I. INTRODUCTION

Quantum Monte Carlo (QMC) methods have contributed to much of our recent knowledge of the properties of interacting quantum-mechanical spin systems, and closely related hard-core boson models. The Greens-function Monte Carlo (GFMC) is one powerful class of approaches which project out the lowest energy many-body eigenfunction. World-line (WLQMC) algorithms constitute another generic class of QMC approaches, and allow the evaluation of finite-temperature properties. Recently, improvements to WLQMC, the loop,1 continuous time,2,3 and duality-based4 techniques, have been developed.

Both GFMC and WLQMC most commonly use a basis labeled by the boson occupation number or position, or, analogously, the $z$ component of spin, in space and imaginary time. The key feature of the approaches is that eigenvalues of the original operators in the Hamiltonian describe the Monte Carlo configurations. In contrast, the preferred techniques for QMC simulations of interacting fermions5 involve the introduction of an auxiliary field. The original fermion operators are integrated out, and the simulation takes place in the space of this abstract auxiliary field.

In this paper we will introduce a new auxiliary field QMC method for interacting quantum mechanical spins and boson systems. Why is such an algorithm interesting? WLQMC and GFMC approaches have very significant weaknesses, including extremely long correlation times and restrictions on the observables which can be measured. While loop algorithms1 have addressed this issue, their efficiency remains problematic in several important cases, for example when interactions are longer range, or disorder is present. Therefore, continued algorithm development is desirable.

The organization of this paper is as follows: We first introduce the Ising model in a transverse field, and briefly review the key issues in its properties. We then describe how an auxiliary field algorithm can be constructed for this model. Although related conceptually to fermion QMC, it differs considerably from analogous fermion techniques in that the resulting traces are over independent single site problems, avoiding the necessity to evaluate the determinants of large matrices in the fermion case. We then give results of our simulations, including a comparison of the approach with existing techniques. We conclude by describing another interacting spin-boson model, the boson-Hubbard model. However, we show that the sign problem is a serious limitation to auxiliary field approaches in this case.

II. TRANSVERSE FIELD ISING MODEL

Two quantum spin–hard-core boson problems of considerably recent issue are the Ising model in a transverse field,6,7 and the boson-Hubbard model.7,8 The former allows one to study in a simple setting many of the key qualitative issues in quantum phase transitions in disordered systems, including the nature of the distribution of correlation functions and the shifts in the values of critical exponents from the clean limit. The latter offers a description of the superconductor-insulator phase transition when preformed pairs exist above the transition, and in the hard-core limit is also formally identical to the quantum-mechanical spin-1/2 $XXZ$ Hamiltonian. In this section we will describe the Ising model in a transverse field, which appears to be the more promising application of the auxiliary field approach.

A. Hamiltonian and algorithm

The transverse Ising model is a transverse field

$$H = \sum_{\langle ij \rangle} J_{ij} S_i^x S_j^x + \sum_i B_i S_i^z,$$ (1)

Here $S_i^\alpha$, $\alpha \in \{x,y,z\}$, are the Pauli matrices obeying the commutation relations: $[S_i^\alpha, S_j^\beta] = \delta_{ij}(\epsilon_{\alpha\beta} S_i^z + \delta_{\alpha\beta})$. The first sum runs over pairs of nearest neighbors, $\langle ij \rangle$. The partition function is given by $Z = \text{Tr} e^{-\beta H}$, and to evaluate it we employ the usual Trotter breakup of noncommuting operators in the Hamiltonian:

$$e^{-\beta H} = (e^{-\Delta \tau H})^{L_N} \prod_{l=1}^N \left( \prod_{j \in NN(i)} e^{-\Delta \tau J_{ij} S_i^z S_j^z} \right) \times e^{\Delta \tau B_i S_i^z} + O(\Delta \tau^2),$$ (2)
with $\Delta \tau L = \beta$. The inner product runs over the $z$ nearest neighbors of $i$.

