

## **On Continuous-Time Self-Avoiding Random Walk in Dimension Four**

**Suemi Rodríguez-Romo<sup>1</sup> and Vladimir Tchijov<sup>1</sup>**

*Received November 11, 1996; final October 24, 1997*

---

We study the distribution of the end-to-end distance of continuous-time self-avoiding random walks (CTRW) in dimension four from two viewpoints. From a real-space renormalization-group map on probabilities, we conjecture the asymptotic behavior of the end-to-end distance of a weakly self-avoiding random walk (SARW) that penalizes two-body interactions of random walks in dimension four on a hierarchical lattice. Then we perform the Monte Carlo computer simulations of CTRW on the four-dimensional integer lattice, paying special attention to the difference in statistical behavior of the CTRW compared with the discrete-time random walks. In this framework, we verify the result already predicted by the renormalization-group method and provide new results related to enumeration of self-avoiding random walks and calculation of the mean square end-to-end distance and gyration radius of continuous-time self-avoiding random walks.

---

**KEY WORDS:** Continuous-time self-avoiding random walk; renormalization-group map; dimerization algorithm; Monte Carlo simulation.

### **1. INTRODUCTION**

Self-avoiding random walk models appeared in chemical physics as models for long polymer chains. Roughly speaking, a polymer is composed of a large number of monomers which are linked together randomly but cannot overlap. This feature is modelled by a self-repulsion term.

To state a self-repulsion term, Flory<sup>(1)</sup> used a self-avoiding random walk (SARW). A self-avoiding random walk of the number of steps  $n$  is a simple random walk which visits no site more than once. Although this

---

<sup>1</sup>Centre of Theoretical Research, UNAM, Campus Cuautitlán, Apdo. Postal 95, Unidad Militar, Cuautitlán Izcalli, Estado de México, 54768 México; e-mail: suemi@servidor.unam.mx, tchijov@servidor.unam.mx.

simple model possesses some qualitative features of polymers, it turns out to be very difficult for obtaining rigorous results and Monte Carlo experiments are commonly used to study this problem. In this paper, we present some results of Monte Carlo experiments for CTRW. CTRW models are useful for studying random walks on random lattices with traps,<sup>(2)</sup> relaxation of complicated systems (e.g., glasses and polymers),<sup>(3)</sup> migration of a classical dynamical system between regions of configuration space,<sup>(4)</sup> energy migration on regular lattices,<sup>(5)</sup> transport of radioactive isotopes in neural membrane channels<sup>(6)</sup> and homogeneous nucleation of vapor condensation.<sup>(7)</sup> Specially, two physical applications, the migration of photons in a turbid medium and the theory of diffusion-controlled reactions in a random medium, suggest that it might be useful to study properties of the CTRW.<sup>(8)</sup>

On the other hand, to obtain analytical results we can take advantage of the several measures on random walks which favor self-avoiding walks and are in the same universality class as the SARWs. In this paper, we use weakly SARW (so called Domb-Joyce model or self-repellent walk). This is a measure on the set of simple walks in which two-body interactions are discouraged but not forbidden. Here, these interactions are penalized by a factor  $e^{-\lambda(\text{measure of (self-)intersection})}$ ,  $\lambda > 0$  being a small constant. This factor is needed to make the process tend to avoid itself.

In Section 2 we use a method already reported in the literature<sup>(9,10)</sup> to study, from an original point of view, the asymptotic logarithmic correction to the end-to-end distance of CTRW in dimension four, weakly self-avoiding, thereby providing a new stochastic meaning to the exponent of the logarithmic correction. We believe that this result can be extended to weakly SARW on a hypercubic lattice. In Section 3, we describe our Monte Carlo experiments on an integer lattice for the CTRW to verify the result predicted in Section 2. In the first case the random walks are not nearest neighbors (this would be trivial because of the hierarchical lattice on which our renormalization group map is implemented), whereas in the second case they are nearest neighbors.

The paper is organized as follows. In Section 2, we present the heuristic procedure to obtain the end-to-end distance of the weakly continuous-time SARW on the hierarchical lattice. We report on the new probabilistic meaning of the result. In Section 3, we present Monte Carlo experiments for continuous-time SARW on a four dimensional integer lattice  $\mathbf{Z}^4$  and verify the goodness of our heuristic approach. In Appendix 1, we discuss the enumeration of SARWs, the corresponding end-to-end distance and gyration radius. Appendix 2 is devoted to a short description of the statistical tools we use to get the best-fit curves. Finally, summary and discussion are presented.

## 2. ASYMPTOTIC END-TO-END DISTANCE

In refs. 9 and 10 we have constructed a map on a hierarchical random walk for SUSY  $\lambda\phi^4$  to study, from the stochastic point of view, the renormalization of this model. In the present paper we intend to use the very same map, through the McKane–Parisi–Sourlas theorem, to give an heuristic explanation to the logarithmic correction of the end-to-end distance,  $d=4$ , for the weakly SARW on a hierarchical lattice.

