Phase Transition in the Two Dimensional Classical XY Model

Jae-Kwon Kim

Center for Simulational Physics and Department of Physics,
The University of Georgia, Athens, GA 30602

Abstract

For the two dimensional classical XY model we present extensive high-temperature-phase bulk data extracted based on a novel finite size scaling (FSS) Monte Carlo technique, along with FSS data near criticality. Our data verify that $\eta = 1/4$ sets in near criticality, and clarify the nature of correction to the leading scaling behavior. However, the result of standard FSS analysis near criticality is inconsistent with other predictions of Kosterlitz’s renormalization group approach.

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The classical XY model is defined by the Hamiltonian

\[ H = -\frac{1}{T} \sum_{<ij>} \vec{s}_i \cdot \vec{s}_j, \]

where \( \vec{s}_i \) is the O(2) spin at site \( i \) and the sum is over nearest-neighbor spins. As a novel statistical model that undergoes a phase transition without long range order, the two dimensional (2D) XY model is interesting in its own right, as well as being a model for 2D layers of either superconducting materials or films of liquid helium.

The mechanism of this kind of phase transition was first illustrated by Berezinskii [1], and by Kosterlitz and Thouless [2] (BKT) based on vortex binding scenario: At low-temperatures spin waves are the only significant fluctuations, and vortices are bound in pairs of zero vortices, thus not affecting the spin-wave description qualitatively; at high temperatures, however, the binding of the vortices decreases. The prediction [3] obtained with a renormalization-group method is that in the high temperature phase the critical properties of correlation length (\( \xi \)) and magnetic susceptibility (\( \chi \)) are given by

\[ \xi(t) \sim \exp(bt - \nu), \]

\[ \chi(t) \sim \xi(t)^{2-\eta}. \]

Here \( t = (T - T_c)/T_c \), and the predicted values of \( \nu \) and \( \eta \) are 1/2 and 1/4, respectively. For \( T \leq T_c \), both \( \xi \) and \( \chi \) diverge identically with such a temperature dependent \( \eta \) that \( \lim_{T \to 0} \eta(T) = 0 \).

Kosterlitz’s renormalization group equations approach was extended to yield the corrections to Eq.\((2)\):

\[ \xi(t) \sim \exp(bt^{-1/2}) \left[ 1 + O(t) \right], \quad \chi(t) \sim t^{-1/16} \exp\left(\frac{7}{4}bt^{-1/2}\right) \]

Accordingly \( \chi(t)/\xi(t)^{7/4} \) increases as \( t \to 0 \).

On the other hand, rigorous studies have established only two things: the existence of a phase transition at a finite temperature [5] and also the existence of an upper bound of the critical temperature [6]. Consequently the validity of Eq.\((2)\) has been questioned both
analytically [7] and numerically [8–10]. A different mechanism, namely “polymerization of the domain walls”, was proposed [9]. Extensive Monte Carlo (MC) studies [11–13] up to \( \xi \simeq 70(1) \) and series expansions studies [14,15] supported Eq.(2) over a pure power-law singularity. But neither the MC data nor the series expansions showed \( \eta = 0.25 \) and \( \nu = 0.5 \) conclusively.

Primary difficulties of various numerical methods in locating the parameters in Eq.(2) are due to four independent parameters involved so that, for example, a determination of \( \nu \) is sharply sensitive to the location of \( T_c \), and vice versa. Thus, most MC studies have determined \( T_c \) by assuming \( \nu = 1/2 \) in Eq.(2), yielding \( 0.890 \leq T_c \leq 0.894 \) [11,13,17–20].

The generic feature that has emerged from those MC studies was that the values of \( \eta \) calculated from the thermodynamic values (TV value in the thermodynamic limit) of \( \xi \) and \( \chi \) are significantly larger than the predicted value [12,13,16].

In this work we present extensive MC data of the thermodynamic values of \( \xi \) and \( \chi \) up to \( T=0.93 \) (\( \xi \simeq 1391(22) \)), indicating for the first time that \( \eta = 1/4 \) holds as \( T \to T_c \). The unconstrained fit of our thermodynamic data are remarkably consistent with the prediction of Kosterlitz, yielding \( \nu \simeq 0.48 \) and \( T_c \simeq 0.893 \). The nature of the corrections to the leading scaling behavior Eq.(3) is clarified. We also attempt to locate \( T_c \) by conventional FSS , i.e., by finding the temperature where \( \chi_L \sim L^{2-\eta} \) holds with \( \eta = 1/4 \) and, at the same time, where the 4th order cumulant ratio [21] is invariant with \( L \). This procedure yields \( T_c \) over the range \( 0.900 < T_c < 0.905 \), being incompatible with that estimated by assuming Eq.(2).

