Introduction to Diagrammatic Approaches

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Autumn School on Correlated Electrons
DMFT – From Infinite Dimensions to Real Materials
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Outline

- Some basics of perturbation theory
- Diagrammatic extensions of DMFT
- Dual fermion approach
  - Formalism
  - Diagram expansion
  - Example approximations
- Applications and illustrative results (1D and 2D)
  - Second-order and ladder approximation
  - Cluster dual fermion
  - Real space dual fermion
  - Dual boson

Some basics

Coherent states $|\phi\rangle$ are eigenstates of the annihilation operator:
$c_\alpha |\phi\rangle = \phi_\alpha |\phi\rangle$

For fermions, the eigenvalues are Grassmann numbers.

Generators of the Grassmann algebra anticommute:
$\phi_\alpha \phi_\beta + \phi_\beta \phi_\alpha = 0 \longrightarrow \phi_\alpha^2 = 0$.

$$|\phi\rangle = e^{-\sum_\alpha \phi_\alpha c_\alpha^\dagger} |0\rangle = \prod_\alpha (1 - \phi_\alpha c_\alpha^\dagger) |0\rangle$$

Adjoint: $\langle 0| \prod_\alpha (1 + \phi_\alpha^* c_\alpha)$

Overlap of two coherent states:

$$\langle \phi | \phi' \rangle = \langle 0| \prod_\alpha (1 + \phi_\alpha^* c_\alpha) \prod_{\alpha'} (1 - \phi_{\alpha'} c_{\alpha'}^\dagger) |0\rangle$$
$$= \prod_\alpha (1 + \phi_\alpha^* \phi_\alpha) = e^{\sum_\alpha \phi_\alpha^* \phi_\alpha}$$

Some basics

Matrix element of *normal-ordered* operator $A[c^\dagger_\alpha, c_\alpha]$

$$\langle\phi|\, A[c^\dagger_\alpha, c_\alpha]\, |\phi\rangle = \langle\phi|\phi\rangle\, A[\phi^*_\alpha, \phi_\alpha] = e^{\sum_\alpha \phi^*_\alpha \phi_\alpha} A[\phi^*_\alpha, \phi_\alpha]$$

Closure relation

$$\int \prod_\alpha d\phi^*_\alpha d\phi_\alpha e^{-\sum_\alpha \phi^*_\alpha \phi_\alpha} \,|\phi\rangle\,\langle\phi| = 1$$

$$\begin{aligned}
\mathrm{Tr}\, A = \sum_n \langle n|\, A\, |n\rangle &= \int \prod_\alpha d\phi^*_\alpha d\phi_\alpha e^{-\sum_\alpha \phi^*_\alpha \phi_\alpha} \sum_n \langle n|\phi\rangle\,\langle\phi|\, A\, |n\rangle \\
&= \int \prod_\alpha d\phi^*_\alpha d\phi_\alpha e^{-\sum_\alpha \phi^*_\alpha \phi_\alpha} \,\langle -\phi|\, A \sum_n |n\rangle\,\langle n|\phi\rangle \\
&= \int \prod_\alpha d\phi^*_\alpha d\phi_\alpha e^{-\sum_\alpha \phi^*_\alpha \phi_\alpha} \,\langle -\phi|\, A\, |\phi\rangle
\end{aligned}$$

Coherent state path integral

$$Z = \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})} = \int \prod_\alpha d\phi_\alpha^* d\phi_\alpha e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} \langle -\phi | \, e^{-\beta(\hat{H}-\mu\hat{N})} \, | \phi \rangle$$

Break imaginary time interval $[0, \beta]$ into M slices of length $\epsilon = \beta/M$, such that $e^{-\beta(\hat{H}-\mu\hat{N})} = (e^{-\epsilon(\hat{H}-\mu\hat{N})})^M$
$H - \mu N$ is in normal-ordered form up to a correction of order ϵ^2:
$e^{-\beta(\hat{H}-\mu\hat{N})} =: e^{-\beta(\hat{H}-\mu\hat{N})} : +\mathcal{O}(\epsilon^2)$.

$$\begin{aligned}
Z &= \int \prod_{k=1}^M \prod_\alpha d\phi_{\alpha,k}^* d\phi_{\alpha,k} e^{-\sum_{k=1}^M \sum_\alpha \phi_{\alpha,k}^* \phi_{\alpha,k}} \prod_{k=1}^M \langle \phi_{\alpha,k} | : e^{-\epsilon(\hat{H}-\mu\hat{N})} : +\mathcal{O}(\epsilon^2) \, | \phi_{\alpha,k-1} \rangle \\
&= \int \prod_{k=1}^M \prod_\alpha d\phi_{\alpha,k}^* d\phi_{\alpha,k} e^{-\sum_{k=1}^M \sum_\alpha (\phi_{\alpha,k}^* \phi_{\alpha,k} - \phi_{\alpha,k}^* \phi_{\alpha,k-1}) - \epsilon \sum_{k=1}^M \sum_\alpha \left\{ H[\phi_{\alpha,k}^*, \phi_{\alpha,k-1}] - \mu \phi_{\alpha,k}^* \phi_{\alpha,k-1} \right\}} \\
&= \int \prod_{k=1}^M \prod_\alpha d\phi_{\alpha,k}^* d\phi_{\alpha,k} e^{-S[\phi_{\alpha,k}^*, \phi_{\alpha,k-1}]}
\end{aligned}$$

$\phi_{\alpha,0} = -\phi_{\alpha,M}$ (antiperiodic boundary conditions)

Action

$$S[\phi^*_\alpha, \phi_\alpha] = \epsilon \left\{ \sum_{k=1}^{M} \sum_\alpha \phi^*_{\alpha,k} \frac{\phi_{\alpha,k} - \phi_{\alpha,k-1}}{\epsilon} - \mu \phi^*_{\alpha,k}\phi_{\alpha,k-1} + H[\phi^*_{\alpha,k}, \phi_{\alpha,k-1}] \right\}.$$

In the limit $\epsilon \to 0$, introduce short-hand notation

$$\phi^*_{\alpha,k} \frac{\phi_{\alpha,k} - \phi_{\alpha,k-1}}{\epsilon} \equiv \phi^*_\alpha(\tau) \frac{\partial}{\partial \tau} \phi_\alpha(\tau), \quad H[\phi^*_{\alpha,k}, \phi_{\alpha,k-1}] \equiv H[\phi^*_\alpha(\tau), \phi_\alpha(\tau)]$$

With

$$H = \sum_\alpha \epsilon_\alpha \phi^*_\alpha \phi_\alpha + V[\phi^*(\tau), \phi(\tau)]$$

Symbolically:

$$Z = \int_{\phi_\alpha(\beta) = -\phi_\alpha(0)} \mathcal{D}[\phi^*_\alpha(\tau), \phi_\alpha(\tau)] e^{-\int_0^\beta d\tau \left\{ \sum_\alpha \phi^*_\alpha(\tau)(\frac{\partial}{\partial \tau} + \epsilon_\alpha - \mu)\phi_\alpha(\tau) + V[\phi^*(\tau), \phi(\tau)] \right\}}$$

Coherent state path integral

[Negele & Orland]

Perturbation expansion

Non-interacting average:

$$\langle \ldots \rangle_0 = \frac{1}{Z_0} \int_{\phi_\alpha(\beta)=-\phi_\alpha(0)} \mathcal{D}[\phi^*_\alpha(\tau), \phi_\alpha(\tau)] e^{-\int_0^\beta d\tau \sum_\alpha \phi^*_\alpha(\tau)(\frac{\partial}{\partial\tau}+\epsilon_\alpha-\mu)\phi_\alpha(\tau)} (\ldots)$$

Perturbation expansion

$$\begin{aligned} G_{\alpha_1\alpha_2}(\tau_1 - \tau_2) &= -\frac{1}{Z} \int \mathcal{D}[\phi^*_\alpha(\tau), \phi_\alpha(\tau)] e^{-S[\phi^*_\alpha(\tau),\phi_\alpha(\tau)]} \phi_{\alpha_1}(\tau_1)\phi^*_{\alpha_2}(\tau_2) \\ &= -\frac{Z_0}{Z} \left\langle e^{-\int_0^\beta d\tau V[\phi^*_\alpha(\tau),\phi_\alpha(\tau)]} \phi_{\alpha_1}(\tau_1)\phi^*_{\alpha_2}(\tau_2) \right\rangle_0 \\ &= -\frac{Z_0}{Z} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau'_1 \ldots \mathrm{d}\,\tau'_n \times \\ &\qquad \times \left\langle V[\phi^*(\tau'_1), \phi(\tau'_1)] \ldots V[\phi^*(\tau'_n), \phi(\tau'_n)] \phi_{\alpha_1}(\tau_{\alpha_1})\phi^*_{\alpha_2}(\tau_{\alpha_1}) \right\rangle_0 \end{aligned}$$

For an instantaneous two-particle interaction

$V[\phi^*(\tau), \phi(\tau)] = V_{\alpha\beta\gamma\delta}\, \phi^*_\alpha(\tau)\phi_\beta(\tau)\phi^*_\gamma(\tau)\phi_\delta(\tau)$

