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Kosterlitz-Thouless transition in the two-dimensional quantum *XY* model

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Convincing numerical evidence is obtained via extensive quantum Monte Carlo simulations on square lattices as large as 96×96 that the spin-$\frac{1}{2}$ *XY* model undergoes a Kosterlitz-Thouless phase transition at $kT_c/J = 0.350(4)$. Correlation length and in-plane susceptibility diverge at T_c precisely according to the form predicted by Kosterlitz and Thouless for the classical *XY* model. The specific heat increases very rapidly near T_c and exhibits a peak around $kT/J = 0.45$.

It is well known now that the two-dimensional (2D) classical (planar) *XY* model undergoes Kosterlitz-Thouless (KT) (Ref. 1) transition at $kT_c/J = 0.898$,[2,3] characterized by exponentially divergent correlation length and in-plane susceptibility. The transition, due to the unbinding of vortex-antivortex pairs, is weak; the specific heat has a finite peak above T_c.

Does the 2D quantum *XY* model go through a phase transition? If yes, what is the type of the transition? This is a longstanding problem in statistical physics. The answers are relevant to a wide class of 2D problems such as magnetic insulators, superfluidity, melting, and possibly to the recently discovered high-T_c superconducting transition. Physics in two dimensions is characterized by large fluctuations. Changing from the classical model to the quantum model, additional quantum fluctuations (which are particularly strong in the case of spin $\frac{1}{2}$) may alter the physics significantly. A direct consequence is that the already weak KT transition could be washed out completely.

The quantum *XY* model was first proposed[4] in 1956 to study the lattice quantum fluids. Later, high-temperature series studies[5] raised the possibility of a divergent susceptibility for the 2D model. For the classical planar model, the remarkable theory of Kosterlitz and Thouless[1] provided a clear physical picture and correctly predicted a number of important properties. However, much less is known about the quantum model. In fact, it has been controversial. Using a large-order high-temperature expansion, Betts and co-workers[6] suggested a second-order transition at $kT_c/J = 0.39$ for spin $\frac{1}{2}$. Later, real-space renormalization-group analysis was applied[7] to the model with contradictory and inconclusive results. De Raedt *et al.*[8] then presented an exact solution and Monte Carlo simulation, both based on the Suzuki-Trotter transformation[9] with small Trotter number m. Their results, both analytical and numerical, supported an *Ising*-like (second-order) transition at the Ising point

$$kT_c/J = \tfrac{1}{2}\ln(1+\sqrt{2}) = 0.567\,,$$

with a logarithmically divergent specific heat. Loh, Scalapino, and Grant[10] simulated the system with an improved technique.[11] They found that the specific-heat peak remains finite and argued that a phase transition occurs at $T_c = 0.4$–0.5 by measuring the change of the "twist energy" from the 4×4 lattice to the 8×8 lattice. The dispute[12] between De Raedt and Lagendijk, and Loh, Scalapino, and Grant, centered on the importance of using a large Trotter number m and the global updates in small-size systems, which move the system from one subspace to another. Recent attempts to solve this problem still add fuel to the controversy.[13,14]

The key to pin down the existence and the type of transition is a study of correlation length and in-plane susceptibility because their divergences constitute the most direct evidence of a phase transition. These quantities are much more difficult to measure and large lattices are required in order to avoid finite-size effects. These key points are lacking in previous works, and are the focus of our study. In this Rapid Communication, we report a simulation on much bigger lattices with much better statistics. Due to the algorithmic advances[15] and extensive use of the parallel supercomputer,[16] we are able to measure spin correlations and thermodynamic quantities accurately on very large lattices (96×96). We report convincing evidence that a phase transition does occur at finite temperature in the extreme quantum case, spin-$\frac{1}{2}$. At the transition point, $kT_c/J = 0.350 \pm 0.004$, the correlation length and susceptibility diverge exactly according to the form of Kosterlitz-Thouless[1] [see Eq. (3)].

The quantum *XY* model

$$H = \sum_{\langle ij \rangle} S_i^x S_j^x + S_i^y S_j^y\,,$$

where $\langle ij \rangle$ goes over all the nearest-neighbor pairs on the square lattice and S_i is the spin operator, is simulated by the quantum Monte Carlo method (see Ref. 15 for details). We performed high-statistics simulations at $T = 0.41$–0.7. We started at $T = 0.7$. As T is lowered, we systematically increase the lattice size to satisfy $L \geq 4\xi$ at every T, so that finite-size effects in our calculation are very small. A similar procedure was used successfully for the classical *XY* model.[3] Over 95% of CPU time is spent on lattices 64×64 and 96×96 at four temperatures. We did two sufficiently long runs at every T. For example, at $T = 0.41$ we run 2×420000 sweeps.

