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Monte Carlo determination of the critical temperature for the two-dimensional XY model

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The critical temperature for the two-dimensional XY model on a square lattice is determined to within a few tenths of a percent by combining Monte Carlo simulations with a lattice size scaling relation.

The two-dimensional (2D) XY model on a square lattice is defined by the Hamiltonian

$$H_{XY} = -\sum_{\langle ij\rangle}\cos(\theta_i - \theta_j) \ , \tag{1}$$

where the indices i and j numerate the lattice sites on a two-dimensional square lattice, the sum is over nearest-neighbor lattice sites, and $\theta_i (0 \le \theta_i < 2\pi)$ is an angle associated with each site. The grand partition function Z, through which the thermodynamic properties of the model may be obtained, is given by

$$Z = \prod_i \int \frac{d\theta_i}{2\pi} e^{-H_{XY}/T} \ . \tag{2}$$

The 2D XY model has been extensively studied due to its interesting phase transition properties.[1] It undergoes a Kosterlitz-Thouless transition at a certain temperature T_c from a low-temperature phase with "quasi"-long-range order to a disordered high-temperature phase.[2-4] No exact solution has so far been found. This means that the qualitative features are by now well understood[1] but that details such as the value of the critical temperature are as yet only approximately known.

An example of an estimate of the critical temperature T_c is the Monte Carlo simulations by Tobochnik and Chester[5] who obtained $T_c \approx 0.89$ with an estimated error of a few percent. An example of an analytical approximation for the same quantity is given by Mattis[6] who, by using a transfer-matrix approach, obtained $T_c \approx 0.883$ but with no estimate of the error.

In the present paper we describe a calculation from which we obtain $T_c \approx 0.887$ with an estimated error of a few tenths of a percent. The point of our calculation is twofold. First of all it gives a very accurate value for T_c against which approximation schemes may be tested. Second, it gives yet another confirmation that the phase transition is indeed of Kosterlitz-Thouless type.

The quantity we focus on is the helicity modulus γ_∞ which may be expressed as $\gamma_\infty = \lim_{N\to\infty}\gamma(N)$ where[7,8]

$$\gamma(N) = -\frac{1}{2N^2}\langle H_{XY}\rangle - \frac{1}{TN^2}\left\langle \left[\sum_{\langle ij\rangle}\sin(\theta_i - \theta_j)\hat{\mathbf{e}}_{ij}\cdot\hat{\mathbf{x}}\right]^2\right\rangle \ , \tag{3}$$

N^2 is the number of lattice sites, $\hat{\mathbf{e}}_{ij}$ is the vector pointing from site j to site i, $\hat{\mathbf{x}}$ is a unit vector of a fixed direction in the lattice plane, and the angle brackets denote thermal averages.[7,8] We calculate the quantity $\gamma(N)$ by a standard Metropolis Monte Carlo method[9,10] with periodic boundary conditions on the lattice.

The Kosterlitz renormalization-group equations[11] lead to the prediction that γ_∞ jumps from the value $(2/\pi)T_c$ to zero at the critical temperature.[7,12] Figure 1 shows results from Monte Carlo simulations of $\gamma(N)$ for two lattice sizes (the lattice sizes in the figure are 8×8 and 64×63). The straight line in the figure represents $(2/\pi)T$ and the crossing point between this line and $\gamma_\infty = \lim_{N\to\infty}\gamma(N)$ gives T_c. Viewed in this way, the problem is the determination of γ_∞ from knowledge of $\gamma(N)$ for some finite lattice sizes N. In order to extract this limit we first observe that the solution of Kosterlitz renormalization-group equations contains the information that, at T_c (or more precisely as T_c is approach from below) and in the limit of large N, the quantity $\gamma(N)$ is given by[14]

$$\gamma(N) = \gamma_\infty\left[1 + \frac{1}{2}\frac{1}{\ln(N) + C}\right] \ , \tag{4}$$

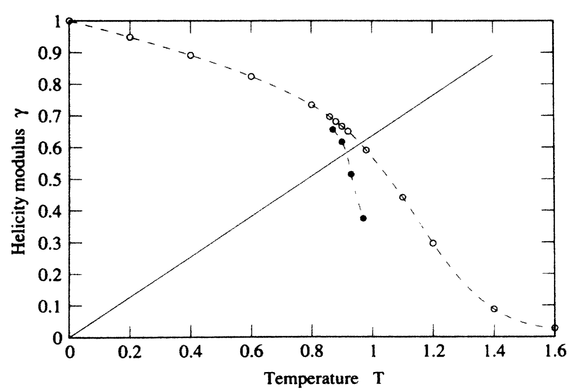


FIG. 1. Monte Carlo simulations of the helicity modulus γ for the XY model. The open circles are results from a 8×8 lattice and the solid circles from a 64×63 lattice (the latter data are from Ref. 13). The dashed curves are guides to the eye. The difference between the values given by the open and solid circles reflects the lattice size dependence of the helicity modulus γ. The solid line is the line $(2/\pi)T$. The crossings between the dashed lines and the solid line give estimates of the critical temperature T_c. This estimate of T_c gets more accurate with increasing lattice size because the thermodynamic limit corresponds to an infinite lattice.

where C is an undetermined constant. Consequently, the validity of Eq. (4) is at least guaranteed for large enough N, provided that the 2D *XY* model undergoes a Kosterlitz-Thouless transition.

