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MONTE CARLO SIMULATIONS OF A POLYMER CHAIN MODEL ON EUCLIDEAN LATTICES

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Abstract: We studied the critical properties of flexible polymers, modelled by self-avoiding random walks, in good solvents and homogeneous environments. By applying the PERM Monte Carlo simulation method, we generated the polymer chains on the square and the simple cubic lattice of the maximal length of N=2000 steps. We enumerated approximately the number of different polymer chain configurations of length N, and analysed its asymptotic behaviour (for large N), determined by the connectivity constant μ and the entropic critical exponent γ. Also, we studied the behaviour of the set of effective critical exponents ν_N, governing the end-to-end distance of a polymer chain of length N. We have established that in two dimensions ν_N monotonically increases with N, whereas in three dimensions it monotonically decreases when N increases. Values of ν_N, obtained for both spatial dimensions have been extrapolated in the range of very long chains. In the end, we discuss and compare our results to those obtained previously for polymers on Euclidean lattices.

Keywords: polymers, Monte Carlo simulations, lattice models, critical exponents.

1. INTRODUCTION

The self–avoiding walk (SAW) is a random walk that must not intersect itself, and on a lattice, it can be formed as a random path of a SAW walker that steps on neighbouring previously non-visited lattice sites. The SAW property of path non-overlapping emulates very well the so-called excluded volume effect of polymers, and the SAW model is widely accepted as the standard model of a linear polymer in a dilute solution [1]. The SAW model can be successfully applied to study a single polymer chain in both good (non-consecutive monomers of a polymer chain do not interact mutually) and poor solvents (there are distinct monomer-monomer interactions within a polymer chain) [2]. In research of statistical properties of SAWs, the special interest is devoted to the critical behaviour of very long SAW chains ($N \to \infty$) described by various critical exponents. It has been shown that the SAW model is equivalent to the n-component spin model in the limit $n \to 0$ [3], so that a correspondence between models of linear polymers and magnetic systems occurs. For most of the studies of statistical properties of SAWs a necessary step is finding the number of different configurations (*i.e.* the number of possible states) for an N-step SAW system. To investigate the asymptotic behaviour of SAWs it is plausible to enumerate SAWs of finite lengths N and then extrapolate the obtained results of related quantities in the limit $1/N \to 0$ of very long chains.

Exact counting of different SAW configurations of the length N on a lattice is very demanding combinatorial task, and so far SAWs of the maximal length N_{max}=79 [4] have been enumerated on the square lattice, whereas on the simple cubic lattice the maximal length is N_{max}=36 [5]. The reached values for N_{max} are still far from the asymptotic region of very long chains, and another method for sampling SAWs for larger N_{max} should be used. To this end various types of Monte Carlo methods have been invented [6], and in this study we utilise the pruned-enriched Rosenbluth-Rosenbluth method (PERM) [7], which is a static Monte Carlo algorithm for SAWs sampling. The PERM enables building of SAWs of different lengths N (up to predefined maximal value), and it appeared to be very efficient for approximate counting of SAW configurations of large length. Also, during the simulation of SAWs with this method it is possible to

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evaluate the averages of various observables within created *N*-step SAWs ensembles, and then, from obtained data, analyse their critical behaviour.

The present paper is organized in the following way. In section 2, we define the main quantities related to the lattice SAW model and expose the basic ideas of the PERM Monte Carlo method for simulation of SAWs on the square and the simple cubic lattice. In section 3 we present the obtained numerical results for critical exponents ν (related to the mean squared end-to-end distance of SAWs) and γ (associated with the total number of distinct SAWs), as well as results for the connectivity constant μ representing the effective coordination number of the SAW (*i.e.* the average number of possible next steps to the walker having already made a large number of steps). In the same section we discuss and compare our findings with those obtained by other methods. Eventually, a short conclusion is given in section 4.

