Self-Avoiding Walks of Continuous Spatial Dimensionality

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The possibility of describing the continuous variation ν_D with D, where ν_D is the shape exponent of self-avoiding walks and D the spatial dimensionality, is investigated. A dimensionality d is associated with the increase of a walk's volume with its length. The value of d is varied at will through an extension (acceleration) of walks on all scales of length. The shape exponent ν_d of such accelerated self-avoiding walks is studied with the help of computer simulation. The results indicate that ν_d reproduces ν_D.

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The average shape of self-avoiding walks (SAW's) deviates from that of ideal walks as the spatial dimensionality D decreases below $D_c = 4$. Theoretical studies envisage a continuous variation of D, especially in connection with the expansion in $\epsilon = 4 - D$.[1] Yet the actual construction of SAW's is carried out in Euclidian space for the integer values $D = 2, 3$, and 4 only. This Letter proposes to simulate the continuous variation of D with the help of modified walks, which are "accelerated" (or decelerated), on all scales of length, so as to vary at will the volume occupied by a walk. The construction of samples of such walks is carried out on a computer, with the help of a modified *dimerization* method. The original dimerization method,[2] proposed some time ago for the construction of conventional (nonaccelerated) SAW's, will be first briefly reviewed: A pair of "monomer" walks of $N = 2$ steps is picked at random from a sample of such walks and linked together (also at random), to yield a "dimer" walk of length $N = 4$. If one-half of the dimer intersects the other, the walk is discarded. If not, the dimer walk $N = 4$ is carried over to the next level of the construction, at which pairs of $N = 4$ monomers are linked together into $N = 8$ dimer walks, which are in turn checked for self-intersections between the two halves, etc. The dimerization procedure provides a very efficient method for the construction of SAW's. It also constitutes a sort of renormalization, the linking being repeated on an ever increasing scale. It is this property which we shall utilize at present for an acceleration of walks on all scales of length. Terminology: Walks which allow self-intersection are called ideal. The ideal walks can be either random, or, accelerated, as described below; similarly, SAW's also can be either random or accelerated.

I first describe the construction of accelerated ideal walks with the modified dimerization procedure. Thus the linking of pairs of monomers of length N into dimers $2N$ is carried out not at random, but with the help of a probability distribution depending on the mutual orientation of the two half walks. Several schemes are possible and the following is adopted here (see Fig. 1). Let $X_{i(1)}$ and $X_{i(2)}$ denote the ith component ($i = 1, \ldots, D$) of the end-to-end vectors for the first and second monomer, respectively. After the linkage, the product $X_{i(1)}X_{i(2)}$ can be larger or smaller than zero. One of these possibilities can be realized through a translation of the origin of the

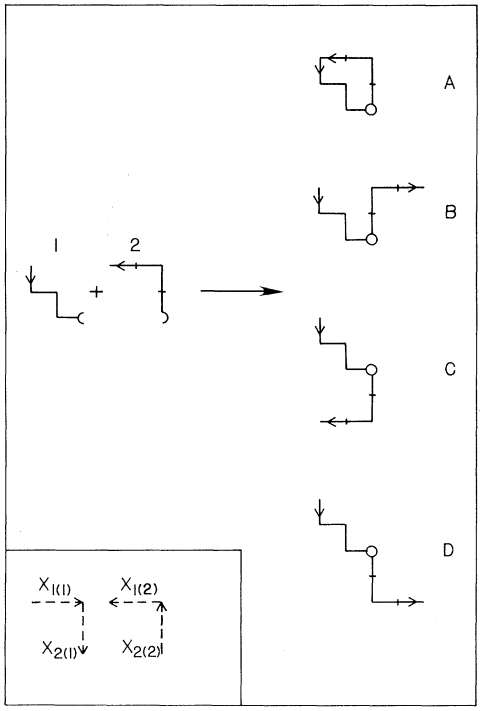

FIG. 1. Dimerization $2\times4\rightarrow8$. The four ways of linking are (A) with no reversal neither of $X_{1(2)}$ nor of $X_{2(2)}$; (B) with a reversal of $X_{1(2)}$; (C) with a reversal of $X_{2(2)}$; and (D) with a reversal of both $X_{1(2)}$ and $X_{2(2)}$.