Our determination of T_c rests on the *empirical* discovery that Eq. (4) is in fact valid to extremely good approximation down to *small* lattice sizes, in fact all the way down to $N=3$ lattices which is the smallest lattice with four different nearest neighbors. For small lattices $\gamma(N)$ can be determined to high accuracy and this in turn makes a high-precision determination of T_c possible.

In our determination of T_c we have used lattice sizes ranging from $N=3$ to $N=12$. Each calculated value of $\gamma(N)$ was based on approximately 10^6–10^7 sweeps through the lattice giving an estimated accuracy of within three or four significant digits depending somewhat on the actual lattice size and temperature.

Our strategy is straightforward and simple: we calculate the $\gamma(N)$ values through Monte Carlo simulations of a sequence of small N lattices for fixed temperature T. We then make least-squares fits to Eq. (4) recast into the form

$$\gamma(N)=\frac{2}{\pi}T\left[1+\frac{1}{2}\frac{1}{\ln(N)+C}\right], \tag{5}$$

using the constant C as the only free parameter. By this procedure our key quantity $\Delta(T)$, the root-mean-square error of the fit as a function of temperature, is obtained.

The quantity $\Delta(T)$ has a sharp and dramatic minimum at a certain temperature as shown in Fig. 2(a). The figure shows the $\Delta(T)$ obtained for a series of sequences $N=3,4,\ldots,N_{\max}$ with $N_{\max}=6$, 7, 8 which in the figure correspond to circles, pluses, and crosses. The solid circles in the figure correspond to the sequence $N=3$, 4, 5, 5, 6, 7, 8, and 12. Figure 2(b) is a blow up of the minimum region of $\Delta(T)$. Figures 2(a) and 2(b) illustrate two things. First of all $\Delta(T)$ in the minimum region $(0.885<T<0.888)$ is extremely small $[\Delta_{\min}(T)\approx 0.0005]$. Second, $\Delta_{\min}$ in the minimum region does apparently vary very little with increasing $N_{\max}$. This is in contrast to temperatures outside the minimum region, where $\Delta(T)$ increases substantially with increasing temperature making the minimum even sharper. Taken together this suggests that Eq. (4) is extremely well obeyed all the way down to $N=3$ lattices (the smallest lattice which has four different nearest neighbors). Since $\Delta(T)$ increases substantially with increasing lattice size for $T\lesssim 0.885$ and $T\gtrsim 0.888$, we may safely conclude that $T_c=0.8865\pm 0.0015$.

One may further note that although the position of the minimum in Fig. 2(b) is at $T=0.886$, the lattice size scaling of $\Delta(T)$ is in fact reversed for the temperature $T=0.887$. This suggests that the minimum in the limit of large N is closer to $T=0.887$ which in turn suggests that the estimate of T_c may be sharpened to $T_c=0.887\pm 0.001$.

One may get some further insight into the lattice size scaling by also comparing with the expected size dependence of γ for $T\neq T_c$ which in the limit of large N is given by [14]

$$\begin{aligned}&\gamma(N)-\gamma_\infty\sim(1/N)^{\alpha_1(T)}\ \text{for}\ T<T_c\ ,\\&\gamma(N)\sim e^{-\alpha_2(T)N}\ \text{for}\ T>T_c\ ,\end{aligned} \tag{6}$$

where $\gamma_\infty>0$ and $\alpha_1(T)>0$ $[\alpha_2(T)>0]$ is decreasing (increasing) with increasing temperature.[14] The lattice size dependence given by Eq. (6) suggests that a $\gamma(N)$ point for a large enough N falls above (below) a fit to Eq. (5) when T is smaller (larger) than T_c. This prediction is illustrated in Fig. 3 which shows the $N=3,4,\ldots,8$ fits to Eq. (5) for $T=0.885$ [Fig. 3(a)] and $T=0.888$ [Fig. 3(b)] plotted as functions of $1/\ln(N)$. The $\gamma(N=12)$ point for $T=0.885$ [denoted by a cross in Fig. 3(a)] was calculated with high accuracy and the positions of this point relative to the fit to Eq. (5) was checked. For $T=0.885$ the $\gamma(N=12)$ point falls a tiny but significant distance above, suggesting that $T=0.885$ is just below T_c