Perturbation theory

Some crucial simplifications

- Wick theorem
- Linked-cluster theorem
- Dyson equation
- Diagram rules

Wick theorem

$$\frac{\int \mathcal{D}[\phi^*,\phi]\phi_{i_1}\phi_{i_2}\dots\phi_{i_n}\phi^*_{j_n}\dots\phi^*_{j_2}\phi^*_{j_1}e^{-\sum_{ij}\phi_i^* M_{ij}\phi_j}}{\int \mathcal{D}[\phi^*,\phi]e^{-\sum_{ij}\phi_i^* M_{ij}\phi_j}} = \sum_{\sigma\in S_n}\mathrm{sgn}(\sigma)M^{-1}_{i_{\sigma(n)},j_n}\dots M^{-1}_{i_{\sigma(1)},j_1}$$

$M_{ij} \to -(\partial_\tau + \epsilon_\alpha - \mu)_{ij}$, $\phi_j \to \phi_{\alpha,k}$:

$$\begin{aligned}
G^0_{\alpha_1\alpha_2}(\tau_1-\tau_2) &= \left\langle \phi_{\alpha_1}(\tau_1)\phi^*_{\alpha_2}(\tau_2)\right\rangle_0 \\
&= -\frac{\int \mathcal{D}[\phi^*_\alpha(\tau),\phi_\alpha(\tau)]e^{-\int_0^\beta d\tau \sum_\alpha \phi^*_\alpha(\tau)(\frac{\partial}{\partial\tau}+\epsilon_\alpha-\mu)\phi_\alpha(\tau)}\phi_{\alpha_1}(\tau_1),\phi^*_{\alpha_2}(\tau_2)]}{\int \mathcal{D}[\phi^*_\alpha(\tau),\phi_\alpha(\tau)]e^{-\int_0^\beta d\tau \sum_\alpha \phi^*_\alpha(\tau)(\frac{\partial}{\partial\tau}+\epsilon_\alpha-\mu)\phi_\alpha(\tau)}} \\
&= -(\partial_\tau+\epsilon_\alpha-\mu)^{-1}_{\alpha_1\tau_1;\alpha_2\tau_2} = G^0_{\alpha_1}(\tau_1-\tau_2)\delta_{\alpha_1\alpha_2}
\end{aligned}$$

Define a contraction

$$\underbracket{\phi_{\alpha_1}(\tau_1)\phi^*_{\alpha_2}}(\tau_2) := \left\langle \phi_{\alpha_1}(\tau_1)\phi^*_{\alpha_2}(\tau_2)\right\rangle_0 = -G^0_{\alpha_1\alpha_2}(\tau_1-\tau_2)\ .$$

$$\left\langle \phi_{\alpha_1}(\tau_1)\phi^*_{\alpha_2}(\tau_2)\dots\phi_{\alpha_n}(\tau_n)\phi^*_{\alpha_n}(\tau_n)\right\rangle_0 = \textbf{Sum over all complete contractions}$$

Example:

$$\begin{aligned}
\left\langle \phi_{\alpha_1}(\tau_1)\phi^*_{\alpha_1'}(\tau_1')\phi_{\alpha_2}(\tau_2)\phi^*_{\alpha_2'}(\tau_2')\right\rangle_0 &= \underbracket{\phi_{\alpha_1}(\tau_1)\phi^*_{\alpha_1'}}(\tau_1')\,\underbracket{\phi_{\alpha_2}(\tau_1)\phi^*_{\alpha_2'}}(\tau_2') \\
&\quad - \underbracket{\phi_{\alpha_1}(\tau_1)\phi^*_{\alpha_2'}}(\tau_2')\,\underbracket{\phi_{\alpha_2}(\tau_1)\phi^*_{\alpha_1'}}(\tau_1') \\
&= G^0_{\alpha_1}(\tau_1-\tau_1')\delta_{\alpha_1\alpha_1'}\,G^0_{\alpha_2}(\tau_2-\tau_2')\delta_{\alpha_2\alpha_2'} \\
&\quad - G^0_{\alpha_1}(\tau_1-\tau_2')\delta_{\alpha_1\alpha_2'}\,G^0_{\alpha_2}(\tau_2-\tau_1')\delta_{\alpha_2\alpha_1'}
\end{aligned}$$

Linked-cluster theorem

$$G_{\alpha_1\alpha_2}(\tau_1-\tau_2) = -\frac{Z_0}{Z}\left\langle e^{-\int_0^\beta d\tau V[\phi^*_\alpha(\tau),\phi_\alpha(\tau)]}\phi_{\alpha_1}(\tau_1)\phi^*_{\alpha_2}(\tau_2)\right\rangle_0$$
$$= -\frac{\left\langle e^{-\int_0^\beta d\tau V[\phi^*_\alpha(\tau),\phi_\alpha(\tau)]}\phi_{\alpha_1}(\tau_1)\phi^*_{\alpha_2}(\tau_2)\right\rangle_0}{\left\langle e^{-\int_0^\beta d\tau V[\phi^*_\alpha(\tau),\phi_\alpha(\tau)]}\right\rangle}$$

Linked-cluster theorem:
Vacuum diagrams cancel out exactly to all orders in perturbation theory

Dyson equation

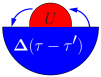
Diagrams can be categorized in reducible and irreducible ones.
Diagrams which cannot be cut in two by cutting a single fermion line are called irreducible.
Define the proper self-energy Σ as the sum of all irreducible diagrams.

$$G = G^0 + G^0 \Sigma G$$

$$G = G^0 + G^0 \Sigma G^0 + G^0 \Sigma G^0 \Sigma G^0 + \ldots$$

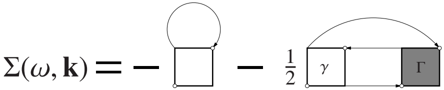
Dyson equation generates all reducible and irreducible diagrams.

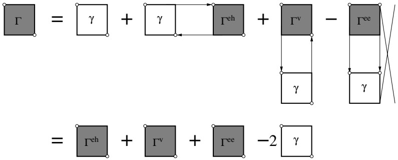
Diagrammatic extensions of DMFT



Impurity model $\Longrightarrow \Sigma_{\nu}^{\text{imp}}$, vertex $\gamma_{\nu\nu'\omega}^{\text{imp}}$

- Include spatial correlations through diagrammatic corrections: second-order, FLEX, Parquet, DiagMC, ...

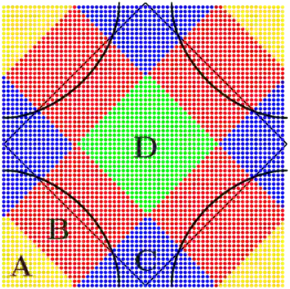




- Examples: DΓA, 1PI, dual fermion, dual boson, TRILEX, ...

[G. Rohringer, H. Hafermann, A. Toschi, A. A. Katanin, A. E. Antipov, M. I. Katsnelson, A. I. Lichtenstein, A. N. Rubtsov, and K. Held, Rev. Mod. Phys. **90**, 025003 (2018).

Complementarity to cluster approaches



Cluster extensions

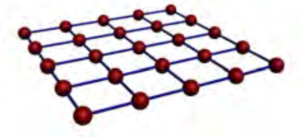
- \+ Control parameter: cluster size
- \+ Rigorous summation of all diagrams on the cluster
- \- Limited cluster size, difficult to converge in practice
- \- Ambiguous interpolation

Diagrammatic extensions

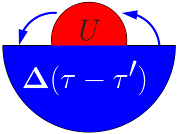
- \+ Long-range correlations
- \+ No sign problem
- \- Approximate at any scale
- \- Truncation of fermion-fermion interaction

Recollection of DMFT

Mapping to impurity problem



$\Longrightarrow$



$$S_{\text{imp}}[c^*, c] = -\sum_{\nu\sigma} c^*_{\nu\sigma}[\imath\nu + \mu - \Delta_\nu]c_{\nu\sigma} + U \sum_{\omega} n_{\omega\uparrow} n_{-\omega\downarrow},$$

$$G_\nu(\mathbf{k}) = \frac{1}{\imath\nu + \mu - \epsilon_{\mathbf{k}} - \Sigma^{\text{imp}}_\nu}$$

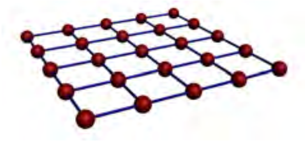
Self-consistency condition

$$g^{\text{imp}}_\nu = \frac{1}{N} \sum_{\mathbf{k}} G_\nu(\mathbf{k})$$

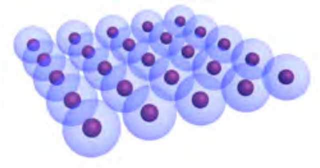
Dual fermions

$$S_{\text{lat}}[c^*, c] = -\sum_{i\nu\sigma} c^*_{i\nu\sigma}[\imath\nu + \mu]c_{i\nu\sigma} + U\sum_{\mathbf{q}\omega} n_{\mathbf{q}\omega\uparrow} n_{-\mathbf{q},-\omega\downarrow} + \sum_{\mathbf{k}\nu\sigma} \varepsilon_{\mathbf{k}} c^*_{\mathbf{k}\nu\sigma} c_{\mathbf{k}\nu\sigma}$$

Introduce impurity problem at each lattice site



$\Longrightarrow$



$$S_{\text{lat}}[c^*, c] = \sum_i S_{\text{imp}}[c^*_{\nu i\sigma}, c_{\nu i\sigma}] - \sum_{\nu\mathbf{k}\sigma} c^*_{\nu\mathbf{k}\sigma}(\Delta_\nu - \epsilon_{\mathbf{k}})c_{\nu\mathbf{k}\sigma}$$

Perturbative treatment of second term?
Complicated: no Wick theorem!

