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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(Received 5 January 1994)

We present simulations of very long two-dimensional polymers near a linear adsorbing boundary which give results in conflict with recent simulations by Meirovitch and Chang [Phys. Rev. E **48**, 1960 (1993)], but agree with earlier studies of very short chains.

PACS number(s): 36.20.Ey, 02.70.−c, 05.70.Jk, 64.60.Kw

Recently, there has been much progress in understanding polymers in two dimensions, partly due to analytical results related to conformal invariance. In this Comment, we shall be concerned with the behavior of self-avoiding walks (SAW's) with one end attached to an attractive surface. The partition sum for an N-step SAW is defined as $Z_N^{(1)} = \sum_{m=0}^{N} C_{N,m} e^{mq}$, where $C_{N,m}$ is the number of configurations having m bonds in the surface, and $q = \epsilon/k_B T$, $\epsilon > 0$ being a binding energy per monomer.

At the special point [1], the exponent γ_1^s defined via $Z_N^{(1)} \sim \mu^N N^{\gamma_1^s - 1}$ is known to be $\gamma_1^s = \frac{93}{64} = 1.4531$ [2], while the crossover exponent ϕ, which governs the scaling of the mean energy, $E_N \sim N^{\phi}$, should be equal to $\phi = \frac{1}{2}$ [3]. These predictions were confirmed both by exact enumerations [4] and by transfer matrix studies [2,5]. On the other hand, a different value $\phi = 0.562 \pm 0.020$ was found in a recent Monte Carlo study with very high statistics [6]. In that paper, a slightly different critical value of q was also found, $q_c = 0.722 \pm 0.004$ as opposed to 0.713–0.715 in Refs. [2,4,5]. Since Monte Carlo simulations use much longer chains than either exact enumerations or transfer matrix methods, this raises the problem of whether there are not large corrections to scaling that were overlooked in [2,4,5].

The longest chains in [6] had $N = 260$. By studying even longer chains, with N up to $N_{\max} = 2000$, we want to show in the present comment that the claims of [6] are wrong, and that the results of [2,4,5] are indeed correct.

To generate SAW's, we use the recursive implementation of the enrichment method described in detail in [7]. It is similar to the recursive method used in [8,9]. Our method generates samples with roughly the same number of walks for all N between 1 and $N_{\max}$, from which we can compute immediately $Z_N^{(1)}$. An important aspect is that it allows for perfect importance sampling with exactly the right thermodynamic bias, i.e., it immediately produces samples in which each chain is included with a probability *exactly* proportional to its Boltzmann weight e^{mq}. Thus all averages are simply unweighted averages without *any* further systematic corrections. This distinguishes it from most other methods as, e.g., the Rosenbluth and Rosenbluth method [10] or the method used in [6]. In these, different configurations can have very different weights, whence thermal averages are dominated by only a few configurations unless one uses huge samples. No such problems arise with our method, unless we use much lower temperatures or much longer chains. Finally, we mention that we used a carefully checked multitap feedback shift register random number generator