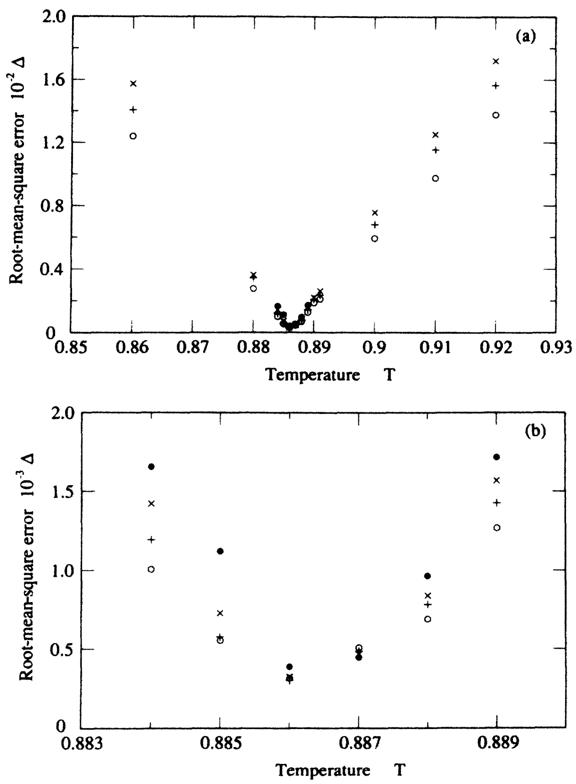
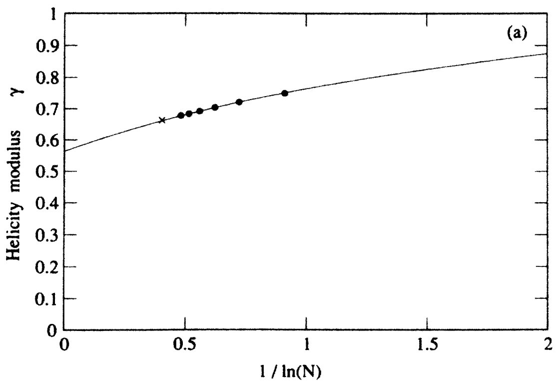


FIG. 2. (a) The root-mean-square error Δ as a function of temperature T. Δ is obtained by fitting the Monte Carlo data for the helicity modulus γ to the lattice size scaling relation given by Eq. (5). The open circles, pluses, crosses, and solid circles correspond to the lattice sequences $N=3$, 4, 5, and 6; $N=3$, 4, 5, 6, and 7; $N=3$, 4, 5, 6, 7, and 8; $N=3$, 4, 5, 6, 7, 8, and 12, respectively. Δ has a dramatic minimum close to $T=0.886$. The position of this minimum determines T_c of the *XY* model. (b) A more detailed plot for the minimum region of the root-mean-square error $\Delta(T)$. The data and symbols are the same as in (a). The figure shows that Δ increases substantially with increasing lattice size for $T\lesssim 0.885$ and $T\gtrsim 0.888$. For $T=0.886$ and $T=0.887$ the lattice size dependence is much smaller. For $T=0.887$ the lattice size dependence of Δ is in fact reversed. This suggests that the true minimum in the limit of large lattice size is close to $T=0.887$.



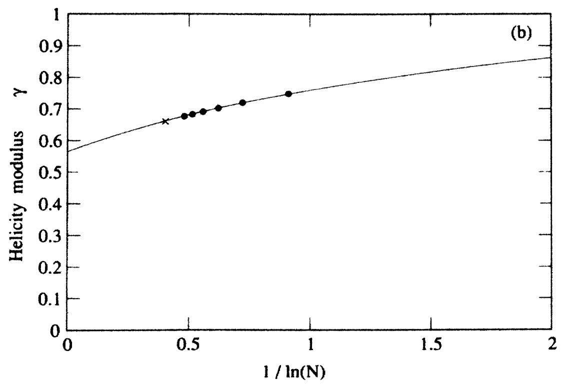


FIG. 3. (a) The helicity modulus γ for $T=0.885$ plotted as a function of $1/\ln(N)$ where $N \times N$ is the size of the square lattice. The six solid circles correspond to the six lattice sizes $N=3$, 4, 5, 6, 7, and 8, respectively. The solid curve is a fit, based on the data given by the six solid circles, to the lattice size scaling relation given by Eq. (5). The cross is the value of γ obtained by Monte Carlo simulations for the lattice size $N=12$. The cross falls a tiny but significant distance above the full line. This suggests that the temperature $T=0.885$ is just below the critical temperature. (b) The helicity modulus γ for $T=0.888$. The six solid circles correspond to the same lattice sizes as in (a) and the solid curve is the corresponding fit to Eq. (5). The cross is the value of γ obtained for the lattice size $N=12$. The cross falls a tiny but significant distance below the full line. This suggests that the temperature $T=0.888$ is just above the critical temperature.