Transformation to Dual Fermions

Decoupling: Hubbard-Stratonovich transformation

$$\exp\left[c^*_{\omega\mathbf{k}\sigma}(\Delta_\omega - \varepsilon_\mathbf{k})c_{\omega\mathbf{k}\sigma}\right] = \det\left[g_\omega^{-1}(\Delta_\omega - \varepsilon_\mathbf{k})g_\omega^{-1}\right]^{-1} \times$$
$$\times \int \exp\left[-f^* g_\omega^{-1}(\Delta_\omega - \varepsilon_\mathbf{k})g_\omega^{-1} f - f^* g_\omega^{-1} c - c^* g_\omega^{-1} f\right] \mathcal{D}[f, f^*]$$

$\rightarrow$ Introduces new fields which mediate coupling between impurities
Coupling of real to dual fields is *local*

Transformed partition function:

$$Z = D_f \int \mathcal{D}[f^*, f] e^{-\sum_{\mathbf{k}\nu\sigma} f^*_{\mathbf{k}\nu\sigma} g_{\nu\sigma}^{-1}(\Delta_{\nu\sigma} - \varepsilon_\mathbf{k})^{-1} g_{\nu\sigma}^{-1} f_{\mathbf{k}\nu\sigma}} \times$$
$$\int \mathcal{D}[c^*, c] e^{-\sum_i \{S_{\text{imp}}[c_i^*, c_i] + S_{\text{cf}}[c_i^*, c_i; f_i^*, f_i]\}}$$

$$S_{\text{cf}}[c^*, c; f^*, f] = \sum_{\nu\sigma} \left(f^*_{\nu\sigma} g_{\nu\sigma}^{-1} c_{\nu\sigma} + c^*_{\nu\sigma} g_{\nu\sigma}^{-1} f_{\nu\sigma}\right)$$

Integrating out the original fermions

$$\int \mathcal{D}[c_i^*, c_i] e^{-S_{\text{imp}}[c_i^*, c_i]} e^{-S_{\text{cf}}[c_i^*, c_i; f_i^*, f_i]} =$$

$$\sum_{\substack{n=0 \\ n \text{ even}}}^{\infty} \frac{(-1)^n}{n!} \left\langle \left(\sum_{\nu\sigma} \left(f_{\nu\sigma}^* g_{\nu\sigma}^{-1} c_{\nu\sigma} + c_{\nu\sigma}^* g_{\nu\sigma}^{-1} f_{\nu\sigma} \right) \right)^n \right\rangle_{\text{imp}}$$

First non-vanishing term:

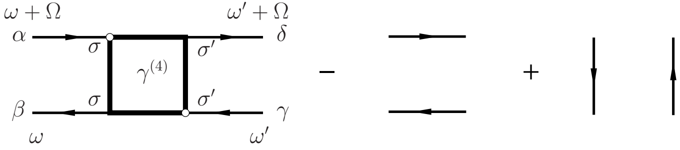
$$\frac{1}{2} \sum_{\nu\sigma} \sum_{\nu'\sigma'} \left\langle f_{\nu\sigma}^* g_{\nu\sigma}^{-1} c_{\nu\sigma} c_{\nu'\sigma'}^* g_{\nu'\sigma'}^{-1} f_{\nu'\sigma'} + c_{\nu\sigma}^* g_{\nu\sigma}^{-1} f_{\nu\sigma} f_{\nu'\sigma'}^* g_{\nu'\sigma'}^{-1} c_{\nu'\sigma'} \right\rangle_{\text{imp}}$$

$$= \sum_{\nu\sigma} \sum_{\nu'\sigma'} g_{\nu\sigma}^{-1} g_{\nu'\sigma'}^{-1} \left\langle c_{\nu\sigma} c_{\nu\sigma}^* \right\rangle_{\text{imp}} \delta_{\nu\nu'} \delta_{\sigma\sigma'} f_{\nu\sigma}^* f_{\nu'\sigma'} = -\sum_{\nu\sigma} f_{\nu\sigma}^* g_{\nu\sigma}^{-1} f_{\nu\sigma}$$

The vertex function

Next non-vanishing-term involves two-particle Green's function

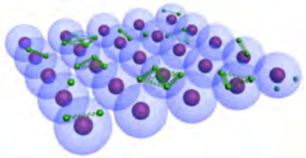
$$g^{\sigma\sigma\sigma'\sigma'}_{\nu\nu'\omega} := \left\langle c_{\nu\sigma} c^*_{\nu+\omega,\sigma} c_{\nu'+\omega,\sigma'} c^*_{\nu'\sigma'} \right\rangle_{\text{imp}}$$



Vertex function

$$\gamma^{\sigma\sigma\sigma'\sigma'}_{\nu\nu'\omega} := \frac{g^{\sigma\sigma\sigma'\sigma'}_{\nu\nu'\omega} - \beta g_{\nu\sigma} g_{\nu'\sigma'} \delta_{\omega} + \beta g_{\nu\sigma} g_{\nu+\omega\sigma} \delta_{\nu\nu'} \delta_{\sigma\sigma'}}{g_{\nu\sigma} g_{\nu+\omega,\sigma} g_{\nu'+\omega\sigma'} g_{\nu'\sigma'}}$$

Compute in QMC $\longrightarrow$ Lecture by F. Assaad



Dual action

$$S[f^*, f] = \sum_{\nu\mathbf{k}\sigma} f^*_{\nu\mathbf{k}\sigma} [\tilde{G}^0_{\mathbf{k}\nu}]^{-1} f_{\nu\mathbf{k}\sigma} + \sum_i V[f^*_i, f_i]$$

$$V[f^*_i, f_i] = -\frac{1}{4}\gamma^{(4)}_{1234} f_1 f^*_2 f_3 f^*_4 + \frac{1}{36}\gamma^{(6)}_{123456} f_1 f^*_2 f_3 f^*_4 f_5 f^*_6 \mp \ldots$$

$$\tilde{G}^0_{\mathbf{k}\nu\sigma} = \left[g^{-1}_{\nu\sigma} + (\Delta_\nu - \varepsilon_{\mathbf{k}})\right]^{-1} - g_{\nu\sigma}$$

[A. N. Rubtsov, M. I. Katsnelson and A. I. Lichtenstein, PRB **77** 033101 (2008)]

Relation to DMFT

$$g_\nu = \frac{1}{\imath\nu + \mu - \Delta_\nu - \Sigma_\nu^{\mathrm{imp}}} \qquad G_{\mathbf{k}\nu} = \frac{1}{\imath\nu + \mu - \varepsilon_{\mathbf{k}} - \Sigma_\nu^{\mathrm{imp}}}$$

$$G_{\mathbf{k}\nu} = [g_\nu^{-1} + (\Delta_\nu - \varepsilon_{\mathbf{k}})]^{-1}$$

$$\tilde{G}^0_{\mathbf{k}\nu} = [g_\nu^{-1} + (\Delta_\nu - \varepsilon_{\mathbf{k}})]^{-1} - g_\nu$$

Avoids double counting of DMFT contributions

Self-Consistency & Relation to DMFT

$$\Delta_\nu = \Delta_\nu^{\mathrm{DMFT}} \longrightarrow \tilde{G}^0_{\mathbf{k}\nu} = G^{\mathrm{DMFT}}_{\mathbf{k}\nu} - g_\nu$$

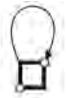
Self-consistency condition for hybridization Δ yields DMFT:

$$\tilde{G}^0_{\mathbf{k}\nu} = 0$$

- DMFT appears as zero-order approximation
- Diagrammatic expansion around DMFT for $\Delta = \Delta_{\mathrm{DMFT}}$

General self-consistency condition:

$$\frac{1}{N}\sum_{\mathbf{k}} \tilde{G}_{\mathbf{k}\nu} = 0 \qquad \Leftrightarrow$$



$= 0$

Eliminates leading-order contribution and an infinite partial series

From dual to physical fermions

$$\tilde{G}^0_{\mathbf{k}\nu} = [g_\nu^{-1} + (\Delta_\nu - \varepsilon_{\mathbf{k}})]^{-1} - g_\nu$$

$\tilde{G}_{\mathbf{k}\nu} \sim 1/\nu^2 \longrightarrow$ not a physical Green function

Exact relations between physical and dual quantities follow from Hubbard-Stratonovich transformation, e.g.

$$\Sigma_{\mathbf{k}\nu\sigma} = \Sigma^{\text{imp}}_{\nu\sigma} + \frac{\tilde{\Sigma}_{\mathbf{k}\nu\sigma}}{1 + \tilde{\Sigma}_{\mathbf{k}\nu\sigma} g_{\nu\sigma}}$$

$$G_{\mathbf{k}\nu} = (\Delta_\nu - \varepsilon_{\mathbf{k}})^{-1} + (\Delta_\nu - \varepsilon_{\mathbf{k}})^{-1} \; g_\nu^{-1} \; \tilde{G}_{\mathbf{k}\nu} \; g_\nu^{-1} \; (\Delta_\nu - \varepsilon_{\mathbf{k}})^{-1}$$

Dual Perturbation Theory

Perturbation expansion

$$\tilde{G}_{12} := -\langle f_1 f_2^* \rangle = -\frac{1}{\tilde{Z}} \int f_1 f_2^* \, \exp(-\tilde{S}[f^*, f]) \, \mathcal{D}[f^*, f]$$

$$\tilde{S}[f^*, f] = -\sum_{k,\,\alpha\beta} f_\alpha^* \, \tilde{G}^{0\;-1}_{\alpha\beta} f_\beta + \sum_i V_i[f_i^*, f_i]$$