We emphasize that the systematic error in our results, due to the finite value of $\Delta\tau = 1/mT$, is very small. The error is of the order of $(\Delta\tau)^2$ and is independent of volume.[9,11,17] We used a large $m = 24$ at all T, so that $\Delta\tau \leq 0.1$ for the temperature range we studied. This is in contrast with De Raedt *et al.*[8] who used $\Delta\tau \sim 1$ and Loh *et al.*[10] who used $\Delta\tau=0.25$ (which appears to be reasonable). Additional support comes from our experience with the Heisenberg model,[15] where at two temperatures ($T=0.3$ and 0.35) correlation lengths measured on large lattices with $m=24$ and 48 agree well within error (see Table I there).

Our main focus is to compute the spin-correlation function

$$C(r)=\frac{4}{L^2}\sum_n \langle S_n^y S_{n+r}^y\rangle \quad (1)$$

and in-plane susceptibility

$$\chi=\left\langle \left(\sum_i S_i^x\right)^2+\left(\sum_i S_i^y\right)^2\right\rangle \Big/ 2L^2=\left\langle \left(\sum_i S_i^y\right)^2\right\rangle \Big/ L^2, \quad (2)$$

where L is the linear size of the system. At large r, $C(r)$ has the asymptotic form $F(r)=Ar^{-\eta}e^{-r/\xi}$, where ξ is the correlation length and η is the algebraic exponent. In practice, we fit to $C(r)=F(r)+F(L-r)$ to incorporate the boundary reflection. The fits to this form are excellent, as shown in Fig. 1. The best fits for ξ and χ are listed in Table I.

As shown in Figs. 2 and 3, ξ,χ increase very fast as T is lowered. They will diverge at some finite T_c. We fit them to the form predicted by Kosterlitz and Thouless for the classical model[1]

$$\xi(T)=Ae^{B/(T-T_c)^\nu}, \quad \nu=\tfrac{1}{2}. \quad (3)$$

The fit is indeed very good (χ^2 per degree of freedom is 0.81), as shown in Fig. 2. The fit for the correlation length gives

$$A_\xi=0.27(3),\ B_\xi=1.18(6),\ T_c=0.350(4). \quad (4)$$

A similar fit for the susceptibility χ is also very good (χ^2 per degree of freedom is 1.06):

$$A_\chi=0.060(5),\ B_\chi=2.08(6),\ T_c=0.343(3), \quad (5)$$

as shown in Fig. 3. The good quality of both fits and the closeness of T_c's obtained are the main results of this work. The fact that these fits also reproduce the expected scaling behavior $\chi\propto\xi^{2-\eta}$ with

$$\eta=2-B_\chi/B_\xi=0.24\pm0.10 \quad (6)$$

is a further consistency check. These results strongly indicate that the spin-$\frac{1}{2}$ XY model undergoes a Kosterlitz-Thouless phase transition at $T_c=0.350\pm0.004$. We note that this T_c is consistent with the trend of the "twist energy"[10] and the rapid increase of vortex density near $T=0.35$–0.40,[10] due to the unbinding of vortex pairs.

TABLE I. A list of temperature, lattice size, correlation length, and susceptibility.

T	Size	ξ	χ
0.7	24×24	1.88(7)	1.93(2)
0.65	24×24	2.41(8)	2.56(3)
0.6	32×32	2.90(8)	3.58(4)
0.55	32×32	3.70(9)	5.72(11)
0.52	48×48	4.53(11)	8.22(16)
0.48	48×48	6.92(14)	16.0(7)
0.45	64×64	11.3(3)	36.3(1.4)
0.43	64×64	17.4(5)	70.1(5.6)
0.42	96×96	22.9(6)	116(11)
0.41	96×96	32.0(1.5)	162(12)

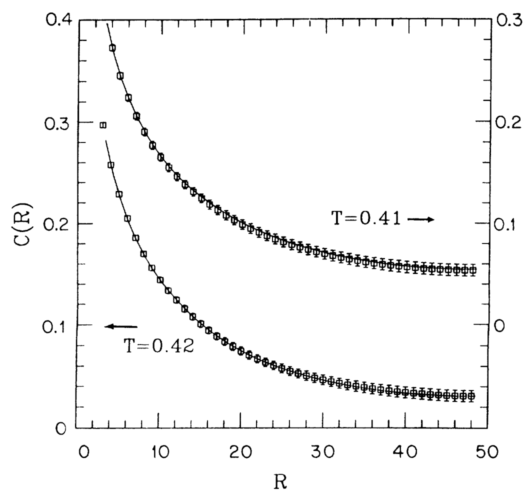

FIG. 1. The correlation functions on 96×96 lattice.