Our extractions of TVs are based on a novel FSS technique [16,22,24] that facilitates drastically the MC measurements of TV. Namely, thermodynamic data can be computed from MC measurements on a much smaller lattice than required for the traditional direct measurements. The technique is based on the fundamental formula of FSS [16],

\[
A_L(t) = A_\infty(t)Q_A(x), \quad x = \xi_L(t)/L.
\]

Here \( A_L \) denotes a multiplicative renormalizable quantity \( A \), defined on a finite lattice of linear size \( L \), and \( Q_A \) is a universal scaling function of a different scaling variable \( \xi_L(t)/L \).
Eq. (5) is supposed to hold even for the 2D XY model [23]. For a detailed description of the technique see Refs. [16, 22, 23], where the TVs extracted by employing the technique are shown to agree completely with those measured traditionally for the 2D and 3D Ising models [23], 2D XY model [16], and 2D Heisenberg ferromagnet [22, 24].

Standard theory of FSS predicts the presence of $L_{\text{min}}$ below which certain corrections to Eq. (5) become non-negligible. It is shown for the 2D and 3D Ising models [23] that at least for $L \geq 16$ Eq. (5) holds (hence, $L_{\text{min}} \leq 16$) within the accuracy of the relative statistical errors of 0.3 percent. For $T$ not so close to the criticality in the high temperature phase of the XY model, Eq. (5) holds with $L_{\text{min}} \simeq 30$ [16]. As will be seen, however, $L_{\text{min}}$ increases as $T \to T_c$. Whether or not $L_{\text{min}}$ will increase endlessly as $T \to T_c$ (thus violating FSS) is not clear at present, although its violation seems unlikely on theoretical grounds [25]. We will assume that Eq. (5) is accurate for any value of $t$ provided $L \geq 80$ [26].

Here the extractions of the TVs of $\xi$ and $\chi$ are made in the range $0.93 \leq T \leq 0.98$, based on available data of $(x, Q_A(x))$ for $T = 1.0$ [13]. The values of $L$ over the range $80 \leq L \leq 480$ are used for our analysis, and most interpolations are made in the range $Q_A(x) \geq 0.1$. We employed Wolff’s single-cluster algorithm [27] for the MC simulations, imposing periodic boundary condition on a square lattice. For a given set of $T$ and $L$, typically 20 - 40 numbers of bins, (5 - 10 bins for the conventional FSS studies near criticality for the location of $T_c$), have been obtained for the measurements. Each bin is composed of 10 000 measurements, each of which is separated by 3-12 consecutive one cluster updating. Accordingly, the relative statistical errors of most raw-data calculated through the jack knife method are typically less than 0.1 percent for the $\chi$ and 0.2 percent for the $\xi$. Correlation lengths are measured by the low-momentum behavior of the propagator [8, 12, 16, 22-24]. A comparison of our thermodynamic data in Table (1) with those obtained from a strong coupling analysis can be found in Ref. [15], which shows good agreement.

Based on the bulk data, $Q_A(x)$ for $A = \xi$ and $\chi$ are plotted in Fig. (1), displaying an excellent data-collapse for $L \geq 80$. The data-collapse verifies Eq. (5) for the given values of $L$ and $T$. The figure also indicates a deviation from the data-collapse for the data point
corresponding to \( T = 0.95 \) and \( L = 60 \). Similar figures including data points with \( L \leq 60 \) will be presented in a detailed paper [28]. They will serve for a clear demonstration for the effect of correction to FSS for these values of \( L \). Fig.(2) depicts \( \chi(T)/\xi(T)^{2-\eta} \) with \( \eta = 1/4 \) as a function of \( \ln(\xi) \). It shows that the effective value of \( \eta \) gradually decreases to \( \eta = 1/4 \) as \( T \to T_c \). Empirical formula obtained from the data in Fig.(2), assuming \( T_c = 0.893 \) (see below), is as follows:

\[
\frac{\chi(t)}{\xi(t)^{7/4}} = a + b|\ln(t)|^r,
\]

where \( a \simeq 1.833 \), \( b = 0.955 \), and \( r \simeq -0.413 \). Note that the slow decrease of \( \chi(t)/\xi(t)^{7/4} \) as \( t \to 0 \) is inconsistent with any positive value of \( r \) such as was predicted in [4]. Without taking account of the corrections to Eq.(3), it turns out, however, that \( \eta \simeq 0.272(8) \). The value of \( \chi^2 \) per degree of freedom \( (\chi^2/N_{DF}) \) for the latter case turns out to be approximately \( 5.4 \times 10^2 \), which is much larger than that for Eq.(6). Accordingly, correction to Eq.(3) is essential.