In order to decouple the interaction terms we recall that any product of two commuting operators can be written as a sum over squares:

$$AB = \frac{1}{4}[(A + B)^2 - (A - B)^2].$$

and a squared operator can be decoupled by the introduction of a Gaussian integration over a classical auxiliary field:

$$e^{(A + B)^2/4} = \pi^{-1/2} \int dx e^{-x^2 + (A + B)x}.$$  \hspace{1cm} (4)

In the present case, one squared operator is sufficient

$$S_i^z S_j^z = \alpha [2(P_{ij}^a)^2 - 1], \quad \text{with } P_{ij}^a = (S_i^z + \alpha S_j^z)/2$$ \hspace{1cm} (5)

and $\alpha = \pm 1$.

Since $(P_{ij}^a)^2$ is a projection operator, i.e. $(P_{ij}^a)^{2k} = (P_{ij}^a)^2$, for $k = 1, 2, \ldots$, one immediately confirms by Taylor expansion that

$$e^{-2\Delta \tau \sigma_{ij} S_i^z S_j^z} \leq \cosh(2\lambda_{ij} P_{ij}^a) = \frac{1}{2} \sum_{\sigma = \pm 1} e^{\sigma \lambda_{ij} (S_i^z + \alpha S_j^z)}$$ \hspace{1cm} (6)

with $\cosh(2\lambda_{ij}) = \exp(-2\Delta \tau \sigma_{ij})$. In order to get real variables one chooses $\alpha = +1$ ($-1$) for $\sigma_{ij} < 0$ ($>0$). Thus a two-valued rather than Gaussian decoupling of the interaction is possible, introducing Ising-type auxiliary spins $\sigma_{ij} = \pm 1$:

$$e^{-\Delta \tau \sigma_{ij} S_i^z S_j^z} = \frac{1}{2} e^{-\Delta \tau \sigma_{ij}} \sum_{\sigma_{ij} = \pm 1} e^{\Delta \tau \sigma_{ij} \sigma_{ij} S_i^z S_j^z}$$ \hspace{1cm} (7)

for $\sigma_{ij} > 0$. This “discrete Hubbard-Stratonovich transformation” was introduced by Hirsch in the fermion case.\(^9\)

The same decoupling holds for any component of the Pauli matrix, hence the extension to $XY$ or (anisotropic) Heisenberg models or, equivalently, hard-core bosonic models, as will be discussed.

The decoupling has to be done for each of the $L$ factors in Eq. (2) giving the auxiliary spins $\sigma_{ij}(l)$ an additional index $l = 1, \ldots, L$. As a result, we have a system of noninteracting Ising spins in a transverse field $B_{i}$ coupled to an auxiliary longitudinal two-valued field, described by $\sigma_{ij}(l)$, which fluctuates in space and imaginary time. For a given configuration, $\{\sigma_{ij}(l)\}$, the original spins are trivially described by a direct product of $2 \times 2$ matrices.

Note that $\sigma_{ij}(l)$ is a bond, not site variable. $i$ and $j$ denote pairs of sites connected by a $J_{ij} \neq 0$. Hence, there are $NzL/2$ auxiliary spins where $z$ is the coordination number of the lattice. Even in the classical limit ($B_{i} = 0$, $L = 1$) the auxiliary spins are not dual to the original ones. An exception is the one-dimensional classical case where original and auxiliary spins are equivalent.

As mentioned above, for a given configuration of auxiliary spins the original spins are independent, the Hilbert space factorizes, and the partition function can be written as

$$Z = \sum_{\{\sigma_{ij}(l)\}} \prod_{i=1}^{N} \prod_{l=1}^{L} \prod_{j \in NN(i)} e^{\lambda_{ij} \sigma_{ij}(l) S_i^z S_j^z}$$ \hspace{1cm} (8)

$$= \sum_{\{\sigma_{ij}(l)\}} w(\{\sigma_{ij}(l)\})$$ \hspace{1cm} (9)

That is, $Z$ is now a sum over the $NzL/2$ auxiliary Ising spins with a weight function proportional to the product of traces of $2 \times 2$ matrices, one for each lattice site.