2. SIMULATION OF SELF-AVOIDING WALKS ON LATTICES WITH PRUNED-ENRICHED ROSENBLUTH-ROSENBLUTH METHOD

In order to describe the statistics of the SAW model on a lattice we assign the weight x (fugacity) to each step of the walk, so that a SAW consisting of N steps has the weight x^N. Thus, the generating function for SAWs of all possible lengths is of the form

$$C(x) = \sum_{N=1}^{\infty} C_N x^N. \quad (1)$$

Here C_N is the total number of distinct N-step SAWs which, in the long chain limit, behaves as

$$C_N \sim \mu^N N^{\gamma-1}, \quad (2)$$

where γ is the entropic critical exponent, and μ is the connectivity constant. Another quantity describing metric properties of *N*-step SAWs is the mean squared end-to-end distance $\langle R_N^2 \rangle$, determined by the scaling law

$$\langle R_N^2 \rangle \sim N^{2\nu}, \quad (3)$$

where ν is the corresponding critical exponent, presuming that the number of steps N is quite large. Here we note that ν and γ are universal critical exponents, that is (for the SAW model) their values only depend on the space dimension of underlying lattice, while the connectivity constant μ is a lattice dependent quantity.

In this paper we apply the PERM Monte Carlo method to calculate the connectivity constant μ and critical exponents γ and ν of flexible SAWs on the square and simple cubic lattice. The PERM method is an improved version of the Rosenbluth-Rosenbluth (RR) chain growth algorithm [8] for sampling SAWs of different lengths on a lattice. Starting from an arbitrary lattice site, in RR method, the SAW chain develops by adding a new step to the existing SAW chain. The added step is chosen randomly from the set of free neighbouring sites, and the process of SAW growth (from the origin, with $N = 0$) is called the tour. The step adding procedure is repeated until the chain reaches the given maximal length N_{max}, or the SAW walker gets stuck (*i.e.* there is no free neighbouring sites for further growth). The SAWs generated in RR method are biased, because the occupied neighbouring sites are not taken into account for the next step random choice, so that the sampled N-step walks have different statistical weights depending on their configuration. This weight, for an N-step SAW in RR method is

$$W_N = \prod_{n=0}^{N-1} a(n), \quad (4)$$

where $a(n)$ is atmosphere of the walk [9], that is the number of free (previously non-visited) neighbouring sites for a growing SAW after n steps ($n < N$). For the square lattice the beginning value for the atmosphere is $a(0) = 4$, while for the simple cubic lattice it is $a(0) = 6$ (see Figure 1). The total number of distinct SAWs C_N in RR method can be evaluated as an average

$$C_N = \langle W_N \rangle = \frac{1}{s_0} \sum_{i=1}^{s_N} W_N^{(i)}, \quad (5)$$

where s_0 is the number of starting SAWs and s_N is the number of SAW samples of length N [10]. Calculation of C_N enables us to find out the values of μ and γ, while the metric critical exponent ν can be extracted from $\langle R_N^2 \rangle$, which in RR method can be calculated as

$$\langle R_N^2 \rangle = \frac{\sum_{i=1}^{s_N} W_N^{(i)} [R_N^2]^{(i)}}{\sum_{i=1}^{s_N} W_N^{(i)}}, \quad (6)$$

where $[R_N^2]^{(i)}$ is the squared end-to-end distance of an N-step SAW sample whose RR weight is $W_N^{(i)}$.

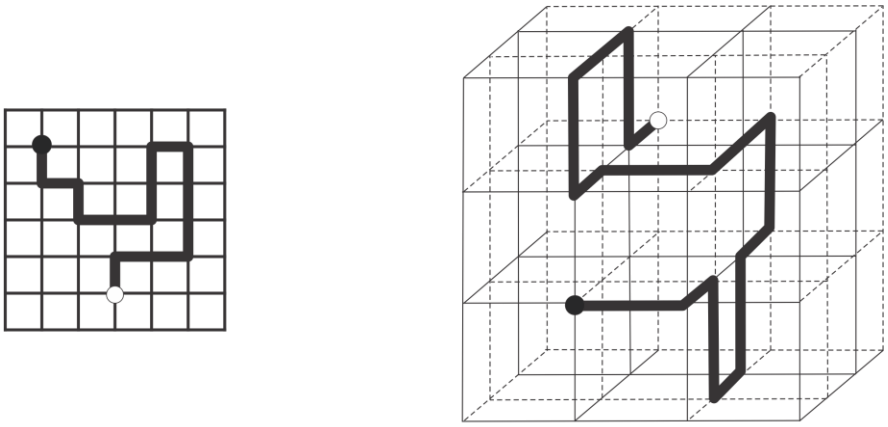

Figure 1. Examples of SAW path on the square (d=2) and on the simple cubic lattice (d=3) with N=14 and N=16 steps, respectively. The full circles are starting, and open ones are ending points of the SAWs. The RR weight of the SAW on the square lattice is $W_{14}= 4 \cdot 3^8 \cdot 2^2 \cdot 3 \cdot 2^2$, *while for the SAW on the simple cubic lattice it is* $W_{16}=6 \cdot 5^4 \cdot 4 \cdot 5^2 \cdot 4^2 \cdot 5 \cdot 4 \cdot 5 \cdot 4 \cdot 5 \cdot 3$.

