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Monte Carlo studies of the quantum XY model in two dimensions

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Monte Carlo simulations are performed for the spin-$\frac{1}{2}$ XY model in two dimensions for large (up to 24×24 sites) lattices. Results are obtained over a wide temperature range which includes the critical temperature T_c, estimated to be 0.4–0.5. The energy, specific heat, vortex density, and derivative of the helicity modulus are given as functions of temperature. As the lattice size is increased, the specific heat per spin approaches a finite value and does not diverge.

Our understanding of the XY model in two dimensions has grown considerably in the last decade. In 1973, Kosterlitz and Thouless[1] explained the phase transition in the classical model in terms of topological order since Mermin and Wagner[2] had already precluded the possibility of conventional long-range order in this system. Numerical work by Tobochnik and Chester,[3] and by van Himbergen and Chakravarty[4] have confirmed some of the expected behavior, and have measured quantities such as the specific heat $C(T)$, the energy $E(T)$, the derivative $\partial(\beta\gamma)/\partial\beta$ of the helicity modulus γ, and the critical temperature T_c. The overall picture is one with bound vortex-antivortex pairs in the low-temperature phase, which break apart at T_c and give rise to a finite peak in the specific heat just above T_c.

Less is known about the corresponding quantum-mechanical spin-$\frac{1}{2}$ problem. Rogiers, Grundke, and Betts[5] used high-temperature series expansions to estimate critical temperatures and exponents. Both Pearson[6] and Suzuki and Miyashita[7] have variational estimates of the ground-state energy. Extrapolations from finite-size lattices also provide approximate values for the ground-state energy, in addition to other quantities such as the susceptibility, vortex density, energy, specific heat, and entropy.[8,9] On the basis of such calculations, attempts have been made to characterize the ground state and the phase transition in the quantum model. A wide variety of real-space renormalization-group approaches, characterized by uncontrolled approximations, have also been applied to this problem.[10] Unfortunately, they have been both inconclusive and contradictory. Finally, Suzuki, Miyashita, and Kuroda[11] have employed Monte Carlo techniques to measure specific heats and susceptibilities. Their results are expected to be valid at high temperatures.

In this paper, recently developed Monte Carlo techniques are used to measure $E(T)$, $C(T)$, and the vortex density $V(T)$. Derivatives of the helicity modulus are utilized to estimate the critical temperature T_c. Results for the energy agree with previous work both at $T=0$ and at high temperatures. The vortex density, meanwhile, is reminiscent of the classical model with the important, though natural, difference that zero-point fluctuations allow for a finite vortex density in the ground state. The specific heat has a sharp, but finite, peak close to the transition temperature, which is estimated to be $T_c=0.4$–0.5.

Following the approach suggested by Suzuki *et al.*,[11] we rewrite the partition function using the Trotter formula. The breakup we use, however, is the checkerboard decomposition employed by Hirsch, Scalapino, Sugar, and Blankenbecler[12] for the fermion problem in one dimension. We write the partition function as

$$Z=\mathrm{Tr}(e^{-\Delta\tau H})^L \ ,$$

where $\beta=L\Delta\tau$ and $\Delta\tau$ will ultimately be taken to be some small number. Next, each of the L exponentials is approximated by

$$\exp(-\Delta\tau H)=\exp(-\Delta\tau H_1)\exp(-\Delta\tau H_2) \ ,$$

where

$$H=H_1+H_2=-\sum_{\langle i,j\rangle}(S_i^xS_j^x+S_i^yS_j^y) \ ,$$

summing only once over near-neighbor pairs $\langle i,j\rangle$. Meanwhile, H_1 and H_2 are each composed of cell Hamiltonians which commute among themselves. Each cell involves only four sites. This breakup is pictured in Fig. 1. The partition function trace is now over a product of $2L$ factors. By introducing complete sets of states between adjacent exponentials, the sum may be thought of as a classical partition function in $2+1$ dimensions. This problem is immediately amenable to Monte Carlo techniques, and one is required to solve no more than the quantum four-site cell sub-Hamiltonian.

