Comment on “High Precision Measurement of the Thermal Exponent for the three-dimensional XY Universality Class”

K. S. D. Beach
Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, MA 02215
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A recent paper [Burovski et al., cond-mat/0507352] reports on a new, high-accuracy simulation of the classical $\phi^4$ model (in the three-dimensional XY universality class). The authors claim that a careful scaling analysis of their data gives $\nu = 0.6711(1)$ for the thermal critical exponent. If correct, this would neatly resolve the discrepancy between numerical simulations and experiments on $^4$He. There is reason, however, to doubt the accuracy of the result. A re-analysis of the data yields a significantly higher value of $\nu$, one that is consistent with other Monte Carlo studies.

Universality is an elegant and powerful concept, but as the basis for any method of data analysis it offers many dangers to the practitioner. For example, it is notoriously difficult to extract critical exponents from data on finite systems. Such an analysis is exquisitely sensitive to the choice of scaling form, to the number of fitting parameters, and to the range of system sizes included in the fit. Worse, it is quite difficult to quantify the uncertainties associated with these factors, so there is a tendency to overstate the accuracy of measured exponents. Reference [1] may suffer from this very problem.

After repeated re-analysis of their experiments on the superfluid transition of $^4$He in microgravity [2, 3, 4], Lipa et al. have concluded that the best experimental value of the thermal critical exponent is $\nu_{exp} = 0.6709(1)$. This value is not in good agreement with numerical simulations of other models also believed to be in the three-dimensional XY universality class. Two recent Monte Carlo studies [3, 4] found $\nu_{mc} = 0.6723(3)$ (8) and 0.67155(27).

In an effort to settle the controversy, Burovski et al. studied the classical $\phi^4$ model [1]

$$\frac{H}{T} = -t \sum_{ij} \phi_i^* \phi_j + \frac{U}{2} \sum_i |\phi_i|^4 - \mu \sum_i |\phi_i|^2$$

(1)

by expanding the partition function in series and sampling the various terms stochastically. They considered two critical points—

point A: $t = -0.0795548(1), \quad U = 0.4101562(14)$
point B: $t = -0.0714288(7), \quad U = 0.3605750(8)$

—the second chosen so as to minimize the subleading corrections to finite-size scaling (although one wonders if this helps or simply makes it harder to pick out the subleading corrections when it comes time to fit the data).

Burovski et al. computed the superfluid stiffness $\rho_s$ and two of its $t$ derivatives for a range of linear systems sizes $L = 4, \ldots, 96$. Their results for $R' = \partial(\rho_s L)/\partial t$, evaluated at the two critical points, are reproduced in Table I. Each of the entries corresponds to $5 \times 10^8$ Monte Carlo sweeps.

| Table I: Derivative of the superfluid stiffness scaling function at critical points A and B computed via Monte Carlo. |
|---|---|---|
| $L$ | $R' = \partial(\rho_s L)/\partial t|_{t=0}$ data set A | $R' = \partial(\rho_s L)/\partial t|_{t=0}$ data set B |
| 4 | 2.6329(9) | 1.9907(3) |
| 5 | 2.8414(5) | 2.7843(7) |
| 6 | 3.7316(4) | 3.6586(1)* |
| 7 | 4.6955(5) | 4.6064(5) |
| 8 | 5.7289(4) | 5.6221(9) |
| 9 | 6.8265(7) | |
| 10 | 7.9848(9) | 7.840(1) |
| 11 | 9.2031(13) | |
| 12 | 10.474(2) | 10.286(1) |
| 16 | 10.764(4) | 15.789(2) |
| 20 | 22.403(4) | 22.020(3) |
| 24 | 29.396(7) | 28.897(3) |
| 32 | 45.095(13) | 44.36(1) |
| 48 | 82.48(3) | 81.15(2) |
| 64 | | 124.57(7)* |
| 96 | 231.56(17) | |

*points of disagreement between Fig. 3 of this paper and Fig. 3 of Ref. [1].

