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Chiral exponents of the square-lattice frustrated $XY$ model:  
A Monte Carlo transfer-matrix calculation

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Thermal and chiral critical exponents of the fully frustrated $XY$ model on a square lattice are obtained from a finite-size scaling analysis of the free energy of chiral domain walls. Data were obtained by extensive Monte Carlo transfer-matrix computations for infinite strips of widths up to 14 lattice spacings. Two transfer matrices were implemented, one for each of the two principal lattice directions. The results of both are consistent, but the critical exponents differ significantly from the pure Ising values. This is in agreement with other recent Monte Carlo simulations. Our results also support the identification of the critical behavior of this model with that along the line of transitions of simultaneous ordering or becoming critical of Ising and planar rotor degrees of freedom in the $XY$-Ising model studied recently.

I. INTRODUCTION

There has been considerable interest, both experimentally and theoretically, in phase transitions of two-dimensional, fully frustrated $XY$ models. Most studies have been motivated by their relevance to Josephson junction arrays in a magnetic field, where these models describe the superconducting-to-normal transition at half a flux quantum per plaquette, but there are also interesting theoretical questions regarding the identification of the universality class. In the standard $XY$ model without frustration the relevant symmetry is the continuous U(1) symmetry which, as is well-known, is responsible for a Kosterlitz-Thouless phase transition. The fully frustrated $XY$ model has a richer behavior with a low-temperature phase with critical fluctuations associated with the U(1) symmetry, accompanied by a broken, discrete $Z_2$ symmetry. In principle, there are two different ordering scenarios: ordering can take place in two stages via separate $XY$ and Ising transitions, or both symmetries can be broken or become critical simultaneously, which yields a single transition, presumably in a new universality class.

On a square lattice the model can be defined by the Hamiltonian

$$H = -\sum_{(ij)} J_{ij} \cos(\theta_i - \theta_j),$$

(1)

where $J_{ij} = J$ ($J > 0$) for horizontal rows and $J_{ij} = \pm J$ for alternating vertical columns. Owing to the presence of an odd number of antiferromagnetic bonds in each plaquette, the model is fully frustrated. This leads to a double degeneracy of the ground state, which is of course accompanied by an additional continuous degeneracy, a manifestation of the U(1) symmetry. One can introduce an Ising-like order parameter $\chi_p$, the local chirality, which measures the sense of rotation of a spin of unit length $s = (\cos \theta, \sin \theta)$ along the sides of a given plaquette $p$. In the ground state there is antiferromagnetic order of the local chiralities ($\chi_p = \pm 1$).

Early Monte Carlo simulations led to the conclusion that the chiral order parameter of the fully frustrated $XY$ model has pure Ising model critical exponents, but more recent estimates of the exponents have differed significantly from the Ising values. In particular, predictions were made for the values of chiral critical exponents of the fully frustrated $XY$ model. These predictions are based on results for the $XY$-Ising model which is expected to describe the critical behavior in these systems. These ideas are supported by recent Monte Carlo simulations. However, in view of results that suggest pure Ising critical exponents, and in the absence of precise agreement among the more recent estimates, the current state of affairs is unsatisfactory from a computational point of view. The additional numerical results presented in this paper may serve to help settle the issue.

We report results of extensive numerical calculations of the chiral domain wall free energy of the fully frustrated $XY$ model in an infinite strip geometry. Because of the continuous nature of the phase variables of this model, the transfer-matrix is intractable for numerically exact computation of its eigenvalues. We therefore use the Monte Carlo transfer-matrix method to obtain the free energy from the largest eigenvalue of the transfer matrix. Exploiting the anisotropy of the Hamiltonian (1) we use two different implementations, a "horizontal" (i.e., column-to-column) and "vertical" (i.e., row-to-row) transfer matrix. These approaches yield results in reasonable agreement. From a finite-size scaling analy-
sis of data for strips of widths up to 14 lattice spacings, we have estimated the thermal exponent $\nu$, the exponent $\eta$ associated with the Ising-like order-order correlation function, and the critical temperature $T_c$. In particular, the result obtained for $\nu$ is quite insensitive of the estimate of $T_c$, as will be discussed in more detail below. We summarize our estimates (with error estimates in parentheses): $\nu = 0.80(4)$, $\eta = 0.38(3)$, and $T_c = 0.454(4)$. Within the errors, these numbers are in agreement, with a Monte Carlo simulation using similar finite-size scaling analysis$^{12}$ and they are also consistent with other Monte Carlo simulations.$^{13}$ However, our value of $\nu$ disagrees with the estimate of $\nu = 1$ by Thijsse and Knop,$^{14}$ who also used the Monte Carlo transfer-matrix method, but with a different method to estimate $\nu$; their estimating deviation is likely an artifact of their fitting procedure.$^{15}$ On the other hand, our value of $\eta$ is in very good agreement with their estimate. Moreover, our results appear to support the identification of the critical behavior of the fully frustrated XY model with the line of single transitions in the XY-Ising model studied recently.$^{11,14}$

