Helicity modulus and specific heat of classical XY model in two dimensions

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A Monte Carlo simulation of the helicity modulus and the specific heat of the classical XY model in two dimensions is presented. In particular, we have investigated the dependence of these quantities with the size of the Monte Carlo sample. The height of the specific-heat peak is found to saturate as the infinite-volume limit is approached. The peak height of the derivative of the helicity modulus is found to grow rapidly with the increase in the size of the system and is located only 7% below the temperature at which the specific heat has the maximum.

I. INTRODUCTION

We now have a fair understanding of the classical XY model in two dimensions, thanks to the work of Kosterlitz and Thouless.[1,2] Their theory of a phase transition driven by the unbinding of vortex pairs has recently been examined in a Monte Carlo simulation by Tobochnik and Chester.[3] The results of this simulation are consistent with the scenario that goes with the theory of Kosterlitz and Thouless. However, a rather intriguing features of this simulation is a sharp specific-heat peak at a temperature $k_B T/J = 1.02$ (J is the nearest-neighbor coupling), 15% above the transition temperature $k_B T_c/J = 0.89$. T_c was determined by fitting the spin-spin correlation function and the susceptibility to the forms of the theory of Kosterlitz and Thouless. In view of this, we have examined the dependence of the height of the specific-heat peak with the size of the Monte Carlo sample. The lengths of the Markov chains employed by us are on the average four to six times longer than those of Tobochnik and Chester. Furthermore, several independent runs were used to improve the statistics. The extensive numerical analysis confirms that the height of the specific-heat peak is independent of the size of the system for a moderately large system of the order of 1600 spins. We then turn to a determination of the helicity modulus as discussed by Fisher, Barber, and Jasnow.[4] This should be an independent check for the transition temperature due to the prediction of Kosterlitz and Nelson.[5] Although we face numerical difficulties for very large systems, the data for systems up to 625 spins indicate quite strongly that the peak of the derivative of the helicity modulus increases quite rapidly as the infinite volume limit is approached. We believe that the specific heat reaches its maximum when *all* the bound pairs of vortices have finally dissociated. Finally, a careful reader may note that the *width* of the specific-heat peak narrows considerably as the infinite volume limit is approached. However, from our numerical work it is difficult to ascertain whether a cusp develops in the specific heat or not, although one cannot in principle rule this out. The cusp in the specific heat will imply an additional transition above the Kosterlitz-Thouless transition. So far we have not found any good reason for this to happen. This question requires a more careful analysis.

II. CALCULATIONAL PROCEDURE

The classical two-dimensional XY model is defined by the following Hamiltonian:

$$\beta H = -\frac{1}{T} \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \ , \tag{2.1}$$

where T is the reduced temperature and is defined to be $k_B T/J$, J is the coupling constant. The sum is taken over nearest-neighbor pairs. To be more specific we have considered square lattices with periodic boundary condition except for the determination of the helicity modulus where we make use of the antiperiodic boundary condition as well.

We have used the time-honored Metropolis Monte Carlo procedure[6] to simulate the system. The maximum change in angle per spin per step was adjusted every pass through the lattice to maintain an acceptance ratio between 0.45 and 0.55. We define a pass conventionally as sequentially stepping through the lattice, turning each spin once.

The calculations were performed on a sequence of 5×5, 7×7, 10×10, 15×15, 25×25, and 40×40 lattices. There are two different ways of computing specific heat, C_v, from a Monte Carlo simulation. One is to calculate it from the fluctuation in the internal energy ($\langle U^2 \rangle - \langle U \rangle^2$) and the other is to calculate the temperature derivative of the computed internal energy $\langle U \rangle$. If one averages over a sufficient number of passes both methods should yield identical results. In practice this is never the case due to the finiteness of the length of the Markov chains. However, in our simulations we have made sure that both of these methods yield practically the same answer. This was one of our guiding principles in estimating the correctness of our simulations. The specific-heat data presented in this paper are from the measurements of the fluctuation of the energy. This way of computing the specific heat turned out to be a little smoother than taking numerical derivatives. For the first four sized lattices mentioned above, we have used 3000 passes to equilibrate and another 15 000 passes to calculate the averages. For the 25×25 and 40×40 lattices we have used once again 3000 equilibration passes but 10 000 expectation value passes. The statistics should be compared to those used by Tobochnik and Chester who used a total of 3000 passes. The expectation values were computed for every pass through the lattice. Furthermore, to improve the statistics we took 6–8 independent runs with different initial conditions for the first five lattice sizes. For the 40×40 lattice we have two independent runs, one for the heating and the other for cooling.