In the case of the Ising model one can choose all local transverse magnetic field values $B_{i}$ to be positive or change their sign by a local spin rotation, respectively. Thus there are only positive matrix elements involved and $w(\{\sigma_{ij}(l)\})$ can serve as a positive definite weight function. This is, however, not general, e.g., in the $XY$ model severe sign problems occur even for small systems (see Sec. III).

To simplify the notation for the following, we denote every factor in the matrix product (8) by

$$B_{i}(l) = \prod_{j \in NN(i)} e^{\lambda_{ij} \sigma_{ij}(l) S_i^z S_j^z}$$ \hspace{1cm} (10)

and define the product over $l$ and its cyclic permutations as

$$A_{i}(l) = B_{i}(l) B_{i}(l+1) \cdots B_{i}(L) B_{i}(1) \cdots B_{i}(l-1)$$ \hspace{1cm} (11)

In fact, the values of the traces do not change under cyclic permutation in the matrix product, i.e., they do not depend on the index $l$ in $A_{i}(l)$, and we can rewrite $Z$ as

$$Z = \sum_{\{\sigma_{ij}(l)\}} \prod_{i=1}^{N} \prod_{l=1}^{L} \text{Tr}A_{i}(l).$$ \hspace{1cm} (12)

The resulting Monte Carlo algorithm is similar to the auxiliary-field methods for lattice fermions,\(^5\) with the key difference that one has the product of traces of $NzL/2$ matrices of dimension $2$ to evaluate, instead of the determinant of a single matrix of dimension the spatial lattice size $N$. Thus the algorithm scales linearly in $N$. It goes as follows:

1. One starts at “time slice” $l = 1$, initializes the auxiliary field $\sigma_{ij}(l)$, and calculates the $2 \times 2$ matrix products $A_{i}(l)$ for each lattice site. The possible matrix elements $[\exp(\pm \lambda_{ij} S_i^z), \exp(\Delta \tau \sigma_{ij} S_i^z)]$ needed to determine $B_{i}(l)$ in Eq. (10) are calculated once and for all at the beginning.

2. At a fixed time slice $l$ try $Nz/2$ single-spin flips, $\sigma_{ij}(l) \rightarrow -\sigma_{ij}'(l)$. Such a flip involves the two lattice sites $i$ and $j$, and is accepted according to the probability ratio

$$p = \frac{\text{Tr} A_{i}(l) A_{j}^I(l)}{\text{Tr} A_{i}(l) A_{j}(l)}.$$ \hspace{1cm} (13)

with the new matrices

$$A_{i}(l) = B_{i}^I(l) B_{i}(l)^{-1} A_{i}(l).$$ \hspace{1cm} (14)

$B_{i}^I(l)$ denotes the matrix (10) with $\sigma_{ij}(l)$ replaced by $\sigma_{ij}'(l)$. Note that it is not necessary to perform the whole product of
L matrices but only a few $2 \times 2$ matrix operations for each spin flip. If accepted the new matrices $A_i(l)$ replace the old ones.

(3) Move to the next time slice, $l + 1$, by calculating

$$A_i(l + 1) = B_i(l)^{-1}A_i(l)B_i(l),$$

(15)

for each lattice site $i$.

(4) Move to the next time slice, $l + 1$, by calculating

$$A_i(l + 1) = B_i(l)^{-1}A_i(l)B_i(l),$$

(15)

for each lattice site $i$.

After $L$ cycles (2–4) one sweep through the $(d+1)$-dimensional system is complete. It takes $\alpha NL(z/2)^2$ multiplications. Step 3 leads to round-off errors, in particular at large $\beta$, so one has to recompute the matrices $A_i(l)$ from scratch from to time, typically after ten time slices.