We also employ the conventional FSS technique to locate \( T_c \) independently. Namely, we measured both \( \chi_L \) and the 4th order cumulant ratio defined as \( U_L = 3 - \langle S^4 \rangle / \langle S^2 \rangle^2 \) with \( S^2 \equiv |\sum_i \vec{s}_i|^2 \). Such well-known standard FSS properties at criticality as the scale invariance of the \( U_L \) and \( \chi_L \sim L^{2-\eta} \) are direct consequences of the fundamental FSS formula, Eq.(5). Therefore those properties should be valid only for \( L \geq L_{\text{min}} \). We would like to stress, moreover, that an additional criterion should be satisfied in order for the former property to be true: a weak hyperscaling relation that the renormalized four point coupling at zero momentum \( (g_R^{(4)}) \) remains a constant in the scaling region [29]. Such a scaling behavior of \( g_R^{(4)} \) has recently been shown numerically [30] for the 2D XY and \( O(3) \) vector models.

We measured \( U_L \) and \( \chi_L \) by varying \( L \) from 20 to 600 for some temperatures over the range \( 0.89 \leq T \leq 0.92 \). Certain non-asymptotic FSS behavior was observed for \( L < 80 \) [28], which seems to be a consequence of the correction to Eq.(3) [31]. Our data with \( L \geq 80 \) fit remarkably well to a standard FSS formula at the criticality.
\[ \chi_L \sim L^{2-\eta} \]  

for \( T \leq 0.905 \) \((\chi^2/N_{DF} < 0.5)\) (Fig.3). The extracted values of \( \eta \) from the linear fit are: \( \eta(T) = 0.260(1), 0.252(0), 0.245(0), \) and \( 0.231(1) \) for \( T = 0.91, 0.905, 0.90, \) and \( 0.89 \) respectively. Thus \( \eta(T_c) = 0.25 \) is consistent with \( 0.90 \leq T_c \leq 0.905, \) most probably \( T_c \simeq 0.904. \) This estimate is also consistent with our data of \( U_L \) (Fig.4). \( U_L(T = 0.92) \) definitely decreases with \( L \) from \( L=80 \) to \( L=240, \) so that \( T_c \) is obviously smaller than \( 0.92. \) At \( T = 0.91 \) and \( 0.905 \) it varies so mildly that some fictitious scale invariance of \( U_L \) appears over a range of \( L \) not too large; nevertheless, it eventually decreases. This fictitious scale invariance may result from an extremely large value of \( \xi \) over the range of temperature. We observe the invariance of \( U_L(T) \) with respect to \( L \) at \( T = 0.90, \) indicating \( T_c \geq 0.90. \)

We carried out a \( \chi^2 \) fit of \( \xi \) data over the range \( 5.01(3) \leq \xi \leq 1391(22) \) (corresponding to \( 0.93 \leq T \leq 1.19 \)) to the exponential singularity, Eq.(2). Our fit, based on down-hill simplex algorithm, is highly non-linear for Eq.(2), so that we have treated \( T_c \) as an input parameter over a reasonable range. The values of \( \chi^2/N_{DF} \) and \( \nu \) as a function of the input \( T_c \) are plotted in Fig.(5). The best fit is obtained for \( T_c \simeq 0.893 \) and for \( \nu \simeq 0.48 \) \((\chi^2/N_{DF} \simeq 0.75)\). \( \nu = 0.5 \) holds at \( T_c \simeq 0.892 \) with \( \chi^2/N_{DF} \simeq 0.80, \) being in agreement with the range of \( T_c \) conventionally accepted. The agreement is gratifying and may be regarded as another verification for Eq.(3) with \( L_{\min} = 80, \) at least for \( T \geq 0.93. \) The results of the unconstrained fit agree extremely well with the prediction in Eq.(2). Notice, however, that \( \eta = 1/4 \) holds for \( T_c \simeq 0.904 \) according to the conventional FSS, being much larger than \( 0.892. \) Assuming \( T_c = 0.904 \) the best fit is for \( \nu \simeq 0.30(1) \) with \( \chi^2/N_{DF} \simeq 6.69; \) assuming both \( T_c = 0.904 \) and \( \nu = 0.5 \) the best fit has \( \chi^2/N_{DF} \simeq 263. \) Therefore, \( \nu = 1/2 \) in Eq.(2) is definitely inconsistent with the prediction of FSS at criticality.