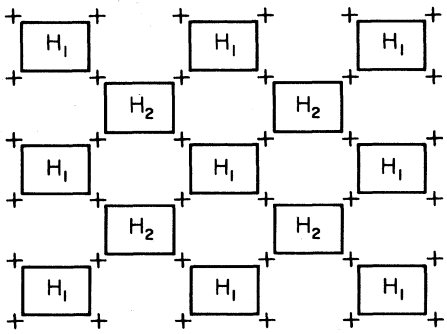

FIG. 1. Breakup of the two-dimensional lattice. Terms in the Hamiltonian are grouped into two parts, H_1 and H_2, each of which is composed of four-site cell sub-Hamiltonians which commute among themselves.

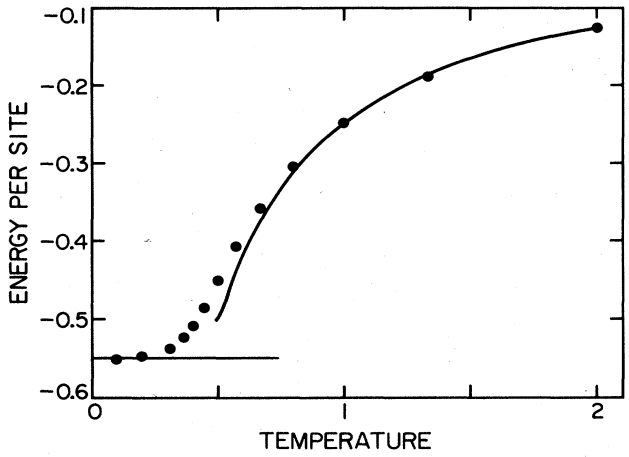

FIG. 2. Energy per site as a function of temperature for the 8×8 lattice with $\Delta\tau=0.25$. Results for the ground-state energy and a simple high-temperature expansion are shown for comparison.

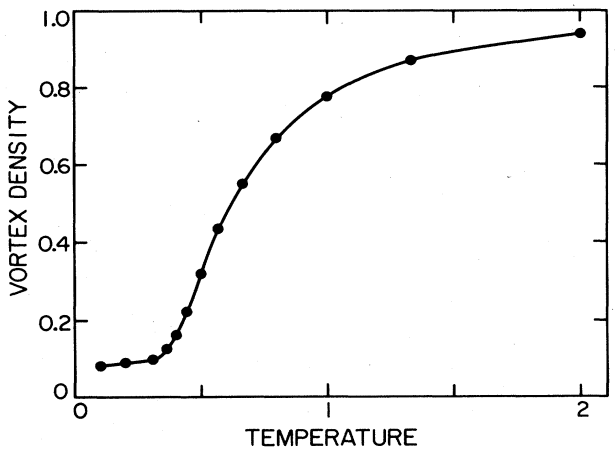

FIG. 4. Swendsen's vortex density vs temperature. The vortex density is nonzero at $T=0$ and exhibits a noticeable increase just below the critical temperature.

The problem was run on an IBM 3081 computer with $\Delta\tau$ usually set to 0.25. Dependence of measurements on $\Delta\tau$ was tested and found to be quite small. Measurements were made 15 000 times, with 2 sweeps of the lattice between measurements. Ten such runs were used to generate each point along with its error bar. Thus, each point represents $10\times15\,000\times2=300\,000$ sweeps of the lattice. Runs on lattices as large as $24\times24=576$ sites were performed, in contrast with exact diagonalizations, which stop around 18 sites. In the τ direction, we have used as many as $L=40$ slices (for $T=0.1$ with $\Delta\tau=0.25$). Suzuki's work used only $L=1$ and 2. Generating measurements of the desired observables at $T=0.5$ ($L=8$) for a 16×16 lattice with a prescribed set of boundary conditions takes just over 3 h.

The energy per site is plotted in Fig. 2. At high temperatures, the curve fits well to the form $E/N\sim-1/4T$, as expected from theory. At low temperatures, E/N goes to -0.543 ± 0.002 (Ref. 13) compared to Pearson's value of -0.550 ± 0.002 and -0.539 ± 0.005, given by both Suzuki and Miyashita and Betts and Kelland, for the ground-state energy. In Fig. 3, the specific heat per spin, computed by measuring fluctuations in the energy, is shown for an 8×8 lattice. Numerical differentiation of the energy curve can be used to reproduce these results. The specific-heat peak occurs at $T=0.5$. The height of this peak clearly levels off, with lattice size at about $C/Nk_B=0.65$, as shown in the inset.

