Diagrammatic Monte Carlo

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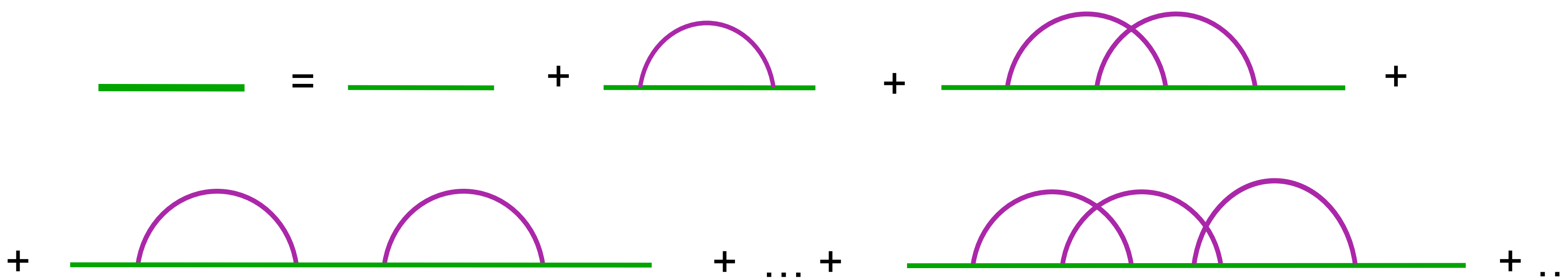
Feynman's Diagrams

Generic structure of diagrammatic expansions:

$$Q(y) = \sum_{m=0}^{\infty} \sum_{\xi_m} \int D(\xi_m, y, x_1, x_2, \ldots, x_m)\, dx_1\, dx_2 \cdots dx_m$$

These functions are visualized with diagrams.

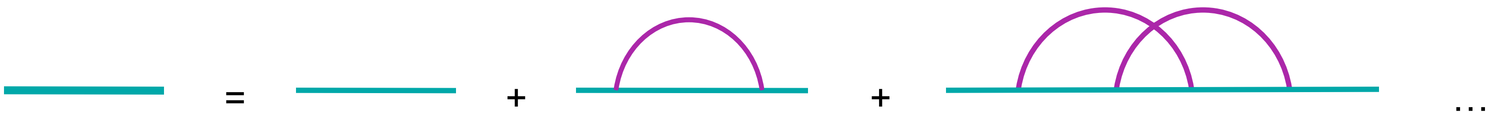
Example:



$Q(y)$ **can be sampled by Monte Carlo** *(Prokof'ev and Svistunov, 1998).*

General principles of Diagrammatic Monte Carlo

Take a diagrammatic series, say the one for polaron Green's function,



and interpret it as a partition function for an ensemble of graphical objects (diagrams). Introduce a Markov process generating ensemble, and calculate corresponding histograms/averages.

The Markov process is organized in the form of pairs of complementary updates. In such a pair, A-B, the update A creates a new graphical element with corresponding continuous variables, while the update B removes the element. For example, A creates a new propagator, while B removes it:

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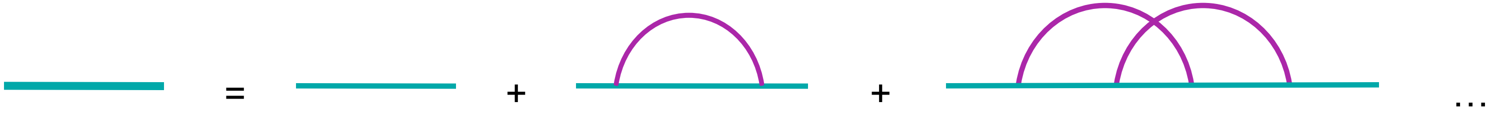

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Balancing diagrammatic Markov process by (generalized) Metropolis-Hastings algorithm

Acceptance ratios for complementary updates A-B

$$R_A\left(\vec{X}\right) = \frac{New\,Diagram}{Old\,Diagram}\,\frac{1}{W\left(\vec{X}\right)}$$

$$R_B\left(\vec{X}\right) = \frac{New\,Diagram}{Old\,Diagram}\,W\left(\vec{X}\right)$$

Arbitrary distribution function for generating particular values of new continuous variables in the update A

The issue of summability: Can an asymptotic series be regularized?

