Diagrammatic extensions of dynamical mean-field theory

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Physics in terms of Feynman diagrammatic series:

\[ \Sigma(p, \tau) = \bigcirc + \bigcirc \bigtriangleup + \bigcirc \bigtriangleup + \ldots \]

For fermions: sign alternation between terms \( \Rightarrow \) diag. series can converge...

Sum the series and see what happens!

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Diagrammatic Monte Carlo in a nutshell: *stochastic sampling of Feynman diagrams*

Configuration space = (diagram order, topology, internal variables)

*Diagrammatic Monte Carlo sampling:* generate diagrams with probability

\[ P \propto |W_v| \]

\( W_v \) - integrand of each term

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Sign alternation \( \Rightarrow \) *SIGN PROBLEM for MC!*
Stochastic summation of all diagrams by DiagMC:

\[ \Sigma(p, \tau) = \bullet + \quad + \quad + \ldots \]

Sign problem \( \Leftrightarrow \) computational complexity scales as

\[ \exp[\#(\text{max. diagram order})] \]

( to be compared to \( \exp[\# V/T] \) in QMC solvers )

Inherent flexibility – full use of analytic “tricks” of diagrammatic technique:

- calculate *irreducible* diagrams (self-energy, vertex functions) + get the rest by *Dyson, Bethe-Salpeter*
- can use *bare* or *skeleton* (bold-line) expansions in different channels (bold Green’s functions, interaction vertices, etc.) + *self-consistency*

Inherent limitations:

- need to enforce diagram order cutoff \( N \) and extrapolate \( N \rightarrow \infty \)
- accessible \( N = 5-10 \)
- how fast does the series converge, if at all?
- if converges, *does it give the correct answer???*
If physics is local -> **non-perturbative solution**: *Dynamical Mean-Field Theory*  

[Georges and Kotliar]

By solving auxiliary quantum impurity problem with a self-consistency condition:

- only approximation: *local self-energy* \( \Sigma(\mathbf{k}, i\omega) \equiv \Sigma(i\omega) \)
- captures strong renormalization effects, e.g, *Mott insulator* physics
- powerful CT-QMC algorithms [E. Gull et al., *RMP*, 2010] for the impurity problem *no sign problem!*

... but can also be written naturally in terms of skeleton diagrams!

\[
\Sigma_{ii}(i\omega_n) = \sum_i G_{ii} \left( i\omega_n \right) = \sum_i \left( i \right) G_{ii} \left( i\omega_n \right) + \left( i \right) \rightarrow \text{local Green's function}
\]
Take advantage of individual strengths of DMFT and DiagMC by combining the two!

Underlying idea:

- use impurity solvers to calculate the *local self-energy* non-perturbatively
- capture *momentum dependence* by summing *only* the *remaining* diagrams using DiagMC to obtain a *controlled solution*

Main gain:

- The *remaining* diagrammatic series for may *converge faster* or may just be *small in certain regimes*
Original proposal [Pollet, Prokof‘ev, Svistunov]:
skeleton (bold-line) series protocol

BUT...

Fails for the Hubbard model for two reasons:

• the map $\Sigma_{\text{imp}} \rightarrow G_{\text{loc}}$ is not invertible: $\Sigma_{\text{imp}}\left[G_{\text{loc}}\right]$ has at least two branches
  -- *the iteration scheme converges to the unphysical branch!*

• the skeleton series for $\Sigma'[G]$ *converges to the corresponding unphysical branch!*

( ill-defined Luttinger-Ward functional for Hubbard interaction: *Michel’s talk* )

[EK, Ferrero, Georges]
Good news: **Bare** series appears to converge to the right answer!

(naturally, as a Taylor series...)

Propose DMFT+DiagMC protocol based on the bare series:

**Step 1.** Represent $\Sigma_{\text{imp}}$ by bare series

(equivalently: take the limit of infinite $D$ in the bare series for the full model):

$$\Sigma_{\text{imp}}(i\omega_n) = \quad \begin{array}{c}
\begin{array}{c}
\text{bare diagrams truncated at order } n
\end{array}
\end{array}
\quad + \quad \begin{array}{c}
\begin{array}{c}
\text{all bare diagrams truncated at order } n
\end{array}
\end{array}
\quad \begin{array}{c}
\begin{array}{c}
\text{bare DMFT diagrams truncated at order } n
\end{array}
\end{array}
\quad + \quad \begin{array}{c}
\begin{array}{c}
\text{full DMFT solution}
\end{array}
\end{array}
\quad + \ldots
$$

**Step 2.** Find the *exact* self-energy from the formal relation:

$$\Sigma_k = \lim_{n \to \infty} \left[ \Sigma_k^{(n)} - \Sigma_{\text{imp}}^{(n)} \right] + \Sigma_{\text{imp}}^{(\text{DMFT})}$$
Hubbard model at half filling (work in progress):
benchmark – determinant diagrammatic MC (DDMC) [Burovski, Prokof’ev, Svistunov, Troyer]

\[ \Sigma_{\text{loc}} = \sum_{\mathbf{k}} \sum_{\mathbf{k}} \]

up to order 4...

\[ \Sigma_{\omega_n} \]

\[ U/t=8, \ T/t=0.5, \ n=1 \]
Hubbard model at half filling (work in progress):
benchmark – determinant diagrammatic MC (DDMC) [Burovski, Prokof’ev, Svistunov, Troyer]

\textit{momentum dependence:}

\textbf{U/t=8, T/t=0.5, n=1}

\textbf{just bare series:} \hspace{0.5\textwidth} \textbf{DMFT+DiagMC:}

\textit{at half-filling the bare series works too good...}
Doped Hubbard model at half filling (work in progress): \( U/t=8, \ T/t=0.5, \ n=1.04(1) \)

bare series: *poor convergence... but...* bare series for DMFT is the same!

\[ \Sigma_{\text{loc}} = \sum_k \Sigma_k \]

\[ \Sigma_k = \lim_{n \to \infty} \left[ \Sigma_k^{(n)} - \Sigma_{\text{imp}}^{(n)} \right] + \Sigma^{(\text{DMFT})}_{\text{imp}} \]

“Regularization” of the bare series by excluding DMFT diagrams!
DMFT+ DiagMC, outlook:

• systematic study of the applicability limits + benchmarks

• also in 3D? – probably works better?

• “algorithmic” improvements to the DiagMC solver
  
  \((\text{together with the Monte Carlo Group...})\)

• the same simplest scheme should work even better with cluster extensions!

\[
\Sigma_k = \lim_{n \to \infty} \left[ \Sigma_k^{(n)} - \Sigma_{\text{imp}}^{(n)} \right] + \Sigma_{\text{imp}}^{(\text{DMFT})}
\]

\[
\Sigma_k = \lim_{n \to \infty} \left[ \Sigma_k^{(n)} - \Sigma_{\text{cluster}}^{(n)} \right] + \Sigma_{\text{cluster}}^{(\text{DCA})}
\]

???