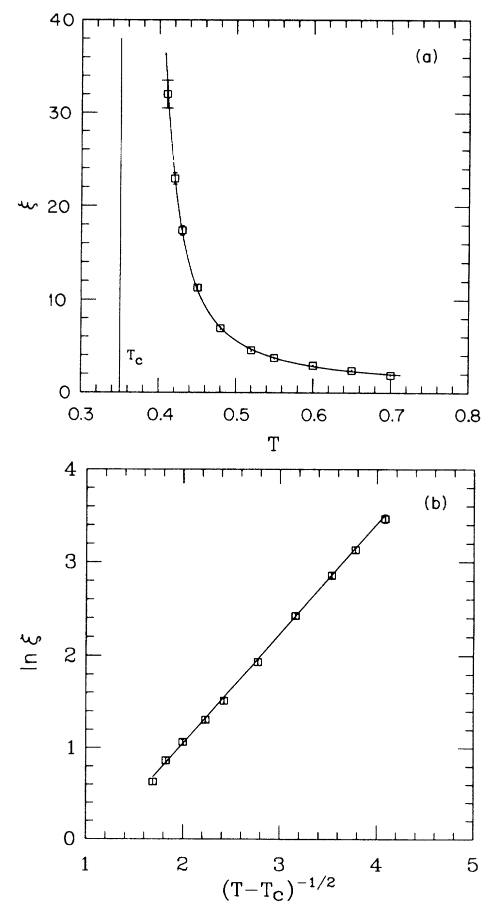

FIG. 2. Correlation length and the fit. (a) ξ vs T. The vertical line indicates ξ diverges at T_c; (b) $\ln\xi$ vs $(T-T_c)^{-1/2}$. The straight line indicates $\nu=\frac{1}{2}$.

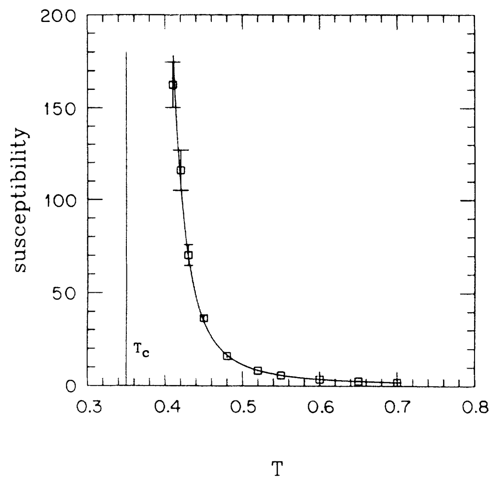

FIG. 3. Susceptibility and the fit.

Figures 2 and 3 also indicate that the critical region ΔT is quite wide ($\sim T_c$), very similar to the spin-$\frac{1}{2}$ Heisenberg model where the $T \rightarrow 0$ behavior holds up to $T \sim 2J$.[15,18] These 2D phenomenon are in sharp contrast to those usual second-order transitions in 3D.

The algebraic exponent η is consistent with the Ornstein-Zernike exponent $(d-1)/2 = \frac{1}{2}$ at higher T. As $T \rightarrow T_c$, η shifts down slightly and shows signs of approaching $\frac{1}{4}$, the value at T_c for the classical model.[1] (Extensive large-lattice simulations[4] indicate that η is slightly bigger than 0.25.) This is consistent with Eq. (6).