From studying the renormalization of the weakly SARW that penalizes two-body interactions (or double-crossing random walks) we can find the stochastic expression for the leading order contribution to the mass or killing rate for the process. In this paper, we use this to build a multiplicative scheme and predict the asymptotic logarithmic correction to the end-to-end distance of the weakly SARW,  $d=4$ . For weakly SARW, we propose the standard scaling factor for local times of the renormalization transformation by including, up to  $O(\lambda)$ , the contribution of the self-repulsion term to renormalized local times. Namely, from the renormalization-group map on weakly SARW, renormalized local times are generated from the interaction. In the field theoretical approach this corresponds to generating mass. Equivalently, we can say that the interaction kills the process at a specific rate. If we take into account only  $O(\lambda)$  contributions to this and follow standard thinking in our multiplicatively renormalization group scheme, the well known asymptotic end-to-end distance for the weakly SARW in  $d=4$  follows. Moreover, from our method, the exponent of the logarithmic correction involved is expressed in terms of conditional expectations for measures of events for random walks inside the smallest hierarchical lattice cosets in the lattice, that upon calculation, give the well known exponent. Recently, an alternative rigorous proof has been given, provided the properties of the Green function are known, in the SUSY field theoretical approach.<sup>(13)</sup> We assume the Green function to be unknown.

Let  $\langle w^\alpha(T) \rangle$  be an  $\alpha$ -moment of a CTRW; it is known that the only finite moments for diffusive random walks on our hierarchical lattice correspond to  $0 < \alpha < 2$ .<sup>(13)</sup> Here  $T$  is the running time of the process. This range of  $\alpha$  values is used to obtain the end-to-end distance in the following proposition.

For  $d=4$ , up to  $O(\lambda)$ , the generated renormalized local times (mass for the field or killing rate for the process), from applying the renormalization-group map on the interaction in a multiplicatively renormalization group scheme, is such that the asymptotic behavior of the end-to-end distance for a weakly SARW that penalizes the intersection of two random walks is  $T^{1/2} \log^{1/8} T$ .

This conjecture comes from the following thinking. After applying ( $p$ ) stages the renormalization-group transformation on  $\langle w^\alpha(T) \rangle^{1/\alpha}$  we have

$$\langle w^\alpha(T) \rangle^{1/\alpha} = \frac{\langle w^\alpha(1) \rangle^{1/\alpha(0)}}{L^p} \quad (1)$$

where  $L \geq 2$ , integer, is a scale (from the hierarchical lattice) used in the renormalization group map. Besides, we have chosen a system of units such that for  $p=0$ ,  $T=1$ . Hereafter,  $\langle w^\alpha(1) \rangle^{1/\alpha(0)} = D$  is a constant called the diffusion constant. Here, we are following the standard procedure for scaling length-type magnitudes.<sup>(16)</sup> Moreover, by  $\langle w^\alpha(T) \rangle^{1/\alpha}$  we mean  $\langle w^\alpha(T) \rangle^{1/\alpha(p)}$ . Since in renormalizing the lattice we divide every length, including the end-to-end distance, by  $L$ , then, upon  $p$  iterations, Eq. (1) follows. This is exactly what is done in scaling correlation lengths but used here on the end-to-end distance, both length-type magnitudes. So Eq. (1) becomes

$$\langle w^\alpha(T) \rangle^{1/\alpha} = L^{-p} D \quad (2)$$

On the other hand

$$T = \frac{1}{L^{2p} \prod_{i=1}^p (1 + \gamma_1^* \lambda^{(i)})} \quad (3)$$

where  $\gamma_1^* = \gamma_1/L^2$ ,  $\gamma_1$  is presented below and by  $T$  we mean  $T^{(p)}$ . Here we have included, up to  $O(\lambda)$ , the contributions to renormalized local times due to two-body interactions in the original random walk (see refs. 9 and 10); namely,  $\gamma_1$  and  $\lambda^{(i)}$ . In this scaling factor, the  $O(\lambda)$  term comes from the leading contribution to the mass (or killing rate of the process) seen as new rescaled holding times.

From this follows

$$\langle w^\alpha(T) \rangle^{1/\alpha} = DT^{1/2} \left( \prod_{i=1}^p (1 + \gamma_1^* \lambda^{(i)}) \right)^{1/2} \sim DT^{1/2} (e^{\gamma_1^* \sum_{i=1}^p \lambda^{(i)}})^{1/2} \quad (4)$$

For  $\beta=2$ ,  $d=4$  and up to order  $(\lambda^{(i)})^2$ , follows  $\lambda^{(i+1)} = \lambda^{(i)} - \beta_2(\lambda^{(i)})^2$  (see ref. 10). Here  $\gamma_1$  and  $\beta_2$  are conditional expectations of two-body interactions (or double crossing in a random walk), one for  $\gamma_1$  and two for  $\beta_2$ , inside the smallest cosets in the hierarchical lattice, provided that renormalization group is applied such that  $\gamma_1$  renormalizes to holding times and  $\beta_2$  renormalizes to two-body interactions (see ref. 10).

Introducing the solution of this recursion into Eq. (4), we obtain

$$\langle w^\alpha(T) \rangle^{1/\alpha} \sim DT^{1/2} e^{(\gamma_1^*/2\beta_2) \ln p} \sim DT^{1/2} (p)^{\gamma_1^*/2\beta_2} \tag{5}$$

In Eq. (5) we have assumed  $p$  (stage we have applied the renormalization group map) to be large enough so  $\lambda^{-1} \ll \beta_1(p)$ . Taking the asymptotic limit  $p \rightarrow \infty$  (i.e.  $p \rightarrow \log T$ ) we rewrite Eq. (5) as

$$\langle w^\alpha(T) \rangle^{1/\alpha} \sim DT^{1/2} \log^{\gamma_1^*/2\beta_2} T \tag{6}$$

which is the asymptotic behavior of the end-to-end distance.