The systematic error due to the Trotter decomposition can be strongly reduced by a third-order decoupling

$$e^{\Delta \tau (A + B)} = e^{\Delta \tau A/2}e^{\Delta \tau B}e^{\Delta \tau A/2} + O(\Delta \tau^3).$$

(16)

while the leading correction in expectation values of Hermitian operators is $O(\Delta \tau^2)$ for both second- and third-order decoupling, the prefactors are typically a lot smaller in the latter case. The implementation is simple. Formally, the matrices (10) are changed to

$$B_i(l) = e^{\Delta \tau h S_i^z/2} \prod_{j \in NN(i)} e^{\lambda_{ij} \sigma_{ij}(l) S_j^z} e^{\Delta \tau h S_j^z/2}.$$

In the product (11), however, there are always two of such factors, $\exp(\Delta \tau B_i S_i^z/2)$, adding to $\exp(\Delta \tau B_i S_i)$, and the remaining factor at the beginning of the product can be shifted to the end since the trace does not change under cyclic permutation. Hence, the Monte Carlo procedure remains completely unchanged, and it is sufficient to replace each local operator $O_i$ by

$$\tilde{O}_i = e^{-\Delta \tau h S_i^z/2}O_i e^{\Delta \tau h S_i^z/2}.$$

(17)

The computational effort for these $2N$ additional $2 \times 2$ matrix multiplications is negligible.

B. Observables

The algorithm allows for the measurement of a variety of static and time-dependent observables. Since measurements for successive time slices are in general correlated they are performed after every full sweep and time.

Interestingly, in the weak-coupling limit ($J_{ij} = 0$), all expectation values become exact, independent on the auxiliary field configuration, i.e., without any sampling. This is not the case if one samples over the original Ising spins. By analogy the auxiliary field approach for fermions exactly solves the noninteracting problem without sampling, while world-line approaches do not, and still require a full Monte Carlo simulation to get observables.

1. Static correlation functions

Most static observables can be expressed in terms of local magnetizations and static correlation functions. The components of the local magnetization $S_i^\alpha$ are given by

$$\langle S_i^\alpha \rangle = \frac{1}{Z} \sum_{\{\sigma_{ij}(l)\}} \left( \prod_{k \neq i} \text{Tr} A_k(l) \right) \text{Tr} \left( S_i^\alpha A_i(l) \right)$$

(18)

with the weight function $w(\{\sigma_{ij}(l)\})$ from Eq. (9). That means we have to sum up the ratio of traces on the right-hand side of Eq. (18) over the auxiliary field configurations. Similar equations hold for static correlation functions. In short,

$$\langle S_i^\alpha S_k^\beta \rangle = \frac{\left( \text{Tr} S_i^\alpha A_i(l) \right) \text{Tr} S_k^\beta A_k(l)}{\text{Tr} A_i(l) \text{Tr} A_k(l)} \langle \cdots \rangle_w$$

(19)

where $\langle \cdots \rangle_w$ stands for the sum over $\{\sigma_{ij}(l)\}$ configurations with proper weight.

2. Static susceptibilities

Susceptibilities, in general, require the calculation of correlation functions in imaginary time. The homogeneous susceptibility for spin component $\alpha$ is defined as

$$\chi^\alpha = N \int_0^\beta d\tau \langle M^\alpha(\tau) M^\alpha(0) \rangle - \beta \langle (M^\alpha)^2 \rangle.$$

(20)

with the magnetization operator

$$M^\alpha(\tau) = e^{-\tau H} M^\alpha(0) e^{\tau H}, \quad M^\alpha = \frac{1}{N} \sum_{i=1}^N S_i^\alpha.$$ 

(21)

In our discrete time approach the integral is replaced by a sum over time slices, yielding

$$\chi^\alpha = \Delta \tau N \sum_{l=1}^L \langle M^\alpha(\Delta \tau l) M^\alpha(0) \rangle - \beta N \langle (M^\alpha)^2 \rangle$$

