25 Advances in the Investigation of the Minus Sign Problem for the Fermionic Case

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Abstract. Recent results in the investigation of the quantum Monte Carlo method for the Hubbard model using auxiliary fields revealed that the minus-sign problem for the fermionic case may be much more benign than conclusions in earlier studies indicated.

25.1 Introduction

In quantum Monte Carlo simulations, the statistical weight P often becomes negative. The sampling of an observable A is then carried out by using $|P|$ as the statistical weight and by reweighting the measurements with the sign S of the corresponding configuration

$$[A] = \frac{\langle AS \rangle}{\langle S \rangle} \,.. \tag{25.1}$$

Generally it is believed that simple averages $\langle A \rangle$ ignoring the sign are different from $[A]$. If the denominator $\langle S \rangle$ approaches zero, the computation of $[A]$ becomes difficult or impossible, a situation which is referred to as the "minus sign problem". From here on, we will limit ourselves to the Hubbard Hamiltonian

$$H = \hat{T} + \hat{U} \tag{25.2}$$

$$= -t_{ij} \sum_{\langle i,j \rangle, \sigma} c^{+}_{i\sigma} c_{j\sigma} + \text{ h.c. } + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \,, \tag{25.3}$$

where $c^{+}_{i\sigma}(c_{i\sigma})$ creates (annihilates) a fermion with spin σ on site i, hopping parameter and the strength of the on-site Coulomb-repulsion are denoted by t and U, respectively. The standard procedure in quantum Monte Carlo starts from decomposing the operator exponentials e.g. in second order as

$$\mathrm{e}^{\tau H} = \mathrm{e}^{\tau \hat{T}/2} \mathrm{e}^{\hat{U}} \mathrm{e}^{\tau \hat{T}/2} + \mathrm{O}(\tau^3) \,. \tag{25.4}$$

This problem has still the dimensionality of the original Hamiltonian. For a many particle problem, the memory requirement is in general too large for

conventional computers. The dimensionality usually increases exponentially with the particle- and system-size, which is the reason why numerical diagonalizations are limited to comparatively small systems. Due to "decoupling" of the parts of the Hamiltonian in (25.4), it is possible to simulate the system as single-particle systems and thereby to reduce the dimensionality considerably. The insertion of complete orthogonal states between the "slices" $\mathrm{e}^{\tau \hat{T}/2}$, $\mathrm{e}^{\hat{U}}$ leads to the so called world-line method, for which the minus sign problem is well established. We will focus here on the auxiliary field method, where the operator product is left intact, and the nature of the minus-sign problem is less clear.

In the auxiliary field method, the interaction is decoupled using usually the discrete Hubbard-Stratonovich (HS) transformation [1]

$$\mathrm{e}^{-\tau n_\uparrow n_\downarrow} = \frac{1}{2} \sum_{s=\pm 1} \mathrm{e}^{2\lambda s (n_\uparrow - n_\downarrow) - \frac{\tau}{2}(n_\uparrow + n_\downarrow)} \,, \quad \lambda = \tanh^{-1} \sqrt{\tanh(\frac{U\tau}{4})} \tag{25.5}$$

for each lattice site, so that Slater-determinants can be used.

25.2 Projector Quantum Monte Carlo

The projector method uses the exponential of the Hamiltonian to filter out the ground state from a trial wave function $|T\rangle$. This can be seen when the trial wave function is written in the energy representation with the basis functions $|n\rangle$, larger n denoting higher energies and $n = 0$ denoting the ground state:

$$\mathrm{e}^{-\beta H} |T\rangle = \mathrm{e}^{-\beta H} \sum_{n} \langle n|T\rangle \cdot |n\rangle \tag{25.6}$$

$$= \mathrm{e}^{-\beta E_0} \langle 0|T\rangle \cdot |0\rangle + \mathrm{e}^{-\beta E_0} \sum_{n>0} \mathrm{e}^{-\beta(E_n - E_0)} \langle n|T\rangle \cdot |n\rangle \,. \tag{25.7}$$

