Monte Carlo study of a two-dimensional quantum ferromagnet

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We present quantum Monte Carlo results for the field and temperature dependence of the magnetization and the spin-lattice relaxation rate $1/T_1$ of a two-dimensional $S = 1/2$ quantum Heisenberg ferromagnet. The Monte Carlo method, which yields results free of systematic errors, is described in detail. The high accuracy of the calculated magnetization allows for stringent tests of recent approximate analytical calculations. We also compare our results with recent experimental data for a $\nu = 1$ quantum Hall ferromagnet, which is expected to be well described by the Heisenberg model. The dynamic response function needed to extract $1/T_1$ is obtained using maximum-entropy analytic continuation of the corresponding imaginary-time dependent correlation function. We discuss the reliability of this approach.

I. INTRODUCTION

The magnetization of a two-dimensional electron gas in the quantum Hall regime has recently been measured.\cite{1,2} The realization that this system represents a novel itinerant ferromagnet has motivated several theoretical studies.\cite{3,4} The system at filling factor $\nu = 1$ should be well described by a two-dimensional Heisenberg ferromagnet, and in a recent publication we presented analytical Schwinger boson and numerical Monte Carlo results for this model.\cite{5} The ferromagnetic Heisenberg model has been much less studied than the antiferromagnetic model, probably because the ground state and lowest excitations are known exactly. At finite temperatures there is, however, no exact analytic solution, and in our first paper we gave a detailed discussion of the calculation of the leading $1/N$ correction to the Schwinger boson mean-field theory. In this second paper we want to give a detailed description of the Monte Carlo calculation and present results for the NMR relaxation rate $1/T_1$. The Monte Carlo technique used is highly efficient and suffers from none of the common systematic errors. The magnetization results are accurate to a relative statistical error of about $10^{-4}$ and to this accuracy they are also free of finite size corrections. This allows for stringent tests of the analytical results. In order to estimate $1/T_1$ we calculate spin correlation functions in imaginary time and continue these to real frequency using the maximum entropy method. We discuss how the results of this approach depend on whether real- or momentum space correlation functions are analytically continued.

We want to emphasize an important technical detail that makes the sampling particularly efficient: the external field is chosen in the $x$-direction, perpendicular to the $z$-direction, in which the basis states are expressed. This automatically causes the simulation to become free of systematic errors, even though only local updates are used. Furthermore, it enables easy access to observables involving both diagonal and off-diagonal operators.

In Sec. II the stochastic series expansion Monte Carlo technique is briefly reviewed and applied to the two-dimensional ferromagnet. The maximum entropy technique used to numerically perform the analytic continuation to real frequency is described in Sec. III. Results for the field and temperature dependence of the magnetization are given in Sec IV. A. and the NMR relaxation rate results are presented in Sec IV. B. Our results and conclusions are summarized in Sec. V.

II. QUANTUM MONTE CARLO

A. Introduction

Over the last few decades, several methods for quantum Monte Carlo calculations have been developed. The most common methods stochastically sample the configurations of the world-line path integral of the system.\cite{6} These methods traditionally suffer from several systematic errors.\cite{7} The Trotter discretization of the imaginary time introduces a systematic error that decreases with decreasing “time slice” width $\Delta \tau$. In principle exact results are obtained by scaling to $\Delta \tau \rightarrow 0$. However, with standard techniques\cite{8} the efficiency of the simulation decreases rapidly as $\Delta \tau$ is decreased and it may therefore be difficult to obtain results completely free of systematic errors. Each configuration can furthermore be labeled by a topological “winding number”. The acceptance rate for moving from one winding number sector to another gets extremely small as the system size increases, thereby making the simulation non-ergodic.\cite{9} In addition, at low temperatures it can be very hard to change the number of particles in fermion or boson simulations, or the total magnetization for spin systems, hence restricting simulations to a canonical ensemble.

Recently there has been much progress in resolving these technical problems, making it much easier to obtain results that are exact within statistical error bars. Nonlocal “loop cluster” moves (analogous to cluster updates for classical systems)\cite{10} have been developed for several
models and can significantly reduce the autocorrelation times of the simulations. They enable sampling of all winding number sectors and all magnetizations. In addition these moves have been formulated in continuous imaginary time, hence eliminating the Trotter error and making the simulation completely free of systematic errors. A related method was recently formulated starting from the standard perturbation expansion in the interaction representation. Within this formulation, new local moves that share some of the advantages of the loop algorithms was introduced.

A different approach to quantum Monte Carlo simulation is[[7]], so called stochastic series expansion (SSE) method (a generalization of Handscomb’s method[[8]]) to a much larger class of models) which does not use the Trotter decomposition as a starting point, but instead samples matrix elements of the exact Taylor expansion of the density matrix \( e^{-\beta H} \). The Trotter error is thus automatically avoided. There are strong formal relationships between the SSE formulation and the continuous-time algorithms was introduced.

Below we will first give a short general overview of the SEE method, and thereafter give a detailed description of the application to the Heisenberg ferromagnet in a magnetic field.