The vortex density is given in Fig. 4. It comes in to a nonzero value at $T=0$, which is qualitatively consistent with Betts, Salevsky, and Rogiers,[14] and is to be expected from quantum zero-point fluctuations. Our value for the

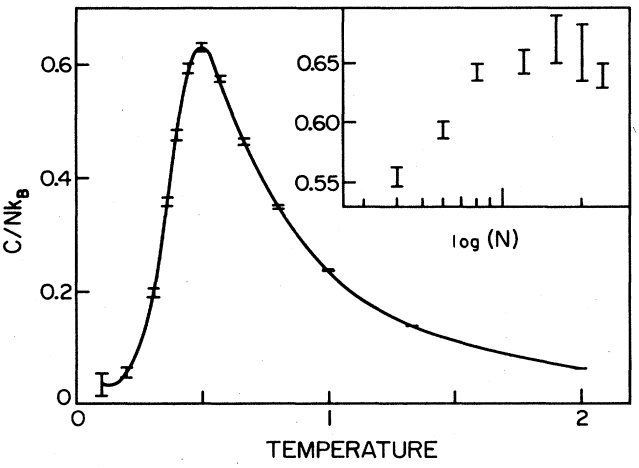

FIG. 3. Specific heat per site as a function of temperature for the 4×4 and 8×8 lattices. Points are found by directly measuring fluctuations in energy. The inset shows the dependence of the peak height on size for 4×4 through 24×24 lattices.

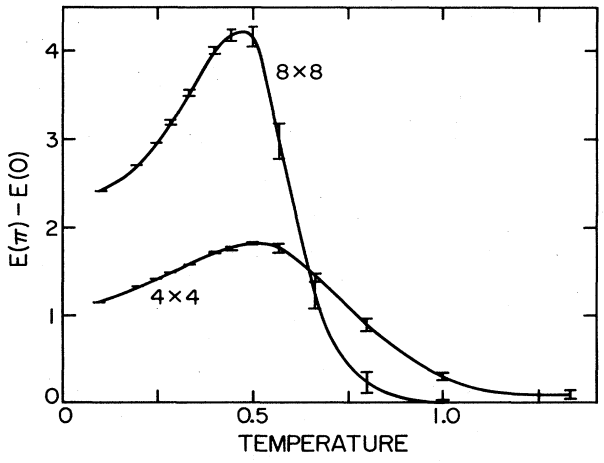

FIG. 5. Increase in the total internal energy due to enforcing a phase twist of π. Since this quantity is proportional to the derivative of the helicity modulus, the spike signals a Kosterlitz-Thouless phase transition.

ground-state vortex density $V(T=0)$ differs from Betts's, since we use Swendsen's vortex-density operator[15]

$$V(T)=\tfrac{1}{4}\sum(1-\sigma_1^x\sigma_3^x-\sigma_1^y\sigma_3^y)(1-\sigma_2^x\sigma_4^x-\sigma_2^y\sigma_4^y)\ ,$$

where σ^x and σ^y are the x and y Pauli spin matrices. The sum is over plaquettes, and the subscripts refer to sites on the vertices of each plaquette numbered in sequential order as one circles around. It is worth noting that $V(T)$ begins to grow noticeably at $T=0.35$–0.40, which is just below where we estimate the phase transition to occur.

The helicity modulus γ has been proposed as a useful quantity for investigating Kosterlitz-Thouless phase transitions in the classical two-dimensional problem,[16] and has been used successfully for this purpose in numerical studies.[4] For a spin system, the modulus is proportional to the spin-wave stiffness, and characterizes the change in the free energy when a slow, in-plane, twist of the spins is made. In models of two-dimensional systems of bosons, it is proportional to the superfluid density. For the classical system, the modulus has a universal jump at the critical temperature.[17] Thus, we expect that the temperature derivative of γ should provide a clear signal of T_c. Fortunately, this derivative is easy to measure, since it is no more than the increase in the internal energy due to a phase twist of π (Fig. 5). The peak occurs at $T=0.4$–0.5, which gives us an estimate of the transition temperature. Rogiers *et al.* give $T_c=0.39\pm0.01$, but claim that the specific-heat peak lies below this temperature, contrary to what we find from our simulations.

We have demonstrated the practicality of our algorithm for performing interesting measurements on two-dimensional quantum spin problems. The method produces reliable results over a wide temperature range, in contrast with previous work, using a variety of different techniques, and can be used for large lattices. Work on the two-dimensional Heisenberg-Ising antiferromagnet is in progress.

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