It only remains to know the value of  $(\gamma_1^*/\beta_2)$ . Actually we can calculate  $\gamma_1^*$  and  $\beta_2$  from their definitions (see Table in ref. 10). We can prove that  $\gamma_1^*/2\beta_2 \sim \frac{1}{8}$ , provided the number of points inside a smallest coset of the hierarchical lattice is larger than the number of jumps performed by the random walk inside the very same coset, even if the second one is large, as we consider it is. Besides, the jumping rate for the process  $r$  is set such that a well defined diffusive Green function follows for this hierarchical lattice, provided the killing rate is introduced critically.<sup>(12)</sup>

In the next Section we test this analytical conjecture on continuous-time weakly SARW by Monte Carlo experiments on continuous-time SARWs on an integer lattice  $\mathbf{Z}^4$ . Both random walk models are in the same universality class, therefore identical logarithmic corrections are expected.

### 3. COMPUTER SIMULATIONS

In this section, we present the results of the Monte Carlo computer simulations we have performed to test the asymptotic behavior of the mean square end-to-end distance and the mean square gyration radius reported in Section 2, as functions of the running time  $T$  for continuous-time self-avoiding random walks with exponentially distributed waiting times on a 4-dimensional hypercubic lattice  $\mathbf{Z}^4$ .

Let  $\omega_n$  be an  $n$ -step self-avoiding random walk with initial point at the origin of the hypercubic lattice  $\mathbf{Z}^4$ . We associate with  $\omega_n$  the *running time*

$$T = \sum_{i=0}^{n-1} t_i$$

where  $t_i$  ( $i=0, \dots, n-1$ ) are exponentially distributed random values—*waiting times* of the sites of a walk, thus producing a continuous-time self-avoiding random walk. We denote a random walk  $\omega_n$  together with its running time  $T$  as  $\omega_{n,T}$ . In order to calculate the distributions of the mean square end-to-end distance and the mean square gyration radius

denoted hereafter as  $\langle \omega^2(T) \rangle$  and  $\langle \omega_g^2(T) \rangle$ , we need at first to introduce the procedure we use to generate self-avoiding random walks on  $\mathbf{Z}^4$ . A method for obtaining  $\langle \omega^2(T) \rangle$  and  $\langle \omega_g^2(T) \rangle$  is described later in this section.

Straightforward algorithms for generating self-avoiding random walks of a given number of steps  $n$ , for example non-reversed simple sampling,<sup>(17)</sup> are impractical since the computer time required to generate a single  $n$ -step self-avoiding walk grows exponentially with  $n$ . In our simulations we use the recursive Alexandrowicz dimerization algorithm<sup>(18)</sup> which is the most efficient known *static* algorithm for generating a single self-avoiding walk in any dimension. This algorithm has been applied to Monte Carlo simulations of self-avoiding random walks in 2- and 3-dimensional calculations.<sup>(19, 20)</sup> In brief, the idea of dimerization algorithm is as follows. If the number of steps  $n$  is less than the “Alexandrowicz length”  $n_0$ , a self-avoiding walk is generated by the non-reversed simple sampling. If  $n \geq n_0$ , two walks of length  $n/2$  are generated and concatenated. If the resulting walk has no self-intersections, it is self-avoiding, otherwise the procedure is resumed from the scratch. The algorithm is recursive: if the subchains of the length  $n/2$  are still longer than  $n_0$ , the subchains themselves are generated using the same algorithm. The main advantage of the dimerization algorithm is that it is *unbiased*, i.e. each possible self-avoiding walk of a given number of steps has the same probability to be generated.<sup>(17)</sup> The estimated computational time for generating a single walk of the number of steps  $n$  is of order  $d_0 n^{d_1 \log_2 n + d_2}$ , where  $d_i$  ( $i = 0, 1, 2$ ) are independent of  $n$ .<sup>(17, 22)</sup> In 4-dimensional case it is expected that  $d_1 = 0$  (if the usual scaling assumptions hold true),<sup>(17)</sup> thus providing a polynomial growth of computational time per single self-avoiding walk. The value  $d_0$  depends upon the “Alexandrowicz length”  $n_0$ . Our simulations show that the usage of  $n_0$  less than 10 significantly slows down the calculations in comparison with larger values of  $n_0$ . On the other hand, if  $n_0$  is comparable with  $n$ , the dimerization algorithm loses its advantage because of the above-mentioned exponential growth of computational time. Hence, there exist some optimal, dimensional dependent values of  $n_0$ . In our simulations we used  $n_0 = 30$ .

A method we use to obtain the distributions of  $\langle \omega^2(T) \rangle$  and  $\langle \omega_g^2(T) \rangle$  utilizes the “windows” refinement introduced in ref. 19. We choose the interval of running times  $[T_{\min}, T_{\max}]$  for which we are going to estimate  $\langle \omega^2(T) \rangle$  and  $\langle \omega_g^2(T) \rangle$ , and divide it into equal-sized “windows”  $[T_i, T_{i+1}]$ ,  $i = 1, \dots, I$ ,  $T_0 = T_{\min}$ ,  $T_I = T_{\max}$ . We specify a “window”  $[T_i, T_{i+1}]$  and, in turn, divide it into  $M$  equal parts. Then, using the dimerization procedure we generate statistical samples of random walks  $\omega_{n, T}$  of all possible number of steps  $n$  (of  $L_c = 100000$  walks for every  $n$ ).