### B. Stochastic Series Expansion

The thermodynamic expectation value for an operator \( A \), at inverse temperature \( \beta \), is

\[
\langle A \rangle = \frac{\text{Tr}\{ A e^{\beta H} \}}{\text{Tr}\{ e^{\beta H} \}} = \frac{1}{Z} \text{Tr}\{ A e^{-\beta H} \}.
\]

Assume that the Hamiltonian consists of \( M \) terms that need not commute, and may be of any order in field operators:

\[
H = - \sum_{i=1}^{M} H_i.
\]

A minus sign has been pulled out of the sum for convenience. The density matrix \( \exp(-\beta H) \) in the expectation value Eq. (1) is Taylor-expanded,

\[
\langle A \rangle = \frac{1}{Z} \sum_{n=0}^{\infty} \sum_{S_n} \frac{\beta^n}{n!} \text{Tr}\{ A \prod_{i=1}^{n} H_{k_i} \},
\]

where \( S_n \) denotes an index sequence \( k_1, \ldots, k_n \) with \( 1 \leq k_i \leq M \), and \( \prod_{i=1}^{n} H_{k_i} \) is an operator string of length \( n \). If the above trace can be analytically calculated the expectation value can be calculated by importance sampling in the space of index sequences. In the original Handscomb’s method, a spin-1/2 system is considered, for which the trace can be evaluated analytically. In the more general SSE method, a complete set of states \( \{|\alpha\rangle\} \) is introduced to calculate the trace, and hence a larger class of problems can be treated:

\[
\langle A \rangle = \frac{1}{Z} \sum_{\alpha} \sum_{n=0}^{\infty} \sum_{S_n} \frac{\beta^n}{n!} \langle \alpha | A \prod_{i=1}^{n} H_{k_i} | \alpha \rangle.
\]

In order to calculate the expectation of the operator \( A \) we assume that a function \( A(\alpha, S_n) \) exists such that Eq. (4) can be re-written as:

\[
\langle A \rangle = \frac{\sum_{\alpha} \sum_{n=0}^{\infty} \sum_{S_n} A(\alpha, S_n) W(\alpha, S_n)}{\sum_{\alpha} \sum_{n=0}^{\infty} \sum_{S_n} W(\alpha, S_n)} = \langle A(\alpha, S_n) \rangle_W,
\]

where the weight function \( W(\alpha, S_n) \) is given by

\[
W(\alpha, S_n) = \frac{\beta^n}{n!} \langle \alpha | \prod_{i=1}^{n} H_{k_i} | \alpha \rangle.
\]

We will assume that \( W(\alpha, S_n) \) is positive definite, which normally is the condition for a stochastic evaluation of \( \langle A \rangle \) to be feasible. One can then carry out a random walk satisfying the detailed-balance principle in the space \( \{|\alpha\rangle \otimes \{S_n, n = 0, \ldots, \infty\} \} \), using \( W \) as a relative probability. One important condition for such a procedure to be feasible in practice is that the operators \( H_i \) in Eq. (2) must be “non-branching”, i.e., the application of any \( H_i \) to a single basis vector should yield a single basis vector (not a linear combination of them),

\[
H_i|\alpha\rangle = h(i, |\alpha\rangle)|\alpha'\rangle, \quad |\alpha\rangle, |\alpha'\rangle \in \{|\alpha\rangle\},
\]

so that the weight factor Eq. (4) can be easily calculated. A scheme can then be constructed in which first an arbitrary allowed operator string and state are chosen. Thereafter relatively simple updating steps (“moves”) are performed that change the number of operators \( (n) \) in the string, the individual operators within the string (thereby changing \( S_n \)), and the state \( |\alpha\rangle \). The acceptances probabilities for the moves are chosen so that the detailed-balance principle is satisfied, using, e.g., the standard Metropolis or heat-bath algorithm.

The Taylor expansion may appear to be a high-temperature expansion, but in principle terms up to \( n = \infty \) are included, and the expansion is equally valid at any temperature. For a finite-size system at a finite temperature only terms of finite length contribute significantly to the trace, and importance sampling includes all relevant terms. This can be compared to the Taylor expansion of the exponential of a simple number, where the factorial \( n! \) in the denominator eventually wins over the numerator. An actual distribution for the order of the series in a typical simulation appears to be close to a normal distribution; see Fig. 1. As will be derived below, the average length of the operator string, \( \langle n \rangle \), equals
\[ P(n) = \begin{cases} 0.04, & n = 60 \text{ to } 120 \\ 0.02, & n = 0 \text{ to } 60 \\ 0.01, & n = 120 \text{ to } 140 \end{cases} \]

\[ n = 60 \text{ to } 140 \]

\[ n = 0 \text{ to } 60 \]

\[ n = 120 \text{ to } 140 \]

\[ \langle A \rangle = \left\langle \frac{1}{n+1} \sum_{p=0}^{n} A[\alpha(p), S_n(p)] \right\rangle_W. \]

In the simplest case where \( A \) is diagonal, \( A|\alpha\rangle = a(\alpha)|\alpha\rangle \), we find that \( A(\alpha, S_n) = a(\alpha) \) and

\[ \langle A \rangle = \left\langle \frac{1}{n+1} \sum_{p=0}^{n} a[\alpha(p)] \right\rangle_W. \]

Next we treat the case where \( A = H_m \), where \( H_m \) is one of the terms in the Hamiltonian, then

\[ \langle A \rangle = \langle H_m \rangle = \frac{1}{Z} \sum_{m=0}^{\infty} \sum_{S_n} \frac{\beta^n}{n!} \langle \alpha | H_m \prod_{i=1}^{n} H_k | \alpha \rangle, \]

and for each index sequence \( S_n \) for the state \( |\alpha\rangle \), there is a sequence \( S_{n+1} \), with \( H_m \) as the last element. Defining

\[ A(\alpha, S_n) = \begin{cases} \frac{\beta}{\beta}, & k_n = m \\ 0, & k_n \neq m \end{cases}, \]

and considering Eq. (10), the expectation value is obtained by counting the number \( N(m) \) of \( H_m \) operators in the sequence,

\[ \langle H_m \rangle = \frac{1}{\beta} \langle N(m) \rangle_W. \]

The energy is the negative sum of all operators \( H_m \), and it therefore follows that

\[ E = -\frac{1}{\beta} \langle n \rangle_W, \]

and we see that the energy is proportional to the average length of the operator sequence. One may argue that this is a strange formula; it seems that one should be able to decrease the average string length by adding a positive constant to the Hamiltonian (thereby increasing the energy). One should even be able to set the energy and average string length to zero! The solution to this paradox lies in the infamous sign problem. Adding a (sufficiently large) positive constant to the Hamiltonian will make it impossible to keep the weight function positive, and hence Eq. (13) is no longer valid. In fact, for most models, a negative constant has to be added to the Hamiltonian in order to make \( W(\alpha, S_n) \) positive definite. Eq. (15) then gives the energy including these constants.