The specific heat as a function of the reduced temperature T is shown in Fig. 1. In Fig. 2 we show how the maximum of the specific heat $C_v^{\max}$ varies as a function of the number of spins N. From this figure it is quite clear that the peak height saturates as the thermodynamic limit is approached. We have found that a reasonable fit to the numerical data is given by

$$C_v^{\max} = C_v^{\infty} + A/N^{\alpha} , \tag{2.2}$$

where $C_v^{\infty} = 1.44$, $A = -10.52$, and $\alpha = 1.07$, the fit is better than 1% on the average.

The error bars in Fig. 2 should be taken as an indication of the uncertainties and not as absolute measures.

A particular way to locate the phase transition in this model is to calculate the helicity modulus, a rather elegant concept introduced by Fisher, Barber, and Jasnow.[4] The free-energy difference between the twisted, ω the angle of twist, and the periodic boundary condition is proportional to the helicity modulus defined by

$$F(\omega) - F(0) = 2\omega^2 (N_2/N_1) \gamma(\beta) , \tag{2.3}$$

where the applied twist is along the x direction of an $N_1 \times N_2$ lattice and $\gamma(\beta)$ the helicity modulus, a thermodynamic function, measures the "rigidity" of an isotropic system under an imposed phase twist. With a bit of care in using lattice gradients, one can also relate $\gamma(\beta)$ to the superfluid density $\rho_s(\beta)$ in helium

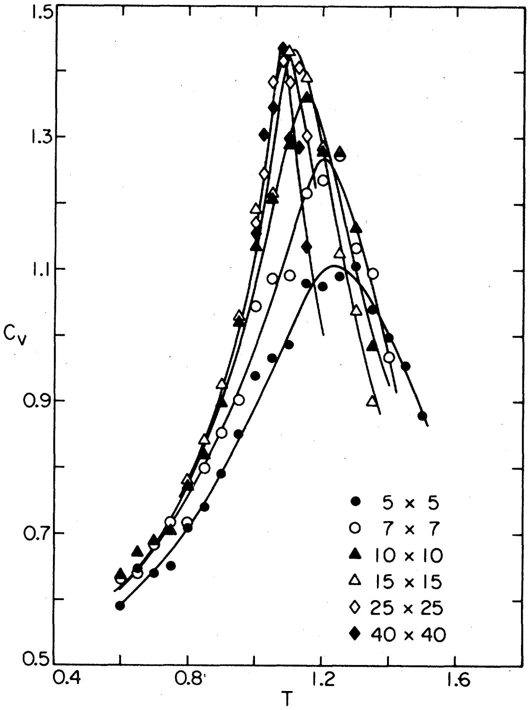

FIG. 1. Specific heat, C_v, as a function of reduced temperature T for different lattice sizes.

films, assuming of course that XY model faithfully represents helium films:

$$\gamma(\beta) = \frac{\hbar^2}{m} \rho_s(\beta) . \tag{2.4}$$

A rather striking prediction of an universal jump in $\rho_s(\beta)$ at the transition by Kosterlitz and Nelson[5] has been verified by Bishop and Reppy.[7] In any case, the *internal* energy difference between antiperiodic boun-