second half to the end of the first half. The other possibility can be realized by reversing $X_{i(2)}$ into $-X_{i(2)}$ through taking the mirror image of the second half in the $D-1$ "plane" perpendicular to i. This is followed by the translation of the origin of the second half to the end of the first. A lottery with probabilities g_i and $1-g_i$ for $X_{i(1)} \times X_{i(2)} > 0$ and < 0, respectively, determines which of the two possibilities is accepted. If $X_{i(1)}X_{i(2)} = 0$ we take $g_i = 0.5$ since the linking is immaterial for acceleration. A sequence of lotteries for $i = 1, \ldots, D$ determines one out of the 2^D possible choices. The probability distribution g_i need not be equal for different i. Let $\langle X_{i,N}{}^2 \rangle$ and $\langle X_{i,2N}{}^2 \rangle$ denote the average square of the ith component on the sample of the monomer and dimer walks, respectively. An expansion coefficient θ_i is defined by

$$2^{\theta_i} = \langle X_{i,2N}{}^2 \rangle / \langle X_{i,N}{}^2 \rangle . \quad (1)$$

Random linking with $g_i = 0.5$ gives $2^{\theta_i} = (\langle X_{i(1)}{}^2 \rangle + \langle X_{i(2)}{}^2 \rangle) / \langle X_{i,N}{}^2 \rangle = 2$, or $\theta_i = 1$. Clearly $g_i > 0.5$ and $g_i < 0.5$ lead to $\theta_i > 1$ and $\theta_i < 1$, respectively. Repeated dimerization $N \to 2N$, $2N \to 4N$, etc., with the help of a given distribution g_i, should lead to a uniformly accelerated ideal walk described by constant θ_i, so that $\langle X_{i,N}{}^2 \rangle \sim N^{\theta_i}$. I focus on the increase of the accelerated walk's volume upon doubling the length:

$$V_{2N}{}^2 / V_N{}^2 = \prod_{i=1}^{D} \langle X_{i,2N}{}^2 \rangle / \langle X_{i,N}{}^2 \rangle = 2^d , \quad (2)$$

where a dimensionality d is defined by

$$d = \sum_{i=1}^{D} \theta_i . \quad (3)$$

For the random ideal walk, $\theta_i = 1$ and $d = D$, whence $V_{2N}{}^2 / V_N{}^2 = 2^D$. This indicates an important advantage: suppose that we wish to study the continuous variation of $V_{2N}{}^2 / V_N{}^2$. In the random case this would require us to define walks in a space of noninteger D. In the accelerated case, however, walks are still defined in the Euclidian space of integer D and the continuous variation of $V_{2N}{}^2 / V_N{}^2$ is effected through varying d.

We now turn to SAW's. The first stage of a dimerization $N \to 2N$ involves the linking of monomers into dimers; at the second stage dimers in which one half intersects the other are eliminated. A ratio of volumes $V_{2N}{}^{2*} / V_N{}^2 = \prod_{i=1}^{D} \langle X_{i,2N}{}^{2*} \rangle / \langle X_{i,N}{}^2 \rangle$ is defined for the first stage, i.e., $\langle X_{i,N}{}^2 \rangle$ and $V_N{}^2$ refer to SAW's of length N but $\langle X_{i,2N}{}^{2*} \rangle$ and $V_{2N}{}^{2*}$ refer to dimers of length $2N$ *prior* to the elimination. Incidentally, the square of the length after the elimination $\langle X_{i,2N}{}^2 \rangle$ is clearly larger than $\langle X_{i,2N}{}^{2*} \rangle$. If the linking is carried out at random, like with the original dimerization method, $\langle X_{i,2N}{}^{2*} \rangle / \langle X_{i,N}{}^2 \rangle = 2$ and $V_{2N}{}^{2*} / V_N{}^2 = 2^D$, precisely like for the random ideal walk. The elimination of non-self-avoiding dimers at the second state and repetition $2N \to 4N$, etc., produces then a random SAW. However, if the linking is carried out with the help of the distribution g_i, viz., with the modified dimerization method, then at the first stage

$$\langle X_{i,2N}{}^{2*} \rangle / \langle X_{i,N}{}^2 \rangle = 2^{\theta_i} \quad (1')$$

and

$$V_{2N}{}^{2*} / V_N{}^2 = 2^d \quad (2')$$

just like for the accelerated ideal walk. The elimination of non-self-avoiding dimers at the second stage and repetition $2N \to 4N$, etc., with given g_i, produces then a uniformly accelerated SAW described by constant θ_i [Eqs. (1'), (2') and (3)]—in brief, an "accelerated SAW of dimensionality d."