Other expectation values, such as products of imaginary-time dependent operators and static susceptibilities can also be easily evaluated with the SSE method. We refer to previous work for the expressions for these more complicated expectation values.

In order to make the simulation code efficient one assumes that only operator strings with a length shorter than \( L \) contribute to the trace. This is not necessary, but by automatically adjusting \( L \) so that the simulation will not reach strings longer than \( L \) in any reasonable
simulation time, only an exponentially small, completely undetectable, error is made. With the length of the operator string limited to \(L\), \((n - L)\) identity operators can introduced in an operator string of length \(n < L\) to make the string length fixed. For every original operator string of length \(n\) there are then \(\binom{L}{n}\) strings of length \(L\), corresponding to all possible insertions of the \((L - n)\) unit operators. The inverse of this factor is included in the Taylor series expansion, where the summation now is over all index sequences of length \(L\), denoted \(S_L\):

\[
\langle A \rangle = \frac{1}{Z} \sum_{\alpha} \sum_{S_L} (-\beta)^n |L - n|! L! \langle \alpha | A \prod_{i=1}^{L} H_{k_i} | \alpha \rangle. \tag{16}
\]

During the simulation the number of these extra unit operators will fluctuate, and hence the previous sum over \(n\) is implied. The advantage with fixing the length in this manner and introducing extra unit operators is that all moves can be defined in solely terms of exchanges, i.e. a set of one or several operators is exchanged for another set of the same number of operators. This simplifies the construction of an updating scheme that satisfies detailed balance.

C. Application to the Heisenberg ferromagnet

In this Section we give a detailed description of how the SSE method is applied to the Heisenberg ferromagnet. The Hamiltonian of this model including a magnetic field is given by

\[
H = -J \sum_{i,\delta(i)} S^z_i \cdot \overrightarrow{S}_{\delta(i)} - h \sum_i S^x(i), \tag{17}
\]

where the coupling constant \(J > 0\), \(h\) denotes the magnetic field strength and \(\delta(i)\) denote the nearest neighbors of site \(i\) (we count each interacting spin pair only once). For reasons that will be explained later, the magnetic field is chosen in the \(x\) direction. The rectangular lattice has \(n = l_1 \times l_2\) sites, where \(l_1\) and \(l_2\) are the linear dimensions of the rectangular lattice. Throughout this work we use periodic boundary conditions, and there are therefore \(m = n\) bonds if \(l_1 = 1\), corresponding to the one-dimensional lattice, and \(m = 2n\) bonds if \(l_1 > 1\), corresponding to the two-dimensional case.

For the purpose of the SSE updating scheme we introduce the following six operators:

\[
\begin{align*}
H_{0,0} &= I \\
H_{1,b} &= I_b \\
H_{2,i} &= I_i \\
H_{3,b} &= 2(S^z_{\delta(b)} S^z_{j(b)} + \frac{1}{2}I_b) \\
H_{4,i} &= S^+_i + S^-_i \\
H_{5,b} &= S^+_j S^z_{k(b)} + S^-_j S^z_{k(b)},
\end{align*}
\tag{18}
\]

where \(i\) denotes a lattice site, \(b\) a bond, \(i(b)\) and \(j(b)\) are the sites connected by bond \(b\), and \(I\) is an identity operator. The unit operators \(I_b\) and \(I_i\), labeled by a site or bond, are introduced to simplify the updating scheme. An algorithm without these could also be formulated.

The Hamiltonian can then be written as

\[
H = -\frac{J}{2} \sum_{b=1}^{m} (H_{1,b} + H_{3,b} + H_{5,b}) - \frac{h}{2} \sum_{i=1}^{n} (H_{2,i} + H_{4,i}) + \frac{3J_m}{4} + \frac{hn}{2}. \tag{19}
\]

Note that the operator \(H_{0,0} = I\) is not considered a term of the Hamiltonian; it is the unit operator employed to augment the operator strings to the fixed length \(L\), as discussed in the previous Section. The constant in the definition of the type-3 operator has been introduced in order to make all its matrix elements positive (or zero), thereby making the weight function positive definite. The introduced constants only shift the energy (and therefore also the mean length of the operator string).

According to an ergodic updating scheme, the six different kinds of operators in the operator sequence are interchanged in such a way that any contributing operator string and basis state can be generated by a series of updates. Before going into the details of these procedures, we will specify our basis states and the weight function, and introduce some notation.

We will work in the \(S^z\) basis \(|S^z_1, S^z_2, \ldots, S^z_n\rangle\), and the non-branching property is satisfied since

\[
\begin{align*}
H_3| \uparrow \downarrow \rangle &= H_3| \downarrow \uparrow \rangle = 0 \\
H_3| \uparrow \uparrow \rangle &= | \uparrow \uparrow \rangle \\
H_3| \downarrow \downarrow \rangle &= | \downarrow \downarrow \rangle \\
H_4| \uparrow \rangle &= | \downarrow \rangle \\
H_5| \uparrow \uparrow \rangle &= H_5| \downarrow \downarrow \rangle = 0 \\
H_5| \downarrow \uparrow \rangle &= | \uparrow \downarrow \rangle.
\end{align*}
\tag{20}
\]