We also checked whether or not the data fit to \( \xi = c_1(1 + c_2t^\theta) \exp(bt^{-\nu}) \) with the input value of \( T_c \) over \( 0.90 \leq T_c \leq 0.905. \) It turns out that they fit to the formula for some negative value of \( \theta \) only (being inconsistent with Eq.(4)), with the value of \( \chi^2/N_{DF} \) being almost insensitive to the choice of \( T_c. \) However, this function has too much freedom to the
fit and gives unstable predictions for the values of both \( T_c \) and \( \nu \).

On the other hand, the data fit very well to a modified second order phase transition (see also Ref. [10]),

\[
\xi = c_1(1 + c_2 t^\theta) t^{-\nu}.
\]  

Assuming \( T_c = 0.904 \) we estimate that \( \nu \simeq 3.10(8), \theta \simeq 1.82(8) \), and \( c_2 \simeq 44.2 \) with \( \chi^2/N_{DF} \simeq 1.2 \) (Fig.(6)). As the value of the fixed \( T_c \) becomes larger, the data fit better to the modified power-law singularity. The large value of \( c_2 \) is unusual, implying that at sufficiently large \( t \) the correction term becomes dominant with an effective exponent of \( \xi \) being equal to \( \nu - \theta \). We note that our effective \( \nu \) for large \( t \) agrees with the prediction in [32]. For \( t \) small enough the correction becomes negligible regardless of the value of \( c_2 \), while over the intermediate \( t \) the effective critical exponent changes gradually.

Assuming \( T_c \simeq 0.904 \), even a modified exponential singularity including correction is unlikely: For a power-law singularity, \( \xi \sim t^{-\nu} \), the FSS of \( U_L(t) \) is given by, \( U_L(t) \sim f_U(L^{1/\nu}t) \) [21]. Using the analyticity of \( U_L \) for a finite \( L \), after a Taylor expansion we get \( U_L(t) \simeq U_L(0) + c L^{1/\nu} t + O((L^{1/\nu} t)^2) \) for a sufficiently small value of the \( L^{1/\nu} t \). An exponential singularity corresponds to \( \nu \to \infty \) so that \( U_L(T) \) at \( T = 0.905 \) (\( t \simeq 10^{-3} \)), for example, would be \( L \) independent regardless of the value of \( L \), contrary to our finding in Fig.(4). Similarly, if an exponential singularity is valid \( \chi_L(T) \sim L^{2-\eta(T_c)} \) would hold identically at any \( T \) close to \( T_c \); in other words, \( \eta \) would remain unchanged over a finite range of \( T \) close to \( T_c \), which again contradicts our data in Fig.(3). In view of this FSS argument, an exponential singularity could be consistent with our data of \( \chi_L \) (Fig.(3)) and \( U_L \) (Fig.(4)) only if \( T_c \) is considerably smaller than 0.904. Assuming a power-law singularity, on the other hand, one can easily check from the expansion of \( \chi_L(t) \) that even for such a modestly large value of \( \nu \) as \( \nu \simeq 3.1 \), \( \ln(\chi_L/L^{7/4}) \) at \( T = 0.905 \) varies very mildly with \( L \) in agreement with our data in Fig.(2) [28].

It remains to be seen, however, whether or not \( L_{\min} \) diverges as \( T \to T_c \). In this case, the conventional FSS analysis at the criticality would be misleading. It is also possible that
the correction to the leading scaling behavior (Eq.(3)) results in a modification to the FSS behavior (at criticality). The conventional analysis then would not give a very accurate estimate of \( \eta(T_c) \). A more detailed account for the possible failure of the standard FSS analysis at the criticality, along with details of our analysis and methods of obtaining our data, will be presented in a longer paper [28].

In conclusion we have reported strong numerical evidence that \( \eta = 1/4 \) sets in at temperatures close to the criticality. The nature of the correction to the leading scaling behavior Eq.(3) has been clarified. The *unconstrained* fit of our high temperature thermodynamic data yields results consistent with the predictions of the BKT for the values of \( \nu \) and \( \eta \). This, nevertheless, does not rule out the possibility of the ordinary second order phase transition. Knowing the *true* critical point is crucial to the resolution of the order of the phase transition in the 2D classical XY model. The critical point obtained from the conventional FSS analysis, however, seems to be incompatible with the conventional exponential singularity.

