Routes to spatial correlations beyond DMFT The one-particle irreducible (1PI) approach

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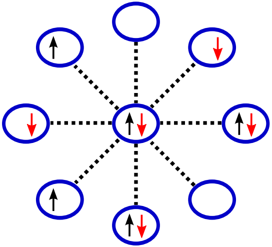
G. R., A. Toschi, H. Hafermann, K. Held, V. Anisimov, A. Katanin, PRB, in press

Outline

1. Introduction
2. Diagrammatic approaches
3. 1PI formalism and results
4. Conclusions and Outlook

When is **DMFT** reliable...

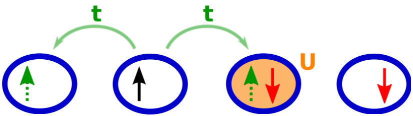
✓ **large number** of neighbors for each site**!**



✓ **high temperatures!**

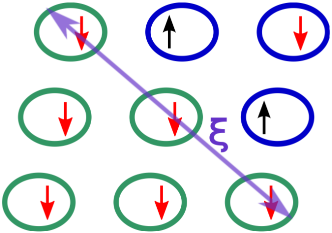
... and when not?

↯ for low-dimensional (d=1,2) systems



e.g.: cuprates, heterostructures

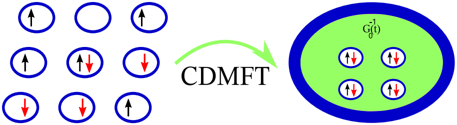
↯ close to (2^{nd}-order) phase-transitions



e.g.: QCP

Spatial correlations

- **cluster extensions of DMFT:**
  (G. Kotliar, S. Y. Sarasov et al., PRL, 2001; T. A. Maier, M. Jarrell et al., Rev. Mod. Phys., 2005)



$\Rightarrow$ **"short" range correlations!**

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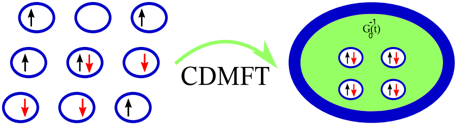

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- **diagrammatic extensions of DMFT:**
  - **1/d-expansion** (A. Schiller, K. Ingersent, PRL 1995)
  - **DMFT+$\Sigma_{\mathbf{k}}$** (E. Z. Kuchinskii, I. A. Nekrasov, M.V. Sadovskii, JETP, 2005)
  - **dynamical vertex(Γ) approximation (DΓA)**$\Rightarrow$ *A. Toschi*
    (A. Toschi, A. Katanin, K. Held, PRB 2007)
  - **DMF^{2}RG** $\Rightarrow$ *C. Taranto*
  - **dual fermion** (A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, PRB 2008)
  - **One-particle irreducible approach (1PI)**
    (G. R., A. Toschi, H. Hafermann, K. Held, V.I. Anisimov, A. A. Katanin, arXiv:1301.7546)

$\Rightarrow$ inclusion of **long range correlations!**

Diagrammatic approaches: General Structure

Starting point: DMFT

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$\Rightarrow$**Local Correlations [$\Sigma_{\mathbf{DMFT}}(\omega)$]** included!

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  - *2-particle vertex* γ^4: **F**, Γ or Λ ($\Rightarrow$ *talk of A. Toschi*)
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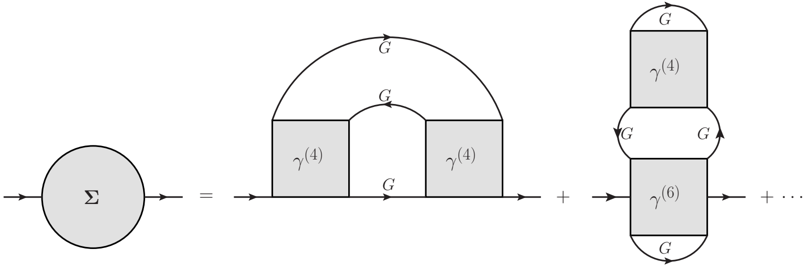

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Resummation of all diagrams (exact solution) not possible!