When non-zero, i.e., if \(|\alpha(L)\rangle = |\alpha(0)\rangle\), the weight function is

\[
W(\alpha, S_L) = \beta^n (L - n)! \left( \frac{J}{2} \right)_{n_1 + n_3 + n_5} \left( \frac{h}{2} \right)_{n_2 + n_4}, \tag{21}
\]

where \(n_k\) is the total number of \(H_{k,i} (i = 1, \ldots, m)\) operators in the operator string. The weight is always positive because all the matrix elements of the operators defined in Eq. (21) are positive or zero. For convenience we now use a two-index notation for the operator-index sequence \(S_L\):

\[
S_L = (k_1)_{j_1} (k_2)_{j_2} \cdots (k_L)_{j_L}, \tag{22}
\]
\begin{align}
|\alpha(0)> & \uparrow \uparrow \uparrow \uparrow \quad (2\ 4) \\
|\alpha(5)> & \uparrow \uparrow \uparrow \uparrow \quad (4\ 2) \\
|\alpha(4)> & \uparrow \uparrow \uparrow \uparrow \quad (4\ 1) \\
|\alpha(3)> & \downarrow \uparrow \uparrow \uparrow \quad (3\ 2) \\
|\alpha(2)> & \downarrow \uparrow \uparrow \uparrow \quad (0\ 0) \\
|\alpha(1)> & \downarrow \uparrow \uparrow \uparrow \quad (5\ 1) \\
|\alpha(0)> & \uparrow \uparrow \uparrow \uparrow 
\end{align}

|FIG. 2. Typical SSE configuration for a four-site system. The propagated states are shown on the left and the operator string to the right. The first operator-index denotes the type of operator \((1 - 6)\) and the second is the bond on which it operates \((1 - m)\), with \(m = 4\) in this case.|

where \(k\) indicates the kind of operator \((k \in \{0, \ldots, 5\})\) and \(j\) indicates which site or bond the operator acts on.

Next we introduce a random walk that satisfies the detailed-balance principle and covers the space \(\{|\alpha\rangle \otimes \{S_n, n = 0, \ldots, L\}\}\). A simulation is started from a random initial state \(|\alpha(0)\rangle\) and an initial sequence of operators \(\{0\}_{1} \{0\}_{2} \cdots \{0\}_{L}\). We define six fundamental moves that together ensure that we cover the full configuration space long enough as long as the magnetic field \(h\) is nonzero. In the absence of a magnetic field, additional moves have to be made, and these will be described later. The moves have to be carefully defined so that the detailed-balance principle is satisfied, generation of zero-weight configurations is not attempted, and so that they can be rapidly executed.

To visualize the seemingly abstract SSE space, a typical configuration for a one-dimensional four-site system is shown in Fig. 2. In the figure we can also see the close resemblance between the SSE method and the standard Euclidean path integral formulations. This relation has been explored in detail.\(^{\text{[2]}}\) Note that only the first state \(|\alpha(0)\rangle\) and the operator string have to be stored in memory. All propagated states can be generated sequentially as needed, and the memory requirements for the method are therefore quite modest.

The first kind of move changes the number of nonzero operators in the string by introducing the unit operator of type 1. Going through the operator string from the first to the last operator, attempts are made to exchange every \(\{0\}_{p}\) operator for a \(\{1\}_{p}\) operator, but only one \(\{1\}_{p}\) operator at a time. This is done by flipping \(\alpha_{i}\) from 0 to 1 or vice versa. The third kind of move attempts to exchange type-1 and type-3 operators.

where \(m\) again is the number of bonds and \(P[\{0\}_{p} \leftrightarrow \{1\}_{p}]\) indicates the \(a\ priori\) probability of the move being carried out, i.e., the probability before any accept/reject probability has been assigned. If the bond \(b\) is chosen at random for a move in the \(\rightarrow\) direction, the \(a\ priori\) probabilities satisfy \(P[\{0\}_{p} \rightarrow \{0\}_{p}] = mp[\{0\}_{p} \rightarrow \{1\}_{p}]\), since there are \(m\) different 1-operators, but only one 0-operator, i.e., every accepted transition from any of the \(b\) 1-operators leads to the same 0-operator, but a transition from the 0-operator only leads to any 1-operator for a given bond with probability \(1/m\). One can easily verify that we satisfy the detailed balance condition by choosing

\[
P\left[\begin{array}{c}
0 \\
0
\end{array}\right]_{p} \rightarrow \left[\begin{array}{c}
1 \\
b
\end{array}\right]_{p} = \frac{m\beta J}{2(L - n)}
\]

\[
P\left[\begin{array}{c}
1 \\
b
\end{array}\right]_{p} \rightarrow \left[\begin{array}{c}
0 \\
0
\end{array}\right]_{p} = \frac{2(L - n + 1)}{Jm\beta},
\]

where a number greater than 1 on the right hand side should be interpreted as probability one.

The second kind of move is very similar, but it exchanges type-0 and type-2 operators. Again the string is sequentially searched for these two kinds of operators, and detailed balance is satisfied with the following exchange probabilities:

The third kind of move attempts to exchange type-1 and type-3 operators. We can see that the weight function is unaffected by this kind of move, and detailed balance is satisfied, but there is a restriction. An attempt to exchange \(\{0\}_{p}\) for \(\{1\}_{p}\) will result in a zero-weight function if the spins on the two sites that are connected to bond \(b\) point in opposite directions. Hence one needs to check the spin configuration before attempting to exchange a 1-operator for a 3-operator, while a 3-operator can always be exchanged for a 1-operator.

The fourth kind of move is slightly more complicated and involves exchanging pairs of 2- and 4-operators. The reason why we have to exchange pairs of operators is that the state of the system has to return to its original state when it has been propagated by the whole operator sequence; \(|\alpha(0)\rangle = |\alpha(L)\rangle\), and if a spin is flipped in an intermediate state it has to be flipped back at a later time. Hence we attempt to make exchanges of the form \(\{0\}_{p}\{1\}_{p}\) \(\leftrightarrow \{1\}_{p}\{0\}_{p}\). But we have to be careful, since this move results in the spin at site \(i\) being flipped in all states
|α(p)⟩, . . . , |α(q − 1)⟩. In case p > q, then |α(0)⟩ will be affected, and we have to flip the spin at site i in the state |α(0)⟩ that we store in the memory. Also, if there is an operator of type (5) r or (5) q, with p < r < q, then this exchange would lead to a zero weight function and the move must not be made. In order to make an efficient updating scheme the operator sequence is divided up into n subsequences, each containing the necessary information to make the above exchange for site i ∈ {1, . . . , n}.