Expansion of Green's function in the interaction:

$$\begin{aligned} \exp\left(-\sum_i V_i[f_i^*, f_i]\right) \quad &= \quad 1 - \sum_i V_i[f_i^*, f_i] + \frac{1}{2!}\left(\sum_i \sum_j V_i[f_i^*, f_i] V_j[f_j^*, f_j]\right) \\ &\quad - \frac{1}{3!}\left(\sum_i \sum_j \sum_k V_i[f_i^*, f_i] V_j[f_j^*, f_j] V_k[f_k^*, f_k]\right) + \ldots \end{aligned}$$

Perturbation expansion

First-order (only those involving $\gamma^{(4)}$ and $\gamma^{(6)}$):

$$\left(-\frac{1}{4}\right)\sum_i \gamma^{(4)}_{i\alpha\beta\gamma\delta}\int f_1 f_2^* f^*_{i\alpha} f_{i\beta} f^*_{i\gamma} f_{i\delta}\ \exp(-\tilde{S}_0[f^*,f])\,\mathcal{D}[f^*,f]$$

$$\left(\frac{1}{36}\right)\sum_i \gamma^{(6)}_{i\alpha\beta\gamma\delta\epsilon\zeta}\int f_1 f_2^* f^*_{i\alpha} f_{i\beta} f^*_{i\gamma} f_{i\delta} f^*_{i\epsilon} f_{i\zeta}\ \exp(-\tilde{S}_0[f^*,f])\,\mathcal{D}[f^*,f]$$

Second-order (only those involving $\gamma^{(4)}$ and $\gamma^{(6)}$):

$$-\frac{1}{2!}\left(-\frac{1}{4}\right)^2\sum_i\sum_j \gamma^{(4)}_{i\alpha\beta\gamma\delta}\gamma^{(4)}_{j\kappa\lambda\mu\nu}\times$$

$$\times\int f_1 f_2^* f^*_{i\alpha} f_{i\beta} f^*_{i\gamma} f_{i\delta} f^*_{j\kappa} f_{j\lambda} f^*_{j\mu} f_{j\nu}\ \exp(-\tilde{S}_0[f^*,f])\,\mathcal{D}[f^*,f]$$

$$-\frac{1}{2!}\left(-\frac{1}{4}\right)\left(\frac{1}{36}\right)\sum_i\sum_j \gamma^{(4)}_{i\alpha\beta\gamma\delta}\,\gamma^{(6)}_{j\kappa\lambda\mu\nu\epsilon\zeta}\times$$

$$\times\int f_1 f_2^* f^*_{i\alpha} f_{i\beta} f^*_{i\gamma} f_{i\delta} f^*_{j\kappa} f_{j\lambda} f^*_{j\mu} f_{j\nu} f^*_{j\epsilon} f_{j\zeta}\ \exp(-\tilde{S}_0[f^*,f])\,\mathcal{D}[f^*,f]$$

$$-\frac{1}{2!}\left(-\frac{1}{4}\right)\left(\frac{1}{36}\right)\sum_i\sum_j \gamma^{(6)}_{i\kappa\lambda\mu\nu\epsilon\zeta}\gamma^{(4)}_{j\alpha\beta\gamma\delta}\times$$

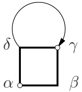
$$\times\int f_1 f_2^* f^*_{i\kappa} f_{i\lambda} f^*_{i\mu} f_{i\nu} f^*_{i\epsilon} f_{i\zeta} f^*_{j\alpha} f_{j\beta} f^*_{j\gamma} f_{j\delta}\ \exp(-\tilde{S}_0[f^*,f])\,\mathcal{D}[f^*,f]$$

$$-\frac{1}{2!}\left(\frac{1}{36}\right)^2\sum_i\sum_j \gamma^{(6)}_{i\alpha\beta\gamma\delta\epsilon\zeta}\gamma^{(6)}_{j\kappa\lambda\mu\nu\rho\eta}\times$$

$$\times\int f_1 f_2^* f^*_{i\alpha} f_{i\beta} f^*_{i\gamma} f_{i\delta} f^*_{i\epsilon} f_{i\zeta} f^*_{j\kappa} f_{j\lambda} f^*_{j\mu} f_{j\nu} f^*_{j\rho} f_{j\eta}\ \exp(-\tilde{S}_0[f^*,f])\,\mathcal{D}[f^*,f]$$

Self-energy diagrams

$$\left(-\frac{1}{4}\right)\sum_i \gamma^{(4)}_{i\alpha\beta\gamma\delta}\int f_1 f_2^* f_{i\alpha}^* f_{i\beta} f_{i\gamma}^* f_{i\delta}\ \exp(-\tilde{S}_0[f^*,f])\,\mathcal{D}[f^*,f]$$



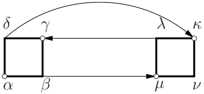
$$+f_1 f_2^* f_{i\alpha}^* f_{i\beta} f_{i\gamma}^* f_{i\delta} = -f_1 f_{i\alpha}^* f_{i\delta} f_{i\gamma}^* f_{i\beta} f_2^* = (-1)^4\ \tilde{G}_{1\,i\alpha}\tilde{G}_{i\beta\,2}\tilde{G}_{ii\delta\gamma}$$

$$\Sigma^{(a)}_{ii\,\alpha\beta} = -\gamma^{(4)}_{i\alpha\beta\gamma\delta}\tilde{G}_{ii\delta\gamma}$$

4 equivalent pairings

Self-energy diagrams

$$-\frac{1}{2!}\left(-\frac{1}{4}\right)^2 \sum_i \sum_j \gamma^{(4)}_{i\alpha\beta\gamma\delta}\gamma^{(4)}_{j\kappa\lambda\mu\nu}\int f_1 f_2^* f_{i\alpha}^* f_{i\beta} f_{i\gamma}^* f_{i\delta} f_{j\kappa}^* f_{j\lambda} f_{j\mu}^* f_{j\nu}\ \exp(-\tilde{S}_0[f^*,f])\,\mathcal{D}[f^*,f]$$



$$+f_1 f_2^* f_{i\alpha}^* f_{i\beta} f_{i\gamma}^* f_{i\delta} f_{j\kappa}^* f_{j\lambda} f_{j\mu}^* f_{j\nu} = -f_1 f_{i\alpha}^* f_{i\beta} f_{j\mu}^* f_{j\lambda} f_{i\gamma}^* f_{i\delta} f_{j\kappa}^* f_{j\nu} f_2^*$$

$$= (-1)^6\ \tilde{G}_{1\,i\alpha}\tilde{G}_{ij\beta\mu}\tilde{G}_{ji\lambda\gamma}\tilde{G}_{ij\delta\kappa}\tilde{G}_{i\nu\,2}$$

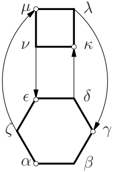
$$\Sigma^{(\mathrm{b})}_{ij\,\alpha\nu} = -\frac{1}{2}\gamma^{(4)}_{i\alpha\beta\gamma\delta}\gamma^{(4)}_{j\kappa\lambda\mu\nu}\tilde{G}_{ij\beta\mu}\tilde{G}_{ji\lambda\gamma}\tilde{G}_{ij\delta\kappa}$$

Nonlocal correction, 16 equivalent pairings

Self-energy diagrams

$$-\frac{1}{2!}\left(-\frac{1}{4}\right)\left(\frac{1}{36}\right)\sum_i\sum_j \gamma^{(4)}_{i\alpha\beta\gamma\delta}\,\gamma^{(6)}_{j\kappa\lambda\mu\nu\epsilon\zeta}\int f_1 f_2^* f_{i\alpha}^* f_{i\beta} f_{i\gamma}^* f_{i\delta} f_{j\kappa}^* f_{j\lambda} f_{j\mu}^* f_{j\nu} f_{j\epsilon}^* f_{j\zeta}\ \exp(-\tilde{S}_0[f^*,f])\,\mathcal{D}[f^*,f]$$

$$-\frac{1}{2!}\left(-\frac{1}{4}\right)\left(\frac{1}{36}\right)\sum_i\sum_j \gamma^{(6)}_{i\kappa\lambda\mu\nu\epsilon\zeta}\,\gamma^{(4)}_{j\alpha\beta\gamma\delta}\int f_1 f_2^* f_{i\kappa}^* f_{i\lambda} f_{i\mu}^* f_{i\nu} f_{i\epsilon}^* f_{i\zeta} f_{j\alpha}^* f_{j\beta} f_{j\gamma}^* f_{j\delta}\ \exp(-\tilde{S}_0[f^*,f])\,\mathcal{D}[f^*,f]$$



$$f_1 f_2^* f_{i\alpha}^* f_{i\beta} f_{i\gamma}^* f_{i\delta} f_{i\epsilon}^* f_{i\zeta} f_{j\kappa}^* f_{j\lambda} f_{j\mu}^* f_{j\nu} = +f_1 f_{i\alpha}^* f_{j\lambda} f_{i\gamma}^* f_{i\delta} f_{j\kappa}^* f_{j\nu} f_{i\epsilon}^* f_{i\zeta} f_{j\mu}^* f_{i\beta} f_2^*$$

