Non-equilibrium analysis of the antiferromagnetic ordering in the half-filled Hubbard Model in two dimensions

Hans-Georg Mattutis, Ito Nobuyasu
Department of Applied Physics, School of Engineering,
The University of Tokyo, Bunkyo-ku, Tokyo 113-8646, Japan

1. Introduction

In the canonical Hubbard Hamiltonian,

$$\hat{H} = -t \sum_{i,j,\sigma} (c_i^+ c_j + c_j^+ c_i) + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

$c_{i\sigma}^+ (c_{i\sigma})$ denotes the electron creators (annihilators), electron densities are written $n_{i\uparrow}, n_{i\downarrow}$, and the hopping parameter and the strength of the on-site Coulomb-repulsion are denoted by t and U, respectively. There is a general agreement that at half-filling, the Hubbard model should exhibit anti-ferromagnetic order in the strong coupling limit. There is nevertheless no clear value given in the literature for which the system can be reliably considered to be in the strong-coupling range. In this paper, we focus on the determination of bounds for the strong coupling limit for finite systems using the nonequilibrium relaxation (NER) method. The NER-method has in the meantime been successfully applied to classical systems[1], quantum spin systems[2] and fermionic systems[3].

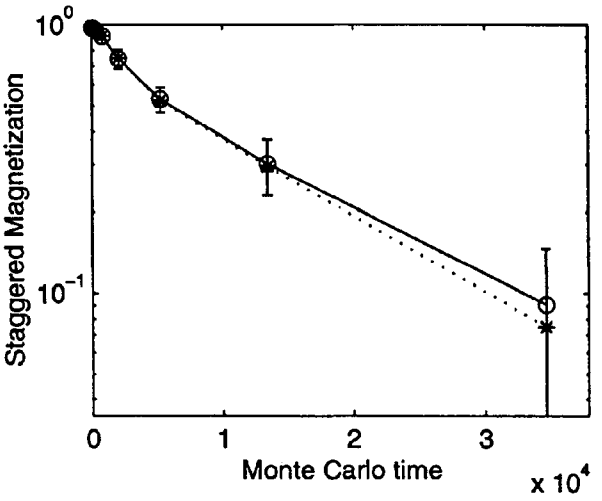

Fig. 1: Relaxation of the staggered magnetization of a 6×6 system with U=4, $\tau = 0.05$ and 120 slices for two different test wave functions (circles: plane waves, stars: anti-ferromagnetic test function).

2. Algorithm

We perform the NER-analysis of quantum Monte Carlo simulations using the auxiliary field ground state algorithm. This "projector formalism" allows to filter the ground-state $|0\rangle$ from a given trial state $|T\rangle$ via the exponential of the system's Hamiltonian,

$$e^{-\theta\hat{H}}|T\rangle = e^{-\theta\hat{H}} \sum_n \langle n|T\rangle \cdot |n\rangle =$$

$$e^{-\theta E_0} \left(\langle 0|T\rangle \cdot |0\rangle + \sum_{n>0} e^{-\theta(E_n - E_0)} \langle n|T\rangle \cdot |n\rangle \right).$$

The excited states $E_i, i > 0$ are exponentially suppressed with respect to the ground-state energy E_0. Though the projection formalism looks very much like a finite time Greens function, the projection parameter θ cannot be interpreted as a temperature. As can be seen from Fig. 1, the

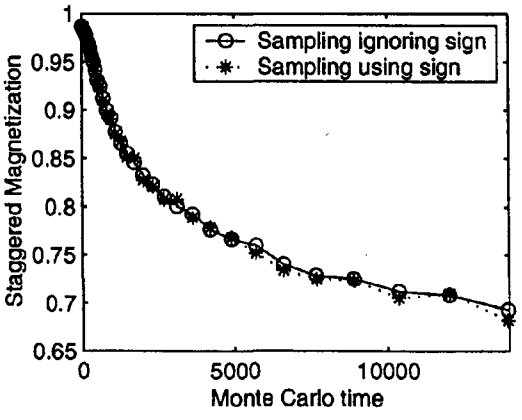

Fig. 2: Relaxation of the staggered magnetization of a 4 × 4 × 4 system with $U = 15$, $\tau = 0.05$ and 160 slices, sampled with (stars) and without sign (circles). The errorbars are of the size of the symbols.

trial wave function has practically no influence on the speed of the relaxation, where both plane waves and anti-ferromagnetic states show the same decay of the staggered magnetization.

