Projects for Computational Physics

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The Hubbard Model in Low-Dimensions

Preparation(**), Implementation(**), Analysis(*)

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1. Project Description

Though the Hubbard Model is one of the simplest ways of modelling the interactions of electrons in solids, it provides great insight into how strong correlations (between electrons) can give rise to insulating, magnetic, and even superconducting phenomena. The Hamiltonian is given by

$$H = -t \sum_{\langle i,j \rangle, s} a_{i,s}^{\dagger} a_{j,s} + U \sum_i n_{i,\uparrow} n_{j,\downarrow} \ ,$$

where $\langle i,j \rangle$ denotes nearest neighbor couplings, s refers to either $\uparrow$ or $\downarrow$, t is the "hopping" parameter that dictates the dynamics of the system, U is the onsite interacting Hubbard term, and

$$n_{i,s} = a_{i,s}^{\dagger} a_{i,s} \ ,$$

is the number operator for spin s at site i. Because we are dealing with fermions, the electron creation ($a_{i,s}^{\dagger}$) and annihiliation ($a_{i,s}$) operators satisfy anti-commutation relations.

For 2 spatial dimensions and higher, surprisingly not much is known analytically about this model, though there have been many numerical studies. For 1 dimension, under the *Bethe ansatz*, the Hubbard model has been solved analytically. For this problem, apply Monte Carlo methods to investigate the Hubbard Model in 1 dimension. If this is too easy, go to 2 dimensions. Good luck!

2. Tasks / hints / interesting problems[1]

- Start small first. Look at the one-site and two-site systems, which can be solved exactly. Calculate the exact correlators in this case.

- Implement your Monte Carlo calculation of this system (what is your multi-dimensional integral in this case?) and compare with your exact solutions.

- Once they agree, crank up the number of sites.

Literature

[1] *The one-dimensional Hubbard model: a reminiscience*, E. Lieb and F. Wu, Physica A: Statistical Mechanics and its Applications **321** (2003) 1-27

[1] *The Hubbard model–an introduction and selected rigorous results*, H. Tasaki, J. Phys.: Condesed Matter **10** (1998) 4353

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[1]These tasks should rather be considered a general guideline than a strict requirement. Besides, the list is by no means complete and could easily be extended