In practice we are restricted to some interval of the number of steps  $n_{\min} \cdots n_{\max}$ . For a given subinterval of length  $\Delta T = (T_{i+1} - T_i)/M$  inside the “window”  $[T_i, T_{i+1}]$ , we calculate the values of  $\langle \omega^2(T) \rangle$  and  $\langle \omega_g^2(T) \rangle$ , taking into account only that walks  $\omega_{n,T}$  whose running times lie within this subinterval. More precisely, denote as  $N_n$  ( $n = n_{\min}, \dots, n_{\max}$ ) the number of  $n$ -step continuous-time self-avoiding random walks (chosen among  $L_c = 100000$  walks generated for given  $n$ ) whose running time lies within the given subinterval  $[T, T + \Delta T]$ , and as  $\omega_{n,T}^{(k)2}$  the mean square end-to-end distance for the  $k$ th walk ( $k = 1, \dots, N_n$ ). Then we can write

$$\langle \omega^2(T) \rangle \approx \left( \sum_{n=n_{\min}}^{n_{\max}} \sum_{k=1}^{N_n} \omega_{n,T}^{(k)2} \right) / \left( \sum_{n=n_{\min}}^{n_{\max}} N_n \right) \quad (7)$$

The similar relationship holds for the distribution of gyration radius  $\langle \omega_g^2(T) \rangle$ .

In practice, the interval  $[T_{\min}, T_{\max}]$  and the above mentioned values  $I, M, n_{\min}, n_{\max}$  are *a priori* arbitrary quantities.<sup>(20)</sup> However, in the model under consideration there exist some reasonable limitations on the choice of  $n_{\min}$  and  $n_{\max}$ . Indeed, given a continuous-time self-avoiding walk  $\omega_{n,T}$  of the number of steps  $n$ , the mean value of its running time  $T$  is also  $n$ , since the mean values of each  $t_i$  are 1, in accordance with the exponential distribution of  $t_i$ . The main contribution to  $\langle \omega^2(T) \rangle$  and  $\langle \omega_g^2(T) \rangle$ , thus, is made by the walks  $\omega_{n,T}$  whose number of steps  $n$  are relatively close to  $T$ . The restrictions on the interval  $[T_{\min}, T_{\max}]$  are imposed by the performance of a computer. We have chosen  $T_{\min} = 40$ ,  $T_{\max} = 180$ ,  $I = 7$ ,  $M = 1000$ . Therefore, we used 1000 subintervals with  $\Delta T = 0.02$  in each of the seven “windows” of length 20. The “windows” on the  $T$  axis, the interval of the numbers of steps of self-avoiding walks  $n_{\min} \cdots n_{\max}$ , and the chain lengths for every  $n$ ,  $n_{\min} \leq n \leq n_{\max}$ , are listed in Table I.

Our programs were written in Borland C++ and run on 60 MHz Pentium system. In order to generate a random choice of the consecutive sites of a self-avoiding walk in the dimerization algorithm, as well as exponentially distributed waiting times  $t_i$  at each site of a walk, we used the pseudo random number generator **ran3**.<sup>(25)</sup> We have performed a test of the subroutine of our main program that generates SARWs by the dimerization algorithm, together with exact enumeration of the SARWs on  $\mathbf{Z}^4$ . The results are presented in the Appendix 1.

The main goal of our Monte Carlo simulations concerning *continuous-time* self-avoiding random walks was to verify the heuristic result of Section 2 on the asymptotic behavior of  $\langle \omega^2(T) \rangle$  and  $\langle \omega_g^2(T) \rangle$ . We have obtained the representative ensembles of the squared end-to-end distances and gyration radii for the continuous-time self-avoiding random walks—

**Table I. Parameters of Computer Experiments**

“Window” <sup>a</sup>	$N_1$	$N_2$	Chain Length
40 ... 60	10	120	50000
60 ... 80	10	200	50000
80 ... 100	10	220	50000
100 ... 120	20	220	50000
120 ... 140	20	240	100000
140 ... 160	20	240	100000
160 ... 180	40	240	100000

<sup>a</sup> “Window” is the interval of length 20 on the  $T$  axis.  $n_{\min}$  and  $n_{\max}$  fix the interval of lengths of SARWs used to obtain the mean values for a given “window.” The column “ $N_n$ ” shows the number of SARWs of each length within the interval  $[n_{\min}, n_{\max}]$  that we generated in our Monte Carlo experiments.