In the quantum Monte Carlo (QMC) formalism, the projector is first decomposed using the Suzuki Trotter decomposition[5], and then the Hubbard-Stratonovich transformation[6] is applied to obtain a description of the problem in terms of auxiliary fields variables with a smaller Matrix size than that of the original Hamiltonian.

We have found in previous studies using large Hubbard-U, it is necessary to use a multi-spin update for the Hubbard Stratonovich configuration. For the single-spin update scheme, the values for the ground-state were consistently off the values for numeric diagonalization results. As the single-spin update scheme imposes a certain time ordering in which the Trotter-slices are updated, this leads to a computationally efficient algorithm, but due to the ordering, the ergodicity is strongly in question.

For the grand-canonical "Hirsch-Algorithm" for finite temperature, it is possible to show that the sign of the half-filled Hubbard Model with nearest-neighbor hopping is strictly positive definite[4]. The proof used the cyclic permutation of the trace, which is not possible for the projector-formalism. As cyclic permutation is not possible for the trace of the ground-state expectation value, the transition probability is not strictly positive. As we had confirmed for other Hubbard systems for the ground-state energy[7] and superconducting correlations functions[8], within the statistical fluctuations observables computed from equal-time Greens functions are the same for sampling with and without sign.

3. NER in Classical and Quantum Systems

There are some aspects of the NER which are different for the Hubbard system than for many classical models. One aspect is that for quantum Monte Carlo simulations, the Trotter direction adds an additional dimension to the system.

The projection parameter θ, which does not exist for classical systems, has to be chosen large enough, so that the contribution of the excited states are effectively suppressed. We chose $\theta = 4$ for the left and the right side, so that the exponential operator computed in total was $\exp(-8H.)$ The Trotter time-step, which does not exist for classical simulations, is not a free parameter, but determines the accuracy of the breakup. When we scan a regime of interactions U, one must keep in mind that the accuracy is lowest for the largest interaction. Due to the the Suzuki Trotter decomposition, the fluctuations will become largest for the largest U, so that bad statistics compensates for the computer time saved in using less Trotter slices. As it turned out that the transitions occurred at rather large U, an additional constraint on the Trotter step became the numerical stabilization after each slice. If the stabilization comes too late (too many or, too large Trotter slice),

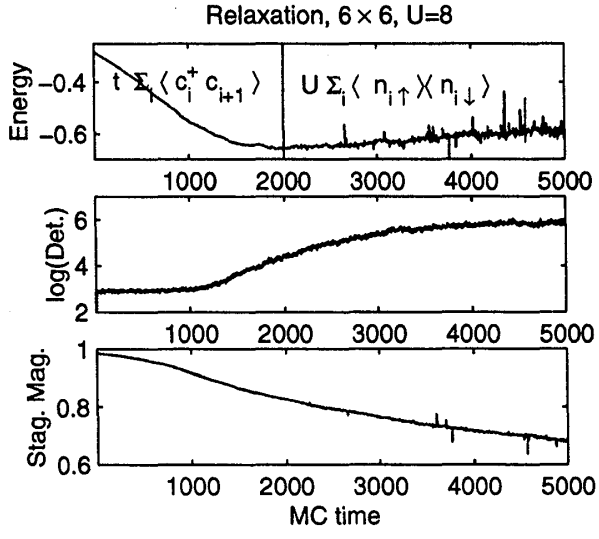

Fig. 3: Relaxation of the Energy (upper graph), transition probability (middle) and staggered magnetization (lower graph) for a 6 × 6 system with U=8.

the result of the simulation is numerically contaminated and therefore meaningless. We verified the parameters (Trotter-time-step and projection parameter) for equilibrium runs of half-filled 4×4 systems for $U = 20$ with numerical diagonalization results.

In classical systems, it is possible to run the NER-method even for a dynamics which does not necessarily guarantee that the equilibrium can be reached. However, it turned out that is was not feasible to obtain faster reliable algorithms by using smaller projection parameters for the non-equilibrium runs than those in the equilibrium simulations.

