MONTE CARLO STUDY OF THE TWO-DIMENSIONAL SPIN-1/2 XY MODEL

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The generalized Trotter formula is used to map the two-dimensional spin-1/2 XY model onto a three-dimensional Ising model with complicated many-spin interactions. This relationship is used to construct an efficient Monte Carlo algorithm. Simulation data for the specific heat and vortex correlation functions give strong evidence for the existence of a phase transition.

Although it is well known that there cannot exist long-range order in the two-dimensional (2D) spin-1/2 XY model at non-zero temperature [1], high-temperature series expansions [2] suggest the existence of critical behavior. Little is known about the quantum model mainly because most techniques which have been successfully applied to the classical model (also referred to as planar rotator model) are very difficult to extend to the quantum case. In particular, quantum renormalization group analysis of the 2D spin-1/2 XY model have given either contradictory or unreliable results [3–8].

An alternative method to calculate the thermodynamic properties of this model is to exploit the formal analogy between d-dimensional quantum spin systems and (d + 1)-dimensional Ising-spin models [9]. Using the generalized Trotter formula [9], Suzuki showed that

$$Z_m = \text{Tr} \left\{ \prod_{i<j} \exp \left[ -\frac{\beta}{m} H_{i,j} \right] \right\}^m,$$

is the mth approximation to the partition function Z, $H_{i,j} = -J (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y)$, $\sigma_i$ is the Pauli spin-operator at site i and the product in (1) runs over some ordered set of nearest neighbor bonds of the square lattice. The basic idea of our approach is to calculate the thermodynamic properties of the approximation (1) and to study the convergence of the results as a function of m. Two of us have already given a rigorous solution of the simplest approximation $Z_1$ for a large class of orderings and it was shown that in this approximation there is a phase transition of unconventional nature (i.e. no spontaneous magnetization but a logarithmic divergence of the specific heat) [10].

A disadvantage of the special class of exactly solvable $m = 1$ approximations is that the construction [10] that maps them onto staggered 8-vertex models...
[11] is difficult to generalize to \( m > 1 \) and, more importantly, it is very difficult and inefficient to perform Monte Carlo simulations with this type of representation. An extensive discussion of the fundamental and technical problems that arise in simulations of 1D spin-1/2 models (XY and Heisenberg models) can be found in ref. [12].

For the \( d \)-dimensional XY model we have found representations of (1) that do not suffer from the problems encountered in simulations of 1D spin-1/2 systems [12]. First we note that (1) remains invariant if we rotate all spins over \( \pi/2 \) about the \( x \)-axis. Working with the XZ instead of XY model solves the problem of constructing algorithms that generate ergodic Markov chains. As this step is essential for the construction of an efficient algorithm, it is clear that our approach for the XY model cannot be used to study the isotropic Heisenberg system. We partition the Hamiltonian in two parts \( H = A + B \) where \( A \) contains all horizontal and \( B \) all vertical bonds. Clearly \( A \) (\( B \)) is a sum of non-interacting XZ chains. We obtain an expression of the form (1) by decomposing \( A \) and \( B \) into blocks of two sites. Having specified the ordering in (1) the next step is to introduce complete sets of states between all the exponential factors in (1). As each spin interacts with four neighbors we need \( 4mN^2 \) (\( N \) is the linear size of the system) Ising-spin variables. To proceed further we calculate the explicit form of the matrix elements of the two-site factors

\[
\langle S_i S_j \exp \left( K_m \left( \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \right) \right) | \sigma_i \sigma_j \rangle = \delta_{i,j} \sinh^{2} K_m^{1/2} \times \exp (\vec{K}_m S_i \sigma_j + K_m S_j S_i),
\]

where \( K_m = \beta J/m \), \( \vec{K}_m = \frac{1}{2} \ln \coth K_m \), \( \sigma_i^x | \sigma_j \rangle = S_i | S_j \rangle \) and \( \sigma_i^y | \sigma_j \rangle = \sigma_i | \sigma_j \rangle \). Finally we sum out \( 2mN^2 \) of the Ising spins analytically [13]. In our simulations we have used two different decompositions for the XZ chains; Suzuki's [9] real-space and Barma and Shastry's [14] checkerboard break-up. For \( m = 1 \) we can show that none of these two choices is in the class of orderings that lead to the rigorous \( m = 1 \) solution [10]. In the case of the real-space decomposition the final expression for \( Z_m \) reads

\[
Z_m = c \sinh^{2} K_m^{1/2} \sum \sum \prod \prod \prod h(j, k) \psi(j, k),
\]