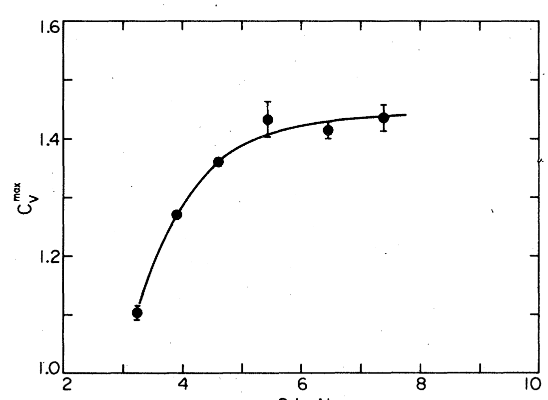

FIG. 2. Height of the specific-heat peak $C_v^{\max}$ as a function of the lattice size.

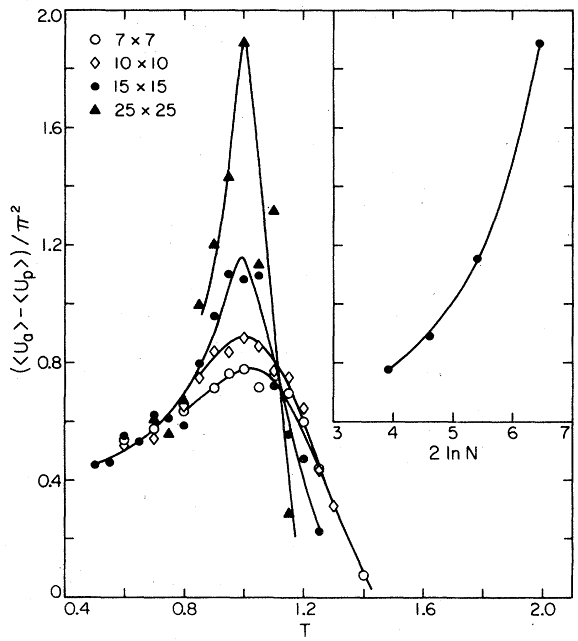

FIG. 3. Derivative of $\frac{1}{2}\beta\gamma(\beta)$ as a function of reduced temperature T for different lattice sizes. The inset shows the height of the peaks as a function of the lattice size.

dary condition $\langle U_a \rangle$ and the periodic boundary condition $\langle U_p \rangle$ gives the derivative of the helicity modulus, namely,

$$\frac{1}{2}\frac{d}{d\beta}[\beta\gamma(\beta)] = \frac{\langle U_a \rangle - \langle U_p \rangle}{\pi^2} , \qquad (2.5)$$

where we have set $N_1 = N_2$. In Fig. 3 we show the Monte Carlo data for the right-hand size of Eq. (2.4) as a function of temperature for different size lattices. The results indicate a sharp change in the superfluid density as the temperature $T = 1$ is approached. The inset of the same figure shows that the derivative of the helicity modulus at $T = 1$ increases quite rapidly as the size of the system increases. The numerical uncertainty also increases quite rapidly as the system size increases and has prevented us from obtaining decent enough data for the 40×40 lattice. We have deliberately restrained ourselves from quoting error bars. These are hard to determine accurately because of the differences between heating and cooling runs due to effects similar to hysteresis. We used on the average 3000 equilibration passes and 10 000 expectation value passes and have averaged over the heating and the cooling runs. For the 25×25 lattice we have used 3000 equilibration passes and 15 000 expectation value passes and have averaged over three independent heating and cooling runs.

III. CONCLUSION

After an extensive numerical analysis it is fair to conclude that the specific-heat peak is independent of the size of the sample for moderately large systems. The peak width, however, narrows and one cannot in principle rule out a cusp in the specific heat. We have also measured the derivative of the helicity modulus and find it to be consistent with a sharp change of the helicity modulus for a moderately large system at the reduced temperature $T \sim 1$ about 7% lower than the peak of the specific heat at about $T \sim 1.07$.

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