It is easiest to actually store three lists: T i, P i and F i, that contain information about the ith site. The list T i = {t 1, . . . , t L(i)} , with t ∈ {2, 4} contains all 2- and 4-operators from the full operator string operating on site i. The list P i = {p 1, . . . , p L(i)} , contains the positions p of these operators in the full operator string. The final list is F i = {f 1, . . . , f L(i)} , where f j ∈ {0, 1} indicates if there are any operators of kind 3 or 5 operating on a bond or all the bonds that start on an even site. Hence the full operator sequence is therefore again divided up into 2 sublists, which can be updated independently. A two-dimensional lattice is divided up into partitions as in move 5. Four different bond partitions of a 6 × 6 lattice with periodic boundary conditions.

FIG. 3. The four different bond partitions of a 6 × 6 lattice.

The final list is S b = {s 1, . . . , s L(i)} , where s i = 1 indicates that the spins connected to bond b are aligned in state |α(p i)⟩, and s i = 0 indicates that they are anti-aligned. The move is identical to the procedure described for the fourth move, except that now the move is canceled if t j ≠ t k or s j = 1.

The sixth move is the most complicated one, because it involves exchanges between three different kinds of operators. It is this move that makes this simulation particularly efficient, since it can generate configurations of non-zero winding number.

The following exchanges are attempted: (3 1) i , (3 5) p ↔ (3 1) q , with p < r < q, where the bond b′ is connected to either of the sites that bond b is connected to. The full operator sequence is therefore again divided up into substrings containing the operators that act on a particular bond and the sites that it is connected to. One can make this kind of move in two different substrings independently of each other, as long as the two bonds do not connect, i.e. as long as they do not have any site in common. The n bonds on a one-dimensional lattice can be partitioned in all the bonds that start at an odd site, or all the bonds that start on an even site. Hence the full operator string is split up two times, each time into n/2 sub-strings, which can be updated independently. A two-dimensional lattice has to be divided into four separate partitions; see Fig. 3.

The updating of the n/2 sublists is very similar to the updating scheme for the fourth move. Four lists are stored this time. The list T b = {t 1, . . . , t L(i)} , with t ∈ {1, 5} contains all 1- and 5-operators from the full operator string operating on bond b. The list P b = {p 1, . . . , p L(i)} again contains the positions p of these operators in the full operator string. The list F b = {f 1, . . . , f L(i)} , where f j ∈ {0, 1} indicates if there are any operators of kind 3 or 5 operating on a bond connected to bond b between the positions p j and p j+1.

The detailed-balance principle is satisfied if

\[ P \left[ \frac{1}{b} \right] \left[ \frac{5}{b} \right] \rightarrow \left[ \frac{4}{i_1} \right] \left[ \frac{4}{i_2} \right] \right] = 2h^2 / J^2 \quad (26) \]

\[ P \left[ \frac{4}{i_1} \right] \left[ \frac{4}{i_2} \right] \rightarrow \left[ \frac{1}{b} \right] \left[ \frac{5}{b} \right] \right] = J^2 / 2h^2. \quad (27) \]

If the last move is excluded one can see that all possible operator sequences are not sampled if periodic boundary conditions are used. To visualize this, we consider a four-site system for which it is easy to realize that the simple string H 5,1 H 5,2 H 5,3 H 5,4 cannot be reached. This is an example of a configuration with a non-zero winding
number (provided that the operator string operates on an appropriate state). In order to make this configuration possible we need to introduce a “ring” move. If we picture each 5-operator as connecting the two sites it acts on, we can see that the configuration \( H_{5,1} H_{5,2} H_{5,3} H_{5,4} \) creates a ring around the system. The ring move is accomplished as follows: starting at a random point in the operator sequence for a \( n \)-site system a search for a set of \( n/2 \) different 5-operators is made. If such a set is found, an attempt to exchange it with its complementary set is made. An example for the 4-site system would be \( H_{5,1} H_{5,3} \rightarrow H_{5,2} H_{5,4} \). If the move is successful the winding number has changed. Whether or not the move can be carried out of course depends on constraints imposed by the states. As the system size is increased beyond about \( L = 16 \) it becomes virtually impossible to perform ring moves.

In a one-dimensional system the ring move is the only move that has to be added if the sixth move is not performed. In two dimensions we can picture a ring around a small part of the system. We can, for example, draw a ring around a \( 4 \times 4 \) square and we realize that we cannot reach a configuration consisting of the 14 5-operators that connect these sites. We therefore introduce a plaquette move. This move changes the 5-operators that act on a single plaquette, which for a two-dimensional square lattice is the smallest square in the lattice. A plaquette move that involves arbitrarily large parts of the system, for example the \( 4 \times 4 \) square considered above, can be reached with these fundamental plaquette moves. The move is identical to the one-dimensional ring move for a 4-site ring.

In higher dimensions, when using periodic boundary conditions, we also have to perform a direct generalization of the one-dimensional ring move. In a two-dimensional system with periodic boundary conditions we can picture making rings around the system in both spatial directions, and in three dimensions we could make the move in all three spatial directions. Apart from performing the move in all spatial directions it is identical to the 1D ring move, and for a linear system size larger than about \( L = 16 \) ring moves are no longer accepted. Note that this ring move can not be accomplished by the above plaquette moves.