The RR method becomes ineffectual when we want to create longer SAW samples, because an accented attrition of starting SAWs appears (*i.e*. large number of SAWs became trapped before reaching a desired length). Besides, the obtained SAW statistics are usually fairly distorted since the SAW samples with very high RR weights (which are infrequent) produce a very large variance in RR weight statistics. To resolve these problems an upgraded version of RR method, called the PERM, has been introduced, where we prune SAWs with low weights and enrich SAWs with large weights [7]. To apply pruning or enriching transformation of an N-step SAW, for the SAW weight we define two milestones $W_N^<$ and $W_N^>$, by the relations

$$W_N^< = \frac{1}{5}\langle W_N \rangle \left(\frac{s_N}{s_0}\right)^2, \quad W_N^> = \langle W_N \rangle \left(\frac{s_N}{s_0}\right)^2. \qquad (7)$$

If $W_N < W_N^<$, the SAW is pruned (killed) with the probability 1/2. If the SAW survives pruning, we double its weight ($1 \cdot W_N \rightarrow \frac{1}{2} \cdot 2W_N$). On the other hand, in the case that $W_N > W_N^>$ we apply the enriching transformation, that is we replace a SAW configuration of the weight W_N with two copies of the halved weight ($1 \cdot W_N \rightarrow 2 \cdot \frac{W_N}{2}$). In this way the N-step SAW weights W_N of different SAW samples stay close to $\langle W_N \rangle$. Here we note that pruning and enriching transformations do not alter the values of C_N and $\langle R_N^2 \rangle$ calculated from (5) and (6).

3. RESULTS AND DISCUSSION

Applying the PERM method, we have created SAW chains of various lengths N (up to $N_{max} = 2000$), on both the square and the simple cubic lattice. In one simulation session, for each N we have made a set of SAW chains consisting of $s_N \simeq 4.37 \cdot 10^8$ SAW samples on the square lattice and $s_N \simeq 1.22 \cdot 10^8$ samples on the simple cubic lattice. To analyse the obtained large sets of data we follow the approach developed in [11], where we have studied semi-flexible polymer chains on the square lattice. Here we expanded the simulation data for flexible polymer chains in two dimensions and extend this study in three dimensions.

Since in our Monte Carlo experiment, we have created SAWs with finite length N, the formula (2) for the total number of different configurations (which is valid for $N \rightarrow \infty$) should be corrected to

$$C_N = A_C \mu^N N^{\gamma-1} \left(1 + \sum_{i=1}^{\infty} \frac{c_i}{N^i} + \sum_{i=0}^{\infty} \frac{c_i'}{N^{\Delta+i}}\right). \qquad (8)$$

The first sum (with integer powers) corresponds to the analytical correction terms, while the second one (where Δ is not an integer) describes the non-analytical correction terms. In two dimensions $\Delta = 3/2 > 1$ [12] and the leading correction term in (8) is analytical $1/N$, while in three dimensions $\Delta = 0.528(12) < 1$ [13] so that the leading correction term is non-analytical $1/N^{\Delta}$. To evaluate the values of μ and γ we analysed the ratio

$$\frac{C_{N+1}}{C_N} = \mu\left(1 + (\gamma - 1)\frac{1}{N} + \cdots\right), \qquad (9)$$

whereupon one can see that the leading correction term is $1/N$ for both $d = 2$ and $d = 3$ case. We notice that, in $d = 2$ the second correction term is $1/N^2$, while in $d = 3$ it is stronger $1/N^{1.528}$. From (9) we see that for large enough N, the ratio $\frac{C_{N+1}}{C_N}$ should display a linear dependence on $1/N$. Since in our Monte Carlo experiment, for various N, we have measured the values of C_N (in accordance with the