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- Generate diagrams by RG-flow $\Rightarrow$ fRG ($\Rightarrow$ *talk of C. Taranto*)

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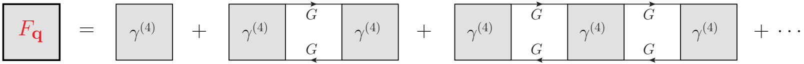

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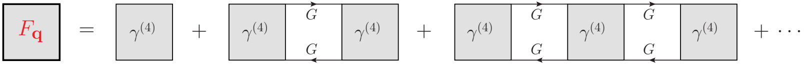

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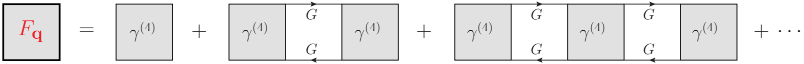

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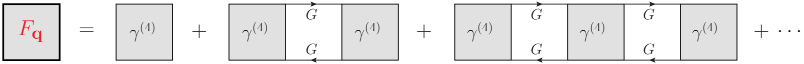

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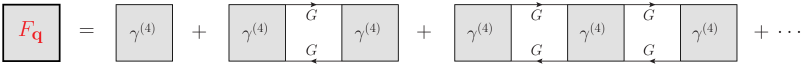

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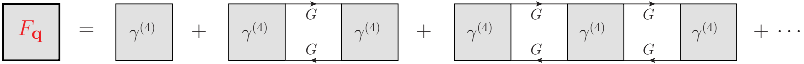

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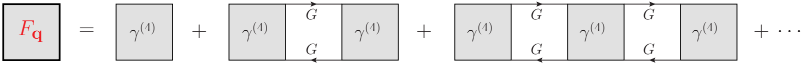

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$$Z = \int D[c_i^+, c_i]\; e^{-\mathcal{S}[c_i^+, c_i]}, \quad \mathcal{S}\ldots\text{Action}, \qquad i_j \widehat{=} (\tau_j/\nu_j, \mathbf{R}_j/\mathbf{k}_j, \sigma_j, l_j, \ldots)$$

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General Idea of 1PI

Separation of **local** and **non-local** degrees of freedom $\Rightarrow$
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Integration of **local** degrees of freedom $\Rightarrow$

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Legendre Transformation ⇒ **1PI-based** theory (cf. fRG)

1PI formalism - Functionals and Actions

Generating functional for the Green's functions:

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AIM (numerically) solvable (1- and 2-particle Green's function, vertices)

1PI formalism - Functionals and Actions

Generating functional for the Green's functions:

$$Z[\eta^+,\eta] = \int D[c^+,c]\; e^{-\mathcal{S}[c^+,c]+\sum_i \int_0^\beta d\tau\, [c_i^+(\tau)\eta_i(\tau)+\eta_i^+(\tau)c_i(\tau)]}$$

$$G_{n,i_1\ldots i_{2n}}(\tau_1,\ldots,\tau_{2n}) = \frac{1}{Z}\frac{\delta^{2n} Z[\eta^+,\eta]}{\delta\eta^+_{i_{2n}}(\tau_{2n})\ldots\delta\eta_{i_1}(\tau_1)}\Bigg|_{\eta^+=0,\eta=0}$$

Action $\mathcal{S}$ is similar for Hubbard model and AIM:

$$\mathcal{S}_{\text{Hub}}[c_i^+,c_i] = \frac{1}{\beta}\sum_{\nu,\mathbf{k},\sigma}[-i\nu+\varepsilon_{\mathbf{k}}-\mu]\, c^+_{\mathbf{k}\sigma}(\nu)c_{\mathbf{k}\sigma}(\nu) + \sum_i H_{\text{int}}[c_i^+,c_i]$$

$$\mathcal{S}_{\text{AIM}}[c^+,c] = \frac{1}{\beta}\sum_{\nu,\sigma}[-i\nu+\boldsymbol{\Delta(\nu)}-\mu]\, c^+_{\sigma}(\nu)c_{\sigma}(\nu) + H_{\text{int}}[c^+,c].$$