In the study of the conventional random SAW's the property investigated is the critical exponent in the scaling law $\langle X_{i,N}{}^2 \rangle \sim N^{2\nu_D}$. A decrease of D decreases $V_{2N}{}^{2*} / V_N{}^2$ enhancing the walk's back-bending and making self-intersection more likely on all scales of length. In the critical region $D < 4$ this causes ν_D to deviate increasingly from the ideal $\nu_D = \frac{1}{2}$. In accelerated SAW's $V_{2N}{}^{2*} / V_N{}^2$ and the back-bending on all scales of length are controlled by d. The dependence of ν_d on d in the accelerated SAW's might therefore reproduce accurately the continuous dependence of ν_D on D in the random SAW's. To formalize this hypothesis I define a unique exponent ν_d for an accelerated SAW of dimensionality d,

$$\langle X_{i,N}{}^2 \rangle \sim N^{2\nu_d \theta_i}; \quad \text{for all } i = 1, \ldots, D. \quad (4)$$

If we can verify the existence of such an exponent ν_d, dependent on d but independent of the particular combination $\sum_{i=1}^{D} \theta_i = d$ and of D [Eq. (3)], then d indeed constitutes a meaningful dimensionality determining the universality class of the accelerated SAW's. Furthermore, one particular combination is $\theta_i = 1$ for all i, giving $d = D$ and corresponding therefore to the conventional random SAW. Fulfillment of Eq. (4) would ensure therefore that for equal integer values of d and D, ν_d of an accelerated SAW is equal to ν_D of the random SAW. But if the equality is established for $d = D = 2$, 3, and 4, there is no special reason for it to break down at intermediate $d = D$. Both requirements will be tested. For example,

the value $d=3$ can be realized with isotropically decelerated walks in $D=4$, having $\theta_1=\theta_2=\theta_3=\theta_4=\frac{3}{4}$; or, with decelerated walks flattened in one direction only having $\theta_1=0$ and $\theta_2=\theta_3=\theta_4=1$; or, with isotropically accelerated walks in $D=2$, having $\theta_1=\theta_2=\frac{3}{2}$. For all these cases we expect the same value of ν_d and furthermore we expect that $\nu_d=\nu_{D=3}\simeq 0.59$.[3] I note that d should not be confused with the fractal or Hausdorff dimensionality[4] $\bar{D}$: In view of $X_N\sim N^{\nu}$, for SAW's $\bar{D}=\nu^{-1}$; one might say that d relates to the cause, $\bar{D}$ to the effect.

Samples of accelerated SAW's on hypercubic lattices of $D=2$, 3, and 4 were dimerized up to $N=2^{14}=16\,384$. Sample size was halved at each level, last size being only about 200. However, θ_i and $\theta_i\nu_d$ values have been computed over internal lengths $\bar{N}\ll N$, which of course are more numerous. $\theta_i\nu_d$ values have been computed from logarithmic plots [Eq. (4)], which were linear in the range $8\lesssim\bar{N}\lesssim N/50$. The combined error of θ_i and $\theta_i\nu_d$ was between ±2% and about ±4%, main sources of error being statistical scatter and unattained convergence with increasing $\bar{N}$, both most pronounced for θ_i far from unity. For that reason θ_i was limited to $\frac{2}{3}\leq\theta_i\leq\frac{3}{2}$. The results are summarized in Fig. 2. On the whole the basic hypothesis of Eq. (4) is supported to within experimental error. Most important support is provided by the approximate reproduction of $\nu_{D=2}=0.75$ (Ref. 5) with decelerated SAW's of $D=3$, and of $\nu_{D=3}\simeq 0.59$,[3] with both decelerated SAW's of $D=4$ and accelerated SAW's of $D=2$. The mutual agreement of ν_d of accelerated and decelerated SAW's in the entire range, for noninteger values of d, also supports the hypothesis. Still as θ_i become appreciably different from 1, there appears to be a systematic tendency for the accelerated SAW's to give a too low value except near to $D=4$ and for the decelerated SAW's to give a too high value. Possibly the control of the back-bending of walks with the help of g_i becomes inadequate: The deviation of SAW's in the sample from the average value of θ_i and even the inhomogeneity inside individual walks become too great. If that is the case, the employment of an alternative procedure of acceleration might improve the agreement for θ_i far away from 1. Another difficulty arises near $D=4$. Extrapolation to $\bar{N}$ becomes inadequate in the range of $\bar{N}$ studied while the use of corrections to scaling seemed unjustified given the scatter of the Monte Carlo results. Thus even the conventional random SAW of $D=4$ extrapolates to $\nu_{D=4}\simeq 0.53$, considerably above the expected value of $\frac{1}{2}$ (recent Monte Carlo results[6] indicate a comparable departure). For that reason our ν_d could not be compared with the theoretical $\nu_\epsilon=\frac{1}{2}+\epsilon/8+\cdots$ $(\epsilon=4-D)$.[1] Incidentally, the accuracy of the dimerization method is entirely satisfacotry,[7] as itself demonstrated by the values $\nu_{D=2}=0.749\pm 0.002$ and $\nu_{D=3}=0.595\pm 0.005$ obtained for random SAW's, in very good agreement with theoretical results.[3,5] Finally, in the range $1.8\leq d<4$ the results agree very closely with the generalized Flory theory $\nu_D=3/(D+2)$, (see Ref. 1, for example). The pronounced departure from Flory's line as d approaches 1 is quite possibly due to the aforementioned unreliability of ν_d for a strong deceleration.