For the simulation, the operator exponential is then decomposed with the methods mentioned in the previous subsection. Denoting a Trotter slice with the HS-decoupled interaction will be denoted as

$$B_{l\sigma}(S) = \mathrm{e}^{\tau K/2} \mathrm{e}^{V(S)_\sigma} \mathrm{e}^{\tau K/2} \,. \tag{25.8}$$

In the PQMC, the wave functions $\langle \psi|$ and $|\phi\rangle$ for m Trotter-slices $B_{l\sigma}$ are computed from the trial function $|0\rangle$ respectively for each spin-direction σ as

$$|\phi_\sigma\rangle = \prod_{i=1,m/2} B_{l\sigma}|0\rangle \quad \text{and} \langle \psi_\sigma| = \Big(\prod_{i=m/2+1,m} B_{l\sigma}|0\rangle \Big)^T \,. \tag{25.9}$$

For n electrons and l sites, $|0\rangle, |\phi\rangle$ and $|\psi\rangle$ are $l \times x$ matrices. The statistical weight P_σ for this configuration is the determinant

$$P_\sigma = \det \langle \psi_\sigma | \phi_\sigma \rangle \,. \tag{25.10}$$

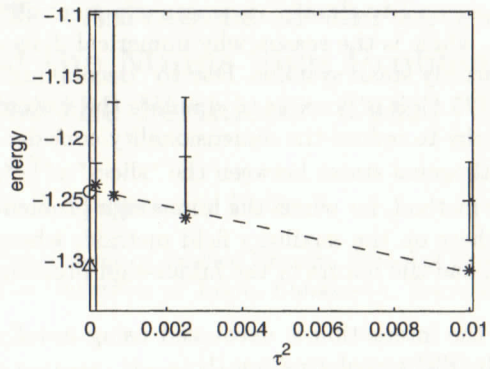

Fig. 25.1. Plot of energy versus the square of the Trotter step τ. Symbols are: Our result for multi site updates, sign taken into account (+), sign ignored (∗), both with errorbars, fit to our data with sign ignored (dashed line), value from numerical diagonalization (circle) and value for sign ignored from Imada et al. [2] (triangle)

As transition-probability P_{Tr}, either $P_\uparrow P_\downarrow$ can be used or its "heat-bath" equivalent $(P_\uparrow P_\downarrow)/(P_\uparrow P_\downarrow + 1)$. The Greens function G_σ is

$$G_\sigma = |\phi_\sigma\rangle^T \left(\langle\psi_\sigma|\phi_\sigma\rangle\right)^{-1} \langle\psi_\sigma|^T . \tag{25.11}$$

In [2], the Hubbard Model for $U = 8$ and 4 electrons on 3×2 sites was examined using single site updates. Significant deviations from diagonalization results were found for the energy value if the Trotter timestep τ was extrapolated to 0. In our recalculation using single-site and multiple-site updates, the deviations were practically insignificant (see Fig. 25.1). As can be seen, the statistics of the data taking the sign into account are much noisier then the one ignoring the sign.

It turned out that the main difference in the codes of Imada et al. was probably the use of different matrix inversion types, a inner product based one in the program of Imada et al. [3], and a Linpack-type [4] one in our case, where the kernel is of the form $y(i) = a * x(i) + y(i)$. For the latter one, pivoting techniques seem to be more effective. As ignoring the sign lead to correct results within the statistical fluctuations, we investigated the correlation between the sign and the energies. We computed the correlation as

$$\frac{\langle A\rangle - [A]}{\langle A\rangle} = \frac{V_{AS}}{\langle A\rangle\langle S\rangle}, \tag{25.12}$$

where V_{AS} denotes the correlation between A and S, that is $V_{AS} = \langle AS\rangle - \langle A\rangle\langle S\rangle$. For (25.12) to be valid, $\langle S\rangle$ may not vanish. Extrapolating from different values of τ, we found that $\langle S\rangle$ approached 0.0775 for $\tau \to 0$. Within the errorbars, the correlation between sign and energy virtually vanish, see Fig. 25.2.