AIM (numerically) solvable (1- and 2-particle Green's function, vertices)

$\Rightarrow$ express $\mathcal{S}_{\text{Hub}}$ in terms of $\mathcal{S}_{\text{AIM}}$

1PI formalism - Hubbard Stratonovich (HS)

$$\mathcal{S}_{\text{Hub}}[c_i^+, c_i] = \frac{1}{\beta} \sum_{\nu, \mathbf{k}, \sigma} [-i\nu + \varepsilon_{\mathbf{k}} - \mu]\, c^+_{\mathbf{k}\sigma}(\nu) c_{\mathbf{k}\sigma}(\nu) + \sum_i H_{\text{int}}[c_i^+, c_i]$$

$$\mathcal{S}_{\text{AIM}}[c^+, c] = \frac{1}{\beta} \sum_{\nu, \sigma} [-i\nu + \boldsymbol{\Delta}(\boldsymbol{\nu}) - \mu]\, c^+_{\sigma}(\nu) c_{\sigma}(\nu) + H_{\text{int}}[c^+, c].$$

Separation: Local ⇔ Non-local

$$\mathcal{S}_{\text{Hub}}[c_i^+, c_i] = \sum_i \mathcal{S}_{\text{AIM}}[c_i^+, c_i]$$

1PI formalism - Hubbard Stratonovich (HS)

$$\mathcal{S}_{\text{Hub}}[c_i^+, c_i] = \frac{1}{\beta} \sum_{\nu,\mathbf{k},\sigma} [-i\nu + \varepsilon_{\mathbf{k}} - \mu]\, c_{\mathbf{k}\sigma}^+(\nu) c_{\mathbf{k}\sigma}(\nu) + \sum_i H_{\text{int}}[c_i^+, c_i]$$

$$\mathcal{S}_{\text{AIM}}[c^+, c] = \frac{1}{\beta} \sum_{\nu,\sigma} [-i\nu + \boldsymbol{\Delta(\nu)} - \mu]\, c_\sigma^+(\nu) c_\sigma(\nu) + H_{\text{int}}[c^+, c].$$

Separation: Local ⇔ Non-local

$$\mathcal{S}_{\text{Hub}}[c_i^+, c_i] = \sum_i \mathcal{S}_{\text{AIM}}[c_i^+, c_i] - \sum_{\mathbf{k}} [\Delta(\nu) - \varepsilon_{\mathbf{k}}]\, c_{\mathbf{k}}^+ c_{\mathbf{k}}$$

⇒ only last term contains non-local degrees of freedom!

1PI formalism - Hubbard Stratonovich (HS)

$$Z[\eta^+,\eta] = \int D[c^+,c]\; e^{-\mathcal{S}[c^+,c]+\sum_i \int_0^\beta d\tau\; [c_i^+(\tau)\eta_i(\tau)+\eta_i^+(\tau)c_i(\tau)]}$$

Separation: Local $\Leftrightarrow$ Non-local

$$\mathcal{S}_{\text{Hub}}[c_i^+,c_i] = \sum_i \mathcal{S}_{\text{AIM}}[c_i^+,c_i] - \sum_{\mathbf{k}} [\Delta(\nu)-\varepsilon_{\mathbf{k}}]\, c_{\mathbf{k}}^+ c_{\mathbf{k}}$$

$\Rightarrow$ only last term contains non-local degrees of freedom!