(22)

$$= \frac{\Delta \tau}{N} \sum_{l=1}^L \sum_{n,m} \langle S_m^\alpha(l) S_n^\alpha(0) \rangle - \beta N \langle (M^\alpha)^2 \rangle,$$

(23)

where $S_m^\alpha(l) = S_m^\alpha(\Delta \tau l)$ means

$$S_m^\alpha(l) = \left( \prod_{l' = 1}^l B(l') \right)^{-1} S_m^\alpha \left( \prod_{l' = 1}^l B(l') \right)^{-1}.$$

(24)

For the time-dependent correlation function we again employ the fact that for a given auxiliary-field configuration operators for different lattice sites commute and we obtain for $m \neq n$:
\[
\chi_{mn}^{\alpha}(l) = \langle S_m^{\alpha}(l) S_n^{\alpha}(0) \rangle = \langle e^{-(\beta - \Delta \tau) H} S_m^{\alpha} e^{-\Delta \tau H} S_n^{\alpha} \rangle \\
= \frac{1}{Z} \sum_{\{\sigma_l\}} \left( \prod_{l \neq m,n} \text{Tr} \mathcal{A}(1) \right) \text{Tr} [S_m^{\alpha}(l)] \text{Tr} [S_n^{\alpha}(0)] \\
= \frac{\text{Tr} [S_m^{\alpha}(l)] \text{Tr} [S_n^{\alpha}(0)]}{\text{Tr} \mathcal{A}(1) \text{Tr} \mathcal{A}(1)} ,
\]

where the operators \((2 \times 2)\) matrices in brackets are defined as
\[
[S_m^{\alpha}(l)] = S_m^{\alpha}(l) \mathcal{A}(1) = \prod_{l'=1}^{l} B_{m}(l') S_m^{\alpha} \prod_{l'=l+1}^{L} B_{m}(l') 
\]

(27)

For the on-site correlation function we obtain similarly
\[
\chi_{mm}^{\alpha}(l) = \frac{\text{Tr} [S_m^{\alpha}(l)] S_m^{\alpha}(l)}{\text{Tr} \mathcal{A}(1)} 
\]

(28)

Equation (27) can be written as a product \(\mathcal{L}_m(l) S_m^{\alpha} \mathcal{R}_m(l)\) where the matrix products on the left- and right-hand side of the spin operator are calculated iteratively:
\[
\mathcal{L}_m(1) = B_m(1), \quad \mathcal{L}_m(l+1) = \mathcal{L}_m(l) B_m(l+1),
\]

\[
\mathcal{R}_m(L) = 1, \quad \mathcal{R}_m(l-1) = B_m(l) \mathcal{R}_m(l).
\]

(30)

For each value of \(l\), the product \(\mathcal{L}_m(l) \mathcal{R}_m(l) = \mathcal{A}_m(1)\). To check for roundoff errors this equality is tested from time to time. No significant deviations were found for the parameters used. \(\chi_{mm}^{\alpha}\) also determines the dynamical susceptibility in imaginary time from which, in principle, the real time dynamics can be extracted by an analytic continuation.

C. Results

1. Random field, random bond transverse Ising chain

The one-dimensional Ising model in a transverse field can be solved exactly using the Jordan-Wigner transformation,\textsuperscript{12,13} and diagonalization of the resulting non-interacting fermion problem. With random bonds and/or random magnetic fields, explicit formulas for finite open chains at finite temperatures were given by Young\textsuperscript{14} which can be used to test the algorithm. We did simulations of open chains of 20 and 100 sites with one disorder configuration, and calculated energy and nearest-neighbor correlation functions (see Fig. 1). The energy values are compared with the numerically exact ones. The convergence with \(\Delta \tau^2\) to the exact values is quite good. The third-order Trotter break-up leads to significantly smaller systematic errors in the energy. In the spin-spin-correlation function, however, the prefactor is somewhat larger.

