Heuristic intro to some Quantum Monte Carlo and selected applications

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Overview

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What MC for what ?

- Spin systems (Heisenberg) ⇒ **SSE**
- Lattice systems ⇒ **Af-QMC**
- (Anderson) Impurity problems ⇒ **CTQMC**

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- CTQMC Coherent States path integrals.
- SSE Taylor expansion in a cleverly chosen basis of H (avoid sign-problem).
- AF-QMC Hubbard-Stratonovich transformation $\Rightarrow$ independent Ising spins "basis".

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2. Calculate the expectation value for the energy with this given wave function.
3. Find a minimum (variational energy) with respect to the variational parameters.
4. Calculate various physical observables with the wave function obtained previously.

$\Rightarrow$ x := "real-space configuration", and $\boldsymbol{\alpha}$:= "variational parameters".

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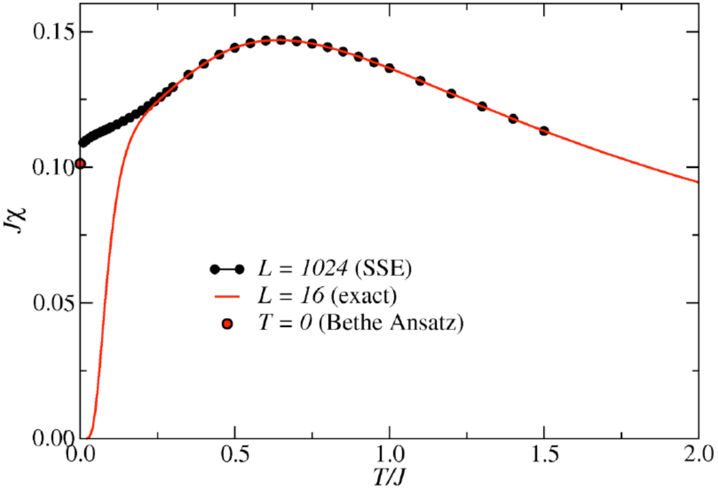
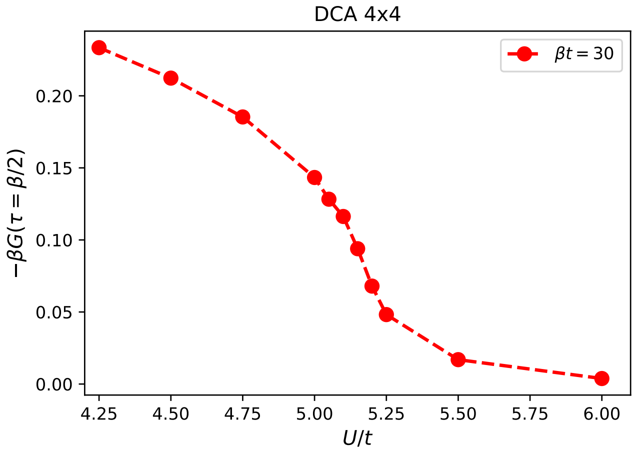
SSE Application : 1D Heisenberg Model

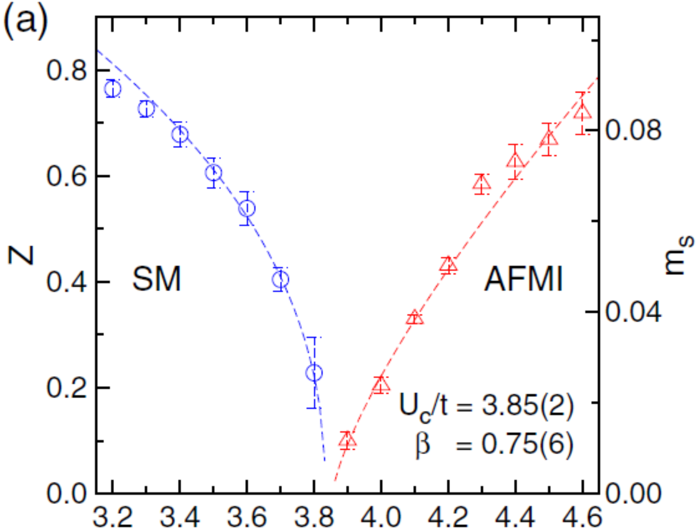


CTQMC Application : Metal-Insulator Crossover on the square lattice



[2].

AF-QMC Application : The ground-state phase diagram for the honeycomb lattice model



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