After the completion of the current work we have become aware of a recent related work by Kenna and Irving [33] that questions the vortex binding scenario in the 2D XY model based on FSS study of Lee-Yang zeros. They argue that Eq.(2) cannot be compatible with \( \eta = 1/4 \) without a certain correction. However, the proposed correction, \( r \simeq 0.02 \) in Eq.(3), is *inconsistent* with our picture in Fig.(2) in that their \( \chi(t)/\xi^{7/4}(t) \) increases as \( t \to 0 \).

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TABLES

TABLE I. The thermodynamic values of $\xi$ and $\chi$ for $0.93 \leq T \leq 0.98$, extracted through our MC FSS technique.

| T  | 0.98 | 0.97 | 0.96 | 0.95 | 0.945 | 0.94 | 0.935 | 0.93 |
|----|------|------|------|------|-------|------|-------|------|
| $\xi$ | 70.4(4) | 100.3(7) | 155.7(1.5) | 262.7(2.9) | 364.5(3.6) | 539.3(4.5) | 846.7(6.4) | 1391(22) |
| $\chi$ | 4284(20) | 7932(30) | 16978(55) | 42295(108) | 74742(206) | 147536(614) | 3.24(1)×10^5 | 7.70(9)×10^5 |
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[26] The violation of Eq.(5) can be easily checked by the observation of a deviation from data-collapse for $L < L_{min}$ when $(x(t), Q_A(x(t)))$ is plotted at different value of $t$. In this manner, it is shown in Fig.(1) that $L_{min} = 80$ is good enough for $T \geq 0.93$. Nevertheless, a similar check for FSS at a temperature much closer to criticality seems infeasible because accurate TVs are much difficult to be measured.

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the vanishing of the critical index of $g_R^{(4)}$.

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Figure Captions:

Fig.(1): $Q_\xi(x)$ (upper data) and $Q_\chi(x)$ (lower data) for $L \geq 60$, calculated with the data from Table(1). It should be clear that for each $T$ a data point with a larger $L$ corresponds to a smaller $x$. For $T = 0.95$ and $L=60$, the deviation from data-collapse is apparent. For the sake of the higher resolution of the data, we show only a lower part of $Q_\xi(x)$; for the upper part, see Ref. [16].

Fig.(2): $\chi(T)/\xi^{7/4}(T)$ versus $\ln(\xi(T))$ for $T$ over the range, $0.93 \leq T \leq 1.25$. The thermodynamic data for $T > 0.98$ are taken from Ref. [10], which agree completely with the data in [11] [12]. The tendency to decrease implies $\eta > 0.25$, but the values of $\chi/\xi^{7/4}$ tend to stabilize at approximately $\ln(\xi) \geq 5$.

Fig.(3): $\ln(\chi L/L^{7/4})$ versus $\ln(L)$ over $80 \leq L \leq 600$. Here the slope of a straight line is related to the value of $\eta$, that is, $\eta = 1/4 - \text{slope}$. Note a slow decrease (increase) of $\ln(\chi L/L^{7/4})$ with respect to $\ln(L)$ for $T=0.905$ ($T=0.90$); hence, $0.90 < T_c < 0.905$ with $\eta = 1/4$.

Fig.(4): $U_L$ as a function of $\ln(L)$ over $80 \leq L \leq 600$, for various temperatures near criticality. $U_L$ is $L$ independent (within small statistical error) over $80 \leq L \leq 150$, and $80 \leq L \leq 360$ for $T = 0.91$ and 0.905 respectively (pseudo scale invariance), although it eventually decreases with $L$.

Fig.(5): The values of $\chi^2/N_{DF}$ (lower) and $\nu$ (upper) as a function of the input parameter $T_c$, which are obtained from the $\chi^2$ fit of the $\xi$ data to Eq.(2).
Fig. (6): $\ln(\xi)$ as a function of $|\ln t|$ assuming $T_c = 0.904$. The circle symbols denote our data in Tab. (1), while the smooth curve represents the modified second order phase transition, Eq. (8), with the values of the parameters reported in the text (except for $c_1 \simeq 2.19 \times 10^{-2}$). The error bars are almost invisible. Here a straight line would represent a pure power-law singularity, with its slope equivalent to the value of $\nu$. Note that for $|\ln t| \geq 2.6$ the data are almost linear, implying that the effect of correction is already not so important in this regime.
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