2. 2D Transverse Ising Model

A second application of the algorithm is the phase transition induced by a transverse magnetic field in the pure (non-random) two-dimensional ferromagnetic Ising model. Figure 2 shows results for one fixed system size at an inverse temperature \(\beta = 10\). All quantities are extrapolated to \(\Delta \tau \to 0\).
order transition. \( M_z \) vanishes around \( B \approx 3.1 \). Spatial lattices of a hundred sites or so are often sufficient to indicate clearly the existence of phase transitions in quantum models, as the data in Fig. 2 demonstrate. A more subtle issue is that of critical exponents. If we assume that the finite system is essentially in its ground state and take the value of the critical magnetic field from high-temperature expansions, 15,16 \( B_c = 3.08 \), then we can fit \( M_z \) near the transition by a power law and get the exponent \( \beta = 0.32 \pm 0.01 \). This is in good agreement with the value for the classical \((d + 1 = 3)\)-dimensional Ising model, \( \beta = 0.325 \pm 0.0015 \),17 which should apply at the quantum critical point (\( T = 0 \)).

Autocorrelation times are short even close to the transition point. At \( B \) near \( B_c \) we observe autocorrelations in \( M_z \), \( E \), and \( \chi_{AF} \) below \( 1/e \) after a few sweeps, and in \( M_x \) after at most 30 sweeps on the largest lattice studied (10 \( \times \) 10 \( \times \) 100). For comparison, a “world-line” approach which uses the eigenvalues of \( S_i^z \) to label the space and imaginary time lattice has autocorrelation times near \( B_c \) in excess of 100 sweeps on a 10 \( \times \) 10 \( \times \) 40 lattice (10 \( \times \) 10 spatial sites and 40 imaginary time slices with \( \Delta \tau = 0.25 \) and \( \beta = 10 \)). For a 10 \( \times \) 10 \( \times \) 100 lattice (10 \( \times \) 10 spatial sites and 100 imaginary time slices with \( \Delta \tau = 0.10 \) and \( \beta = 10 \)) the autocorrelation time exceeds 500 sweeps near \( B_c \). We conclude that, like analogous approaches (“determinant QMC”) for interacting fermion systems, auxiliary field approaches to quantum spin simulations have short correlation times.

III. THE BOSON-HUBBARD (XXZ) MODEL

A. Hamiltonian and algorithm

The boson Hubbard model is

\[
H = -t \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) + V \sum_{\langle ij \rangle} n_i n_j + U \sum_i n_i (n_i - 1) - \mu \sum_i n_i.
\]

(31)

Here \( \hat{a}_i \) and \( \hat{a}_i^\dagger \) are the destruction and creation operators for bosons on site \( i \), and \( n_i = \hat{a}_i^\dagger \hat{a}_i \) is the number operator. The first term is the kinetic energy, and \( V \) and \( U \) are on-site and near-neighbor repulsions between bosons. \( \mu \) is a chemical potential which controls the density of electrons per site, \( \langle n \rangle \), on the lattice.

To briefly illustrate some of the properties of the model, consider the ground-state phase diagram at \( V = 0 \). As the chemical potential is raised, the density of bosons on the lattice increases smoothly from zero. However, if \( U \) is large, then when the density goes through \( \langle n \rangle = 1 \), the chemical potential takes a sudden jump, since at that point lattice sites become doubly occupied at the cost of the big on-site repulsion \( U \). Similar jumps occur at all integer fillings. These jumps represent a gap in the many-body energy spectrum, and reflect the fact that the system is insulating at strong coupling. If \( U \) is sufficiently small, the kinetic energy dominates, and the gap vanishes. Therefore, as \( U/t \) is changed, the boson-Hubbard Hamiltonian undergoes a quantum phase transition between superfluid and insulating states at commensurate \( \langle n \rangle \). Away from integer filling, the system is a superfluid at any ratio of \( U/t \). Nonzero \( V \), or the introduction of disorder, likewise allow for interesting new phases at \( T = 0 \).