relation (5)), we have been able to study the ratio $\frac{C_{N+1}}{C_N}$, as function of N and $1/N$ (see Figure 2), for both square ($d = 2$) and simple cubic ($d = 3$) lattice. We see that the function $\frac{C_{N+1}}{C_N}(1/N)$ is linear, so that using (9) one can determine μ and γ fitting the obtained Monte Carlo data, presented in Figure 2. The fitting technique is similar to the one applied in [11]. We constitute sets of data $\left\{\frac{1}{N}, \frac{C_{N+1}}{C_N}\right\}$ where N belongs to the range $[N_{min}, N_{max}]$ with fixed N_{max}=1999. Then we change incrementally the value of N_{min} to get the set of estimates $\mu(N_{min})$ and $\gamma(N_{min})$, obtained by weighted linear fits of data $\left\{\frac{1}{N}, \frac{C_{N+1}}{C_N}\right\}$, in the range $[N_{min}, 1999]$. These estimates are presented in Figure 3 as functions of N_{min}, for both the square and the simple cubic lattice. From these data (obtained from one simulation session) the final results for $\mu \pm \Delta\mu$ and $\gamma \pm \Delta\gamma$ we obtain as an average of $\mu(N_{min})$ (as well as $\gamma(N_{min})$) in a region where they appeared to be stable (see Figure 3). We repeat this analysis from data collected from n_S independent Monte Carlo sessions ($n_S = 26$ for the square lattice and $n_S = 22$ for simple cubic lattice) obtaining n_S results: $\mu^{(i)} \pm \Delta\mu^{(i)}$ and $\gamma^{(i)} \pm \Delta\gamma^{(i)}$, $(i = 1, \ldots, n_S)$, for μ and γ. The final numerical assessment of the connectivity constant μ and the entropic critical exponent γ is calculated as a weighted mean of $\mu^{(i)}$ and $\gamma^{(i)}$, respectively. The evaluated numerical values are given in Table 1.