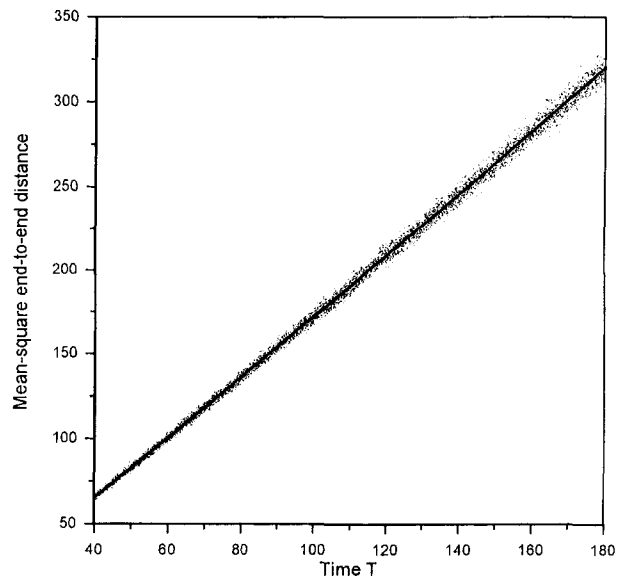


Fig. 1. Mean square end-to-end distance for continuous-time self-avoiding random walks with exponentially distributed waiting times, as a function of running time  $T$ , in dimension four. Each small dot represents the value of the mean square end-to-end distance obtained by averaging over about 2000 walks whose running times lie within the subinterval of length  $\Delta T = 0.02$ . The figure depicts 7000 points obtained in our Monte Carlo experiments, and the best-fit curve  $DT(\ln T)^\alpha$  with  $D = 1.1780$  and  $\alpha = 0.2508$  (solid line).



about 2000 walks for each of the subintervals of the length  $\Delta T = 0.02$  on the interval  $[T_{\min}, T_{\max}]$ . Using Eq. (7), we calculated the values of  $\langle \omega^2(T) \rangle$  and  $\langle \omega_g^2(T) \rangle$ . The variances of the squared end-to-end distances and gyration radii for all of the mentioned subintervals were also recorded (see Appendix 2).

To test the result obtained in Section 2, we fitted our data to the functional relationships

$$\langle \omega^2(T) \rangle \sim DT(\ln T)^\alpha$$

$$\langle \omega_g^2(T) \rangle \sim D_g T(\ln T)^{\alpha_g}$$

with the *a priori* unknown parameters  $D$ ,  $\alpha$ ,  $D_g$ , and  $\alpha_g$ , having applied the nonlinear weighted least-square method and the Levenberg–Marquardt minimization procedure with additive damping.<sup>(26)</sup> We have got the following values of the parameters:  $\alpha = 0.2508 \pm 0.0059$ ,  $D = 1.1780 \pm 0.0107$ ,  $\alpha_g = 0.2531 \pm 0.0037$ ,  $D_g = 0.1932 \pm 0.0011$  (99% confidence intervals). The

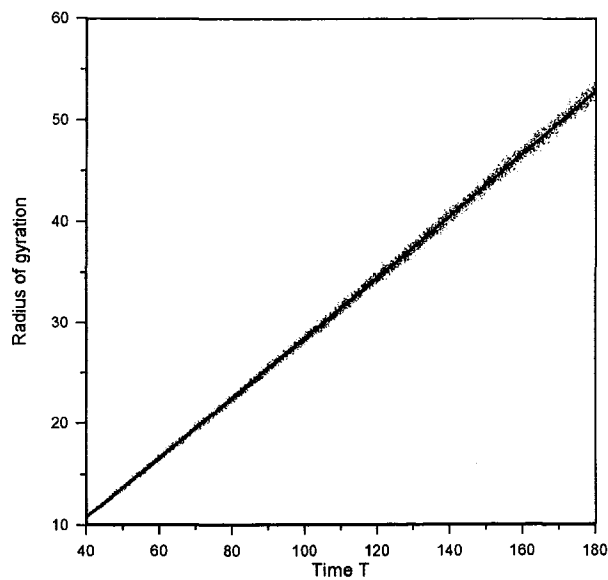


Fig. 2. Mean square gyration radius for continuous-time self-avoiding random walks with exponentially distributed waiting times, as a function of running time  $T$ , in dimension four. Each small dot represents the value of the mean square gyration radius obtained by averaging over about 2000 walks whose running times lie within the subinterval of length  $\Delta T = 0.02$ . The figure depicts 7000 points obtained in our Monte Carlo experiments, and the best-fit curve  $D_g T(\ln T)^{\alpha_g}$  with  $D = 0.1932$  and  $\alpha = 0.2531$  (solid line).

goodness of the fit of the models<sup>(25)</sup> was estimated as 0.639 and 0.138, respectively. Figures 1 and 2 reproduce our numerical data and the best fit curves with the above mentioned values of  $\alpha$ ,  $D$ ,  $\alpha_g$ , and  $D_g$ . We remark that the value of  $\alpha = 0.2508$  is in very good agreement with its theoretical counterpart 0.250 obtained in Section 2 of the present paper.

#### 4. SUMMARY AND DISCUSSION

In this paper, we use a real space renormalization-group map on the space of probabilities<sup>(10)</sup> to study the asymptotic end-to-end distance of a continuous-time weakly SARW that penalizes the (self-)intersection of two random walks on a hierarchical lattice, in dimension four. From this, a conjecture of the end-to-end distance for a weakly continuous-time SARW on a hierarchical lattice is derived. This gives a new probabilistic meaning to the exponent of the logarithmic correction based on physical intuition.