HS-Trafo: $e^{\frac{1}{\beta}[\Delta-\varepsilon]c_{\mathbf{k}}^+ c_{\mathbf{k}}} \propto \int D[f^+,f]\; e^{[c_{\mathbf{k}}^+ f_{\mathbf{k}}+f_{\mathbf{k}}^+ c_{\mathbf{k}}]} e^{-B_{\mathbf{k}} f_{\mathbf{k}}^+ f_{\mathbf{k}}}$

1PI formalism - Hubbard Stratonovich (HS)

$$Z[\eta^+,\eta] = \int D[c^+,c]\; e^{-\mathcal{S}[c^+,c]+\sum_i \int_0^\beta d\tau\, [c_i^+(\tau)\eta_i(\tau)+\eta_i^+(\tau)c_i(\tau)]}$$

Separation: Local $\Leftrightarrow$ Non-local

$$\mathcal{S}_{\text{Hub}}[c_i^+,c_i] = \sum_i \mathcal{S}_{\text{AIM}}[c_i^+,c_i] - \sum_{\mathbf{k}} [\Delta(\nu)-\varepsilon_{\mathbf{k}}]\, c_{\mathbf{k}}^+ c_{\mathbf{k}}$$

$\Rightarrow$ only last term contains non-local degrees of freedom!

$$\begin{cases} \text{HS-Trafo: } e^{\frac{1}{\beta}[\Delta-\varepsilon]c_{\mathbf{k}}^+ c_{\mathbf{k}}} \propto \int D[f^+,f]\; e^{[c_{\mathbf{k}}^+ f_{\mathbf{k}} + f_{\mathbf{k}}^+ c_{\mathbf{k}}]} e^{-B_{\mathbf{k}} f_{\mathbf{k}}^+ f_{\mathbf{k}}} \\ \text{Parseval: } \sum_{\mathbf{k}} c_{\mathbf{k}}^+ f_{\mathbf{k}} + f_{\mathbf{k}}^+ c_{\mathbf{k}} = \sum_i c_i^+ f_i + f_i^+ c_i \end{cases}$$

1PI formalism - Hubbard Stratonovich (HS)

$$Z[\eta^+,\eta] = \int D[c^+,c]\; e^{-\mathcal{S}[c^+,c]+\sum_i \int_0^\beta d\tau\, [c_i^+(\tau)\eta_i(\tau)+\eta_i^+(\tau)c_i(\tau)]}$$

Separation: Local ⇔ Non-local

$$\mathcal{S}_{\text{Hub}}[c_i^+,c_i] = \sum_i \mathcal{S}_{\text{AIM}}[c_i^+,c_i] - \sum_{\mathbf{k}} [\Delta(\nu)-\varepsilon_{\mathbf{k}}]\, c_{\mathbf{k}}^+ c_{\mathbf{k}}$$

⇒ only last term contains non-local degrees of freedom!

Generating functional

Generating functional in terms of f^+ and f:

$$Z[\eta^+,\eta] \propto \int D[f^+,f]\; e^{-\sum_{\mathbf{k}} B_{\mathbf{k}}[f_{\mathbf{k}}^+-\eta_{\mathbf{k}}^+][f_{\mathbf{k}}-\eta_{\mathbf{k}}]+\sum_i \ln Z_{\text{AIM}}[f_i^+,f_i]}$$

1PI formalism - DF vs. 1PI

What is the physical content of the new fields f^+ and f?

$$\widetilde{\mathcal{S}}[f^+, f] =$$

Dual Fermion

1PI

1PI formalism - DF vs. 1PI

What is the physical content of the new fields f^+ and f?

$$\widetilde{\mathcal{S}}[f^+, f] = \sum_{\mathbf{k}} B_{\mathbf{k}} f^+_{\mathbf{k}} f_{\mathbf{k}}$$

Dual Fermion

- Non-interacting part: $B_{\mathbf{k}} \sim [G_{\text{DMFT}}(\nu, \mathbf{k}) - G_{\text{loc}}(\nu)]^{-1}$

1PI

1PI formalism - DF vs. 1PI

What is the physical content of the new fields f^+ and f?

$$\widetilde{S}[f^+, f] = \sum_{\mathbf{k}} B_{\mathbf{k}} f^+_{\mathbf{k}} f_{\mathbf{k}} - \sum_i \ln Z_{\text{AIM}}[f^+_i, f_i]$$

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- Non-interacting part: $B_{\mathbf{k}} \sim [G_{\text{DMFT}}(\nu, \mathbf{k}) - G_{\text{loc}}(\nu)]^{-1}$
- Interacting part: expansion of $\ln Z_{\text{AIM}}[f^+_i, f_i] \Rightarrow$ connected, *one-particle reducible*, vertex functions (At 2P-level: F)!