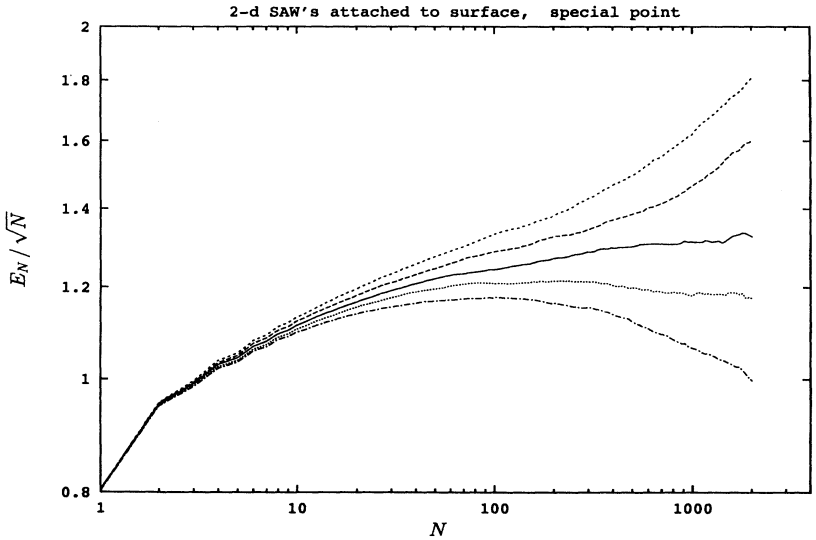

FIG. 1. Log-log plot of $E_N/\sqrt{N}$ against N, for five equally spaced values of q in the range 0.706 (lowest curve) to 0.722 (highest).

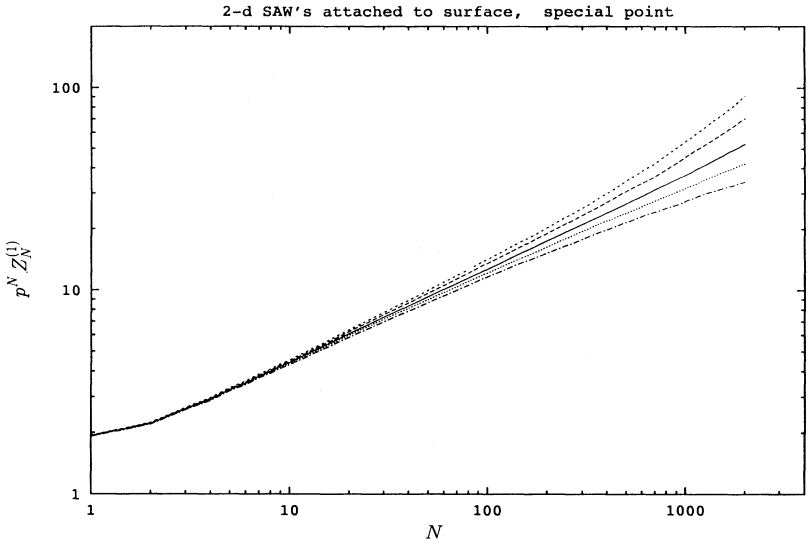

FIG. 2. Log-log plot of $Z_N^{(1)}/\mu^N$ against N, for the same values of q as in Fig. 1.

(RNG) [11], as simpler RNG's perform poorly in similar problems [9].

We have performed runs at five different values of q (0.706,0.71, . . . , 0.722), with ca. 1.5×10^6 walks for each q. Within each run, the walks are not statistically independent, as discussed in [7]. But data for different q's are strictly independent, whence the consistency between different curves in Figs. 1–3 gives a direct hint as to the size of our statistical errors. The number of *independent* SAW's of length N in each sample decreases asymptotically as $\sim 1/N$. For each value of q it is larger than 6000 at $N=N_{\max}$. This number might sound very modest, but we verified that statistical errors were indeed inversely proportional to its square root, with coefficients of order 1. The total CPU time was 60 h on a fast workstation (HP730), compared to more than 2000 h on an IBM 340/6000 (which has roughly half the speed of an HP730) in [6].

In [6], the value of q_c was estimated from a plot of $\ln(E_N/N)$ against $\ln N$. In Fig. 1 we show a similar plot (we assume $k_B T=1$). We see that indeed the straightest curve in the interval $10<N<260$ (the range used in [6]) would be obtained with $q\approx0.722$, and this would give $\phi\approx0.56$. But taking our full range we see that this estimate would be wrong due to large corrections to scaling. Our estimate from Fig. 1 is instead $q_c=0.713\pm0.002$, $\phi=0.50\pm0.01$, in perfect agreement with [2,4,5].