where for periodic boundary conditions

\[
\begin{align*}
  h(j, k) &= \cosh \left( K_m \left( S_1^j \sigma_i^1 \sigma_j^1 + \ldots \right. \\
  &+ S_1^j \ldots S_N^j \sigma_i^j \sigma_j^j \right) \\
  &+ K_m \left( S_1^j \sigma_i^j \sigma_j^j \right. \\
  &+ S_1^j \ldots S_N^j \sigma_i^j \sigma_j^j \right) \\
  &\times \exp \left( K_m \left( S_1^j \sigma_i^j \sigma_j^j + \ldots \right. \\
  &+ S_1^j \ldots S_N^j \sigma_i^j \sigma_j^j \right) \\
  &+ S_1^j \ldots S_N^j \sigma_i^j \sigma_j^j \right) + S_{N-1}^j \sigma_i^j \sigma_j^j \right) \\
  c &= \text{an unimportant numerical constant and } \psi(i, k) \text{ can be obtained from } h(j, k) \text{ by substituting } S_1^j \sigma_i^1 \sigma_j^1 \text{ and } \sigma_i^j \sigma_j^j \text{ for } S_1^j \sigma_i^j \sigma_j^j \text{ and } S_{N-1}^j \sigma_i^j \sigma_j^j. \\
\end{align*}
\]
Fig. 1. Specific heat per site of the 2D spin-1/2 \(XY\) model in the \(m = 1\) approximation for lattices of different size. Solid line: rigorous staggered 8-vertex solution; broken line: high-temperature expansion. For most temperatures full squares cover open triangles. Statistical errors are of the size of the symbols.

and found excellent agreement with results obtained by summing all terms in (3) and by diagonalizing the full hamiltonian. At high temperatures \(T \geq 4\), our simulation results for the energy and specific heat are in very good agreement with those obtained from high-

Fig. 2. Specific heat per site of the 2D spin-1/2 \(XY\) in the \(m = 1\) approximation. Solid line: rigorous staggered 8-vertex solution; broken line: high-temperature expansion. Comparison with the data of fig. 1 shows that in the critical region the \(m\)-dependence is very weak.

Fig. 3. Minus the energy per site (full symbols) and specific heat per site (open symbols) as a function of \(1/m\) for the \(12 \times 12\) system. Circles: \(T/J = 1\); squares: \(T/J = 2\) and triangles \(T/J = 2.25\). The arrow gives the Pearson's estimate of the ground-state energy.
for $T/J > 2$ the specific heat, which from the point of view of convergence is the most difficult quantity to calculate [13], depends weakly on the particular value of $m$. Except for $2 \leq T \leq 2.5$ the size dependence of the energy per site and specific heat per site is small. More convincing evidence that the convergence of the energy and specific heat is very good is given in fig. 3. In the critical region ($T/J \approx 2.27$) the $m$-dependence of physical quantities is very weak. Therefore it might be tempting to assume that to a good approximation the critical properties of the 2D spin-$1/2$ $XY$ model are that of the $m = 1$ representation. Although our numerical data is not inconsistent with this assumption we take the point of view that the subtle $\beta/m$ dependence of the approximants could change the critical behavior. Furthermore it is obvious that it is impossible to prove or disprove by means of Monte Carlo data that some physical quantity is continuous or divergent.

To elucidate the nature of the transition we calculate spin-correlation functions which are sensitive to the occurrence of vortex-like excitations. In particular we study the quantum version of Swendsen’s vortex detector [17]

$$D = N^{-2} \sum_{\text{plaquettes}} \langle (1 - \sigma_i^z \sigma_j^z - \sigma_i^x \sigma_j^x) \rangle \times (1 - \sigma_k^z \sigma_l^z - \sigma_k^x \sigma_l^x),$$

where $i(j)$ and $k(l)$ label the opposite corners of an elementary square. Simulation data for the approximant $D_m$ are shown in fig. 4. As for the energy and specific heat the $m$-dependence of $D_m$ is very weak. The rapid change of the disorder-parameter $D$ as $K$ approaches $K_c$ strongly suggests that there is a phase transition.

To demonstrate the versatility of our method we have also carried out simulations for systems with $N = 8, 16$ and $1 \leq m \leq 32$ for temperatures down to $T/J = 0.5$. Within the statistical accuracy of the simulation data (which for the energy is less than one percent), we find that for $0.5 \leq T/J \leq 1.5$, the energy is constant. The extrapolated ground state energy per site $\approx -2.2$ which is in agreement with estimates given by Pearson [18].

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