Dyson's argument: *The perturbative series has **zero convergence radius** if changing the sign of interaction renders the system pathological.*

BUT

1. Fermions can be put on a lattice…

2. Bosons can be represented as pairs of fermions…

3. Other regularization tricks seem to be possible.

Sign PROBLEM and Sign PROBLEM

Extensive configurational space

$$\text{Complexity} \propto e^{V/V_0}$$

V is the configuration volume

V_0 is the correlation volume

$$V/V_0 \sim 10^2$$

Diagrams (intensive configurational space)

$$\text{Complexity} = C\,(N!)^m$$

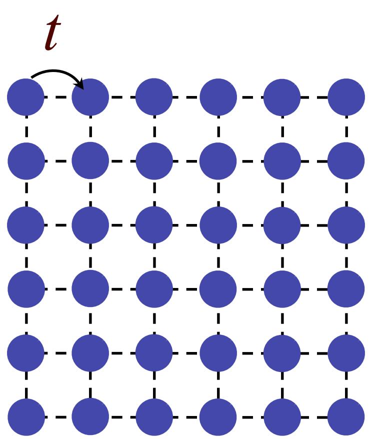
$N \lesssim 10$ is the diagram order

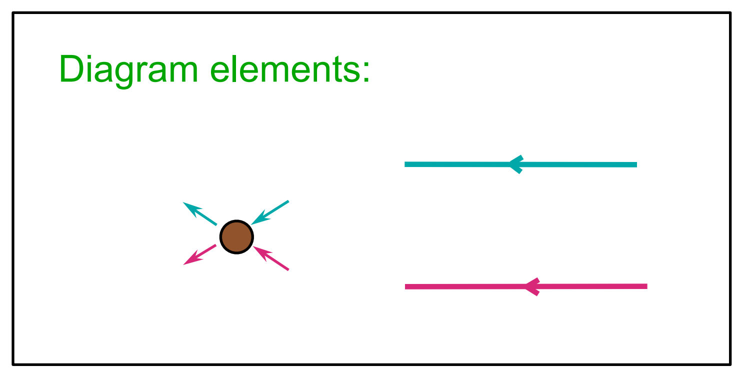
$$m \sim 1, \qquad C \sim 1$$

C can be significantly reduced by partial summation

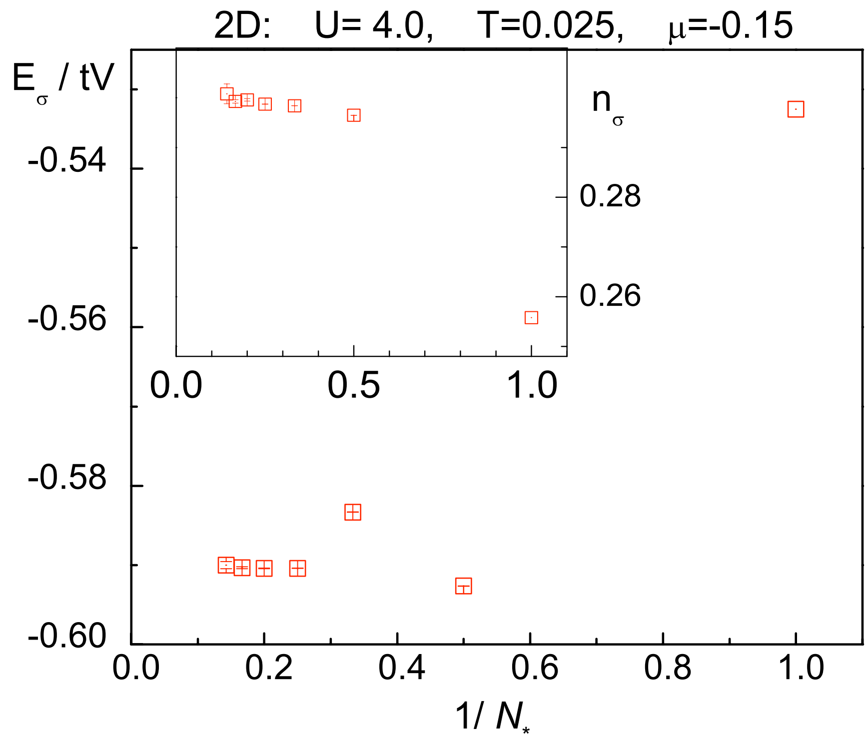
Hubbard model

$$H = -t \sum_{\substack{<ij> \\ \sigma=\uparrow,\downarrow}} a^{+}_{\sigma i}\, a_{\sigma j} + U \sum_{i} n_{\uparrow i}\, n_{\downarrow i}\,, \qquad n_{\sigma i} = a^{+}_{\sigma i} a_{\sigma i}$$