In order to check this and to estimate γ_1^s, we show in Fig. 2 our values of $Z_N^{(1)}/\mu^N$. Here we used for μ the very precise estimate of [12], $\mu=2.638\,159(1)$. We find roughly the same critical value of q as above, giving us our final estimate $q_c=0.712\pm0.001$ and $\gamma_1^s=1.46\pm0.01$. If we would insist on $q_c=0.722$, we could produce a nearly straight plot by increasing μ to a value close to 2.639. Such a value was indeed measured in [6], but the very large error bar given it there would have suggested that the precise value of μ is not important for the analysis of the data. Again we see that this might be true for the

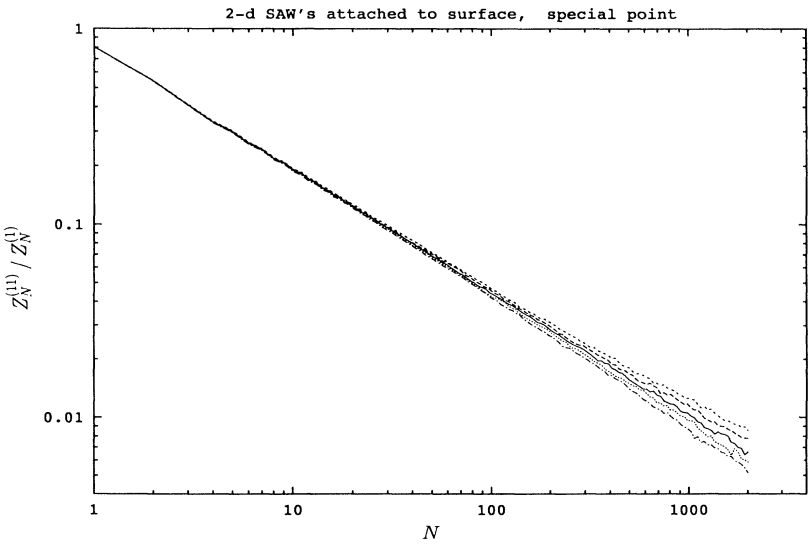

FIG. 3. Similar to Fig. 1, but for the ratio $Z_N^{(11)}/Z_N^{(1)}$.

moderately long chains of [6], but that it is definitely not true anymore for the chains studied in the present work.

Finally, we show in Fig. 3 the ratio $Z_N^{(11)}/Z_N^{(1)}$, where $Z_N^{(11)}$ is the number of walks having both ends on the surface. It follows a scaling law similar to that for $Z_N^{(1)}$, but with γ_1^s replaced by another exponent γ_{11}^s. From Fig. 3 we can read off $\gamma_1^s-\gamma_{11}^s=0.64\pm0.01$. Together with the above value for γ_1^s and the exact values of the exponents γ and ν for two-dimensional (2D) SAW's in the bulk, this gives perfect agreement with the Barber scaling relation [13] $2.10\pm0.014=2\gamma_1^s-\gamma_{11}^s=\gamma+\nu=\frac{43}{32}+\frac{3}{4}=2.094$.

Our conclusion thus is that the critical exponents for the special point in two-dimensional polymer adsorption agree with their theoretical predictions. There are strong corrections to scaling, but they were correctly taken into account in the exact enumeration and transfer matrix studies of [2,4,5], where the absence of statistical fluctuations allows very sophisticated extrapolations. In order to obtain similarly good results in a Monte Carlo study, one has to take *much* longer chains. Though the chains in [6] were roughly an order of magnitude longer than those in the exact enumerations of [4] and had very high statistics, this was not enough. Only by adding another order of magnitude in the chain length were we able to see them clearly—in spite of much lower statistics. This demonstrates that it is important to simulate very long chains. Thus a method like that used in [6] (whose efficiency decreases exponentially with chain length, albeit slowly, and which puts unequal weights on different chains) is inherently less suitable than the present one, whose efficiency decreases as $1/N$ and which puts the same weight on each chain—though it can be very useful in other circumstances.

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