In the hard-core limit, the occupations are \( n_i = 0.1 \). Then \( U \) drops out of the problem and with the usual mappings

\[
\hat{a}_i - \rightarrow S_i^+ = (S_i^x + iS_i^y)/2,
\]

\[
\hat{a}_i - \rightarrow S_i^- = (S_i^x - iS_i^y)/2,
\]

\[
n_i - \rightarrow S_i^z + 1/2,
\]

(32)

Eq. (29) transforms into the spin-1/2 XXZ model,

\[
H = -t/2 \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) + V \sum_{\langle ij \rangle} \left( S_i^z + \frac{1}{2} \right) \left( S_j^z + \frac{1}{2} \right) - \mu \sum_i S_i^z + \frac{1}{2}.
\]

(33)

An occupied site is hence identified with a spin up, etc., and the issues discussed above for the boson-Hubbard model can be reformulated in spin language. For example, the competition between superfluid and insulating phases corresponds to the competition between magnetic order in the \( XY \) plane and along the \( Z \) axis.

As mentioned above, the auxiliary-field decoupling (7) can be performed for different spin components independently. In the case of the \( z \) component it is useful to extract a trivial factor of \( \hat{S}_z \) in order to avoid complex matrix elements. Alternatively, by using the relations

\[
(a_i^\dagger)^2 = a_i^2 = 0,
\]

\[
a_i^\dagger a_i + a_i a_i^\dagger = 1,
\]

(34)

valid in the hard-core limit, one can directly decouple the kinetic energy term in Eq. (31):

\[
\exp{\Delta \tau a_i^\dagger a_i} = 1 + \Delta \tau a_i^\dagger a_i
\]

\[
= 1 + \frac{\Delta \tau}{2} (a_i^\dagger + a_i)^2
\]

\[
= \cosh{[\sqrt{\Delta \tau}(a_i^\dagger + a_i)]}
\]

\[
= \frac{1}{2} \sum_{\sigma = \pm 1} \exp{\sqrt{\Delta \tau}(a_i^\dagger + a_i)\sigma}.
\]

(35)

The same decoupling is used for the Hermitian conjugated term \( a_i^\dagger a_i \), yielding, together with the \( S_i^x S_j^y \) decoupling, three auxiliary Ising-type fields for the XXZ model which can be treated in analogy to the algorithm described in Sec. II.

B. Results

In order to check the algorithm and the code we calculate the nearest-neighbor spin-spin-correlation function of the isotropic antiferromagnetic (AF) Heisenberg model on a \( 2 \times 2 \) lattice. First, we did a full enumeration over all possible auxiliary spin configuration for several values of \( \Delta \tau \). Figure 3 shows the transverse and longitudinal correlation...
function vs $\Delta \tau^2$. Apparently they converge quadratically with $\Delta \tau$ to the exact value, however with different prefactors.

Even for very small systems at relatively high temperature severe minus-sign problems occur. Figure 4 shows the average sign $\langle \sigma \rangle$ of $w$ vs $\beta$ for systems with four sites. $\langle \sigma \rangle$ vanishes exponentially with $\beta$. Values of $\langle \sigma \rangle$ below approximately 0.2 preclude an efficient Monte Carlo sampling. The values of $\langle \sigma \rangle$ do not much differ for the two different decouplings, Eqs. (7) and (35), of the $XY$ contribution. Hence the algorithm does not appear to be suitable for models with couplings in more than one spin component.

IV. CONCLUSIONS

We have formulated an auxiliary field Quantum Monte Carlo algorithm for spin and hard-core boson systems. In boson language, it is based on a Hubbard-Stratonovich decoupling of the kinetic energy term, leaving a set of independent one-site problems in a fluctuating external field. Such a procedure has been used in analytic studies of the boson-