II. MONTE CARLO TRANSFER MATRIX

The Monte Carlo transfer-matrix method introduced by Nightingale and Blöte$^{15}$ is particularly useful when, as is the case in the model under consideration, the continuous nature of the spin variables does not allow a numerically exact diagonalization of the transfer matrix. The method is a stochastic version of the well-known power method of calculating the dominant eigenvalue of a matrix or integral kernel. More specifically, the dominant eigenvector $\psi^0$ is approximated by a Monte Carlo time average over weighted walkers representing row (or column) configurations. The basic idea is that the (weighted) frequency of occurrence of a particular row (or column) configuration, say $S = (s_1,s_2,\ldots,s_L)$, is proportional to the magnitude of the corresponding component $\psi^0_S$ of the dominant eigenvector $\psi^0$. The key elements of the algorithm are the following.

Walkers are generated in subsequent generations labeled by an index $t$. The generation at time $t$ consists of a sequence of a number of $r_t$ walkers $[(S_{i,1},w_{i,1,t}),(S_{i,2},w_{i,2,t}),\ldots,(S_{i,r_t},w_{i,r_t,t})]$, where the $S_{i,t}$ are row (or column) configurations of the form $S$ introduced above, and the $w_{i,t} > 0$ are statistical weights. This sequence represents a (generally extremely) sparse vector $\psi$ with components

$$\psi_S = \sum_{i=1}^{r_t} \delta_{S,S_i} w_{i,t},$$

(2)

where $\delta$ is the Kronecker $\delta$ function. One can write

$$\psi'_S = \sum_S T(S'|S)\psi_S = \sum_S P(S'|S)D_S \psi_S,$$

(3)

where $D_S = \sum_{S'} T(S'|S)$ and $P(S'|S) = T(S'|S)/D_S$. Since by construction $P$ is a stochastic matrix, multiplication by the transfer matrix of a vector of the form $\psi$ can be implemented as a stochastic process with transitions from $S$ to $S'$ with probability $P(S'|S)$. That is, to update generation $t$ to $t+1$, new walker states are sampled with probability $P(S_{t+1}|S_t)$, while in each transition the weight of walker $i$ is updated to $w_{i,t+1} = D_S w_{i,t}/c_{t+1}$. For reasons of efficiency the weights are kept close to unity by duplicating walkers with great statistical weights and by eliminating walkers with low weights. To ensure that $r_{t+1}$ remains close to its initial value $r_0$, one can choose $c_{t+1} = \lambda t r_t/r_0$, where $\lambda$ is a moving or cumulative average estimate of the dominant transfer-matrix eigenvalue. Assuming that the generation counter $t$ is reset to unity upon equilibration, the largest eigenvalue can be estimated from a sequence of $T$ generations as

$$\lambda = \sum_{t=1}^{T} c_{t+1} W_{t+1} \bigg/ \sum_{t=1}^{T} W_t,$$

(4)

where $W_t = \sum_{i,t} w_{i,t}$ denotes the total statistical weight of all walkers of generation $t$. It should be noted that this estimator of the dominant eigenvalue suffers from a bias due to the correlations of the population control constants $c_t$ with the weights $W_t$. These correlations have the effect of suppressing large contributions to the estimator (4) and enhancing small ones.$^{17}$ As a result, the estimator tends to underestimate the exact transfer-matrix eigenvalue, but this effect can be reduced by choosing a large target number of walkers, $r_0$. Further algorithmic details, such as how to correct for this bias without increasing the average population size, and an alternative, sometimes better choice of the population control constant $c_t$ can be found in Refs. 18–20. In applying this method to the fully frustrated XY model, we have performed extensive calculations using, typically, $r_0 = 30,000$ walkers and $150,000$ Monte Carlo steps which corresponds to $4.5 \times 10^6$ attempts per site.