1PI

1PI formalism - DF vs. 1PI

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1PI

Legendre transform of $\ln Z_{\text{AIM}}[f_i^+, f_i] \Rightarrow \Gamma_{\text{AIM}}[\phi^+, \phi]$

1PI formalism - DF vs. 1PI

What is the physical content of the new fields f^+ and f?

$$\tilde{S}[f^+, f] = \sum_{\mathbf{k}} B_{\mathbf{k}} f^+_{\mathbf{k}} f_{\mathbf{k}} - \sum_i \ln Z_{\text{AIM}}[f_i^+, f_i]$$

Dual Fermion

- Non-interacting part: $B_{\mathbf{k}} \sim [G_{\text{DMFT}}(\nu, \mathbf{k}) - G_{\text{loc}}(\nu)]^{-1}$
- Interacting part: expansion of $\ln Z_{\text{AIM}}[f_i^+, f_i] \Rightarrow$ connected, *one-particle reducible*, vertex functions (At 2P-level: F)!

1PI

Legendre transform of $\ln Z_{\text{AIM}}[f_i^+, f_i] \Rightarrow \Gamma_{\text{AIM}}[\phi^+, \phi]$

- Non-interacting part: $[G_{\text{DMFT}}(\nu, \mathbf{k}) - G_{\text{loc}}(\nu)]^{-1}$, $[G_{\text{loc}}(\nu)]^{-1}$

1PI formalism - DF vs. 1PI

What is the physical content of the new fields f^+ and f?

$$\widetilde{\mathcal{S}}[f^+, f] = \sum_{\mathbf{k}} B_{\mathbf{k}} f^+_{\mathbf{k}} f_{\mathbf{k}} - \sum_i \ln Z_{\text{AIM}}[f^+_i, f_i]$$

Dual Fermion

- Non-interacting part: $B_{\mathbf{k}} \sim [G_{\text{DMFT}}(\nu, \mathbf{k}) - G_{\text{loc}}(\nu)]^{-1}$
- Interacting part: expansion of $\ln Z_{\text{AIM}}[f^+_i, f_i] \Rightarrow$ connected, *one-particle reducible*, vertex functions (At 2P-level: F)!

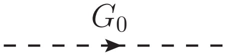
1PI

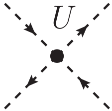
Legendre transform of $\ln Z_{\text{AIM}}[f^+_i, f_i] \Rightarrow \Gamma_{\text{AIM}}[\phi^+, \phi]$

- Non-interacting part: $[G_{\text{DMFT}}(\nu, \mathbf{k}) - G_{\text{loc}}(\nu)]^{-1}$, $[G_{\text{loc}}(\nu)]^{-1}$
- Interacting part: expansion of $\Gamma_{\text{AIM}}[\phi^+, \phi] \Rightarrow$ connected, *one-particle irreducible*, vertex functions (At 2P-level: F)!

1PI formalism - Dual Fermion approach(I)

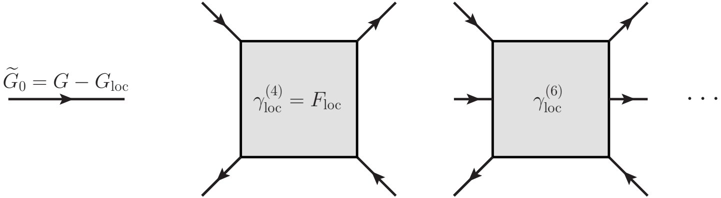
Diagrammatic Elements: for **“real” electrons**