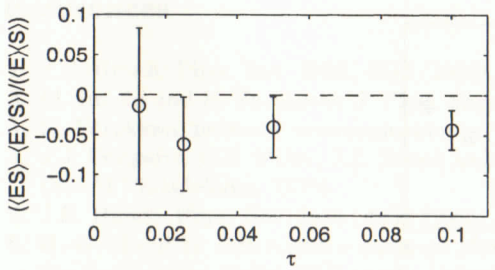

Fig. 25.2. Correlation between the average sign $\langle S\rangle$ and the energy $\langle E\rangle$, given as $(\langle ES\rangle - \langle E\rangle\langle S\rangle) / (\langle E\rangle\langle S\rangle)$, versus the Trotter-parameter τ for a system with 4 electrons and 3×2 sites at $\beta = 8$. The line is drawn to guide the eye

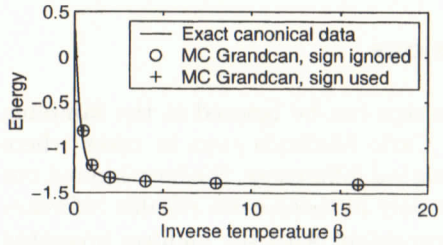

Fig. 25.3. Temperature dependence of the energy for a system of 3×2 sites with a filling corresponding to 4 electrons

25.3 Finite Temperature Quantum Monte Carlo

For the investigation of finite temperature properties, we use a grand canonical method after [5]. We compare simulational results from the grancanonical method with data from numerical diagonalization. for 3×2 sites ad $U = 4$ and (on average) 4 electrons. Though the system is small, the canonical and grand canonical data are in good agreement, and the sign does not seem to affect the measurement, see Fig. 25.3. For stronger interaction ($U = 8$), the behavior is different, but still unaffected by the sign. Both for $U = 8$ and $U = 4$, for large β the energy approaches the value for the ground state energy. Furthermore, we compared the d_{xy} equal time superconducting correlation function, which is quite sensitive to statistics and parameters, in a 8×8 system with 50 electrons and $U = 2$, $t = 1$ and a next nearest neighbor hopping term $t' = -0.22$ and time slice $\tau = 1/8$. The groundstate data take the sign into account (with projection parameter $\beta = 8$,), for the grand canonical data (inverse temperature $\beta = 15$) the sign is ignored. The data show good agreement between the different methods.

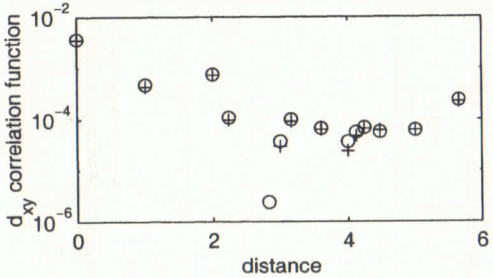

Fig. 25.4. The d_{xy} superconducting correlation function for a 8×8 system in the groundstate (circles) and for a grand canonical ensemble at finite temperature $T = 1/15$ (+) is shown [6]

25.4 Summary and Conclusions

We have shown cases where the minus sign can be ignored in the sampling process for the auxiliary field Monte Carlo Methods even in cases where previous publications had proclaimed marked differences. We have limited our investigation to small systems because only in these cases reliable reference data exists. Larger system sizes were consistent with the findings presented here [8].

For implementations where observables taking the sign into account turn out more accurately than if the sign is ignored, we suspect that the quantum Monte Carlo sampling procedure in (25.1) seems to provide a certain degree of error compensation. Due to the multi-linear nature of the determinant, numerically problematic values will be indefinite in sign and are counted as "positive" or "negative" with equal probability, so that correct estimates can be obtained for observable computations using observables of the form $\langle c^+_{i\uparrow} c_{j\uparrow} \rangle$ and $\langle c^+_{i\downarrow} c_{j\downarrow} \rangle$. We are not sure whether this effect is also present in larger systems, and exists also for observables of the form $\langle c^+_{i\uparrow} c_{j\uparrow} c^+_{k\downarrow} c_{l\downarrow} \rangle$ like superconducting correlation functions.

Within our investigation, for time independent observables we have not yet detected a case where the sign of the determinant has to be taken into account. We are currently investigating the influence of the sign on the computation of time-dependent greens functions, especially the example given in [7]. No clear picture has yet evolved, but it seems that numerical details of the stabilization process seem to have larger effect than the ignoring or taking into account the sign.

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