To apply this Monte Carlo method it is necessary to sample configurations $S'$ from the distribution $P(S'|S)$ for arbitrary $S$ and to evaluate the quantity $D_S$ at each elementary Monte Carlo step. One way to do this is to factor the transfer matrix in a way that amounts to building up the square lattice by, e.g., first adding bonds perpendicular to the transfer direction and then adding new sites and bonds along the transfer direction. The algorithm given above is then applied to both factors in succession. The first of these operations corresponds to multiplication by a diagonal matrix. This leaves the row (or column) configurations unchanged while the weight factors are calculated trivially: they consist of one term each. The second matrix factor, which adds $L$ new sites, has a direct product form. Sampling and reweighting problems in this case reduce to simple one-site problems. In principle, this method works, but it yields an inefficient Monte Carlo process: the simple factorization generates row (or column) configurations with variables that are too weakly correlated in the sense that, as it is added to the lattice, each variable is sampled independently from a distribution with direct correlations only to one other nearest-neighbor variable. True many-site correlations are subsequently recovered via multiplication by
strongly fluctuating weight factors. This, however, causes
strong fluctuations in the number of walkers, which re-
results in frequent elimination and duplication of walkers
and enhances correlations between walkers within each
generation, which reduces the overall Monte Carlo sam-
ing efficiency.

The alternative we have used in this paper requires
helical boundary conditions. In that case the lattice
can be constructed by repetition of identical elementary
steps, each of which adds one site at a time. This implies
that the states $S'$ and $S$ in the transition matrix $P(S'|S)$
consist of lattice sites all of which coincide with the
exception of one site. Consequently only a small number
of states $S'$ can be reached from any given state $S$, i.e.,
$P$ is sparse in this case. The degrees of freedom that
are added will have direct correlations with those at two
neighboring lattice sites, one in the horizontal and one
in the vertical direction for the square lattice. In prin-
ciple, given an approximate dominant eigenvector, one can
transform the transfer matrix and incorporate even more
correlations of the weights and eigenvalue estimates. We
will return to this later on.

Use of helical boundary yields a more efficient Monte
Carlo process, but the method has the disadvantage of
producing a lattice with a surface that has a step defect,
as is unavoidable when one cuts across a screw. One
would expect the presence of this defect to lead to unnec-
essary corrections to scaling, which may adversely affect
finite-size convergence, but in practice this appears not
to be a serious problem.

In fact, the method used in this paper requires use of
a transfer matrix of somewhat more complicated form
than the one of Eq. (3), in that this equation has to be
replaced by

$$
\psi''_{S'} = \sum_{S',S} T^{(1)}(S'|S)T^{(2)}(S'|S)\psi_S.
$$

Although this is no real complication—one can simply
devide a stochastic process with steps alternating in corre-
spondence to the two matrices $T^{(1)}$ and $T^{(2)}$—it has
prevented our use of approximate trial eigenvectors to
reduce the noise of the stochastic process. In principle,
this variance reduction scheme works as follows. Equa-
tion (3) can be replaced by the equivalent equation