Without the external field in the \( x \)-direction, the Hamiltonian conserves the total magnetization in the \( z \)-direction; \( M_z = \sum_i S_i^z \), and the operator string updates alone therefore sample only within a fixed magnetization sector. In order to sample in the grand canonical ensemble, one then has to carry out an update that changes the magnetization of the state \( |\alpha\rangle \) in Eq. 11. A spin \( S_i^z \) in \( |\alpha\rangle \) can be flipped, without change in the weight, if there are no operator \( \langle \delta \rangle \) or \( \langle \gamma \rangle \) in \( S_L \) with \( b \) a bond connected to spin \( i \). The probability of this being the case approaches zero rapidly as \( T \) is lowered, and hence this update can be carried out only at relatively high temperatures. With an external field in the \( x \) direction the magnetization is no longer conserved and the simulation is automatically grand canonical. It is nevertheless useful to carry out the single-spin flips at high temperatures.

With the field present in two dimensions, the sixth move also makes plaquette and ring moves unnecessary. This can be understood since the sixth move introduces single 5-operators, and through a series of moves any configuration of 5-operators can be generated. Had we chosen the field in the \( z \)-direction this would not have been possible. Having the field in the \( x \)-direction therefore makes the simulation particularly efficient by introducing single-spin flipping operators. Strictly speaking we do not need to make the fifth move either, but especially at small fields it may be good to include this move to shorten the auto-correlation time and speed up the thermalization of the system.

Another advantage of choosing the \( x \)-direction for the field is that we can then easily measure spin-spin correlations both parallel and perpendicular to the field. The perpendicular correlation functions are diagonal in our chosen basis, and can be evaluated according to Eq. (14). The parallel correlations involve expectation values of products of the number of field operators in \( S_L \) as discussed in Refs. [17]. We are particularly interested in the perpendicular correlations for this model, since they are the ones required to calculate the relaxation rate \( 1/T_1 \). The magnetization \( M = \langle S_i^z + S_i^- \rangle / 2 \) is according to Eq. (14) proportional to the average total number of field operators \( H_{L,i} \) in the sequence; \( M = \langle n_4 \rangle / (N \beta h) \).

A complete Monte Carlo step for the two-dimensional lattice, as used in this work, consists of

1. Move 1, \( \langle 0 \rangle_p \leftrightarrow \langle 1 \rangle_p \), attempted at all positions \( p = 1, \ldots , L \) in the sequence \( S_L \).
2. Move 2, \( \langle 0 \rangle_p \leftrightarrow \langle 7 \rangle_p \), attempted at all positions \( p = 1, \ldots , L \) in \( S_L \).
3. Move 3, \( \langle 1 \rangle_p \leftrightarrow \langle 3 \rangle_p \), attempted at all positions \( p = 1, \ldots , L \) in \( S_L \).
4. The sequence is split up into \( n \) sub-sequences and in each sequence move \( 4, \langle 2 \rangle_p \leftrightarrow \langle 5 \rangle_q \) is attempted, whereafter the full operator sequence is restored.
5. The operator string is split up 4 times into \( n/2 \) different sub-sequences. In each sub-sequence the fifth move, \( \langle 4 \rangle_p \leftrightarrow \langle 5 \rangle_q \) is then attempted a number of times of the order of the length of the subsequence. The updated sub-sequences are recombined into the full string.
6. The operator string is split up 4 times into \( n/2 \) different sub-sequences and in each sub-sequence the sixth move, \( \langle 4 \rangle_p \leftrightarrow \langle 5 \rangle_q \), is attempted. The sub-sequences are recombined to the full string.
7. All spins that are not acted on by any interaction operators \( \{ \mathcal{H}_{\text{int}} \} \) or \( \{ \mathcal{H}_{\text{int}} \} \) are flipped with probability \( 1/2 \).

\[
C_{M_x}(t) = \frac{\langle M_x(i)M_x(i+t) \rangle - \langle M_x \rangle^2}{\langle M_x^2 \rangle - \langle M_x \rangle^2},
\]

where \( M_x(i) \) is the value of the magnetization estimator, \( n_k/(N\beta h) \), at the \( i \)th Monte Carlo step. We show results for \( 8 \times 8 \) lattices at two different temperatures and three different field strengths. Note that the long-time correlations decrease with decreasing temperature. This is related to the fact that the distribution of magnetization values becomes broader. For example, for \( h/J = 0.05 \) at \( T/J = 1 \), the magnetization essentially fluctuates between two values, corresponding to configurations with 0 or 2 field operators, as shown in Figure 4. The system spends long times in states with no field operators and occasionally short times with 2 operators. These two time scales are reflected in the autocorrelation function, which shows a rapid decay at short times, but a very slow decay at longer times (the asymptotic exponential decay time is several hundred Monte Carlo steps). At the lower temperature the short-time behavior shows a less rapid decay, but also a faster asymptotic decay, as the fluctuations in the distribution of the number of field operators \( n_k \) is now broader, and the likelihood of a fluctuation by \( \pm 2 \) in the simulation is higher. At \( h/J = 0.2 \), the time dependence of \( n_k \) shows fluctuations on much shorter time-scales, and the autocorrelation function accordingly decays considerably faster.

III. THE MAXIMUM ENTROPY TECHNIQUE

It is notoriously difficult to obtain dynamic information from quantum Monte Carlo simulations. One of the presently most common and promising methods is the maximum entropy technique, which we used to calculate the spin-lattice relaxation rate. In this section we will discuss various ways to use the method, compare results to exact diagonalization and show some of the limitations of the procedures.

The nuclear magnetic resonance spin-lattice relaxation rate is given by

\[
\frac{1}{T_1} = \frac{1}{N} \sum_q |A_q|^2 S(q, \omega_N),
\]

where \( A_q \) is the Fourier transform of the hyperfine coupling. The resonance frequency \( \omega_N \) is so small compared to other energy scales that we consider the limit \( \omega \to 0 \). From now on we assume that \( A_q = 1 \). The dynamic structure factor \( S(q, \omega) \), which measures transverse spin correlations, can be obtained from the imaginary time dependent correlation function...
by inverting the expression

$$C(q, \tau) = \sum_r e^{iqr} C(r, \tau) = \sum_q e^{iqr} \left\langle S_i^z(\tau)S_{i+r}^z(0) \right\rangle$$

Calculating the local imaginary time correlation function is therefore in principle sufficient for determining the relaxation rate, after performing a maximum entropy inversion. For reasons that will become clear below, we did, however, also measure the spatial dependence of the correlation function.