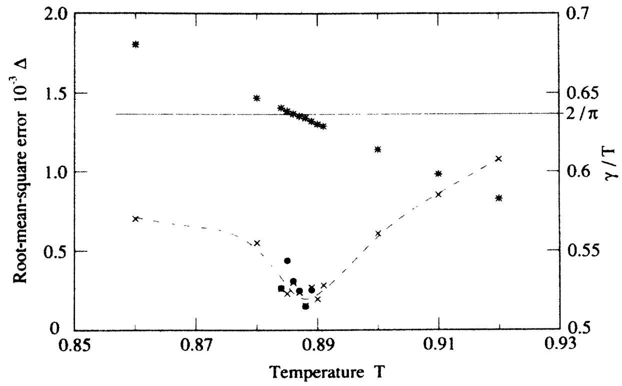


FIG. 4. The root-mean-square error Δ obtained by fitting the Monte Carlo data to the scaling relation given by Eq. (4) using both γ_∞ and the constant C as free parameters. The crosses correspond to the lattice size sequence $N=3$, 4, 5, 6, 7, and 8 and the solid circles to the sequence $N=3$, 4, 5, 6, 7, 8, and 12. The dashed curve represents a fit to the data given by the crosses and the solid circles. The minimum of Δ occurs within the interval $0.884 < T < 0.891$ giving the corresponding T_c estimate $0.884 < T_c < 0.891$. The asterisks give the values of γ_∞/T corresponding to the crosses. The horizontal line is the value $2/\pi$ which is the prediction from Kosterlitz renormalization-group equations for the quantity γ_∞/T precisely at the critical temperature. From the data given by the asterisks together with the T_c estimate given by the crosses and the solid circles, one may conclude that $\gamma_\infty/T_c = 2/\pi$ to within roughly a percent error.

[the distance from the fit is a factor 3 larger than the $\Delta(T)$ of the fit]. For $T=0.888$ the $\gamma(N=12)$ point [denoted by a cross in Fig. 3(b)] falls a tiny but significant distance below, suggesting that $T=0.888$ is just above T_c [the distance from the fit is a factor 2 larger than the $\Delta(T)$ of the fit]. These results are entirely in accord with the earlier estimate $T_c = 0.8865 \pm 0.0015$ based on Figs. 2(a) and 2(b).

One may also note that the fact that Eq. (4) is extremely well obeyed may, *ipso facto,* be taken as a verification that the phase transition is of Kosterlitz-Thouless type. This is further illustrated in Fig. 4. The figure shows the root-mean-square error $\Delta(T)$ of the case when both γ_∞ and C in Eq. (4) are treated as free parameters. The crosses in the figure correspond to fits to the sequence $N=3$, 4, 5, 6, 7, and 8 and the solid circles to the sequence $N=3$, 4, 5, 6, 7, 8, and 12. The dashed line in the figure is a fit to the Monte Carlo data given by the crosses and the solid circles. The position of the minimum of $\Delta(T)$ is by this procedure determined to be within the interval $0.884 < T < 0.891$. The corresponding values of the quantity γ_∞/T obtained by the fits to Eq. (4) (denoted by asterisks in Fig. 4) are $0.63 < \gamma_\infty/T < 0.64$ for $0.884 < T < 0.891$. This means that by this method γ_∞/T_c is determined to be $\gamma_\infty/T_c = 2/\pi \pm 0.008$. Or in other words, the prediction from Kosterlitz renormalization-group equations[7,11,12] $\gamma_\infty/T_c = 2/\pi$ is confirmed to within roughly a percent error. This way of determining the actual value of γ_∞ at the phase transition for *XY*-type models we have found to be quite useful in order to determine whether or not a particular model has a Kosterlitz-Thouless transition, which will be further described in a forthcoming publication.

In summary, we have, by combining Monte Carlo simulations with the scaling relations given by Eqs. (4)–(6), determined T_c to $T_c = 0.887$ with an estimated error of a few tenths of a percent. We observe that this estimate of T_c is consistent with, but much more narrow than, the estimate given by Tobochnik and Chester.[5] We also conclude that the transfer-matrix approximation by Mattis[6] which gave $T_c = 0.883$ is indeed a very good approximation.

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