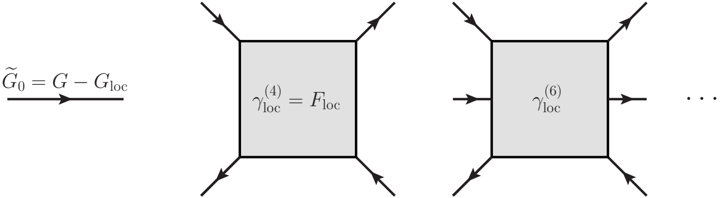
1PI formalism - Dual Fermion approach(I)

Diagrammatic Elements: for **dual electrons**



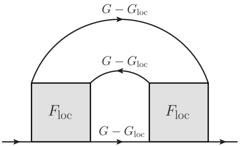
1PI formalism - Dual Fermion approach(I)

Diagrammatic Elements: for **dual electrons**

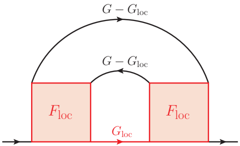


Second order diagrams:

in DF at the 2P level:



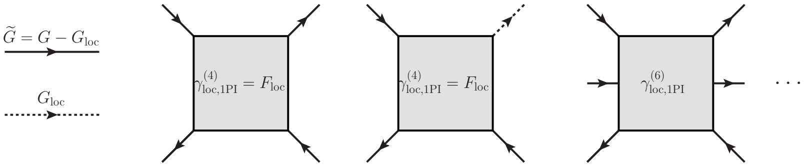
not in DF at 2P level:



+other technical problems (A. Katanin, J.Phys.A, 2013)

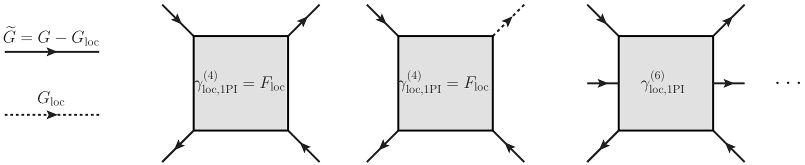
1PI formalism - 1PI Diagrammatics

Diagrammatic Elements: for **1PI**



1PI formalism - 1PI Diagrammatics

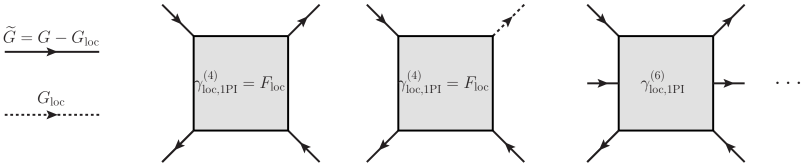
Diagrammatic Elements: for **1PI**



- **Local** propagator available!

1PI formalism - 1PI Diagrammatics

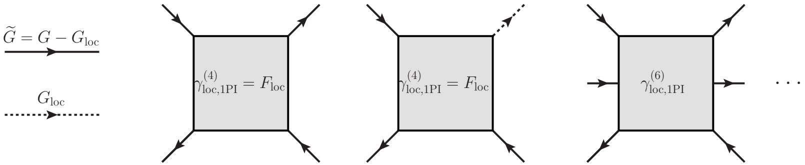
Diagrammatic Elements: for **1PI**



- **Local** propagator available!
- Technical problems are **solved**!

1PI formalism - 1PI Diagrammatics

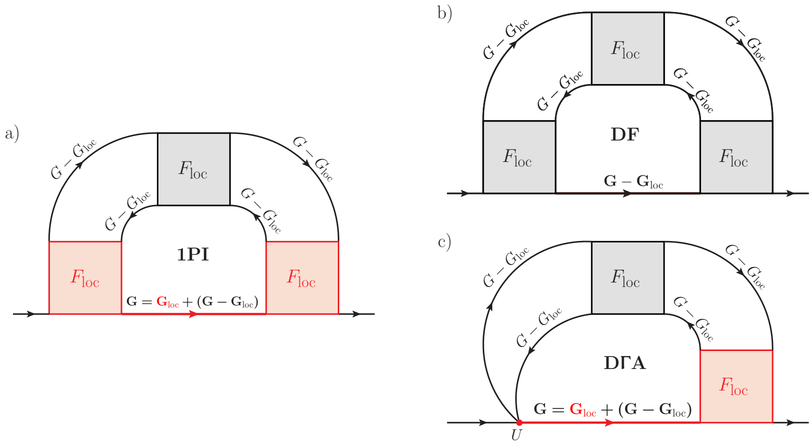
Diagrammatic Elements: for **1PI**



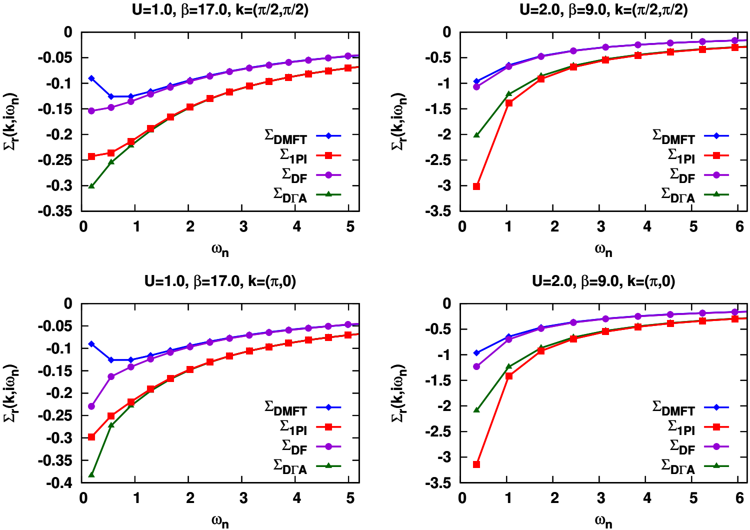
- **Local** propagator available!
- Technical problems are **solved**!
- **Unifying** aspect: Diagrams of **DΓA** and **DF**:

1PI formalism - 1PI Diagrammatics

Diagrammatic Comparison between 1PI, DF and DΓA

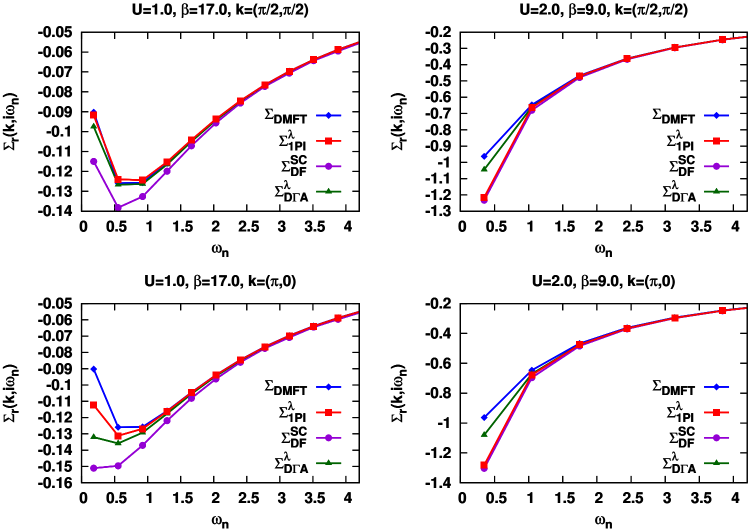


1PI formalism - One shot numerical Results



Hubbard model, simple cubic lattice, nearest neighbor hopping, half-filling

1PI formalism - Self-consistent numerical Results



Hubbard model, simple cubic lattice, nearest neighbor hopping, half-filling

Conclusions and Outlook

Conclusions

- Complementary methods of Cluster extensions of DMFT

$\Downarrow$

diagrammatic approaches

$\Downarrow$

based on the **local vertex**

$\Downarrow$

DΓA, DMF^{2}RG, DF, **1PI**

- **1PI** $\Rightarrow$ potential for a unifying formulation of diagrammatic extension of DMFT

Outlook

- Selfconsistency in 1PI
- Parquet based implementation
- Benchmark with cluster calculations/exact results