We have performed Monte Carlo computer simulations of continuous-time self-avoiding random walks in dimension four. The main goal of these computer experiments was to test our conjecture of Section 2 on the asymptotic behavior of the mean square end-to-end distance  $\langle \omega^2(T) \rangle$  and gyration radius  $\langle \omega_g^2(T) \rangle$  as functions of the running time  $T$  of the stochastic process. Our simulations have covered the interval of running times  $40 < T < 180$ . We have fitted our data on  $\langle \omega^2(T) \rangle$  and  $\langle \omega_g^2(T) \rangle$  to the functions  $DT(\ln T)^\alpha$  and  $D_g T(\ln T)^{\alpha_g}$  respectively. The best fit was obtained at  $\alpha = 0.2508 \pm 0.0059$ ,  $D = 1.1780 \pm 0.0107$ ,  $\alpha_g = 0.2531 \pm 0.0037$ ,  $D_g = 0.1932 \pm 0.0011$  (99% confidence intervals).

In general, the problem of establishing the asymptotics of such quantities as the mean square end-to-end distance is not easy in four dimensions. Grassberger *et al.*<sup>(27)</sup> have recently presented the results regarding the behavior of the mean square end-to-end distance for *discrete-time* SARWs on  $\mathbf{Z}^4$ . In the model studied in ref. 27 there is no other parameter associated with SARW except for the number of steps  $n$ . Given a set  $\{\omega_n^{(k)}\}$  ( $k = 1, \dots, N_n$ ) of  $N_n$  computer-generated SAWRs of the number of steps  $n$ , the mean square end-to-end distance as a function of  $n$  was calculated in ref. 27 as

$$\langle \omega^2(n) \rangle \approx \frac{1}{N_n} \sum_{k=1}^{N_n} \omega_n^{(k)2} \quad (8)$$

It was shown in ref. 27 that the subleading corrections to the leading asymptotic  $\langle \omega^2(n) \rangle \sim n(\ln n)^\alpha$  noticeably affect upon the value of  $\alpha$  for which the best fit to the data of computer simulations may be obtained.

However, in the present paper we deal with a distinctly different stochastic model. Indeed, there is an additional parameter in our model associated with a SARW—the running time  $T$  as a sum of exponentially distributed waiting times. To obtain the distribution of the mean square end-to-end distance  $\langle \omega^2(T) \rangle$  as a function of  $T$ , we average the values of the squares of end-to-end distances for the SARWs of *various* numbers of steps provided that their running times lie within the given interval  $[T, T + \Delta T]$  (see Eq. (7)). By contrast, in the model<sup>(27)</sup> the averaging is performed over all generated walks with the *fixed* number of steps  $n$  (see Eq. (8)). Our aim in the present work was to find the best fit of the form  $DT(\ln T)^\alpha$  (which was conjectured in Section 2) for the *continuous-time* SARWs, so we did not analyze the subtle details of possible logarithmic corrections to this leading asymptotic, if any. Note, however, that theoretical predictions of the behavior of  $\langle \omega^2(T) \rangle$  are in very good agreement with the results of our computer Monte Carlo simulations. This, together with the analytic results on hierarchical lattices,<sup>(13)</sup> lead us to think of the form  $DT(\ln T)^\alpha$  for  $\langle \omega^2(T) \rangle$  as highly probable. Further computer studies may help to understand the role of possible corrections to the formula  $DT(\ln T)^\alpha$ . They require the investigation of a larger interval of running times  $T$  than the one studied here, and more powerful hardware than the 60 MHz Pentium system.

## APPENDIX 1

In order to test our main computer program and pseudo random number generator **ran3**<sup>(25)</sup> we have performed the exact enumeration of discrete-time self-avoiding random walks  $\omega_n$  on a hypercubic lattice  $\mathbf{Z}^4$ . To this end, yet another program has been developed to specify the exact values of mean square end-to-end distance  $\langle \omega^2 \rangle$ , mean end-to-end distance  $\langle \omega \rangle$ , mean square radius of gyration  $\langle \omega_g^2 \rangle$ , and mean radius of gyration  $\langle \omega_g \rangle$  for random walks of number of steps  $n = 6 \dots 12$ . In this program we utilize the simple symmetry reasons that it suffices to take into account only that walks on  $\mathbf{Z}^4$  whose first step is made in the positive X-direction (this reduces running time of a program by factor 8) and second step is made only in the positive X-direction or in the positive Y-direction (thus decreasing the running time of a program about 7/2 times more). The results of exact enumeration are listed in Table II. The total number of self-avoiding random walks (first column in Table II) is consistent with the data of other authors.<sup>(22–24)</sup> However, the exact values of  $\langle \omega^2 \rangle$ ,  $\langle \omega \rangle$ ,  $\langle \omega_g^2 \rangle$ , and  $\langle \omega_g \rangle$  were not computed in refs. 22–24. We have performed the calculation of these values along with the enumeration of self-avoiding random walks. These values are given in the columns of the Table II named

**Table II. Exact Enumeration in Four Dimensions and Comparison with Results Produced by Self-Avoiding Walk Generator Used in Our Monte Carlo Experiments<sup>a</sup>**