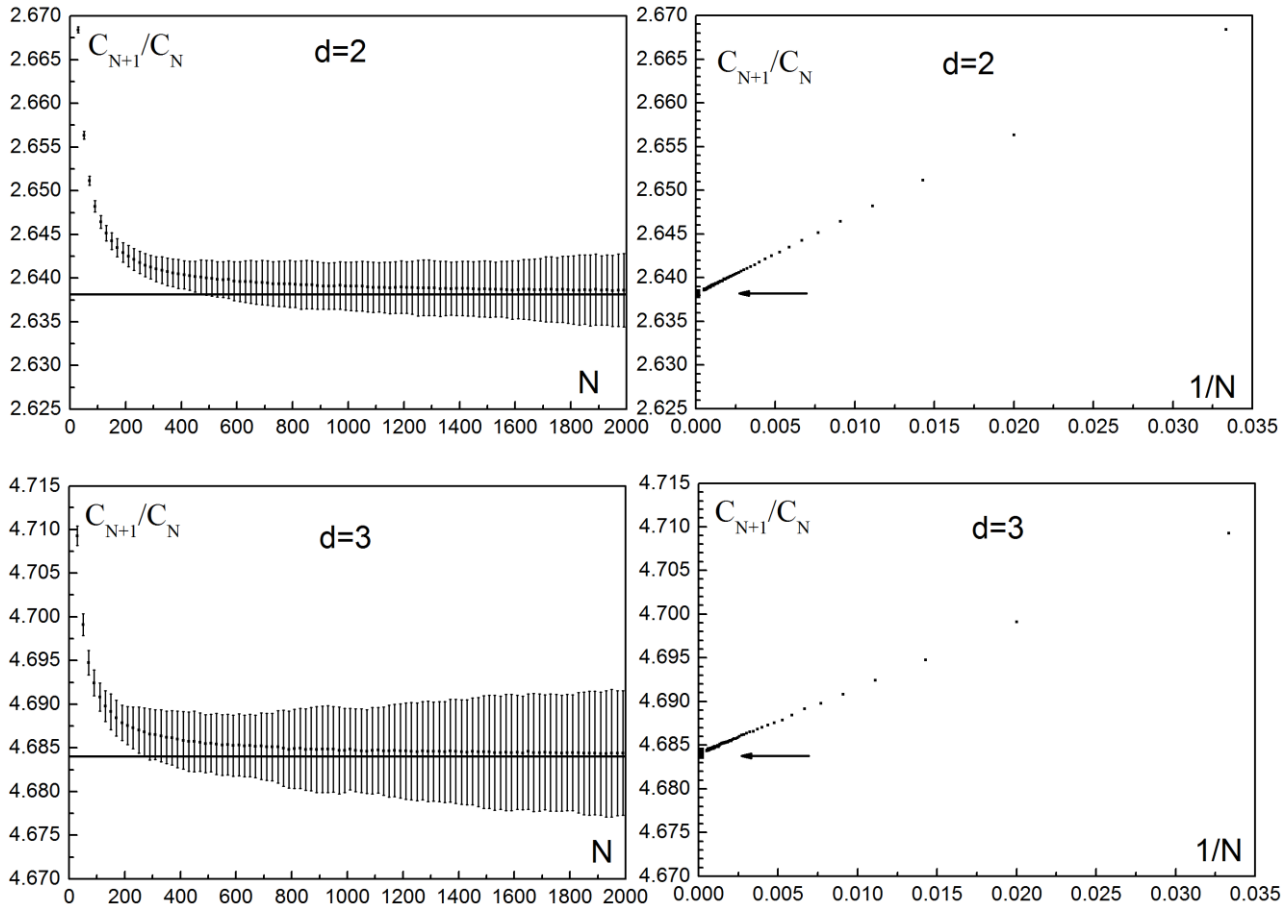

Figure 2. Values of the ratio C_{N+1}/C_N for SAWs on the square (d=2) and the simple cubic (d=3) lattice presented as a function of chain length N (left panels), and 1/N (right panels). Also, we have depicted the error bars related to C_{N+1}/C_N (on the left panels), while horizontal lines (on left panels) and arrows (on right panels) correspond to the extrapolated values in the limit $N \to \infty$.