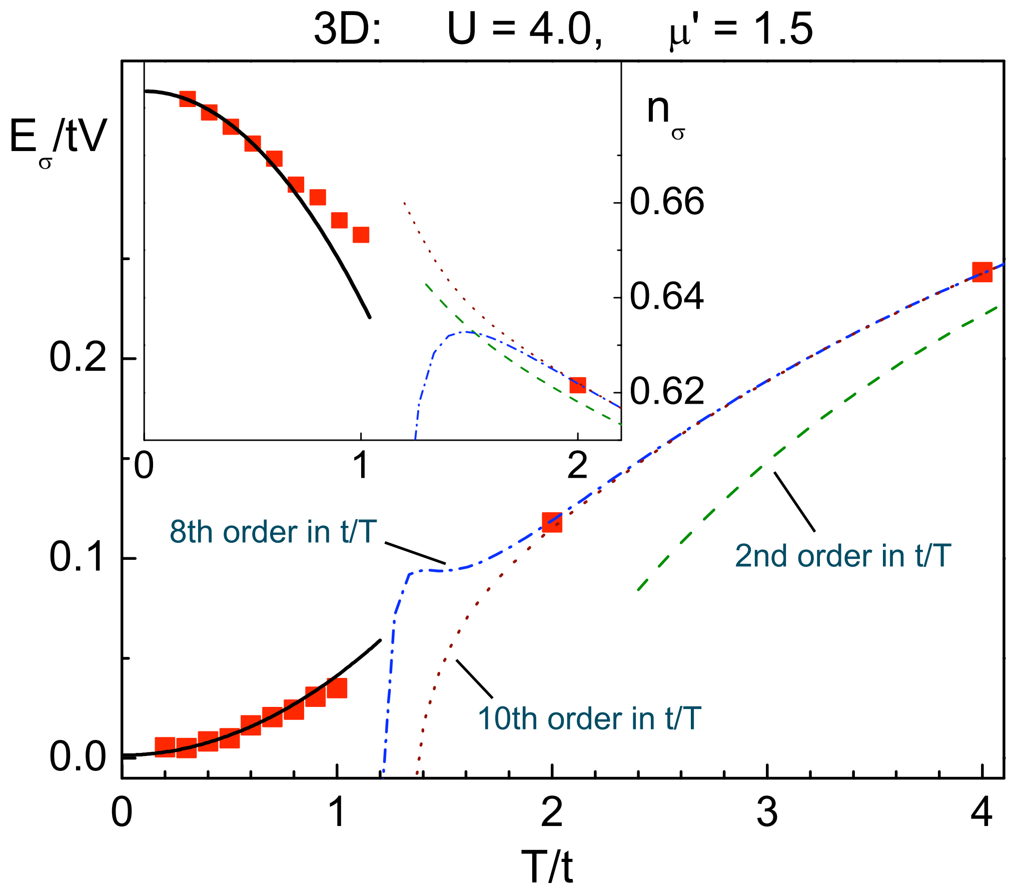




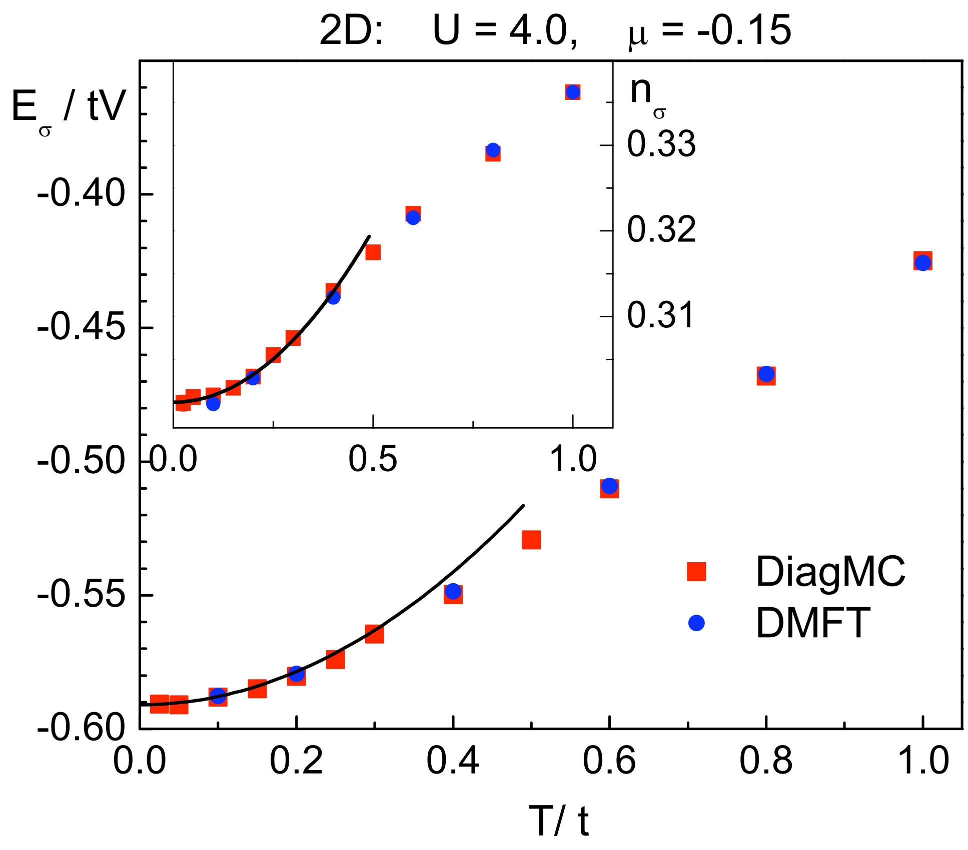
The Convergence



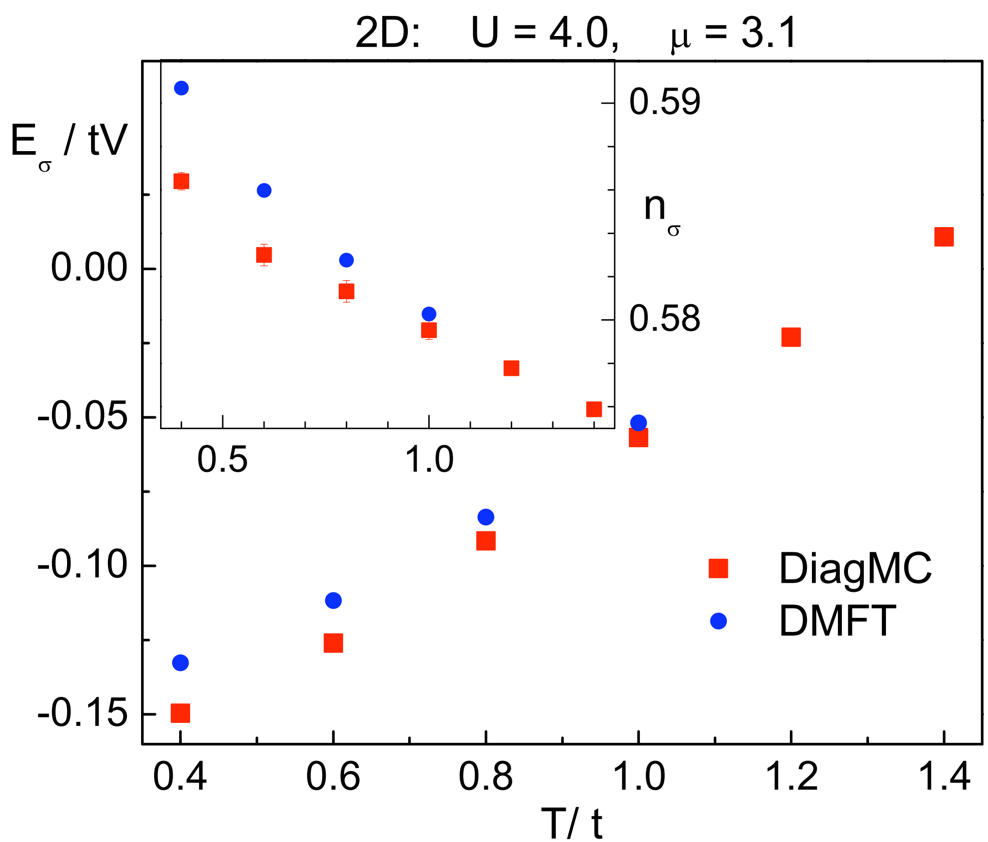