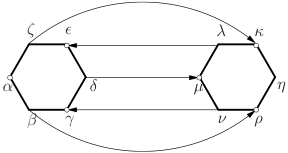
$$= (-1)^6\,\tilde{G}_{1\,i\alpha}\,\tilde{G}_{ji\lambda\gamma}\,\tilde{G}_{ij\delta\kappa}\,\tilde{G}_{ji\nu\epsilon}\,\tilde{G}_{ij\zeta\mu}\,\tilde{G}_{i\beta\,2}$$

$$\Sigma^{(c)}_{ii\,\alpha\beta} = \left(\frac{1}{4}\right)\sum_j \gamma^{(6)}_{i\alpha\beta\gamma\delta\epsilon\zeta}\,\gamma^{(4)}_{j\kappa\lambda\mu\nu}\,\tilde{G}_{ji\lambda\gamma}\,\tilde{G}_{ij\delta\kappa}\,\tilde{G}_{ji\nu\epsilon}\,\tilde{G}_{ij\zeta\mu}$$

36 equivalent pairings

Self-energy diagrams

$$-\frac{1}{2!}\left(\frac{1}{36}\right)^2 \sum_i \sum_j \gamma^{(6)}_{i\alpha\beta\gamma\delta\epsilon\zeta}\gamma^{(6)}_{j\kappa\lambda\mu\nu\rho\eta}\int f_1 f_2^* f^*_{i\alpha} f_{i\beta} f^*_{i\gamma} f_{i\delta} f^*_{i\epsilon} f_{i\zeta} f^*_{j\kappa} f_{j\lambda} f^*_{j\mu} f_{j\nu} f^*_{j\rho} f_{j\eta}\ \exp(-\tilde{S}_0[f^*, f])\,\mathcal{D}[f^*, f]$$



$$f_1 f^*_{i\alpha} f_{i\beta} f^*_{i\gamma} f_{i\delta} f^*_{i\epsilon} f_{i\zeta} f^*_{j\kappa} f_{j\lambda} f^*_{j\mu} f_{j\nu} f^*_{j\rho} f_{j\eta} f_2^*$$

$$= + f_1 f^*_{i\alpha} f_{i\beta} f^*_{j\rho} f_{j\nu} f^*_{i\gamma} f_{i\delta} f^*_{j\mu} f_{j\lambda} f^*_{i\epsilon} f_{i\zeta} f^*_{j\kappa} f_{j\eta} f_2^*$$

$$= (-1)^7\, \tilde{G}_{1\,i\alpha}\, \tilde{G}_{ij\beta\rho}\, \tilde{G}_{ji\nu\gamma}\, \tilde{G}_{ij\delta\mu}\, \tilde{G}_{ji\lambda\epsilon}\, \tilde{G}_{ij\zeta\kappa}\, \tilde{G}_{j\eta\,2}$$

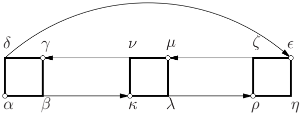
$$\Sigma^{(\mathrm{d})}_{ij\,\alpha\eta} = \left(\frac{1}{12}\right)\gamma^{(6)}_{i\alpha\beta\gamma\delta\epsilon\zeta}\gamma^{(6)}_{j\kappa\lambda\mu\nu\rho\eta}\, \tilde{G}_{ij\beta\rho}\, \tilde{G}_{ji\nu\gamma}\, \tilde{G}_{ij\delta\mu}\, \tilde{G}_{ji\lambda\epsilon}\, \tilde{G}_{ij\zeta\kappa}$$

216 equivalent pairings: $(1/2)(1/36)^2 \times 216 = 1/12$

Self-energy diagrams

$$+\frac{1}{3!}\left(-\frac{1}{4}\right)^3 \sum_i \sum_j \sum_k \gamma^{(4)}_{i\alpha\beta\gamma\delta}\,\gamma^{(4)}_{j\kappa\lambda\mu\nu}\,\gamma^{(4)}_{k\epsilon\zeta\rho\eta}\times$$

$$\times\int f_1 f_2^* f^*_{i\alpha} f_{i\beta} f^*_{i\gamma} f_{i\delta} f^*_{j\kappa} f_{j\lambda} f^*_{j\mu} f_{j\nu} f^*_{k\epsilon} f_{k\zeta} f^*_{k\rho} f_{k\eta}\ \exp(-\tilde{S}_0[f^*,f])\,\mathcal{D}[f^*,f]$$



$$f_1 f^*_{i\alpha} f_{i\beta} f^*_{i\gamma} f_{i\delta} f^*_{j\kappa} f_{j\lambda} f^*_{j\mu} f_{j\nu} f^*_{k\epsilon} f_{k\zeta} f^*_{k\rho} f_{k\eta} f_2^*$$

$$= - f_1 f^*_{i\alpha} f_{i\beta} f^*_{j\kappa} f_{j\nu} f^*_{i\gamma} f_{i\delta} f^*_{k\epsilon} f_{j\lambda} f^*_{k\rho} f_{k\zeta} f^*_{j\mu} f_{k\eta} f_2^*$$

$$= (-1)^8\, \tilde{G}_{1\alpha}\, \tilde{G}_{ij\beta\kappa}\, \tilde{G}_{ji\nu\gamma}\, \tilde{G}_{ik\delta\epsilon}\, \tilde{G}_{jk\lambda\rho}\, \tilde{G}_{kj\zeta\mu}\, \tilde{G}_{\eta 2}\ ,$$

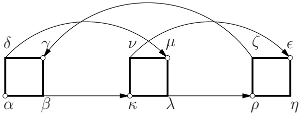
$$\Sigma^{(e)}_{ik\,\alpha\eta} = (-1)\sum_j \gamma^{(4)}_{i\alpha\beta\gamma\delta}\,\gamma^{(4)}_{j\kappa\lambda\mu\nu}\,\gamma^{(4)}_{k\epsilon\zeta\rho\eta}\, \tilde{G}_{ij\beta\kappa}\, \tilde{G}_{ji\nu\gamma}\, \tilde{G}_{ik\delta\epsilon}\, \tilde{G}_{jk\lambda\rho}\, \tilde{G}_{kj\zeta\mu}$$

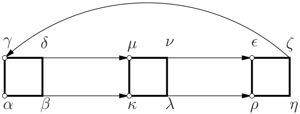
384 equivalent pairings

Self-energy diagrams

$$+\frac{1}{3!}\left(-\frac{1}{4}\right)^3 \sum_i \sum_j \sum_k \gamma^{(4)}_{i\alpha\beta\gamma\delta}\,\gamma^{(4)}_{j\kappa\lambda\mu\nu}\,\gamma^{(4)}_{k\epsilon\zeta\rho\eta}\times$$

$$\times \int f_1 f_2^* f_{i\alpha}^* f_{i\beta} f_{i\gamma}^* f_{i\delta} f_{j\kappa}^* f_{j\lambda} f_{j\mu}^* f_{j\nu} f_{k\epsilon}^* f_{k\zeta} f_{k\rho}^* f_{k\eta}\; \exp(-\tilde{S}_0[f^*, f])\,\mathcal{D}[f^*, f]$$





$$f_1 f_{i\alpha}^* f_{i\beta} f_{i\gamma}^* f_{i\delta} f_{j\kappa}^* f_{j\lambda} f_{j\mu}^* f_{j\nu} f_{k\epsilon}^* f_{k\zeta} f_{k\rho}^* f_{k\eta} f_2^*$$

$$= - f_1 f_{i\alpha}^* f_{i\beta} f_{j\kappa}^* f_{k\zeta} f_{i\gamma}^* f_{i\delta} f_{j\mu}^* f_{j\lambda} f_{k\rho}^* f_{j\nu} f_{k\epsilon}^* f_{k\eta} f_2^*$$

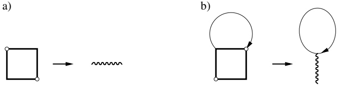
$$= (-1)^8\, \tilde{G}_{1\,i\alpha}\, \tilde{G}_{ij\,\beta\kappa}\, \tilde{G}_{ki\,\zeta\gamma}\, \tilde{G}_{ij\,\delta\mu}\, \tilde{G}_{jk\,\lambda\rho}\, \tilde{G}_{jk\,\nu\epsilon}\, \tilde{G}_{k\eta\,2}$$

$$\Sigma^{(f)}_{ik\,\alpha\eta} = \left(-\frac{1}{4}\right) \sum_j \gamma^{(4)}_{i\alpha\beta\gamma\delta}\,\gamma^{(4)}_{j\kappa\lambda\mu\nu}\,\gamma^{(4)}_{k\epsilon\zeta\rho\eta}\, \tilde{G}_{ij\,\beta\kappa}\, \tilde{G}_{ki\,\zeta\gamma}\, \tilde{G}_{ij\,\delta\mu}\, \tilde{G}_{jk\,\lambda\rho}\, \tilde{G}_{jk\,\nu\epsilon}$$

96 equivalent pairings

Diagram rules

- Include a factor $1/n!$ for each tuple of *equivalent* lines
- Determination of the sign: closed loop yields factor (-1)



- Symmetry factor for n-th order vacuum amplitude diagrams: $1/(2n)$
  cyclic permutations of $(1, 2, \ldots n)$ and $(n, \ldots, 2, 1)$

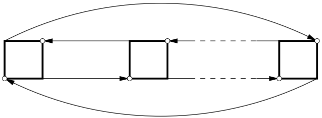
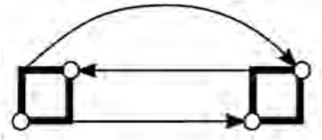


Diagram rules

Self-energy diagrams in momentum space

- Draw all topologically distinct, connected irreducible diagrams involving any n-body interaction $\gamma^{(2n)}$
- Connect the vertices with directed lines
- With each line associate a dual Green function $\tilde{G}_{\mathbf{k}\nu}$
- Assign a frequency, momentum, orbital and spin label to each endpoint
- Sum / integrate over all internal variables taking into account energy- momentum- and spin-conservation at each vertex
- For each tuple of n equivalent lines, associate a factor $1/n!$
- Multiply the expression by $(T/N)^m S^{-1} \times s$, where m counts independent frequency / momentum summations and S and s are the symmetry factor and sign described above.