Using conservation of momentum it is possible to obtain finite temperature exact diagonalization results for system sizes up to $4 \times 4$. Below we will show diagonalization data compared to Monte Carlo + maximum entropy results.

First a few words concerning the default model needed in the maximum entropy method. All data shown in this paper have been generated using a flat default model as defining zero entropy. Much has been written about how to choose a good default model but from our experience it seems that unless something very specific and very accurate is known about the solution (in which case it probably is unnecessary to use Monte Carlo + maximum entropy), one should use a flat default model. If only general features, obtained from, for example, perturbation theory or some analytical mean field solution, are known about the function, then one introduces a bias towards one approximate model by placing peaks at frequencies that are only approximate. If the answer is very dependent on what default model one uses, then the accuracy of the results should be viewed with caution. Using good data and a flat default model is optimal in the sense that no prior bias has been used to construct features in the spectral function; the default model only has a regularizing effect. We worked extensively with Gaussian default models, where we determined all the parameters of the default model through sum rules that could be calculated in the Monte Carlo simulation. In some cases this worked fairly well, but in those cases a flat default model worked almost equally well. In other cases the maximum entropy solution would be very close to the Gaussian default model, but far from the exact diagonalization results. This clearly shows that the problem is ill-posed. In these instances it was our experience that a flat default model resulted in better agreement with exact diagonalization.

We now turn to actual comparisons with exact diagonalization results. At low temperatures the spectral function is dominated by a delta function for each magnon, and this extreme limit will first be considered to illustrate some weaknesses and strengths of the maximum entropy solution. In Fig. 6 we show results for a $4 \times 4$ system at inverse temperature $T/J = 0.25$ and field strength $h/J = 0.25$. As usual, the exact diagonalization result really only consists of a series of delta peaks, but the spectrum has been divided into bins of finite width in order to illustrate the result more clearly. The first peak is at exactly $\omega = h/J = 0.25$ and is the response of the $q = (0,0)$ momentum. This peak will remain a delta function even at finite temperatures since the spin-correlation function then will contain the total spin raising and lowering operators, and hence transitions can occur only between levels within the same spin multiplet. These levels are all separated by the Zeeman splitting, which is independent of temperature. Therefore the delta peak at the Zeeman energy will not get broadened by temperature. For finite q-values there will be transitions between different spin multiplets causing transition energies that differ from the Zeeman energy.

In order to be able to directly study the different momenta we have measured the full spatial dependence of the correlation function and we can therefore either analytically continue each momentum and then average the spectrum, or first average the correlation function and then do the analytic continuation. In Fig. 6 both methods are demonstrated. The dotted curve shows the result when analytically continuing each momentum separately. We notice two important features. First, the maximum entropy method resolves each peak, and secondly, the resolution of the peaks decreases with frequency, as can be expected, since the factor $e^{-\tau \omega}$ makes the inversion insensitive to high frequency features. The dashed curve shows the result when the average over all momenta is continued. We notice immediately that the maximum entropy method has difficulty in resolving more than one peak and tends to smear the result out. Focusing on the limit $\omega \to 0$ we notice that because of the $q = (0,0)$ peak

\[ \sum_q C(q, \tau) = \int d\omega \sum_q S(q, \omega) e^{-\tau \omega} = C(r = 0, \tau). \]
at \( \omega = \hbar / J = 0.25 \), an estimate of \( 1/\langle T \rangle \) would be too high, since the weight of the \( q = (0,0) \) peak is smeared out all the way to \( \omega = 0 \). To remedy this effect we can average over all momenta, except \( q = (0,0) \). The results are shown in the dot-dashed curve, and we see that this certainly affects the solution close to \( \omega = 0 \), where there is now correctly, no weight.

We are, however, interested in results for large system sizes, for which the spectral function should be smooth on a reasonably fine frequency scale. We cannot compare our results to diagonalization results for more than \( 4 \times 4 \) sites. We can, however, study this system at higher temperatures, for which the spectral function is fairly smooth. In Fig. 8 the same parameter values as in the previous figure are shown, but at a higher temperature, \( T / J = 2.0 \). We see that the diagonalization results are much smoother and we can analyze the maximum entropy results. The dashed curve shows all momenta separately continued. \( 1/\langle T \rangle \) is grossly overestimated since the \( q = (0,0) \) peak is smeared out at this higher temperature. Removing the \( q = (0,0) \) peak gives a much better estimate; see the dotted curve. Continuing the average of all momenta again places too much weight at low frequencies, because of the \( q = (0,0) \) peak, as can be seen from the dot-dashed curve. Removing the \( q = (0,0) \) momentum from the average improves the result a great deal; see the long dashed curve.

We found that the optimal use of the maximum entropy method in our case was to continue the average of all momenta, excluding the \( q = (0,0) \) momentum. For this momentum we know the exact analytic result, and including it in the continuation leads to an over-estimate of \( 1/\langle T \rangle \). The reason for not continuing each separate momentum, which worked miraculously well in Fig. 6, is that at intermediate temperatures this method also leads to an overestimation of \( 1/\langle T \rangle \), since peaks close to the origin will be smeared out, and much of their weight will be incorrectly placed at \( \omega = 0 \).

To conclude this Section, we have found that the maximum entropy method is a useful method to obtain real time data from imaginary time quantum Monte Carlo data for the Heisenberg ferromagnet. We believe that the specific recipe for how to use the method probably varies from system to system, but for the case we have considered here we found the most useful default model to be flat, and we also found that we had to separate out the \( q = (0,0) \) momentum before carrying out the analytic continuation.