$$
\tilde{\psi}'_{S'} = \sum_{S} \tilde{T}(S'|S)\tilde{\psi}_S
$$

where $\tilde{T}(S'|S) = \gamma S T(S'|S)/\gamma S$ and $\psi$ and $\psi'$ are
similarly similarity transformed. As long as the components
of $\gamma$ are all of one sign and do not vanish, the same Monte
Carlo method can be applied to $\tilde{T}$ instead of $T$. This
approach satisfies the following zero-variance principle: in
the ideal limit where $\gamma$ is the dominant left eigenvector
of $T$, the largest eigenvalue of $T$ can be estimated with
vanishing statistical error. More realistically, as this limit
is approached the variance of the Monte Carlo process
decreases. In practical applications, one chooses a trial
vector $\gamma(p_1, p_2, \ldots)$ which depends on variational param-
eters $p_i$. These are optimized by minimization of the vari-
ance over $S$ of $\sum_{S'} \gamma S T(S'|S)/\gamma S$ with states selected
with probability proportional to $\gamma S$. This minimization
is accomplished approximately by minimizing the variance
over a relatively small set of states $S$ generated by Monte
Carlo. For a transfer matrix of the form of Eq. (5) the
same process is still possible in principle, but it is more
complicated. In fact there are two alternatives. One can
define a Kramers–product-like, two-site transfer matrix
$T^{(1)}(S', S', S', S) = T^{(1)}(S'|S)T^{(2)}(S'|S)$ and base the
Monte Carlo process on the derived stochastic matrix
$P(S'', S', S, S) \propto \gamma_{S',S'} T^{(1)}(S'', S'|S')/\gamma_{S',S'}$.
where ideally $\gamma_{S',S'}$ is the dominant left eigenvector of $T^{(1)}$. We
note that the pairs $(S'', S')$ and $(S', S)$ differ at two lat-
etic sites, and therefore this approach requires simultane-
ous sampling of two site variables, which renders the algo-
rum unnecessarily slow. The alternative is to employ—
as we have done in this paper—a matrix product of two
single-site transfer matrices rather than a single two-
site transfer matrix, but this approach requires two trial
vectors. In terms of these, one defines $\tilde{T}(S'|S) =
\gamma S' T^{(1)}(S'|S)/\gamma S$, and $\tilde{\gamma}_{S',S} = \gamma S' T^{(2)}(S'|S)/\gamma S$.
It is straightforward to construct a transformed process
which again has a zero variance principle. This time
it requires that $\gamma^{(1)}$ be the dominant left eigenvector
of the product matrix $T^{(1)} T^{(2)}$ and that $\gamma^{(2)}$ be the
dominant left eigenvector of $T^{(2)} T^{(1)}$. Again adjustable pa-
rameters of $\gamma^{(1)}$ and $\gamma^{(2)}$ can be chosen by minimization
of the (appropriately weighted) sum of the variances
$\sum_{S'} \gamma S T(S'|S)/\gamma S$ and $\sum_{S'} \gamma S T(S'|S)/\gamma S$. In con-
trast with the alternative of a two-site transfer matrix, the
choice of two matrices slows down the algorithm only
in the initial stage of parameter optimization with this
approach.

III. CHIRAL DOMAIN WALL FREE ENERGY

For an infinite strip of width $L$, the reduced free energy
$f$ per lattice site can be obtained from the largest trans-
fer matrix eigenvalue, $\lambda(L, K)$, via the relation $f = -\ln \lambda$,
where $K = J/k_B T$ is the reduced coupling constant. For
any given $L$ this quantity, $f$, depends on the choice of
boundary conditions. By suitable choice of the latter,
as specified in detail below, the chiral domain wall free
energy can be obtained from the free energy difference,
denoted by $\Delta f$. For finite-size analysis, a convenient
quantity is the domain wall energy per $L$ lattice units
of length:

$$
\Delta F(K, L) = L^2 \Delta f(K, L).
$$

Since the fully frustrated $XY$ model is spatially
anisotropic, one can devise two different types of bound-
ary conditions to compute the domain wall free energy.
These two types are associated with two different transfer
matrices obtained by choosing the transfer direction to
be either horizontal or vertical, as shown in Fig. 1. If the
transfer direction is horizontal [Eq. 1(a)], one is forced
to use helical boundary conditions with a pitch of two
measured in lattice units, so as to match up the vertical
antiferromagnetic bonds, which have a periodicity of two in the transfer direction. This is the construction used in Ref. 10. As indicated in Fig. 1(a), only strips with \( L \) even will match the antiferromagnetic pattern of the local chiralities \( \chi_p \) in the ground state; for strips with odd \( L \) the boundary conditions will introduce a chiral domain wall along the infinite horizontal direction. Calculation of the domain wall energy requires that the boundary conditions be varied at constant \( L \). With the horizontal transfer matrix this can be done approximately only, and we chose to use the difference of the free energy computed directly for \( L \), and the free energy obtained by linear interpolation between sizes \( L - 1 \) and \( L + 1 \). This still leaves two possibilities, depending on whether \( L \) is odd or even. As an alternative we also performed calculations using a vertical transfer matrix illustrated in Fig. 1. In this case one has a choice between helical boundary conditions with a pitch of one or two lattice units. For each value of \( L \) precisely one of these two boundary conditions will force the presence of a domain wall and this offers a convenient way to determine the chiral domain free energy without interpolation.