Second-order approximation DF$^{(2)}$

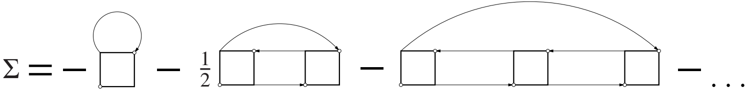


DF$^{(2)}$ self-energy in momentum space:

$$\tilde{\Sigma}_{\mathbf{k}\nu\sigma} = -\frac{1}{2}\frac{T^2}{N^2}\sum_{\mathbf{k}'\mathbf{q}}\sum_{\nu'\omega}\sum_{\sigma'}\gamma^{\sigma\sigma\sigma'\sigma'}_{\nu\nu'\omega}\,\tilde{G}_{\mathbf{k}+\mathbf{q}\nu+\omega\sigma}\,\tilde{G}_{\mathbf{k}'+\mathbf{q}\nu'+\omega\sigma'}\,\tilde{G}_{\mathbf{k}'\nu'\sigma'}\gamma^{\sigma'\sigma'\sigma\sigma}_{\nu'\nu\omega}$$
$$-\frac{1}{2}\frac{T^2}{N^2}\sum_{\mathbf{k}'\mathbf{q}}\sum_{\nu'\omega}\gamma^{\bar{\sigma}\sigma\sigma\bar{\sigma}}_{\nu\nu'\omega}\,\tilde{G}_{\mathbf{k}+\mathbf{q}\nu+\omega\sigma}\,\tilde{G}_{\mathbf{k}'+\mathbf{q}\nu'+\omega\sigma'}\,\tilde{G}_{\mathbf{k}'\nu'\sigma'}\gamma^{\bar{\sigma}\sigma\sigma\bar{\sigma}}_{\nu'\nu\omega}$$

Includes non-local, but rather short-range correlations

Ladder approximation



Generate infinite series through Bethe-Salpeter equations:

$$\tilde{\Gamma}^{\sigma\sigma\sigma'\sigma'}_{\mathbf{q}\nu\nu'\omega} = \gamma^{\sigma\sigma\sigma'\sigma'}_{\nu\nu'\omega} - \frac{T}{N}\sum_{\mathbf{k}''\nu''\sigma''} \gamma^{\sigma\sigma\sigma''\sigma''}_{\nu\nu''\omega}\, \tilde{G}_{\mathbf{k}''+\mathbf{q}\nu''+\omega}\, \tilde{G}_{\mathbf{k}''\nu''}\, \tilde{\Gamma}^{\sigma''\sigma''\sigma'\sigma'}_{\mathbf{q}\nu''\nu'\omega}$$

$$\tilde{\Gamma}^{\sigma\bar{\sigma}\bar{\sigma}\sigma}_{\mathbf{q}\nu\nu'\omega} = \gamma^{\sigma\bar{\sigma}\bar{\sigma}\sigma}_{\nu\nu'\omega} - \frac{T}{N}\sum_{\mathbf{k}''\nu''} \gamma^{\sigma\bar{\sigma}\bar{\sigma}\sigma}_{\nu\nu''\omega}\, \tilde{G}_{\mathbf{k}''+\mathbf{q}\nu''+\omega}\, \tilde{G}_{\mathbf{k}''\nu''}\, \tilde{\Gamma}^{\sigma\bar{\sigma}\bar{\sigma}\sigma}_{\mathbf{q}\nu''\nu'\omega}$$

Multiple scattering of particle-hole pairs with defined spin projection S_z
First equation mixes spin components of vertices $\longrightarrow$ total spin S is not conserved in scattering processes
Second equation has $S = 1$

Ladder approximation

Spin diagonalization:
Equations decouple in terms of linear combinations

$$\gamma^{d(m)}_{\nu\nu'\omega} = \gamma^{\uparrow\uparrow\uparrow\uparrow}_{\nu\nu'\omega} \overset{+}{(-)} \gamma^{\uparrow\uparrow\downarrow\downarrow}_{\nu\nu'\omega}$$

$$\tilde{\Gamma}^{\alpha}_{\mathbf{q}\nu\nu'\omega} = \gamma^{\alpha}_{\nu\nu'\omega} - \frac{T}{N} \sum_{\mathbf{k}''\nu''} \gamma^{\alpha}_{\nu\nu''\omega} \tilde{G}_{\mathbf{k}''+\mathbf{q}\nu''+\omega} \tilde{G}_{\mathbf{k}''\nu''} \tilde{\Gamma}^{\alpha}_{\mathbf{q}\nu''\nu'\omega}$$

Describes collective spin and charge excitations:

γ^{d}: density, $S = 0$, $S_z = 0$ $(\langle n_\sigma n_\uparrow \rangle + \langle n_\sigma n_\downarrow \rangle = \langle n_\sigma n \rangle)$
γ^{m}: magnetic, S=1, $S_z = 0$ $(\langle n_\sigma n_\uparrow \rangle - \langle n_\sigma n_\downarrow \rangle = \langle n_\sigma S_z \rangle)$
Paramagnetic case: result independent of $S_z \longrightarrow$
$\gamma^{\uparrow\uparrow\uparrow\uparrow}_{\nu\nu'\omega} - \gamma^{\uparrow\uparrow\downarrow\downarrow}_{\nu\nu'\omega} = \gamma^{\uparrow\downarrow\downarrow\uparrow}_{\nu\nu'\omega}$

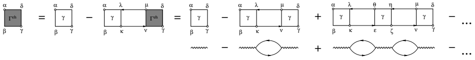
Ladder approximation

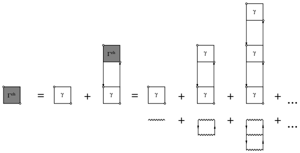
Solution by matrix inversion

$$[\tilde{\Gamma}^{\alpha}_{\mathbf{q}\omega}]^{-1}_{\nu\nu'} = [\gamma^{\alpha}_{\omega}]^{-1}_{\nu\nu'} + (T/N)\sum_{\mathbf{k}} \tilde{G}_{\mathbf{k}+\mathbf{q}\nu+\omega}\tilde{G}_{\mathbf{k}\nu}\delta_{\nu\nu'}$$

Similar to a geometric series $\Gamma = \gamma(1 - q + q^2 - q^3 + \ldots)$
with $q = GG\gamma$

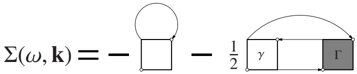
Caution: series may diverge!





Ladder approximation

Schwinger-Dyson equation



Approximate the lattice vertex as $\tilde{\Gamma} \approx \tilde{\Gamma}^{\mathrm{eh}} + \tilde{\Gamma}^{\mathrm{v}} - \gamma$
Neglects particle-particle scattering; double counting correction γ

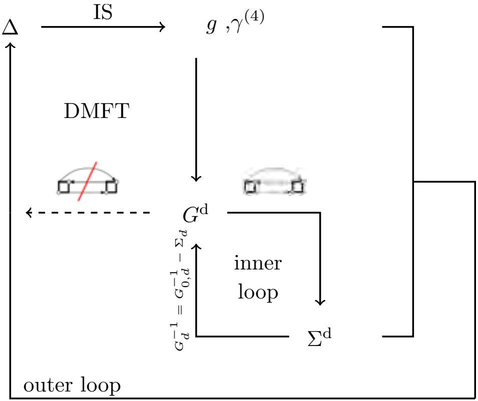
Horizontal and vertical electron-hole channel contribute equally to ladder self-energy:

$$\tilde{\Sigma}_{\mathbf{k}\nu} = -\frac{T^2}{N^2} \sum_{\mathbf{k}'\mathbf{q}} \sum_{\nu'\omega} A_\alpha \gamma^{\alpha}_{\nu\nu'\omega} \tilde{G}_{\mathbf{k}+\mathbf{q}\nu+\omega} \tilde{G}_{\mathbf{k}'+\mathbf{q}\nu'+\omega} \tilde{G}_{\mathbf{k}'\nu'} \left[\tilde{\Gamma}^{\mathrm{h},\alpha}_{\nu'\nu\omega} - \frac{1}{2}\gamma^{\alpha}_{\nu'\nu\omega} \right]$$

$A_{\mathrm{d}} = 1$ and $A_{\mathrm{m}} = 3$ accounts for spin degeneracy ($S_z = 0, \pm 1$)

