Monte Carlo results for three-dimensional self-avoiding walks

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We discuss possible sources of systematic errors in the computation of critical exponents by renormalization-group methods, extrapolations from exact enumerations and Monte Carlo simulations. A careful Monte Carlo determination of the susceptibility exponent $\gamma$ for three-dimensional self-avoiding walks has been used to test the claimed accuracy of the various methods.

1. Possible sources of systematic errors in the computation of critical exponents

The major problem in a high-precision determination of critical parameters is the presence of corrections to scaling. Indeed they are \textit{a priori} unknown and cause a systematic error which is usually difficult to detect. The problem appears in extrapolations from exact enumerations, where one is forced to use higher-order differential approximants which however give stable results only for long series. The problem arises in Monte Carlo (MC) simulations as well. Because the correlation length is necessarily much smaller than the lattice size $L$ to avoid finite-size effects, the simulation is done in a region of temperatures so far from the critical point that neglecting the unknown corrections to scaling can deeply affect the final estimates. A clear example of this effect can be found in the history of the estimates of the critical exponent $\nu$ for three-dimensional SAWs: the first MC simulations [1] with quite short walks suggested an exponent in agreement with the Flory theory $\nu = 3/5$, while a recent simulation [2] with very long walks (corresponding to a correlation length of $\xi(\beta) \approx 340$) gave the much lower estimate $\nu = 0.5877 \pm 0.0006$ which is in good agreement with renormalization-group (RG) estimates. It is clear that only a careful analysis of the Monte Carlo data can prevent from underestimating the error bars.

On the other hand, a possible source of systematic errors in the field-theoretic approach to critical phenomena could be the presence of non-analyticities on the real axis in the $\beta$-function. Consider the critical behaviour of the coupling constant and of the mass of a generic system. If one includes, beside the dominant correction to scaling with exponent $\Delta_1$, generic subleading ones with exponents $2\Delta_1$, $\Delta_2$ and analytic corrections, etc., one finds for the $\beta$-function

$$W(g) = \frac{M(T)}{\frac{dM}{dT}} = \frac{\Delta_1}{\nu} [(g - g^*) + a (g - g^*)^2$$
$$+ b (g - g^*)^{2\Delta_1} + c (g - g^*)^{\frac{\Delta_2}{\Delta_1}} + \cdots].$$

One can easily see that confluent singularities on the real axis arise naturally if no specific hypothesis on the form of the corrections to scaling is made. In this situation the usual summation method [3] based on a Borel transformation and a complex-plane mapping, in which the request of analyticity of the $\beta$-function on the real axis plays a crucial role, will converge very slowly.

Nickel [4] suggested a new type of analysis, consisting in fitting the $\beta$-function with functions with the expected cut singularity on the real axis, such as hypergeometric functions. With this type of analysis one finds [5], for the $O(n)$ $\sigma$-model analytically continued to $n = 0$, that the zero of the $\beta$-function is at $g^* \approx 1.39$, which is a value sensibly lower than the one obtained using the usual

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type of analysis, $g^* = 1.421 \pm 0.008$. This fact reflects itself on the estimate of the critical exponent $\gamma$ in the following way:

1. the well-known value given by the standard analysis [3] is
   \[ \gamma = 1.1616 \pm 0.01 (g^* - 1.421) \pm 0.0004 \quad (2) \]

2. the one obtained with the analysis suggested by Nickel [5] is
   \[ \gamma = 1.1569 \pm 0.10 (g^* - 1.39) \pm 0.0004 \quad (3) \]

This last value is in perfect agreement with our MC simulation [7], as shown below.

2. The Monte Carlo simulation

One can hope to be able of discriminating between the two proposed types of analysis by means of a Monte Carlo simulation. The SAW is the best possible test-case because the simulations are not affected by finite-size effects and there are algorithms which have autocorrelation times much smaller than those of the algorithms which are available for other systems. To give an idea, for our algorithm the autocorrelation time in CPU units scales as $\tau \sim \xi^4$, which can be compared with the best algorithms for the Ising model, for which $\tau \sim \xi^{d+z}$, with $z \approx 0.4$. A detailed description of the algorithm used in this work can be found in [6] . The algorithm works in the ensemble of pairs of walks with fixed total length $N_{tot}$. One can make inferences on the value of $\gamma$ from the observed distribution of length of one of the two walks, which is in our case

\[ \pi(N_1) = \frac{c_{N_1} c_{N_{tot} - N_1}}{Z(N_{tot})}, \quad (4) \]

where $c_{N_1}$ denotes the number of walks of length $N_1$ and $Z = \sum_{N_{tot}} c_{N_1} c_{N_{tot} - N_1}$.

Instead of making an a priori hypothesis on the form of the corrections to scaling to fit the MC data, we prefer to keep only the leading term in the scaling law for $c_N$

\[ c_N \approx \mu^N N^{\gamma - 1} \quad (5) \]

and make a type of analysis which is sensible to the presence of corrections to scaling, in the following way. We progressively reject those walks with length shorter than a certain length $N_{min}$ and greater than $N_{tot} - N_{min}$ . Of course the estimated values of $\gamma$, $\hat{\gamma}(N_{tot}, N_{min})$, depending on the range of allowed lengths and on $N_{tot}$, converge for $N_{tot} \rightarrow \infty$ and $N_{min} \rightarrow \infty$ to the correct value.

High-statistics runs at different total length, giving an idea of how strong the effect of correction to scaling can be, are shown in Table 1. The run at $N_{tot} = 200$ shows a strong dependence on the cut $N_{min}$, but is in agreement, for large values of the cut, with [3] and with previous MC simulations [8]. For $N_{tot} = 2000$, the estimated values are lower and much flatter, but still sensibly biased by corrections to scaling. For the final estimate we used a weighted average of the estimates obtained using walks of length $N_{tot} = 20000$ and $N_{tot} = 40000$. The effective exponents are shown in Figure 1, where the last point on the right denotes the final estimate with its error bar. The estimates reported in Fig. 1 show a very small dependence on $N_{min}$ but, of course, one cannot conclude that the estimates are not biased by corrections-to-scaling effects. Indeed to understand the residual systematic effects we must compare estimates with different values of $N_{tot}$. Assuming that the corrections to Eq. (5) scale with a subleading exponent $\Delta \geq 0.5$, one confirms that our data at the larger values of $N_{tot}$ have a systematic bias which is less than the statistical error. A very conservative way of determining the residual systematic error consists in making the hypothesis that the effective estimates $\hat{\gamma}$ tend toward the true value following the law

\[ \hat{\gamma} = \gamma + \frac{B}{N_{tot}^\Delta}. \quad (6) \]

Fitting our data to this law, requiring that (6) reproduces the highest estimated exponent for $N_{tot} = 2000$ and the lowest one for $N_{tot} = 40000$ with $\Delta = 0.5$, we estimate $B \approx 0.06$. This result clearly leads to an overestimate of the systematic error if $\Delta > 0.5$. With this type of analysis of the
Table 1

Estimates of $\gamma$ for $N_{tot} = 200$ and $N_{tot} = 2000$. $N_{iter}$ is the number of iterations.

<table>
<thead>
<tr>
<th>$N_{min}$</th>
<th>$\hat{\gamma}$</th>
<th>$N_{min}$</th>
<th>$\hat{\gamma}$</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>1.15288 ± 0.00011</td>
<td>1</td>
<td>1.15782 ± 0.00013</td>
</tr>
<tr>
<td>10</td>
<td>1.15808 ± 0.00021</td>
<td>100</td>
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<td>300</td>
<td>1.15838 ± 0.00071</td>
</tr>
<tr>
<td>40</td>
<td>1.15999 ± 0.00084</td>
<td>400</td>
<td>1.1598 ± 0.0011</td>
</tr>
<tr>
<td>50</td>
<td>1.1605 ± 0.0014</td>
<td>500</td>
<td>1.1584 ± 0.0019</td>
</tr>
</tbody>
</table>

$N_{iter}$ $5 \cdot 10^8$ $N_{iter}$ $6.2 \cdot 10^8$

<table>
<thead>
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<th>$\hat{\gamma}(N_{min})$</th>
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<tbody>
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<td>2000</td>
</tr>
<tr>
<td>4000</td>
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<tr>
<td>6000</td>
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Figure 1. Estimates of $\gamma$ obtained from the weighted average of the results with $N_{tot} = 20000$ (number of iterations $N_{iter} = 10^8$) and $N_{tot} = 40000$ ($N_{iter} = 8.5 \cdot 10^8$). For clarity the statistical error is reported only in two cases. The dotted line and the rightmost point indicated by a diamond is our final estimate with its error bar.

3. Conclusions

The present work indicates that the previous estimate of the critical exponent $\gamma$ obtained from the RG $g$-expansion is significantly biased upward, possibly because of the presence of strong confluent singularities of the $\beta$-function on the real axis at $g^*$. We hope that further analytic work can be done in this direction to clarify this point. Previous Monte Carlo and exact enumeration determinations appear to be incorrect as well, showing how important and difficult is the determination of the systematic error due to corrections to scaling.

REFERENCES

7. S. Caracciolo, M. S. Causo and A. Pelissetto, preprint SNS/PH/1997-02, cond-mat/9703250