We measured energy and specific heat C_V (for $T \leq 0.41$ we used a 32×32 lattice). The value of energy is in general agreement with Refs. 10 and 13. The specific heat is shown in Fig. 4. We found that C_V has a peak above T_c, at around $T = 0.45$. The peak clearly shifts away from $T = 0.52$ on the much smaller 8×8 lattice.[10] De Raedt *et al.*[8] suggested a logarithmic divergent C_V in their simulation, which is likely an artifact of their small m values. One striking feature in Fig. 4 is a very steep increase of C_V at $T \approx T_c$. The shape of the curve is asymmetric near the peak. These features of the C_V curve differ from that in the classical XY model.[2,3]

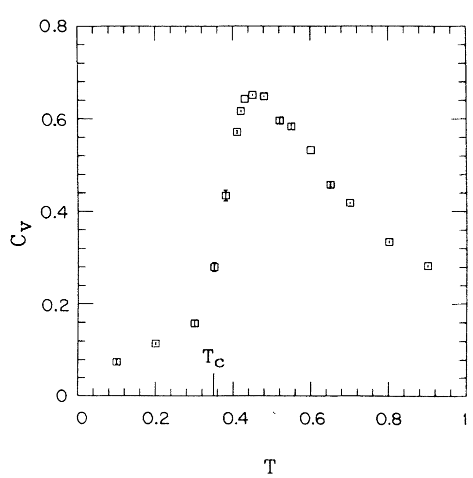

FIG. 4. Specific heat C_V. Lattice sizes are listed in Table I for $T \geq 0.41$. For $T < 0.41$, lattice size is 32×32.

A few comments are in order. Quantum fluctuations are capable of pushing the transition point from $T_c = 0.898$ (Ref. 3) in the classical model down to $T_c = 0.35$ in the quantum spin-$\frac{1}{2}$ case, although not strong enough to push it down to zero. They also reduced the constant B_ξ from 1.67 in the classical case[3] to 1.18 in the spin-$\frac{1}{2}$ case.

The critical behavior in the quantum case is of KT-type as in the classical case. This is a little surprising, considering the differences regarding the spin space. In the classical case, the spins are confined to the X-Y plane (thus the model is conventionally called the "planar rotator" model). This is important for the topological order in KT theory. The quantum spins are not restricted to the X-Y plane, due to the presence of S^z for the commutator relation. The KT behavior found in the quantum case indicates that the extra dimension in the spin space (which does not appear in the Hamiltonian) is actually unimportant. This interpretation is supported by the behavior of the correlation functions between S^z components listed in Table II. These correlations are very weak and short-ranged. The out-of-plane susceptibility remains a small quantity in the whole temperature range.

Our results for the XY model, together with recent work[15] on the quantum Heisenberg model, which was found to behave essentially like its classical counterpart at finite T, strongly suggest that, although quantum fluctuations at finite T can change the quantitative behavior of these nonfrustrated spin systems with *continuous* symmetries, the qualitative picture of the classical system persists. This could be understood following universality arguments that near the critical point, dominant behavior of the system is determined by long wavelength fluctuations which are characterized by symmetries and dimensionality. The quantum effects only change the short-range fluctuations which, after integrated out, only enter as renormalization of the physical parameters, such as B_ξ.

Our data also show that, for the XY model, the critical exponents are spin-S independent, in agreement with universality. More specifically, ν in Eq. (3) could in principle differ from its classical value $\frac{1}{2}$. Our data are sufficient to detect any systematic deviation from this value. For this purpose we plotted ξ in Fig. 2(b), using $\ln(\xi)$ vs $(T-T_c)^{-1/2}$. As expected, data points all fall well on a straight line (except the point at $T = 0.7$ where the critical region presumably ends). A systematic deviation from $\nu = \frac{1}{2}$ would lead to a slightly curved line instead of a straight line. In addition, the exponent η at T_c

TABLE II. $4\langle S_0^z S_r^z \rangle$ at several temperatures.

	r			
T	0	1	2	3
0.55	1	−0.1145(1)	−0.0016(1)	−0.0002(1)
0.45	1	−0.1353(2)	−0.0030(1)	−0.0007(1)
0.35	1	−0.1516(2)	−0.0051(2)	−0.0012(2)
0.2	1	−0.1647(1)	−0.0073(1)	−0.0027(1)

seems to be consistent with the value for the classical system.

In conclusion, by studying the correlation lengths and susceptibility of the spin-$\frac{1}{2}$ XY model via a large-scale simulation, we found convincing evidence that the Kosterlitz-Thouless transition occurs at finite T_c. The general picture of the quantum model remains essentially that of the classical model. The specific heat exhibits a steep rise in the vicinity of T_c and a finite peak about 28% above T_c.

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