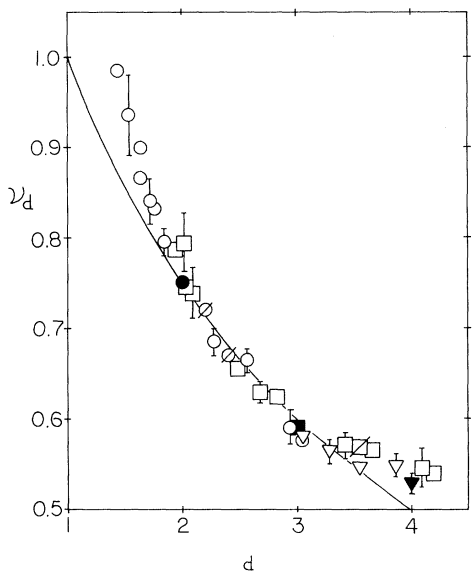

FIG. 2. ν_d, the shape exponent of accelerated SAW'S, as a function of dimensionality d. Open circles, open squares, and open triangles describe isotropic acceleration (deceleration) of walks of Euclidian dimensionality $D=2$, 3, and 4, respectively; circles with slash and square with slash describe acceleration of one component only. Filled circle, filled square, and filled triangle describe conventional exponents ν_D of random SAW's, of $D=2$, 3, and 4, respectively. Solid line describes Flory's theory for continuous D.

In conclusion it appears that accelerated SAW's permit one to study, at least to within a reasonable approximation, the continuous dependence of ν_D on D in random SAW's. Furthermore, the accelerated ideal walk offers an intriguing geometrical construction which takes us continuously from $\theta=2$ (a line), via $\theta=1$ (random walk), to $\theta=0$ (a point), either through an isotropic variation, or through the flattening of particular com-

ponents.

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Theory of Enhanced Migration of Interstitial Aluminum in Silicon

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Self-consistent electronic structure calculations are reported for Al at two interstitial locations in silicon. On the basis of these calculations, a novel mechanism for enhanced interstitial migration is proposed in which electron capture can cause a barrier lowering appreciably greater than E_G, the energy gap. The model and the present numerical results are in good agreement with recent measurements by Troxell *et al.*

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The migration of interstitial atoms in semiconductors is a long-standing problem.[1-4] In particular, the phenomenon of recombination-enhanced migration has been recognized as an important feature of defect reactions and device degradation. Detailed experimental measurements of enhanced diffusion exist for some systems, e.g., the aluminum interstitial in silicon,[5] and qualitative models for understanding the process have been proposed and discussed. Nevertheless, a basic understanding of the migration process and the detailed role played by the capture of the carriers is still lacking. The present calculations provide additional theoretical insight into these questions.

These calculations are the first, to our knowledge, in which the change in the barrier against migration is calculated. We can obtain the change in barrier height by inspecting the change in transition-state eigenvalues, even without a full calculation of the total energy, for the following reason: Recall that E_T, the total energy of the defect system, depends on Q, the configuration of the system, and on N, the number of electrons residing on the defect. If Q_1 designates the equilibrium configuration of the defect for both charge states $N=N_1$ and $N=N_2$, and if Q_2 designates the saddle-point configuration of the system, then the barrier against migration in charge state N is $V_B(N)=E_T(Q_2,N)-E_T(Q_1,N)$. The *change* in barrier height is

$$\Delta V_B \equiv V_B(N_2)-V_B(N_1)=[E_T(Q_2,N_2)-E_T(Q_1,N_2)]-[E_T(Q_2,N_1)-E_T(Q_1,N_1)]$$
$$=[E_T(Q_2,N_2)-E_T(Q_2,N_1)]-[E_T(Q_1,N_2)-E_T(Q_1,N_1)].$$

Recall also that the one-electron *levels* of the system are given by the differences in total energy caused by the addition of a *single* electron at some fixed configuration: $\epsilon_Q(N+1/N)=E_T(Q,N+1)-E_T(Q,N)$. Thus

$$E_T(Q,N_2)-E_T(Q,N_1)=\sum_{N=N_1}^{N=N_2-1}\epsilon_Q(N+1/N)$$

and the *change* in barrier height is given by the sum from N_1 to N_2 over occupied levels at Q_2, minus a similar sum at $Q=Q_1$. The electron level $\epsilon_Q(N+1/N)$ is, within local density theory, approximately the Slater transition-state eigenvalue, calculated at configuration Q and occupation $N+\frac{1}{2}$. Calculating the barrier height itself