Calculations of the free energy using the horizontal and vertical transfer matrices were performed as a function of strip width in a very narrow range of couplings \( \Delta K = 0.04 \) around the estimate of the critical coupling obtained by Monte Carlo simulations of Lee, Kosterlitz, and Granato.\(^{12} \) Note that the range we use is about ten times smaller than the range used in Ref. 10. The data for the chiral domain wall free energy using both implementations of the transfer matrix are shown in Figs. 2 and 3.

**IV. FINITE-SIZE SCALING ANALYSIS**

To determine the critical temperature and critical exponents, we make use of the following finite-size scaling relation for the domain wall free energy

\[
\Delta F(K, L) = A(L^{1/\nu} \Delta K),
\]

where \( A \) is a scaling function and \( \Delta K = K - K_c \) is the deviation of the coupling constant from its critical value \( K_c \). For sufficiently small values of its argument, the scaling function can be expanded as

\[
\Delta F(K, L) = a_0 + a_1 L^{1/\nu} \Delta K + a_2 (L^{1/\nu} \Delta K)^2 + \cdots,
\]

which shows that \( \Delta F(K, L) \) is constant as a function of \( L \) for \( K = K_c \), but for that value of the coupling constant only. This behavior is apparent in Figs. 2 and 3 for
at least $L \geq 8$ if we attribute the deviations for smaller system sizes to corrections to scaling. To the extent that the quadratic and higher-order terms in Eq. (9) can be neglected, the critical exponent $\nu$ can be obtained from the condition that $\Delta F(K, L)$ be linear in $L^{1/\nu}$ for fixed $\Delta K$. In fact, in this approximation, $\nu$ can be obtained from the slope of a log-log plot of $S = \partial \Delta F(K, L)/\partial K$ vs $L$, which gives $1/\nu$. From the data of Figs. 2 and 3, we have obtained $S$ as a function of $L$ for the horizontal and vertical transfer matrix using this procedure. The results are indicated in Fig. 4. The slopes of the straight lines in the log-log plot, corresponding to the results for vertical and horizontal transfer matrices, agree within the errors, as one would expect, providing a check to the consistency of our data. From this plot we can estimate $\nu = 0.80(4)$. It is interesting to note that within the linear approximation—as is the case for the free energy barrier in the histogram of chirality in the Monte Carlo simulations, where a similar finite-size scaling is possible—the estimate of the critical temperature $T_c = 1/K_c$, and the estimate of the thermal exponent $\nu$ are in fact independent, but this property is preserved only approximately in our generalized finite-size analysis, where we fitted the domain wall energies to the form of Eq. (9) with as fitting parameters $K_c$, $\nu$, and $a_i$ with $i = 0, 1$, and 2, as obtained by truncation of the scaling function beyond second order. Note that the correlation function exponent $\eta$ can be obtained from the universal amplitude $a_0$ in Eq. (9) using the results of conformal invariance in two dimensions: $a_0 = \pi \eta$.

The results of the finite-size scaling based on Eq. (9) fits are summarized in Table I and the corresponding scaling plots are shown in Figs. 5 and 6. The table contains estimates of the statistical errors associated with the least-squares procedure. In some cases the $\chi^2$ were too large to be attributable to chance and as consequence these statistical error estimates are to be treated with suspicion. This is also evident from the discrepancies between the various independent estimates. Under the circumstances all we can do is to take the mutual differences of various estimates as (admittedly unsatisfactory) error estimates. Thus we obtain our estimates: $T_c = 0.454(3)$, $\nu = 0.80(5)$, and $\eta = 0.38(2)$. This result for $\nu$ is inconsistent with the pure Ising value of $\nu = 1$, but it is in agreement with the result $\nu = 0.85(3)$ from a similar finite-size scaling analysis of the free energy barrier in the histogram of chirality from other Monte Carlo simulations. Our estimate also agrees with a recent estimate $\nu = 0.875(35)$ based on a finite-size scaling analysis of correlation functions. We therefore conclude that the estimate of $\nu = 1$ obtained by Thijsen and Knops is likely to be an artifact of their fitting procedure.