$N$	Number of SARWs	$\langle \omega^2 \rangle_{EE}$	$\langle \omega \rangle_{EE}$	$\langle \omega_g^2 \rangle_{EE}$	$\langle \omega_g \rangle_{EE}$	$\langle \omega^2 \rangle_{DA}$	$\langle \omega \rangle_{DA}$	$\langle \omega_g^2 \rangle_{DA}$	$\langle \omega_g \rangle_{DA}$
6	127 160	7.938(34)	2.715(96)	1.399(38)	1.172(61)	7.9958	2.719	1.401	1.173
						7.953	2.719	1.401	1.173
						7.955	2.717	1.400	1.173
7	871 256	9.418(19)	2.949(55)	1.639(71)	1.268(25)	9.419	2.949	1.640	1.268
						9.419	2.949	1.640	1.268
						9.409	2.947	1.640	1.268
8	5 946 200	10.942(84)	3.176(05)	1.885(13)	1.358(95)	10.948	3.179	1.885	1.359
						10.972	3.183	1.888	1.360
						10.952	3.180	1.885	1.359
9	40 613 816	12.463(57)	3.383(48)	2.132(04)	1.444(34)	12.454	3.382	2.131	1.444
						12.464	3.382	2.132	1.444
						12.463	3.382	2.132	1.444
10	276 750 536	14.018(89)	3.585(86)	2.382(96)	1.526(21)	14.016	3.585	2.382	1.526
						14.013	3.584	2.382	1.526
						14.020	3.585	2.382	1.526
11	1 886 784 200	15.570(44)	3.774(49)	2.635(06)	1.604(18)	15.592	3.776	2.637	1.605
						15.568	3.773	2.635	1.604
						15.596	3.777	2.637	1.605
12	12 843 449 288	17.150(04)	3.959(25)	2.890(56)	1.679(03)	17.138	3.959	2.890	1.679
						17.142	3.959	2.891	1.680
						17.124	3.957	2.888	1.679

<sup>a</sup> The values of mean square end-to-end distance, mean end-to-end distance, mean square gyration radius, and mean gyration radius obtained by exact enumeration are given in the columns of the table named  $\langle \omega^2 \rangle_{EE}$ ,  $\langle \omega \rangle_{EE}$ ,  $\langle \omega_g^2 \rangle_{EE}$ , and  $\langle \omega_g \rangle_{EE}$ , respectively. The Monte Carlo estimations of the above mentioned values by generating 100000 SARWs for  $n = 6$  and 500000 SARWs for  $n = 7 \dots 12$  (3 runs for each  $n$ , to observe statistical deviations) are given in the columns named  $\langle \omega^2 \rangle_{DA}$ ,  $\langle \omega \rangle_{DA}$ ,  $\langle \omega_g^2 \rangle_{DA}$ , and  $\langle \omega_g \rangle_{DA}$ .

$\langle \omega^2 \rangle_{EE}$ ,  $\langle \omega \rangle_{EE}$ ,  $\langle \omega_g^2 \rangle_{EE}$ , and  $\langle \omega_g \rangle_{EE}$ , respectively. To test our main computer program (specifically, the subroutine that generates self-avoiding random walks), we have also performed Monte Carlo estimations of  $\langle \omega^2 \rangle$ ,  $\langle \omega \rangle$ ,  $\langle \omega_g^2 \rangle$ , and  $\langle \omega_g \rangle$  by dimerization algorithm for statistical samples of 100000 self-avoiding walks for  $n=6$  and of 500000 walks for  $n=7 \dots 12$ . To observe statistical deviations, we run our program three times for every  $n$ , each time recording the above mentioned mean values. The results of Monte Carlo estimations are given in Table II in the columns named  $\langle \omega^2 \rangle_{DA}$ ,  $\langle \omega \rangle_{DA}$ ,  $\langle \omega_g^2 \rangle_{DA}$ , and  $\langle \omega_g \rangle_{DA}$ . One can see a good agreement between theoretical and estimated values of  $\langle \omega^2 \rangle$ ,  $\langle \omega \rangle$ ,  $\langle \omega_g^2 \rangle$ , and  $\langle \omega_g \rangle$ , which confirms the correctness of the computer program and of the pseudo random number generator that we used in our simulations.

**APPENDIX 2**

In this paper we use the dimerization algorithm to generate self-avoiding random walks on  $\mathbf{Z}^4$ . It has been rigorously proved<sup>(17)</sup> that this algorithm produces *statistically independent* SARWs  $\omega_n$ , uniformly distributed on the set of all SARWs of a given number of steps  $n$ . This is the advantage of the dimerization procedure: other highly efficient methods of SARW generation (such as the pivot algorithm<sup>(21)</sup> or the recursive and randomized implementation of the enrichment method<sup>(27)</sup>) give a sequence of self-avoiding random walks that are *not* statistically independent. Statistical independence of a sequence of SARWs implies that simple standard methods for estimating the mean values of random variables and their variances apply.

Let  $\xi$  be a real-valued random variable (for instance, the square end-to-end distance of a SARW) with mean  $\langle \xi \rangle$  and  $x_1, \dots, x_n$  be a sample of its  $n$  independent observations. The random variable

$$\bar{x}^{(n)} = \frac{1}{n} \sum_{i=1}^n x_i \tag{9}$$

(the sample mean) is the natural estimator of  $\langle \xi \rangle$ ; its variance can be estimated as

$$\text{var}(\bar{x}^{(n)}) \approx \frac{1}{n} V^{(n)}$$

where

$$V^{(n)} = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x}^{(n)})^2 \tag{10}$$