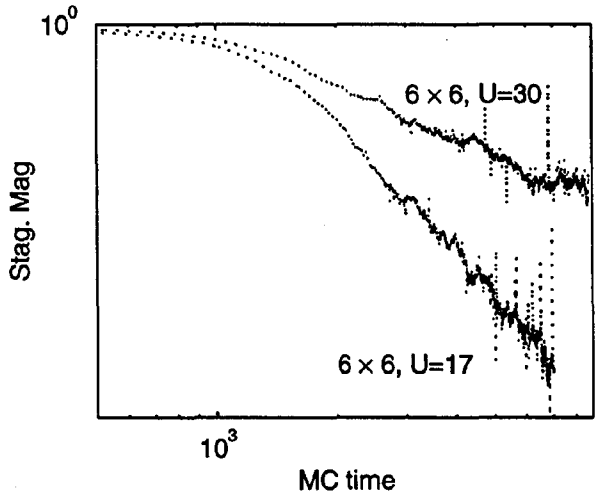

Fig. 4: NER of the two-dimensional half-filled Hubbard-model for a 6 × 6 system at U=17 and U=30.

A curious result of the simulation can be seen in Fig. 3. In a classical spin system, the energy determines the transition probability, and, as in a nearest-neighbor interaction system, there is only a single time-scale, the energy behaves monotonically. In the Hubbard system, the relaxations of the interaction energy and the kinetic energy occurs on different time-scales, and for the parameters shown in Fig. 3, a relative minimum in the relaxation occurs. In contrast, the transition probability, which is computed from the Fermion determinant, behaves monotonically. The spatial system size has a rather strong influence on the observables in computer simulations of classical systems at the critical point. For a quantum system, the Trotter-dimension contributes the quantum character of the simulation, and additionally increases the number of the degrees of freedom. Whereas in a classical two-dimensional system with 6×6 spins, only 36 spins have to be flipped to "invert" a configuration, in a Hubbard system of 6×6 sites and 400 Trotter slices, there number of Hubbard-Stratonovich spins is 14400, corresponding to the number of spins in a classical 120×120. Therefore, in a situation with two "stable" magnetizations, the simulation will hardly ever visit the "down"-state if it was initialized in the up-state.

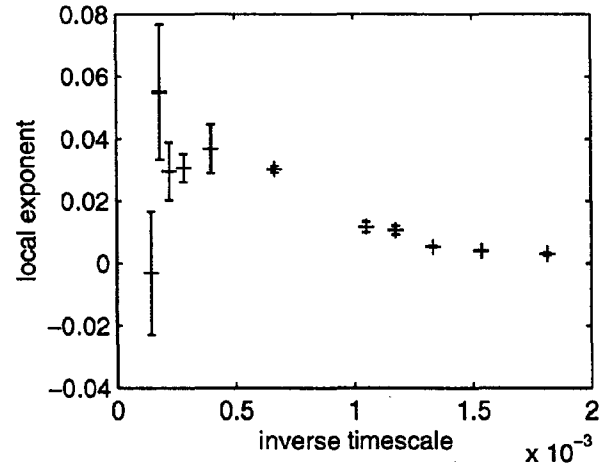

Fig. 5: Local exponent analysis for for a 6 × 6 system at U=30.

4. Results and Conclusion

For the 6×6, reliable saturation of the staggered magnetization could be only achieved for a Hubbard interaction of $U = 30$, see Fig. 4. For up to $U = 20$, the staggered magnetization decayed monotonically for system sizes between 4×4 and 8×8 (not shown). Currently, we try to narrow the interaction regime for which the system shows ferromagnetic ordering. The current data allow the NER-Local exponent analysis for $U = 30$, which shows that

for large times (small inverse times), the local exponent within error bars is zero,see Fig. 5, and the saturation of the magnetization could be confirmed.
We have presented NER data for the fermionic Hubbard model, which to our knowledge is the first case in the literature. It turned out that the NER-analysis is also applicable to the fermionic quantum Monte Carlo algorithms, and auxiliary quantities like projection parameter, Trotter-stepsize and trial wave functions, which are absent in classical simulations, pose no fundamental obstacle for the application of the method. It turned out that the anti-ferromagnetic transition of the two-dimensional Hubbard model occurs at a surprising high interaction strength.

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