Recently, the phase diagram of the two-dimensional $XY$-Ising model defined by the Hamiltonian

\begin{table}[h]
\centering
\begin{tabular}{c c c c c c}
$T_c$ & $\nu$ & $\eta$ & $L$ & Transfer & $\chi^2$
\hline
0.4544(3) & 0.77(5) & 0.378(3) & 10, 14 (2) & $v$ & 11
0.4555(2) & 0.83(4) & 0.369(2) & 8, 14 (2) & $v$ & 14
0.4538(2) & 0.83(5) & 0.394(1) & 8, 12 (2) & $h$ & 1
\end{tabular}
\caption{Results for critical temperature and critical exponents, obtained from finite-size scaling analysis of domain wall energies. Standard errors are indicated parenthetically. As explained in the text, these standard errors reflect only statistical uncertainties, which are presumably considerably smaller than the errors due to corrections to scaling. The column labeled $L$ indicates which system sizes were used in the fits: $L_1, L_2 (\Delta L)$ stands for sizes from $L_1$ to $L_2$ in steps of $\Delta L$. Horizontal and vertical transfer matrices are indicated by $v$ and $h$ under the heading transfer. The last column is the $\chi^2$ per degree of freedom.}
\end{table}
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\[ f(K_c, L) = f_{\infty} + \frac{\pi c_{3/2}}{6L^2} \]  

(11)

which is valid asymptotically for large \( L \). Fitting the data for \( f(K, L) \) closest to the estimated critical temperature \( T_c \), we obtain \( c = 1.61(3) \) from the strips of \( 8 \leq L \leq 14 \) using both horizontal and vertical Monte Carlo data. This result agrees with the estimate of the central charge first obtained by Thijssen and Knops,\textsuperscript{10} also using Monte Carlo transfer-matrix calculations, and appears to be significantly larger than \( c = 3/2 \), which would be expected if the transition was single, but decoupled.\textsuperscript{28} However, one cannot be certain of this value unless calculations are done at sufficiently large \( L \) such that small-\( L \) corrections to the above asymptotic expression are negligible. Using only the Monte Carlo transfer-matrix data for \( 6 \leq L \leq 14 \) may not allow us to extrapolate to the \( L \) large limit and it is quite likely that this estimate of \( c \) is subject to systematic errors. In fact, recent large \( L \) calculations for the related \( XY \)-Ising model\textsuperscript{29} show a significant decrease of \( c \) with increasing \( L \). Unfortunately, our data for the fully frustrated \( XY \) model for \( L > 14 \) turn out to be rather noisy. This problem can be remedied in principle by using variance reductions techniques,\textsuperscript{20–22} but as discussed this is complicated in the case of the square lattice fully frustrated \( XY \) model because of the presence of both ferromagnetic and antiferromagnetic bonds. The case of the triangular lattice is more straightforward in this respect.

V. CONCLUSION

We have studied the finite-size behavior of the chiral domain wall free energy of the square lattice fully frustrated \( XY \) model on an infinite strip, using the Monte Carlo transfer matrix. From a finite-size scaling analysis of data for strip widths up to 14 lattice spacing, we have estimated the critical temperature and chiral critical exponents. The latter appear to be significantly different from the pure Ising values and in agreement with other recent Monte Carlo simulations. The results are also consistent with the identification of the critical behavior of the fully frustrated \( XY \) model with that of a point of the line of single transitions in the \( XY \)-Ising model studied recently.\textsuperscript{30} The value of the central charge \( c = 1.61(3) \) is found to be consistent with the estimate first obtained by Thijssen and Knops, but we cannot rule out the possibility that all results obtained for this and similar models are skewed by large, slowly decaying corrections to scaling.

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