0 \Rightarrow T^{pp/eh} = \text{HF} \quad (\text{for } t \to 0)$$

- **Removal/addition energies**

screened pp T
improves satellites



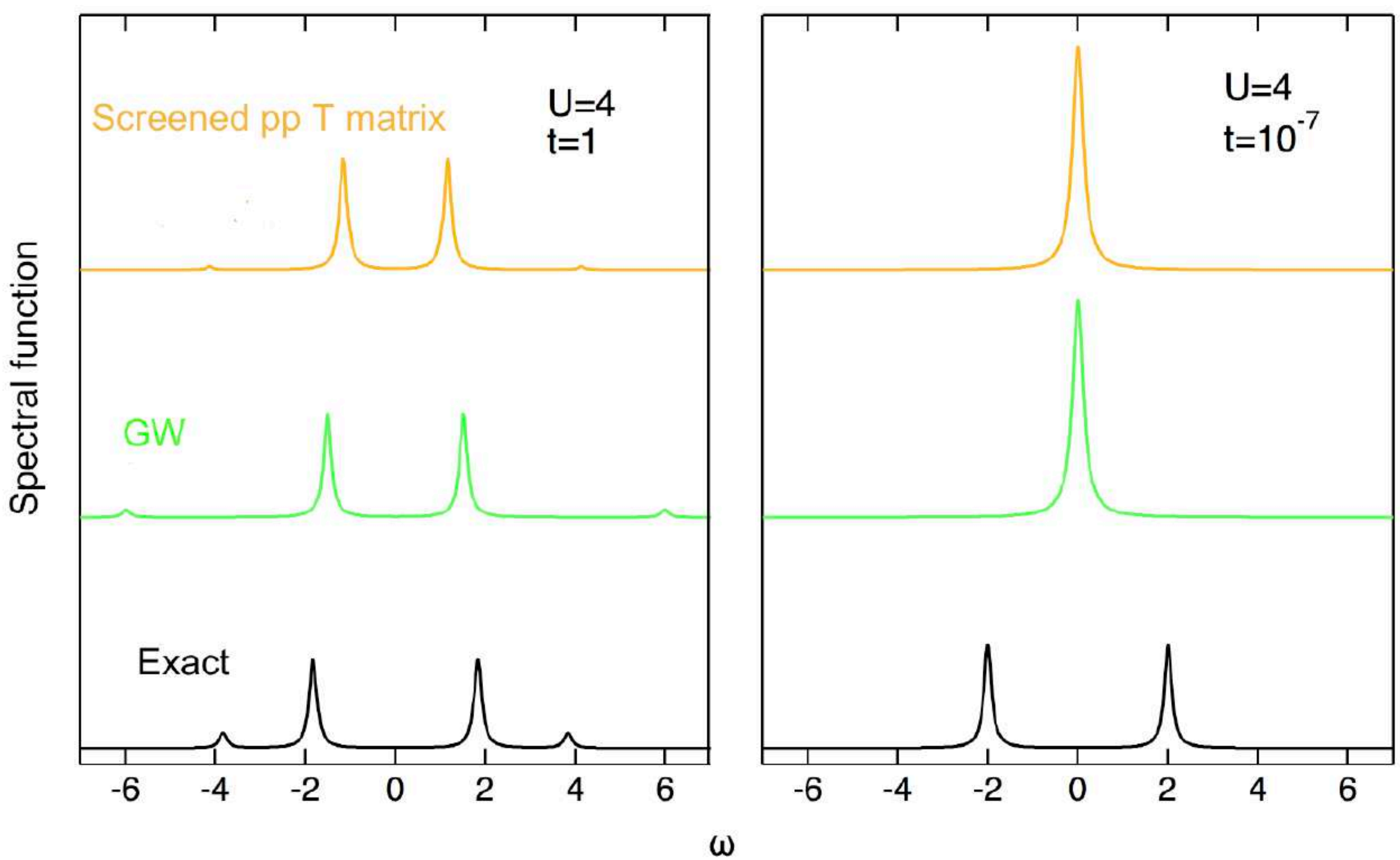
The Hubbard dimer: T-matrix solution



$L^{pp/eh} \neq 0 \Rightarrow T^{pp/eh} \neq$ HF (for $t \neq 0$)

$L^{pp/eh} = 0 \Rightarrow T^{pp/eh} =$ HF (for $t \to 0$)

- **Spectral function**



Atomic limit remains a challenge!

Conclusions

- **GW suffers from two shortcomings:**
  - self-screening (extra poles in 1e-, non symmetric addition/ removal energies 1e-/2e-)
  - incorrect atomic limit (no gap in the Hubbard dimer)
- **pp T matrix makes the one-electron case exact**
- **Screened pp T matrix improves the satellite description over a wide range of the interaction for the two-electron case**
- **Atomic limit remains a challenge**

Open questions

- Why in the atomic limit is the pp screened T matrix exact for one electron but not for two electrons?

- Which approximation in the derivation of the T-matrix self-energy is harmless for the one-electron case, but dramatic for the two-electron case? And why?

- Will realistic systems be more forgiving than the Hubbard dimer when the screened pp T-matrix approximation is used?

Thanks

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Universität Jena

References

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