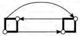
Applications

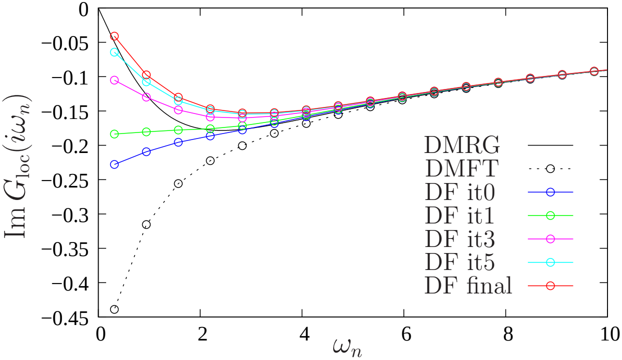
Self-consistency



$$\Delta_{\text{new}} = \Delta_{\text{old}} + g^{-1} G^{\mathrm{d}}_{\text{loc}} G^{-1}_{\text{loc}}$$

1D Hubbard model

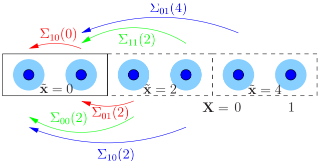
$U/t = 6,\ T/t = 0.1,\ h_{\mathbf{k}} = -2t\cos(ka)$, $\Sigma^{\mathrm{d}} =$ 

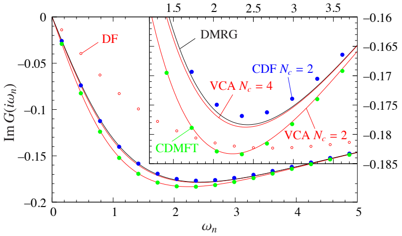


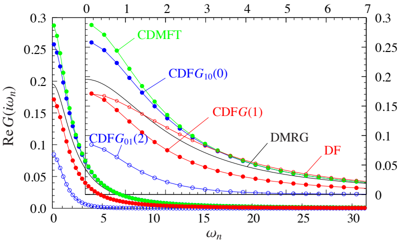
- Model is insulator for any finite U
- Nonlocal correlations change the environment (Δ)

1D Hubbard model

Cluster Dual Fermion





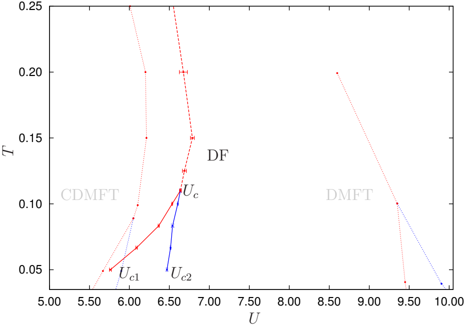


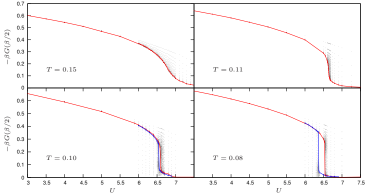
Significant improvement of the single-site solution

Diagrams have a tendency to restore translational invariance

2D Hubbard model: Mott transition

Second-order DF





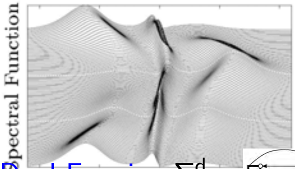
- Strong reduction of U_c compared to DMFT
- Short-range correlations reduce entropy of the Mott insulator

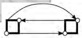
Method	U_c
DMFT(Park *et al.*, 2008)	9.35
CDMFT(Park *et al.*, 2008) (2×2)	6.05
DCA(Werner, 2013) (16 sites)	6.53
DF (this study)	6.64

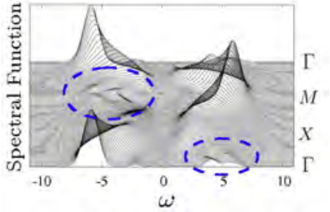
2D Hubbard model: Spectral function $A(\mathbf{k}, \omega)$

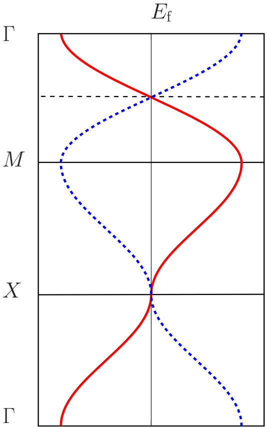
paramagnetic calculation $U/t = 8$, $T/t = 0.235$

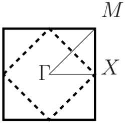
DMFT



Dual Fermion $\Sigma^{\mathrm{d}} =$ 







$\mathbf{Q} = (\pi, \pi)$

$\epsilon_{\mathbf{k}+\mathbf{Q}} = -\epsilon_{\mathbf{k}}$

- Strong modifications through *dynamical* AF short-range correlations

[S. Brener, HH, A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein PRB **77**, 195105 (2008)]

Convergence Properties

What are the small parameters?

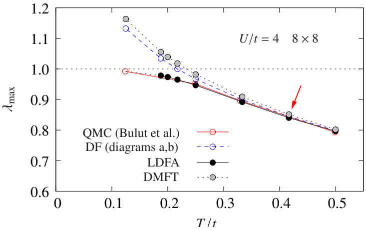
- Weak coupling limit ($U \to 0$): $\gamma^{(4)} \sim U\ , \gamma^{(6)} \sim U^2\ , \ldots$
- Strong coupling limit ($t \sim \varepsilon_{\mathbf{k}} \to 0$); atomic limit ($\Delta \equiv 0$):

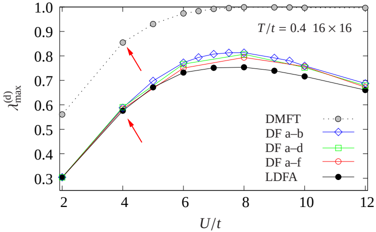
$$\tilde{G}^0_\nu(\mathbf{k}) = g_\nu \left[g_\nu + (\Delta - \varepsilon_{\mathbf{k}})^{-1} \right]^{-1} g_\nu \approx g_\nu \, \varepsilon_{\mathbf{k}} \, g_\nu$$

Large d-limit:

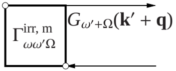
- Scaling $t \sim 1/\sqrt{d}$
- $\tilde{G}_{ii} = 0,\ \tilde{G}_{i\neq j} \sim 1/\sqrt{d}$
- Ladder diagrams leading at order $\sim 1/\sqrt{d}$

2D Hubbard model: ladder approximation





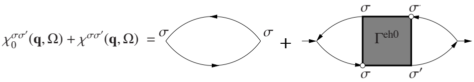
$$-\frac{T}{N}\sum_{\nu'\mathbf{k}'}\Gamma^{\text{irr, m}}_{\nu\nu'\omega=0}\, G_{\nu'}(\mathbf{k})\,G_{\nu'}(\mathbf{k}+\mathbf{Q})\,\phi_{\nu'} = \lambda\phi_{\nu'}$$

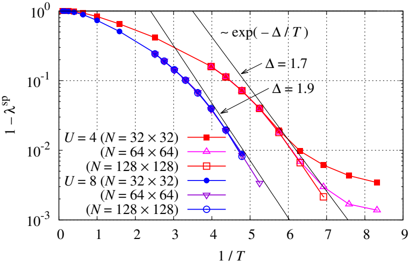


DF: $\Gamma^{\text{irr}} = \gamma^{(4)}$, $G = G^{\text{d}}$ DMFT: $\Gamma^{\text{irr}} = \gamma^{\text{irr}}_{\text{imp}}$, $G = G^{\text{DMFT}}$

[HH, G. Li, A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, H. Monien PRL **102**, 206401 (2009)]

2D Hubbard model: ladder approximation



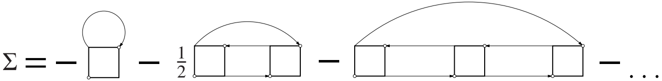


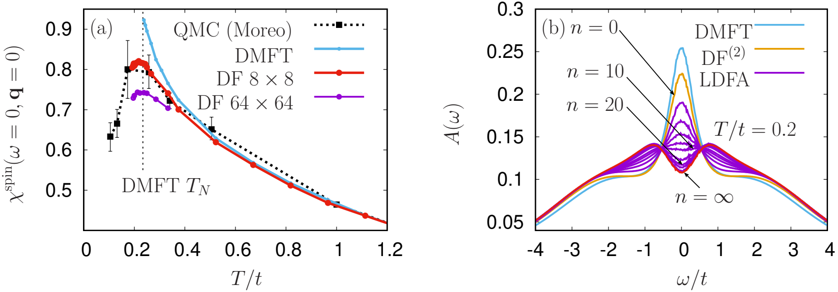
In the critical regime for $T \to 0$, $\chi \sim e^{\beta\Delta} \longrightarrow 1-\lambda \sim e^{-\beta\Delta}$

Néel temperature $T_{N=0}$ as required by Mermin-Wagner theorem

[Junya Otsuki, HH, Alexander I. Lichtenstein, Phys. Rev. B **90**, 235132 (2014)]

2D Hubbard model: ladder approximation



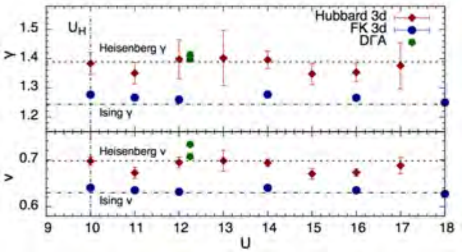


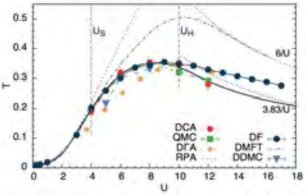
Downturn of susceptibility due to spin correlations (super-exchange)