Denote  $\bar{x}^{(k)}$  and  $V^{(k)}$  the values (9) and (10) applied to the first  $k \leq n$  elements of the sample  $x_1, \dots, x_n$ . It can easily be shown that the following recurrent relationships hold true for  $k = 2, \dots, n$ :

$$\bar{x}^{(k)} = \frac{k-1}{k} \bar{x}^{(k-1)} + \frac{x_k}{k} \quad (11)$$

$$V^{(k)} = \frac{k-2}{k-1} V^{(k-1)} + \frac{1}{k} (\bar{x}^{(k-1)} - x_k)^2 \quad (12)$$

with  $\bar{x}^{(1)} = x_1$ ,  $V^{(1)} = 0$ . In our computational experiments we utilized Eq. (11) and Eq. (12) to calculate the distributions of the mean square end-to-end distance  $\langle \omega^2(T) \rangle$  and gyration radius  $\langle \omega_g^2(T) \rangle$  for continuous-time self-avoiding random walks. We note that the recurrent relationships (11) and (12) substantially reduce the hardware requirements since it is not necessary to keep large arrays of the square end-to-end distances and gyration radii in the memory of a computer in order to estimate their variances. Once the values  $\langle \omega^2(T) \rangle$  and  $\langle \omega_g^2(T) \rangle$  and their variances are computed for all subintervals of the length  $\Delta T = 0.02$  on the interval  $[T_{\min}, T_{\max}]$ , a nonlinear least-square method can be applied to calculate the covariance matrix and then to find the values of the fitting parameters and their confidence intervals.<sup>(25, 26)</sup>

## ACKNOWLEDGMENTS

S.R.R. wishes to thank CONACYT, México for partial support under contract REF 4336E9406. V.T. is grateful to CONACYT for support through Cátedra Patrimonial Nivel II, contract 940395.

## REFERENCES

1. P. Flory, *J. Chem. Phys.* **17**:303 (1949).
2. Ch. Wen and F. S. Lui, *Acta Phys. Sinica* **35**:43 (1986).
3. J. T. Bendler and M. F. Shlesinger, *The wonderful world of stochasticity*, Stud. Statist. Mech., XII (North-Holland, Amsterdam-New York, 1985).
4. R. Zwanzig, *J. Stat. Phys.* **30**:255 (1983).
5. A. Blumen and G. Zumofen, *J. Chem. Phys.* **77**:5127 (1982).
6. M. F. Shlesinger and U. Landman, "Solution of physical stochastic processes via mapping onto ideal defective random walk lattices" Collection: Applied stochastic processes (*Proc. Conf. Univ. Georgia, Athens*, 6a 1978), 151.
7. D. T. Gillespie, *J. Chem. Phys.* **74**:661 (1981).
8. G. H. Weiss and Sh. Halvin, *J. Stat. Phys.* **63**:1005 (1991).
9. S. Rodríguez-Romo, *Int. J. Modern Phys. A* **12**:963 (1997).
10. S. Rodríguez-Romo, *RG96 JINR Dubna Proceedings*, 1996.

11. E. Brézin, J. C. Le Guillou, and J. Zinn-Justin, Field theoretical approach to critical phenomena, in “*Phase Transitions and Critical Phenomena*” (C. Domb and M. S. Green, Ed.), Vol. 6 (Academic Press, London–New York–San Francisco, 1976); P. G. De Gennes, *Physics Lett.* **38A**:339 (1970).
12. D. Brydges, S. N. Evans, and J. Z. Imbrie, *Ann. Probab.* **20**:82 (1992).
13. J. Imbrie, Mathematical Quantum Theory Summer School, University of British Columbia, Vancouver Canada, Summer 1993. J. Imbrie, *Centre de Recherches Mathématiques, Proceedings* **7**:191 (1994).
14. B. Duplantier, *J. Stat. Phys.* **54**:581 (1984).
15. A. J. McKane, *Phys. Lett. A* **76**:22 (1980). G. Parisi, *J. Phys. Lett.* **43**:744 (1979); G. Parisi, *J. Phys. Lett.* **41**:L403 (1980).
16. L. D. Kadanoff, *Physics* **2**:263 (1966). K. G. Wilson and J. Kogut, *Phys. Rep.* **12C**:75 (1974). J. J. Binney, N. J. Dowrick, A. J. Fisher, and M. E. J. Newman, “*The Theory of Critical Phenomena. An Introduction to the renormalization group*” (Oxford Science Publications, 1992).
17. N. Madras and G. Slade, *The Self-Avoiding Walk* (Birkhauser, Boston, 1993).
18. Z. Alexandrowicz, *J. Chem. Phys.* **51**:561 (1969).
19. J. Dayantis and J.-F. Palierne, *J. Chem. Phys.* **95**:6088 (1991).
20. R. Everaers, I. S. Graham, and M. Z. Zuckerman, *J. Phys. A: Math. Gen.* **28**:1271 (1995).
21. N. Madras and A. D. Sokal, *J. Stat. Phys.* **50**:109 (1988).
22. M. E. Fisher and D. S. Gaunt, *Phys. Rev.* **133**:A224 (1964).
23. A. J. Guttmann, *J. Phys. A: Math. Gen.* **11**:L103 (1978).
24. D. MacDonald, D. L. Hunter, K. Kelly, and N. Jan, *J. Phys. A: Math. Gen.* **25**:1429 (1992).
25. W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical recipes in C: The art of Scientific Computing* (Cambridge University Press, Cambridge, 1988).
26. M. Lampton, *Computers in Physics* **11**:110 (1997).
27. P. Grassberger, R. Heggert, and L. Schafer, *J. Phys. A: Math. Gen.* **27**:7265 (1994).
28. P. G. de Gennes, *The scaling concepts in Polymer Physics* (Ithaca, Cornell University Press, NY, 1979).