DiagMC vs HTSE



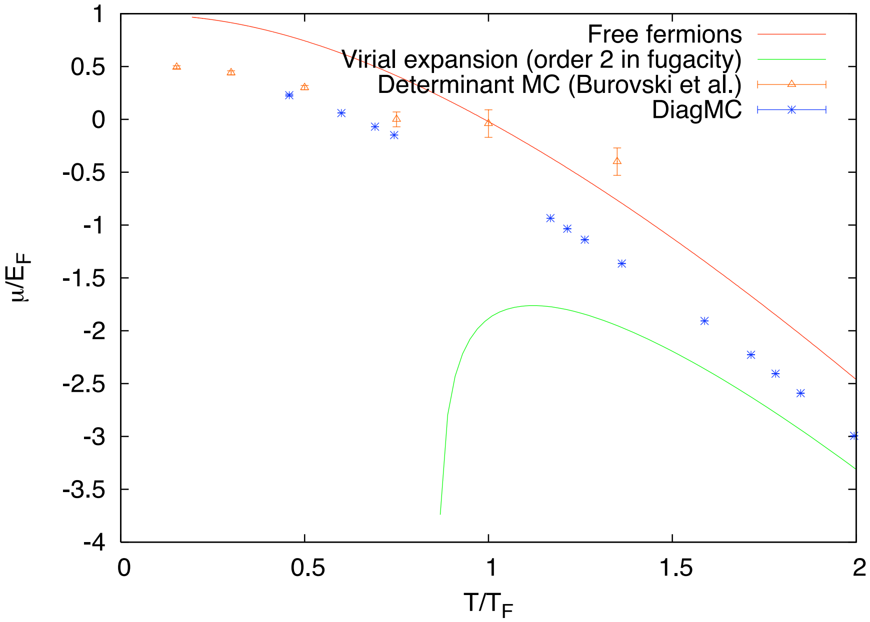
DiagMC vs DMFT

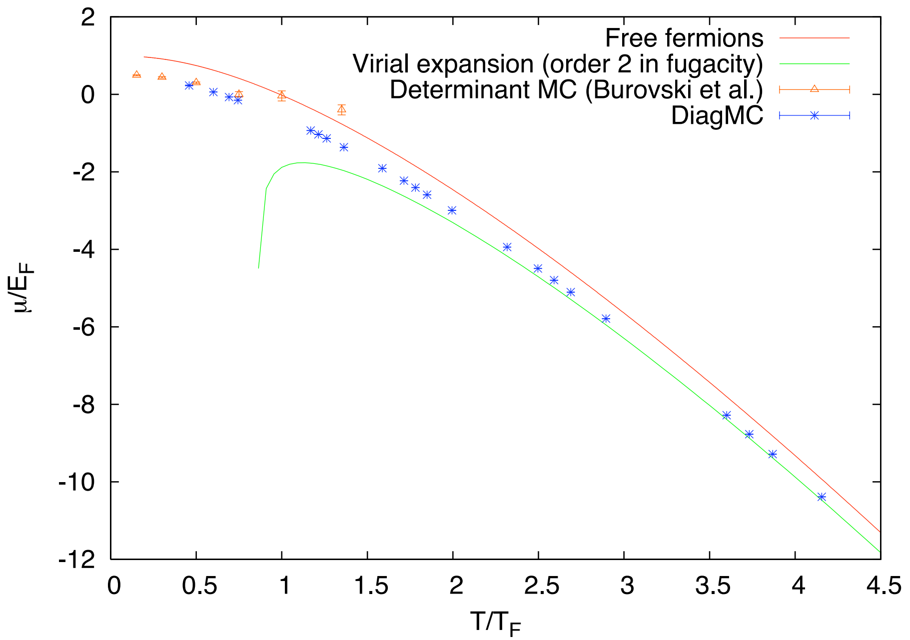


DiagMC vs DMFT (continued)



Resonant Fermions at unitarity: Equation of State





immediate application to experiments in a trap:

thermometry through the wings