Significant size-dependence

No more pinning of spectral function at Fermi level

[E. van Loon, HH, M. I. Katsnelson, Phys. Rev. B **97**, 085125 (2018)]





Critical exponents describe universal behavior of physical quantities near continuous phase transitions

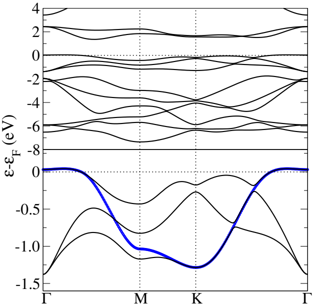
Fluctuations penetrate the entire system

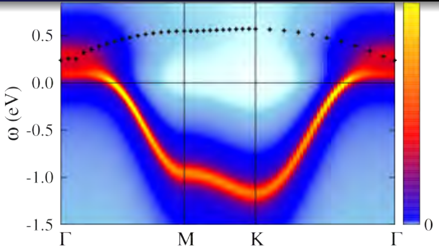
DΓA and DF reproduce the Heisenberg critical exponents

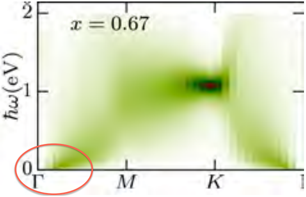
[A. Antipov, E. Gull, S. Kirchner, Phys. Rev. Lett. **107**, 256402 (2011)]
[G. Rohringer, A. Toschi, A. Katanin, K. Held, Phys. Rev. Lett. **112**, 226401 (2014)]
[D. Hirschmeier, HH, E. Gull, A. Lichtenstein, A. Antipov, Phys. Rev. B **92**, 144409 (2015)]

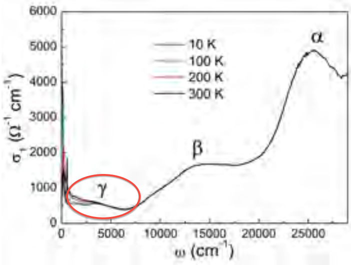
See lecture by K. Held on Friday

Spin polarons in Na_xCoO_2









Ladder approximation describes bound states between quasiparticles and paramagnons

[L. Boehnke, F. Lechermann, Phys. Rev. B **85**, 115128 (2012)]

[A. Wilhelm, F. Lechermann, HH, M. I. Katsnelson, A .I. Lichtenstein, Phys. Rev. B **91**, 155114 (2015)]

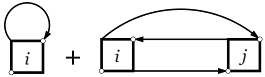
Real space dual fermion (RDF)

Real-space formulation for inhomogeneous systems

$$G_\nu^{\mathrm{RDMFT}} = \begin{pmatrix} i\nu_n+\mu-[\Sigma_\nu^{\mathrm{imp}}]_{11} & -t & 0 & \cdots & -t \\ -t & i\nu_n+\mu-[\Sigma_\nu^{\mathrm{imp}}]_{22} & -t & \cdots & 0 \\ 0 & -t & i\nu_n+\mu-[\Sigma_\nu^{\mathrm{imp}}]_{33} & \cdots & 0 \\ & & & \ddots & \\ -t & 0 & 0 & \cdots & i\nu_n+\mu-[\Sigma_\nu^{\mathrm{imp}}]_{NN} \end{pmatrix}$$

$$\begin{aligned}
&[\hat{\Sigma}^{\mathrm{d}}_{\nu\sigma}]_{ij} = \\
&-\frac{1}{2}T^2\sum_{\nu',\omega,\sigma'}\gamma^{\sigma\sigma\sigma'\sigma'}_{i\,\nu\nu'\omega}[\hat{G}^{\mathrm{d}}_{\nu+\omega\,\sigma}]_{ji}[\hat{G}^{\mathrm{d}}_{\nu'+\omega\,\sigma'}]_{ij}[\hat{G}^{\mathrm{d}}_{\nu'\,\sigma'}]_{ji}\gamma^{\sigma'\sigma'\sigma\sigma}_{j\,\nu'\nu\omega} \\
&-\frac{1}{2}T^2\sum_{\nu',\omega}\gamma^{\bar{\sigma}\sigma\sigma\bar{\sigma}}_{i\,\nu\nu'\omega}[\hat{G}^{\mathrm{d}}_{\nu+\omega\,\bar{\sigma}}]_{ji}[\hat{G}^{\mathrm{d}}_{\nu'+\omega\,\bar{\sigma}}]_{ij}[\hat{G}^{\mathrm{d}}_{\nu'\,\sigma}]_{ji}\gamma^{\bar{\sigma}\sigma\sigma\bar{\sigma}}_{j\,\nu'\nu\omega}.
\end{aligned}$$

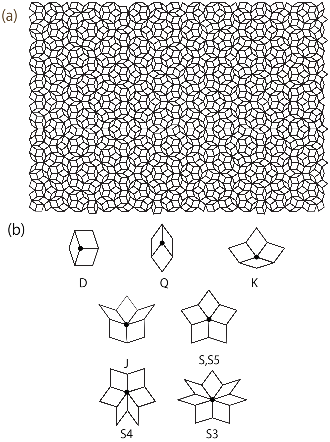
$$[\hat{\Sigma}_\nu]_{ij} = [\hat{\Sigma}^{\mathrm{imp}}_\nu]_{ii}\delta_{ij} + [(\hat{1}+\hat{\Sigma}^{\mathrm{d}}_\nu\hat{g}_\nu)^{-1}\hat{\Sigma}^{\mathrm{d}}_\nu]_{ij}.$$

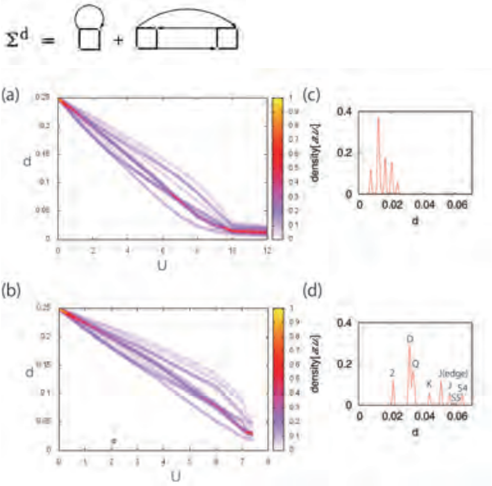
$\Sigma^{\mathrm{d}}_{i,j} =$ 

Diagrammatic extension of real-space DMFT (RMDFT)

Real space dual fermion

Quasicrystals: the Penrose lattice





coordination numbers

3 (D,Q), 4 (K), 5 (J, S, S5), 6 (S4) and 7 (S3)

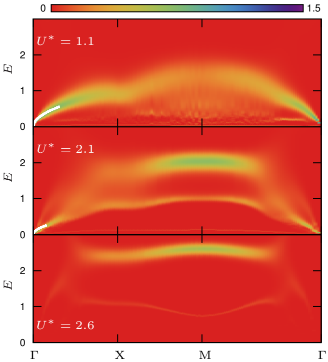
$T = 0.1$, $U = 10.0$ for RDMFT, $U = 7.2$ for RDF

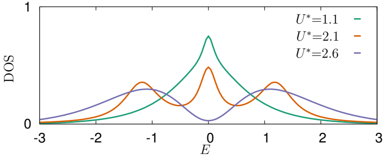
RDF double occupancy not only depends on coordination number, but also on coordination of neigbors

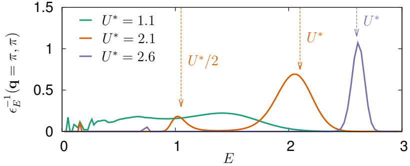
[Nayuta Takemori, Akihisa Koga, HH, J. Phys.: Conf. Ser. **683**, 012040 (2016); arXiv:1801.02441]

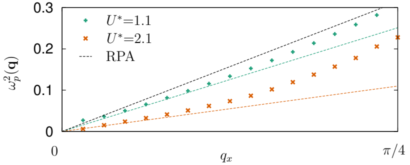
Dual bosons: surface plasmons ($V_{\mathbf{q}} = V/q$)

Conserving description of plasmons in the correlated state









Spectral weight transfer and renormalized dispersion !

[E. van Loon, HH, A. I. Lichtenstein, A. N. Rubtsov, M. I. Katsnelson, PRL **113**, 246407 (2014)]

What's missing?

Did not cover applications to following models

- Extended Hubbard model
- Kondo lattice model
- Falikov-Kimball model

and scenarios

- Non-equilibrium systems
- Disordered systems
- Symmetry broken phases
- Multi-orbital systems
- ...

Can be combined with clusters, weak-coupling approaches (Diagrammatic Monte Carlo, functional RG, ...)

[Rev. Mod. Phys. **90**, 025003 (2018)]

What's next?

Combination of diagrammatic extensions of DMFT with electronic structure methods

- Realistic treatment of spatial correlations in materials
- Restricted to single-band models so far
- Technically challenging but highly rewarding

Many interesting open questions:

- Role of multi-particle interactions?
- What are good approximations (in terms of relevant physics, conservation laws, diagrams . . .)?

Further reading:

- Comprehensive review: Rev. Mod. Phys. **90**, 025003 (2018).
- Textbook: e.g. Negele & Orland.
- Technical derivations: PhD thesis $\rightarrow$ please send me an email.

Stay curious!