Similar calculations of NMR relaxation rates have previously been carried out also for various quantum antiferromagnets. In that case the differences between maximum entropy calculations based on momentum and real-space correlations were less pronounced than what we have found here. The ferromagnetic case appears to be more difficult since the field induces additional structure in the frequency dependence. Also, at low temperatures independent magnons are exact excitations of the ferromagnet, which causes further sharp features in the spectral function.

IV. RESULTS

A. Magnetization

The Heisenberg model is one of the basic non-trivial models of a quantum ferromagnet. A detailed knowledge of the field dependence of the magnetization is therefore of interest for comparisons both with analytical and experimental results. In this Section we will show the general field dependence of the magnetization for the two-dimensional model. We will also compare our Monte Carlo results to exact diagonalization results and show the nature of the finite size corrections. We also compare the results to recent experimental results for the \( \nu = 1 \) quantum Hall state.

In Fig. 8 we show a comparison of exact diagonalization and Monte Carlo data for a \( 4 \times 4 \) system. We have verified the agreement to a relative error of \( 10^{-4} \). To this degree of accuracy the results for the largest system sizes shown \((16 \times 16) \) and \( 32 \times 32 \) have also converged. We did additional test runs for systems of size \( 64 \times 64 \), and the results were within error bars of the above results. From Fig. 8 we notice that the finite size effects are largest at intermediate temperatures, which is easily understood since in the limit of very low temperatures the magnetization will be fully saturated independently of the lattice.
size, while in the high temperature limit the magnetization will vanish independently of the system size.

FIG. 8. Monte Carlo results for the magnetization vs temperature for $L \times L$ systems with $L = 4, 8, 16$ and $32$, and exact diagonalization results for $L = 4$. The magnetic field $h = 0.1$.

FIG. 9. Magnetization vs temperature for the 2D Heisenberg ferromagnet in magnetic fields of strengths $h = 1.00, 0.80, 0.60, 0.40, 0.20, 0.10$ and $0.05$, from top to bottom. The results were calculated using lattices sufficiently large (typically $32 \times 32$) to eliminate finite-size effects almost completely.

In Fig. 8 we present a plot of the magnetization as a function of temperature for a range of field strengths. We have tried to scale the data as a function of $T/h^\alpha$ for different values of the exponent $\alpha$. Such scaling does not collapse the data onto a single curve, however. Analytical calculations have also suggested that there is no scaling in $T$ and $h$ for this model.

We also show a comparison of recent magnetoabsorption measurements performed on the $\nu = 1$ quantum Hall state compared to quantum Monte Carlo data and Schwinger boson calculations in Fig. 10. There are no adjustable parameters in this comparison, since $J$ can be calculated exactly for the zero-width well using the exactly known spin wave dispersion for the quantum Hall ferromagnet, and estimated for the actual experimental system. The excellent agreement shows that this itinerant ferromagnet is well described by an effective Heisenberg model. As discussed in our previous paper, the comparison with the analytical Schwinger boson solutions showed that the $1/N$ corrections to the $O(N)$ model agrees well with Monte Carlo and experimental results at moderate and intermediate temperatures, while the low-temperature result was better reproduced by the $SU(N)$ model. For a more comprehensive discussion of the Schwinger boson results and the experimental data, we refer to our previous paper.

B. Spin-lattice relaxation rate

In Fig. 11 we compare mean-field results for the nuclear magnetic relaxation rate $1/T_1$, to numerical results obtained by analytic continuation of imaginary time Monte Carlo data, as described previously. As we have discussed, the maximum entropy results have to be viewed with some caution. The error bars are obtained using the bootstrap technique. They do not strictly correspond to a statistical likelihood that the estimated relaxation rate is within error bars of the true relaxation rate, since there is also an unknown systematic error due to the bias of the maximum entropy procedure. The error bars do contain information about how sensitive the results are to the variations in the MC data.

We notice a fairly good agreement between the analytic and numerical results and, as in the case for the magnetization, the $O(N)$ theory appears to be somewhat closer to the numerical results. Notice that this
time the numerical results do not lie between the O(N) and SU(N) solutions, which was the case for the magnetization. At zero temperature the relaxation rate is zero, since no spins flip in the ordered ferromagnet and therefore the nuclear spins cannot relax. At low temperatures the rate is activated and caused by thermally activated spin waves.

Not enough experimental data is available for the relaxation rate to make a comparison with the above numerical results. Because results for the Heisenberg model agreed very well with experimentally measured magnetization, it would be of interest to compare the relaxation rate, to see if the Heisenberg model also captures the correct dynamic behavior of the $\nu = 1$ quantum Hall ferromagnet.

V. SUMMARY AND CONCLUSION

We have described an approximation-free quantum Monte Carlo technique and applied it to a two-dimensional ferromagnet in a magnetic field. We have shown that applying the field in the transverse direction causes the simulation to become free of systematic errors although only local Monte Carlo moves are made. The transverse field also enables easy access to transverse spin correlation functions. We have calculated the temperature dependence of the magnetization for a range of field strengths and discussed finite-size effects. Some results have previously been compared to measurements of the $\nu = 1$ quantum Hall state and analytical Schwinger Boson calculations. The high relative accuracy ($10^{-4}$) of the Monte Carlo results made it possible to make statements about the relative merits of the SU(N) and O(N) solutions. We have, in addition, calculated the spin-lattice relaxation rate $1/T_1$ using a maximum entropy method, and compared also these results with the Schwinger boson results. The role of the maximum entropy default model was discussed, and for the 2D Heisenberg model we argued that a flat default model works best. We further discussed advantages and problems arising when applying the maximum entropy procedure to imaginary time correlation functions in real space and momentum space.

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