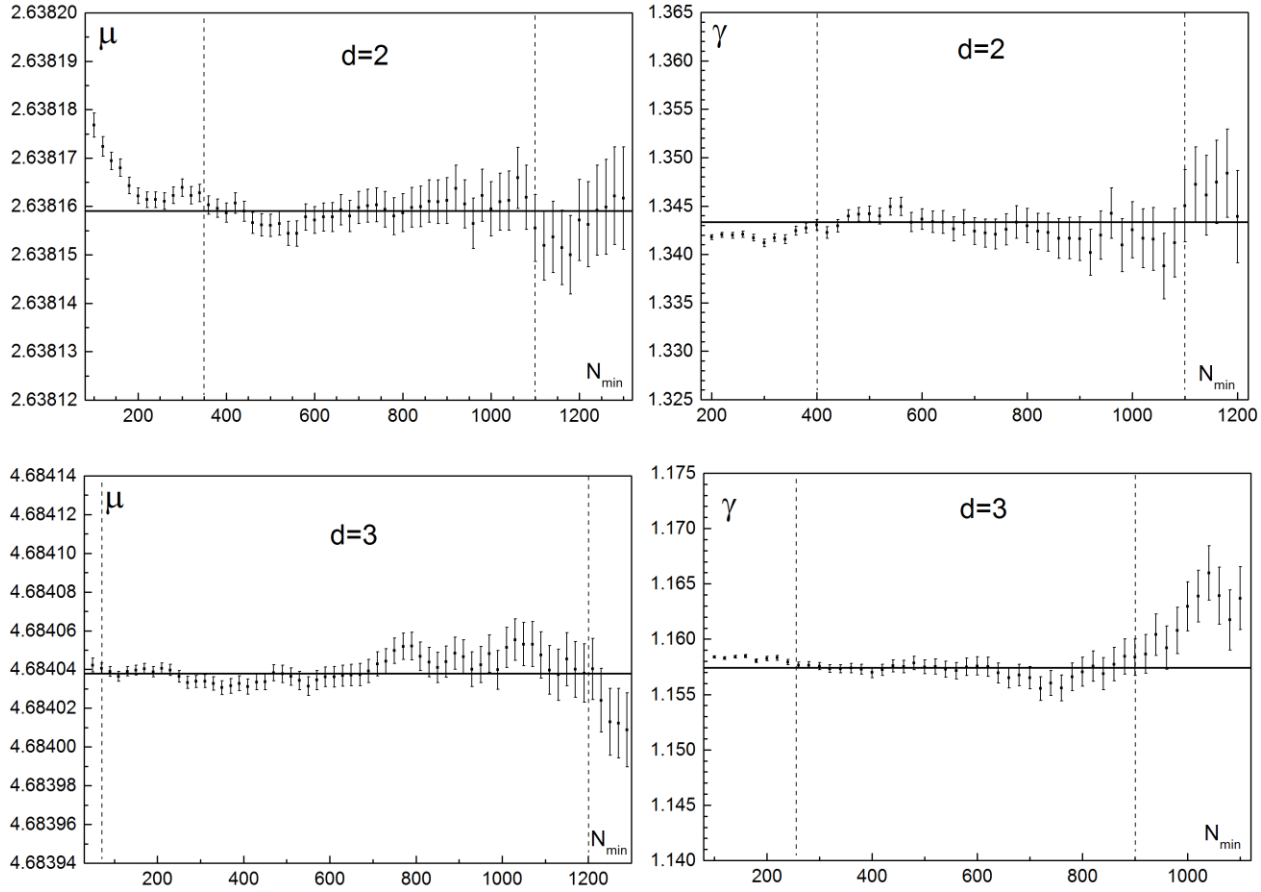

Figure 3. Numerical results for the connectivity constant μ *and the critical exponent* γ *as functions of* N_{min}*, obtained from weighted least squares linear fit of* C_{N+1}/C_N *against 1/N. The upper panels correspond to the square lattice (d=2), and the lower to the simple cubic lattice (d=3). The pairs of vertical dotted lines denote the range of* N_{min} *where analysed data are stable, whereas full horizontal lines represent the average values of data covered by corresponding intervals.*

Table 1. Values of the connectivity constant μ and critical exponents γ and ν, obtained via PERM Monte Carlo simulation method for the square (d=2) and the simple cubic (d=3) lattice. The figures in the brackets are single standard errors connected with the last two digits of the main results.

	μ	γ	ν
d=2	2.6381586(14)	1.3433(05)	0.74999(02)
d=3	4.6840399(09)	1.1578(02)	0.58785(07)

First, we discuss results for the square lattice. Our Monte Carlo result for the critical exponent γ=1.3433(05) is very close to the exact value 43/32=1.34375 proposed by Nienhuis [14], and deviates from it 0.034%. The result for the connectivity constant μ=2.6381586(14) is more precise then the value μ=2.63818(3) obtained previously using the same PERM method [15]. Also, our finding for μ agrees very well with high precision estimates 2.63815853035(2) [16] and 2.63815853032790(3) [17] obtained recently utilising very efficient transfer matrix methods. On the simple cubic lattice, our result for entropic critical exponent γ=1.1578(02) is consistent with numerical ones obtained by Monte Carlo simulations γ=1.1573(02) [18], exact enumeration method γ=1.15698(34) [5] and conformal field theory γ=1.1588(26) [19]. Finally, our estimate for the connectivity constant μ=4.6840399(09) is more precise then existing exact enumeration result μ=4.6840401(50) [5] and Monte Carlo estimate μ=4.6840386(11) [20].

Next, we study the critical exponent ν. The scaling relation (3) is valid in the asymptotic region of very long SAWs ($N \to \infty$). For SAWs of finite length *N*, we must consider the correction terms, so that we use the scaling equation

$$\langle R_N^2 \rangle = A_R N^{2\nu} \left(1 + \sum_{i=1}^{\infty} \frac{r_i}{N^i} + \sum_{i=0}^{\infty} \frac{r_i'}{N^{\Delta+i}}\right), \qquad (10)$$

which is analogous to (8), with the same values for the exponent Δ describing non-analytical correction terms (for the square lattice $\Delta = 3/2$ and for the simple cubic lattice $\Delta = 0.528(12)$). To estimate ν from obtained Monte Carlo data of $\langle R_N^2 \rangle$, we define a set of effective critical exponents [21] with the formula

$$\nu_N = \frac{1}{2}\log_2 \frac{\langle R_N^2 \rangle}{\langle R_{N/2}^2 \rangle}, \tag{11}$$

which are calculated up to $N_{max} = 2000$, with step 2 for *N*, for both *d*=2 and *d*=3. To analyse the behaviour of ν_N for large *N* we insert (10) in (11). For the square lattice (*d*=2) we obtain

$$\nu_N = \nu - \frac{r_1}{\ln 4}\frac{1}{N}, \tag{12}$$

whereas for the simple cubic lattice (*d*=3) it follows

$$\nu_N = \nu - \frac{0.44\, r_0'}{\ln 4}\frac{1}{N^{0.528}}. \tag{13}$$

From (12) we may perceive that in two dimensions ν_N should behave as a linear function of 1/*N*, while from (13) we see that in three dimensions ν_N should behave as a linear function of $1/N^{0.528}$. The expected behaviour of ν_N against $1/N$ ($1/N^{0.528}$) for the square (simple cubic lattice) is depicted on the left panels of Figure 4. From $d = 2$ graph one can see that in two dimensions ν_N monotonically increases with *N* and approaches the limiting value $\nu = \lim_{N\to\infty} \nu_N$ from below, which implies that $r_1 > 0$ in equation (12). On the other hand, in three dimensions ($d = 3$) one may observe that ν_N decreases with *N*, which in (13) brings about $r_1' < 0$.

