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

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We agree that our simulations of the two-dimensional quantum XY model differ from those of De Raedt and Lagendijk and argue that our results—a finite specific-heat peak and a conclusively nonzero vortex density at zero temperature—are the correct ones, agreeing with other work on this model.

We agree that the results of our numerical simulations[1] of the quantum $(S=\frac{1}{2})$ XY model differ from those of Ref. 2.

Using a finite-size scaling analysis, we found that the height of the specific-heat peak saturates at a value of $0.65k_B$/spin. This peak height agrees with Kelland's extrapolations from finite-size lattices[3] as well as recently published results on the XY model using a different Monte Carlo algorithm.[4] This saturation with increasing lattice size is similar to the Monte Carlo analysis of the specific-heat peak for the classical model[5] and, along with the behavior we found for the helicity modulus, leads us to the conclusion that the 2D quantum XY model undergoes a Kosterlitz-Thouless-like transition. This is in contrast with the work reported in Ref. 2 which claims that the specific-heat peak grows slowly with the lattice size "in concert with the $m=1$ (1 time slice) solution which predicts a logarithmic divergence of the specific heat." We believe that the many-time-slice quantum problem is qualitatively different than the single-time-slice problem. As we point out in Ref. 1, our results for the specific heat are the same both when measured directly and when calculated from energy-fluctuation measurements. As an additional check, we have integrated the specific heat divided by the temperature, obtaining the entropy of the system. As shown in Fig. 1, the entropy calculated in this way maps smoothly onto the high-temperature limit $S(T)\sim\ln(2)-1/8T^2$.

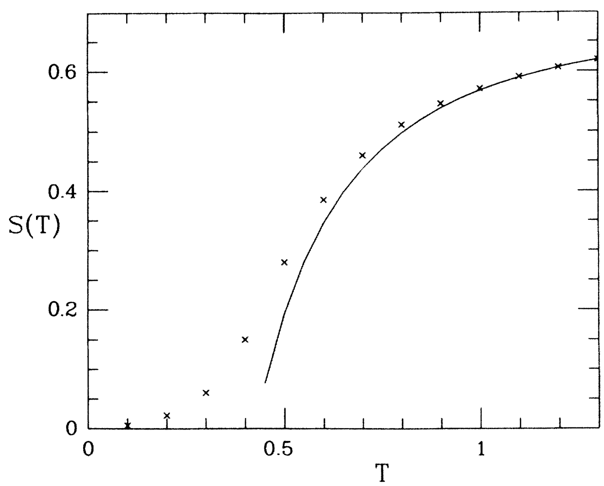

FIG. 1. Entropy as a function of temperature. Our Monte Carlo data for the specific heat, obtained by integrating $\int_0^T C(T)/T dT$, are shown as the points $(\times)$. The high-temperature expansion $\ln(2)-1/8T^2$ is shown as the solid curve.

The "vortex density" plotted in Fig. 4 of our work is $4V(T)$ and hence should correspond directly to $D(T)=4V(T)$, shown in Fig. 4 of Ref. 2. The factor of 4, which unfortunately was not mentioned in the figure caption, was chosen so that at high temperatures the data would go asymptotically to 1. New results,[6] based on a Monte Carlo method for studying ground states of quantum spin models without decomposing the Hamiltonian, give $4V(T=0)=0.071\pm0.006$, which is consistent with the value of the zero-temperature vortex density reported in Ref. 1. These results are indeed significantly larger than the value given in Ref. 2.

Finally, ensemble restrictions are unimportant in the thermodynamic limit. Indeed, a large system with some quantity fixed is no more than several smaller systems in a bath with each other.

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