Comments

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Comment on "Monte Carlo studies of the quantum XY model in two dimensions"

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We point out that some of the simulation results on the two-dimensional spin-$\frac{1}{2}$ XY model of Loh, Scalapino, and Grant are not in agreement with previous work.

In a recent paper, new Monte Carlo results have been presented for the two-dimensional (2D), quantum ($S=\frac{1}{2}$) XY model.[1] We wish to draw attention to differences between the new results and previous work.[2] The data seem to disagree for two important observables: the specific heat and the vortex detector.

(i) According to Ref. 1 the specific heat exhibits a maximum at $T_c^{(1)} \approx 0.5$ (temperature units of Ref. 1, which differ by a factor of 4 from that used in Ref. 2), and saturates as a function of the lattice size (for lattices up to 24×24), the height of the specific-heat peak being approximately $C_{\max}^{(1)} \approx 0.65$. Previous simulations[2,3] show that for lattices up to 32×32 the specific heat peaks at $T_c^{(2)} \approx 0.55$, having a maximum $C_{\max}^{(2)} \approx 1.9$ (for a 24×24 lattice). Consequently, $C_{\max}^{(2)} \approx 3C_{\max}^{(1)}$, a disagreement which seems too large to be accounted for by purely "statistical noise."

(ii) The estimates for the "vortex detector" denoted by $V(T)$ in Ref. 1, and by D in Ref. 2 also differ. This quantity has a nonzero value at $T=0$ because of quantum fluctuations. From Fig. 4 of Ref. 1 one estimates $V(T=0.1) \approx 0.08$. This value is about three times larger than the estimate derived from Ref. 2.

We will discuss some aspects of both simulation studies. Both the old and the new simulations rely on the equivalence of a d-dimensional $S=\frac{1}{2}$ model and a $(d+1)$-dimensional Ising Model with multispin interactions.[4] It has been proven rigorously that, independent of the breakup used, the results obtained from the $(d+1)$-dimensional system converge to the exact results.[4] In practice, the size of the system in the additional direction (hereafter referred to as the number of "time slices") has to be chosen such that the systematic errors, introduced by the mapping, disappear in the statistical noise. In Ref. 1 the Barma and Shastry checkerboard breakup[5] is used to decompose the Hamiltonian into blocks of four spins, whereas in Refs. 2 and 3 two spins per block were taken. The approach used in Ref. 1 treats four spins exactly and it may be expected that compared to the latter, fewer time slices are needed to bring the systematic errors due to the breakup down to a prescribed level. However, in the regime of interest, the temperature is relatively high, and for the decomposition used in Refs. 2 and 3, four time slices were sufficient, as was tested by sampling systems having up to 32 time slices. In the temperature range of interest, there is hardly any difference for the specific-heat data obtained from simulations with the number of time slices varying from 1 through 32 time slices for the same lattice size.[2,3] It is therefore of interest to compare the simulation data with a class of rigorous solutions for the one-time-slice model.[6] This rigorous solution of a class of one-time-slice models predicts a critical temperature at the 2D Ising model critical temperature $\sinh(1/2T_c)=1(T_c \approx 0.55)$.

We now give a possible explanation for the observed discrepancies. In Ref. 1 an additional approximation, not present in Refs. 2 and 3, has been made. In Ref. 1 it is implicitly assumed (see Ref. 7) that simulation of a system using a restricted ensemble, i.e., an ensemble with fixed total magnetization, will yield correct results for the full problem. In general, the assumption that it is sufficient to compute physical properties for a fixed magnetization only, is unjustified as can easily be seen by considering spin susceptibilities. It may be argued that for many quantities and in the thermodynamic limit, these restricted ensemble calculations will give the correct answer; this argument must be used with great care if one uses simulation techniques to compute physical quantities, since simulations necessarily have to be done on relatively small lattices. The approach used in Ref. 1 suffers from the drawback that reliable results for the spin problem can only be obtained in the thermodynamic limit, as can for instance be verified by performing calculations for exactly solvable Ising spin models. In addition, the argument that a quantity from the restricted ensemble, introduced in Ref. 1, and the one obtained from the full ensemble used in Refs. 2 and 3 become equal in the thermodynamic limit is, for practical purposes, useless in the regime where critical behavior is observed. In our opinion, this extra approximation used in Ref. 1 is one, possibly the main, source of the differences discussed above.

Another approximation which may look somewhat technical but is of equal importance is that even in the restricted ensemble approach used in Ref. 1, the Monte Carlo algorithm employed is not ergodic, i.e., it cannot generate all states of the subspace of spin states considered (see Ref. 7). As it is not known how the results of the Metropolis Monte Carlo simulation are modified when this basic requirement of ergodicity of the Markoy chain[8] is not satisfied, the procedure used in Ref. 1 is equivalent to making an uncontrollable approximation.

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