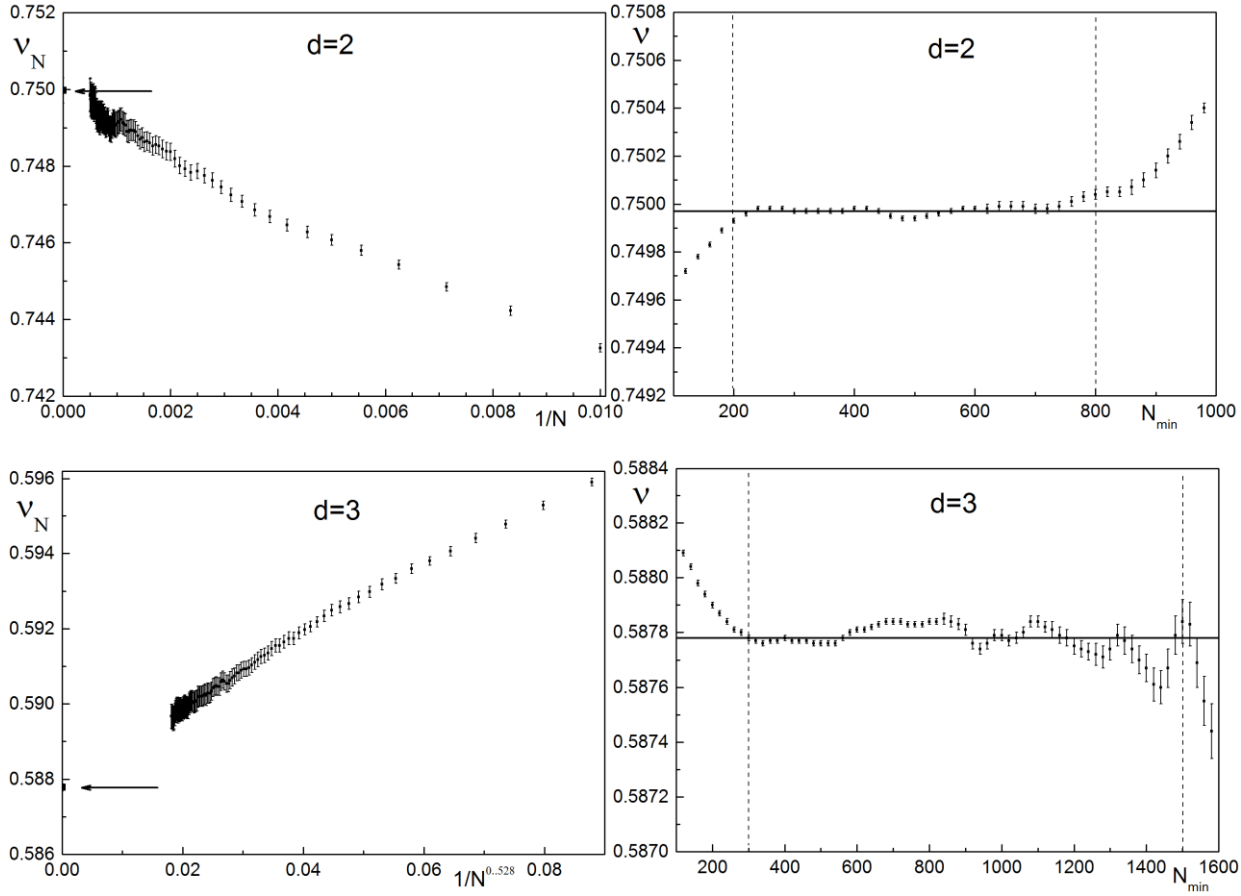

Figure 4. On the left panels we have presented Monte Carlo results for the effective critical exponent ν_N for SAWs on the square (d=2) and simple cubic (d=3) lattice as function of $1/N$ (for d=2) and $1/N^{0.528}$ (for d=3). On right panels we presented estimates of the critical exponent ν (together with their error bars) as functions of N_{min}, obtained from weighted least squares linear fit of $\{1/N, \nu_N\}$ for d=2 and $\{1/N^{0.528}, \nu_N\}$ for d=3, in the range $[N_{min}, 2000]$. The pairs of vertical dotted lines denote the range of N_{min} where estimates of $\nu(N_{min})$ emerge to be stable. The arrows (on left panels) as well as full horizontal lines (on right panels) designate extrapolated values of ν_N for $N \to \infty$.

