Numerical studies of Correlated Materials with Diagrammatic Monte Carlo Techniques

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Diagrams & Monte Carlo

\[ H = H_1 + H_2 \]

Hamiltonian \( H \) for finite system at non-zero temperature, split into two parts: convenient / noninteracting / exactly known part \( H_1 \); ‘rest’ \( H_2 \). Convergent interaction expansion of \( H_2 \) with respect to \( H_1 \).

Infinite sum of terms (‘diagrams’) with varying number of tau points (and potentially) internal indices. Traditionally: pick some ‘relevant’ or low-order terms, sum them up analytically, neglect the rest.

Here: perform importance sampling of diagrams: randomly generate all of them with the weight that they contribute to \( Z \). Exact answer within Monte Carlo error, convergence guaranteed by central limit theorem.

Interaction Expansion

‘Standard’ method for cluster dynamical mean field theory on clusters with more than four sites.

Choose \( H_1 \) as the non-interacting term, \( H_2 \) as the interaction. In practice limited to density-density interactions, simple band structures, best near particle hole symmetry (Hubbard models).

Ideally coupled to embedding scheme (DCA, DMFT, etc); up to 100 lattice sites at high \( T \); on small Hubbard systems (8-site, 16-site clusters) results down to \( T \sim T_c \).

Hybridization Expansion

‘Standard’ method for ‘real materials’ DMFT (LDA+DMFT, GW +DMFT, etc) for quantum impurity systems.

Choose \( H_1 \) as the local term, \( H_2 \) as the hybridization term of the impurity with its bath. In practice limited to ~5–7 impurity orbitals but fully general local interactions, band structures.

Complementary to interaction expansion: efficient where local physics important, hybridization weak.

Inchworm Expansion

Keep diagram expansion order as low as possible (e.g. to simplify normalization to analytic results, reduce sign problem).

Simulate (exact) propagator up to some time as (exact) propagator propagates to a shorter time + corrections. If time difference is small, few correction diagrams.

Works well for real-time expansions of quantum impurity problems, allows access to long-time behavior at quadratic (rather than exponential) cost.

Convergence

- Not necessarily ‘weak coupling’
- Typical diagram orders strongly problem dependent, maximum average order ~3000
- No explicit truncation of diagram order
- Typical order \( \sim \beta(H_2) \)

Often sequence of finite systems followed by TL extrapolation.

Finite size? \( \beta \gg L \).

Careful near phase transitions!

Maximum Fluctuations

Where in \( U/n \) space is the (high-\( T \)) \( \delta \)-wave susceptibility of the single orbital Hubbard model the largest?

8-site DCA, calculation of the vertex function, inversion of the Bethe Salpeter equation.

Data obtained at \( T \sim 2 \, T_{\text{max}} \) for different \( U \).

What about other types of superconductivity?

The ‘sign problem’

Diagrammatic expansion is just a Taylor series! There is no guarantee that terms are positive. In practice, this leads to the ‘sign’ problem.

Most algorithms are exponential in cost (in \( U, 1/T, \) system size, real time, …) away from high symmetry points (though still numerically exact). In practice: how far can an algorithm be pushed in the presence of a sign problem?

Details matter. Often:
1. Embedding (cluster DMFT) helps
2. Changing/rotating basis may help
3. Explicitly respecting symmetries helps
4. Adapt the algorithm to the problem at hand.

Kondo Voltage Splitting

\[ g \]

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Maximum Fluctuations

- For the same problem: problem size reduced by \( \sim 10^0 \).
- Corresponds to time speedup of factor \( 30 \sim 27000 \) or >25 years of Moore’s law

Speed & Accuracy

- Same problem solved more accurately
- Elimination of bias and systematic errors (Trotter discretization errors)

Bold Line Expansion

Often analytic diagrammatic results are available (and easy to get). Use them as a starting point for the numerical Examples: RPA, the non-crossing approximation, the one-crossing approximation, etc.

Stochastically sample corrections to analytics.

- If analytics is good: corrections are small, Monte Carlo converges instantly.
- If analytics is decent: Monte Carlo can provide the exact result.

- If diagrammatically diagrams irrelevant: Monte Carlo will need to work as hard as bare expansion, will still always get right result.

Spectral Functions

\[ W_{\text{av}} = \min \left( 1, \frac{w(c')}{w(c)} \right) \]

DIY DiagMC

1. Find a convergent diagrammatic expansion (finite-\( T \), finite system size, finite real time, etc)
2. Write the partition function in the form
3. Write the observables of interest as functions of \( c \)
4. Define a sequence of updates; given a configuration \( c \), generate a new configuration \( c' \) by changing part of \( c \) (adding a new interaction vertex, changing a time, adding/moving time, etc).
5. Make sure any diagram can be reached from any other diagram in a finite number of steps.
6. Perform a Metropolis sampling: