Reply to "Comment on 'Surface critical exponents of self-avoiding walks on a square lattice with an adsorbing linear boundary: A computer simulation study' "

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We respond to some statements made in the Comment [Phys. Rev. **51**, 2674 (1995)], and argue that exact enumeration results for short chains are not conclusive and that the claimed accuracy of the simulation results is not supported by the data, due to the relatively small samples.

In their Comment the authors Grassberger and Hegger (GH) [1] apply a relatively new simulation technique to a numerically controversial problem—the critical behavior (at the special point) of a self-avoiding walk on a square lattice anchored to an adsorbing linear "surface." They simulate much longer chains than those treated in our study [2] and find agreement with theory; they claim that the deviation of our results from the theoretical predictions is due to finite size effects.

Before discussing their method and results we would like to respond to several statements made in the Comment. The authors state (second paragraph) that the theoretical predictions "were confirmed by both exact enumerations and by transfer matrix studies," which have found the critical temperature q_c within the range 0.713–0.715, and add (last paragraph and Abstract) that the strong corrections to scaling "were correctly taken into account in the exact enumeration and transfer matrix studies." Indeed, the transfer matrix calculations [3–5] (which, however, use the theoretical values $\nu = \frac{4}{7}$) are equal to the theoretical values $\phi = 0.5$ and $\gamma = 1.453\ldots$ within relatively small error bars. However, their estimates of q_c lie within the range 0.711–0.717, where the latter upper bound is close to our [2] lower bound, 0.718. On the other hand, the exact enumeration results are less conclusive and depend on the analysis technique used. For example, the central values for ϕ ($\phi = 0.55 \pm 0.1$ and 0.55 ± 0.15) obtained in the earlier work of Kremer [6] are close to our estimate, but the large errors cover also the theoretical result. The same is true for most of the results obtained by Zhao, Lookman, and De'Bell [7], who have applied the partial differential approximation to several models. For the present model they have found $q_c = 0.72 \pm 0.05$, $\phi = 0.50 \pm 0.09$, and $\gamma_1 = 1.45 \pm 0.05$, while for a model (on the square lattice) based on site (rather than bond) attraction they have obtained $\phi = 0.52 \pm 0.03$ and $\gamma = 1.40 \pm 0.05$, and for the triangular lattice, $\phi = 0.50 \pm 0.01$ and $\gamma_1 = 1.4 \pm 0.1$. It should be pointed out that these results could not be obtained independently and they are based on the best known result for μ and the theoretical value of γ_1 (for details see [7]). Moreover recently [8] results with significantly smaller errors, $q_c = 0.715 \pm 0.001$ and $\gamma_1 = 1.460 \pm 0.004$ (but no result for ϕ) have been obtained

with another analysis method; it is not clear, however, whether γ_1 has been obtained independently.

We also would like to respond to the GH comparison of the CPU times required by their calculations and ours. First, it should be stressed that in general such a comparison is not easy due to unknown factors, such as the efficiency of the code and the number and type of quantities calculated. Our simulations would require ~ 900 CPU/h on a HP730 work station (used by GH), they provide results for 20 temperatures (rather than five in the Comment), and the samples are significantly larger than those generated by GH (50–100 million vs 1.5 million). Another statement that should be corrected is "that with the scanning method thermal averages are dominated by only few configurations...." Thus, a special discussion is devoted in our paper [2] to the *accepted chains,* which are the *different* chains in the sample that contribute significantly to the averages, and results presented in Table I, reveal that even for a chain length $N = 250$ their number is ~ 7 million. Finally, it should be added that the explanation of the GH method and more importantly, the discussion about its efficiency are too sketchy in the Comment as well as in their other works ([9,10] and Ref. [7] of the Comment). Fortunately, Garel and Orland [11] proposed earlier the ensemble (or chain) growth method (EGM), which is very similar in nature to the GH method, and applied it to several systems, Ising models, polyelectrolytes, and peptides [12–14]. These papers provide a detailed account of the whole approach, including a thorough discussion about efficiency.

The GH method is an extension of the enrichment [15] and the Redner and Reynolds (RR) [16] techniques and is also related to the Berretti-Sokal (BS) procedure [17]; these methods, in principle, enable one to generate relatively long self-avoiding walks (SAW's). Thus, even in the early 1960s and 1980s SAW's of up to 2000 and 1000 steps have been generated by the enrichment [18] and the RR [16] methods, respectively. The problem, of course, is to determine the extent of correlations among the chains. An efficient application of the enrichment method requires working under the conditions in which the enrichment exactly offsets the attrition. However, for long chains it is difficult to balance these two opposing effects and typically large fluctuations between produc-

tion of short chains and population explosion of highly correlated long chains occur. This is probably the reason why in later applications of this method SAW's of only several hundred steps have been generated [19–22]. Similar difficulty is also expected with the BS and RR methods. The efficiency of these three methods for SAW's in the bulk has been estimated under certain assumptions by Sokal [23]. He finds that the CPU time required to generate a statistically independent chain is $\sim N^p$, where $2 \le p \le 1 + \gamma$ (for the RR and BS methods $\langle N \rangle$ replaces N). This efficiency is better than that of the scanning method. However, as far as we know, only BS have verified this estimate by calculating from the simulation the autocorrelation functions of various quantities. For SAW's with finite attractive or repulsive interactions and in the presence of geometrical constraints (such as an impenetrable surface) it becomes difficult to assess the effect of the temperature and the constraints on the efficiency (see discussion below). GH (Ref. [7] of Ref. [1]) estimate the effect of temperature on the efficiency but they do not provide detailed computational data to support their theoretical predictions (see also the Appendix of Ref. [12]).

One of the difficulties in simulating SAW's with attractions is that configurational space consists typically of regions that are small (and therefore hard to be reached by the simulation) while contributing significantly to the partition function; an extreme example is protein folding. Since the GH (and EGM) construction procedure is determined by short-range interactions (i.e., looking only one step ahead), highly probable chains that are based on long-range attractions (i.e., large loops) will be generated with very low probability and practically will be missed. In this respect the scanning method is advantageous, since at each step all the future continuations of the chain up to some cutoff length are scanned and thus at least important medium-range loops are taken into account. In fact, in an initial application of the scanning method to an off lattice model of polyglycine [24] only three steps ahead were scanned and the most stable structure found was the α helix. In a later study five future steps were considered and a structure was generated with much lower energy than that of the α helix [25]. Therefore, for such models the best one can do is to verify that the results become stable for increasing sample sizes. Indeed, for the present model [2] we have found that for chains of $N \sim 200$ a sample size of $n_{accept} \sim 13$ million accepted chains is necessary in order to gain stability. (Notice that the sample size that correctly represents an accepted sample is smaller than n_{accept}; the two sample sizes approach each other as the acceptance rate increases.)

In this respect the work described in the Comment is very unsatisfactory and its significance is questionable: The samples used are extremely small (between 6000 and 15 000 independent chains for $N = 2000$). In particular, the samples of chains with two ends on the surface, which lead to Z^{11} and to the exponent γ_{11}, are even smaller. We have found (Table I of [2]) that already for $N = 250$ they constitute only $\sim 0.9\%$ of the total number of chains and therefore 0.34% for $N = 2000$ (due to the $N^{\gamma_{11} - \gamma_1}$ decrease in the ratio of these populations). GH state that their statistical errors are inversely proportional to the square root of the sample sizes; however this behavior should be verified for much larger samples in order to claim stability.

GH agree that our results for $N \le 200$ are reliable due to the very high statistics; therefore if their calculations are reliable they should lead to our results in the range $50 \le N \le 200$ (our results were derived at $40 \le N \le 200$). However, a careful examination of Fig. 1 in the Comment reveals that already in this range the best straight line is obtained for $q = 0.714$, as compared to 0.722 found by us, and the corresponding value of ϕ is ~ 0.53 with an error $\sim \pm 0.03$ (due to the lack of simulations for $0.710 < q < 0.714$). This means that satisfactory agreement with the theoretical predictions is obtained from the GH simulations already for $N \le 200$ without the need to study chains of up to $N = 2000$. This conclusion applies also to the other two figures, where both γ_1 and $\gamma_1 - \gamma_{11}$ can be obtained from $N \le 200$. (Notice that for estimating the γ's, GH use the best value for μ known from exact enumeration studies, while we estimate μ, γ_1, and γ_{11} from our data.)

In summary, the sample size of GH is relatively small and their claimed accuracy is not supported by the data, as discussed above. Obviously, in order to reduce correction to scaling effects, it is very important to develop methods that would enable one to investigate longer chains than those studied by us. It seems that the GH method has the potential to become such a tool (at least for certain models), however a thorough study of its efficiency should be carried out.

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