They simultaneously fit the two data sets, assuming a scaling form

$$R' = (\text{const.}) L^{1/\nu} [1 + (\text{const.}) L^{-\omega}]$$

(2)

The constants were allowed to take on different values at critical points A and B, whereas the exponents $\nu$ and $\omega$ were assumed to be universal ($\nu = \nu_A = \nu_B$, etc.). On the basis of a known irrelevant exponent, the fit was constrained such that $|\omega - 0.795| < 0.03$; data for system sizes below $L_{\text{cutoff}} = 12$ were discarded. Final fit values of $\omega = 0.796(3)$ and $\nu = 0.6711(1)$ were reported.

Is this value of $\nu$ convincing? Such a high degree of confidence in the fourth digit is probably not warranted. It is clear even to the eye—in Figs. 2 and 3 of Ref. [1]—that the data allows considerable leeway in the slope and offset of the fit. Moreover, two aspects of the data analysis are troubling:

1. It is not particularly useful to restrict the value of the scaling exponent. While it is true that the
FIG. 1: (Top panel) The data from Table I are plotted exactly as in Fig. 3 of Ref. [1]. The two black squares mark the data points in Fig. 3 (at \(L = 6\) and \(L = 64\)) that do not coincide with those shown here. The solid lines denote the best fits for critical points A (red) and B (pink) with \(L_{\text{cutoff}} = 12\) and \(\omega = 0.796\) fixed. Best fits for \(L_{\text{cutoff}} = 4, 5, 6, 7, 8, 9, 10, 11\) are drawn dotted and those for \(L_{\text{cutoff}} = 16, 20, 24\) are drawn dot-dashed. (Bottom panel) The optimal \(\nu\)—computed with both \(\omega\) held fixed and \(\omega\) left free to vary—is plotted as a function of the lower size cutoff. The corresponding values of \(\omega\) are shown in the figure inset. The violet band indicates one standard deviation above and below \(\nu_{\text{exp}}\) from Ref. [4]. The Monte Carlo results from Refs. [2] and Ref. [6] are marked by the cyan and hatched regions.

The lowest-order subleading correction arises from an irrelevant scaling field with exponent \(\omega_{\text{irr}} \sim 0.8\), that correction coexists with other contributions analytic in \(L^{-1}\) [which are not explicitly included in Eq. (2)]. In practice, \(\omega\), as it appears in Eqs. (4) and (6) of Ref. [1], is an effective exponent that approximates the subleading behaviour over some range of \(L\).

2. More important, the authors have failed to quantify the effect of \(L_{\text{cutoff}}\) on their fit. If, as I believe is true in this case, the optimal \(\nu\) depends sensitively on the choice of the lower size cutoff, then some convincing criterion must be advanced to justify choosing one value of \(L_{\text{cutoff}}\) over another.

In the top panel of Fig. 1, I have replotted the superfluid stiffness data of Burovski et al. alongside my own best fits. These fits were generated using exactly the procedure outlined in Ref. [1] for a range of \(L_{\text{cutoff}}\), with and without constraints on \(\omega\). The large variability in \(\nu\), as seen in the bottom panel of Fig. 1, suggests that an uncertainty of \(\pm 0.0001\) is overly optimistic. Moreover, contrary to the authors primary claim, it appears that (for \(6 \lesssim L_{\text{cutoff}} \lesssim 20\)) \(\nu\) is largely consistent with the result of Campostrini et al. and not significantly closer to the experimental value. There is little compelling evidence for a value as low as 0.6711.

It is important to note that there is a curious disagreement (in two data points from the B data set) between Fig. 1 of this paper and Fig. 3 of Ref. [1]. In Fig. 3, the \(L = 6\) data point has the same position, but a larger errorbar; the \(L = 64\) data point is placed considerably higher. The origin of this discrepancy is somewhat mysterious. It may simply be a consequence of minor typographical errors in Table I. In that case, Burovski et al. are fitting to slightly different data set than I am. Nonetheless, it is telling that minor changes on the order of one or two standard deviations to two of twenty-eight data points could have such a disruptive effect. It suggests that \(\nu = 0.6711(1)\) is an unrealistic estimate of the thermal critical exponent.

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