The limiting values $\nu = \lim_{N\to\infty} \nu_N$ for both dimensions ($d = 2$ and 3) are determined applying the weighted linear fit of data presented on the left panels of Figure 4. To accomplish this task, we follow the procedure applied in the case of μ (for details see caption of Figure 4) and our definitive estimates for ν are listed in Table 1. For $d = 2$ we can compare our Monte Carlo estimate with the exact result 3/4 [14]. One can see that our finding ν=0.74999(02) is quite close to 3/4 (with relative error 0.001%), and it is more accurate than ν=0.7489(21) [22] recently obtained by Monte Carlo method that used non-reversed random walk algorithm to generate SAWs.

On the other hand, for $d = 3$ our finding ν=0.58785(07) coincides with numerical ones obtained by Monte Carlo methods ν=0.58765(20) [18], ν=0.587597(7) [13], ν=0.5876(14) [22], exact enumeration method ν=0.58772(17) [5] and conformal field theory ν=0.5877(12) [19].

Overall, we may infer that the applied PERM Monte Carlo algorithm came out to be very efficient method for sampling long polymer chains in order to learn numerical values of quantities describing critical properties of linear polymers. Especially, our numerical findings for the connectivity constant μ and the critical exponents γ and ν, studied on Euclidean lattices, appeared to be very accurate and consistent with the results obtained by other methods utilised in studies of polymer statistics.

4. CONCLUSION

We have applied the PERM Monte Carlo chain growth algorithm to simulate polymer chains, modelled by self-avoiding random walks (SAWs), in two and three dimensions. Particularly, on the square and the simple cubic lattice, for SAWs of the maximal length of 2000, we have enumerated approximately the number of different SAW configurations and we have studied the behaviour of effective critical exponents ν_N for the end-to-end distance of a polymer chain of finite length *N*. We have found out that on the square lattice ν_N monotonically increases, whereas on the simple cubic lattice it monotonically decreases with *N*. Also, we analysed the asymptotic region of large chains ($N \to \infty$), for which we have evaluated the values of critical exponents ν and γ that govern the mean squared end-to-end distances of polymer chains and total number of different SAW configuration, respectively, as well as the connectivity constant μ (representing the effective coordination number of the SAW, for very long chains). Our results (given in Table 1) are consistent with the results previously obtained with other methods. The performed study has been made for a limited length of polymer chains (up to 2000 steps) and we believe that our result may be additionally improved simulating SAWs of larger length.

5. ACKNOWLEDGMENT

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МОНТЕ КАРЛО СИМУЛАЦИЈЕ МОДЕЛА ПОЛИМЕРНОГ ЛАНЦА НА ЕУКЛИДСКИМ РЕШЕТКАМА

Сажетак: Проучаване су критичне особине флексибилних полимера, моделованих самонепресецајућим случајним шетњама, у добрим растварачима и хомогеним срединама. Примењујући PERM Монте Карло метод, симулирани су полимерни ланци на квадратној и простој кубичној решетки, максималне дужине N = 2000 корака. Апроксимативном методом пребројаван је укупан број полимерних конфигурација дужине N, и анализирано је његово асимптотско понашање (за велико N), одређено константом повезаности μ и ентропијским критичним експонентом γ. Такође је проучавано понашање скупа ефективних критичних експонената ν_N, који одређују растојање између крајева полимерног ланца дужине N. Установљено је да у дводимензионом случају ν_N монотоно расте са порастом N, док у три демензије ν_N монотоно опада када N расте. За обе димензије вредности за ν_N екстраполиране су за област ланаца јако великих дужина. Добијени резултати су дискутовани и поређени са раније добијеним резултатима за полимере на еуклидским решеткама.

Кључне речи: полимери, Монте Карло симулације, модели на решеткама, критични експоненти.

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