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Asymptotic Distributions for Self-Avoiding Walks Constrained to Strips, Cylinders, and Tubes

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A transfer matrix method for treating self-avoiding walks on a lattice is developed. Single walks confined to infinitely long strips, cylinders, or tubes are considered, particularly in the limit where the length of the walk becomes infinite compared to the transverse dimensions. In this case relevant distributions are demonstrated to be asymptotically Gaussian. Explicit numerical results are given for a few of the narrower systems. Similar results for self-avoiding cycles are indicated, too. Finally, the behavior of the various distributions as a function of strip width is discussed.

KEY WORDS: Polymer statistics; self-avoiding random walks.

1. INTRODUCTION

Self-avoiding walks on various lattices have been extensively employed as models for chain polymers. Here we develop a formally exact transfer matrix technique for treating such self-avoiding walks. The technique is applied here to pseudo-one-dimensional systems, including strips, cylinders, and tubes, such as have already become a topic of interest in the recent literature.[(1–4),3] As pointed out in this previous work, these or related model systems are of interest in connection with thin polymer films or fibers, with polymers confined to capillaries or pores, with the stabilization of colloids, and perhaps even with the solubilities of biopolymers in lipid bilayers.

Attention is here directed toward the asymptotic behavior of the number of walks with a given (horizontal) end-to-end separation x and with a given number of steps l. Two different asymptotically Gaussian distributions are found, depending on whether x or l is held constant while the other is varied.

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Formulas for parameters and moments of these distributions are given in terms of eigenvalues, eigenvectors, etc., of a "transfer" matrix. Indeed, the technique is similar in some respects to earlier[(6),4] applications of transfer matrices in other contexts. Numerical results are given for a number of simpler cases, extending earlier exact results by Wall *et al.*[(1)]

To accomplish these results we consider in Sections 2–5 a rather special subclass of self-avoiding walks (in pseudo-one-dimensional systems). In Section 7 it is shown how to deal with the complete class of self-avoiding walks, and in addition it is argued that the asymptotic results are the same for the subclass and the complete class. Section 3 deals with the distribution for varying the walk length l while holding the end-to-end separation x constant. Section 4 then utilizes some of these results and techniques to obtain the (perhaps more physically relevant) distribution for varying x at constant l. Numerical results are given in Section 5. Section 6 points out how a parallel development allows one to treat self-avoiding cycles in these pseudo-one-dimensional systems, and some numerical results are given. In treating the complete class of self-avoiding walks in Section 7, results from all the preceding sections are utilized; in particular from the numerical results of Sections 5 and 6 it is shown that the numerical results of Section 5 also describe the asymptotic behavior of the complete class of self-avoiding walks. Section 8 considers evidence and arguments concerning the dependence of the various distributions on strip width. The appendices present some auxiliary material and relevant theorems.

Finally, we note that the present technique is of somewhat wider applicability than that pursued here. Different weights (or energies and Boltzmann factors) may be assigned to different chain conformations, by making simple modifications of the transfer matrices. Also, the transfer matrices may be utilized for the exact enumeration of shorter walks. Further, the same techniques apply even when more than one chain is present. Possibly even the transfer matrix for a full two-dimensional lattice can be utilized to yield some exact properties for self-avoiding walks in this case.

2. TRANSFER MATRIX AND GENERATING FUNCTION FOR CHAINS WITH FIXED ENDS

First we consider the problem for self-avoiding walks with the ends fixed in horizontal positions at the left and right extremes of the walk. In Section 7 we shall return to the more general problem with free ends, which may be

[4] Transfer matrices arise in the popular rotational-isomeric model of polymer chains and are described by Flory.[(7a)] This model involves so-called "second-order" walks, but transfer matrices for higher-order walks have also been studied, for instance, in Refs. 7b–7h. Transfer matrix ideas are also extensively used in the theory of Markov processes, as discussed by probability theorists, whence the transfer matrix is often termed a transition matrix.

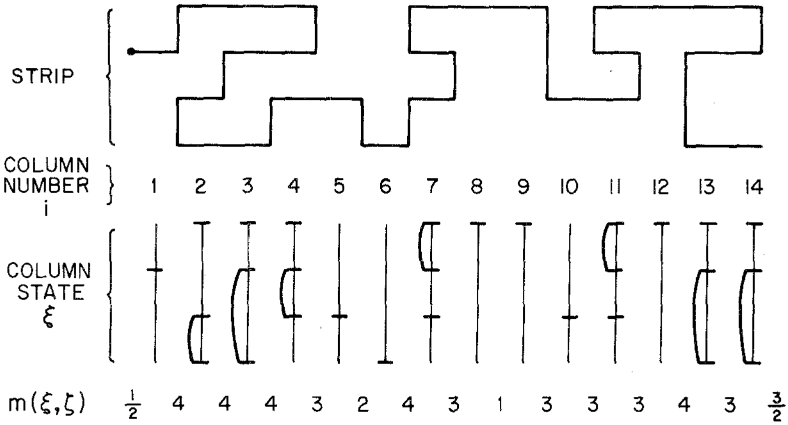

Fig. 1. An example of a self-avoiding walk of length $l = 44$ and horizontal span $x = 14$ on a strip of width $D = 4$. The columns are numbered and the associated column states indicated. Also, the number of steps needed in going from a column state ζ to the following column state ξ are given.

treated by an extension of the method for chains with fixed ends. For explicitness and simplicity of presentation we initially restrict attention to a horizontal strip, say of width D, from a square planar lattice. Now a particular self-avoiding walk on this strip will be designated by a sequence of *column states*, the ith column state being associated with the ith column of horizontal lattice links through which the walk passes. Such a column state is specified by (a) a designation of which lattice links the walk passes over, and (b) a designation of which pairs of so-occupied lattice links are connected together by a sequence of steps in the walk, all located to the left of column i. An example of a self-avoiding walk and its designation via column states is illustrated in Fig. 1. Because of the fixed-end feature of the self-avoiding walks, each column state must have exactly one lattice link occupied by the walk, yet paired to no other; also, this dangling end must not occur between two occupied and connected lattice links. Further, we see that a sequence of such column states uniquely determines a self-avoiding walk. For the $3 \times \infty$ strip, there are just five (presently allowable) column states required for the

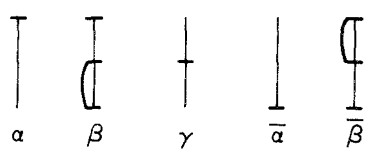

Fig. 2. The five column states arising on a strip of width $D = 3$. The states $\bar{\alpha}, \bar{\beta}$ are obtained from α, β via a reflection about the center of the column.

designation of any self-avoiding walk (with fixed ends). These five states, denoted $\alpha, \beta, \gamma, \bar{\alpha}$, and $\bar{\beta}$, are illustrated in Fig. 2. The number of column states for general strip widths is given in Appendix A.

Generally now, for a given ith column state, only certain ones can follow in the $(i+1)$th column. For example,

$$\begin{aligned} &\alpha \to \alpha, \beta, \gamma, \bar{\alpha} \\ &\beta \to \beta, \bar{\alpha} \\ &\gamma \to \alpha, \gamma, \bar{\alpha}, \quad 3 \times \infty \text{ strip} \\ &\bar{\alpha} \to \alpha, \gamma, \bar{\alpha}, \bar{\beta} \\ &\bar{\beta} \to \alpha, \bar{\beta} \end{aligned} \tag{2.1}$$

Further, each such transformation may involve a different number of steps in the walk. This we may keep track of by introducing a dummy parameter t raised to a power $m(\xi, \zeta)$ taken to be the[5] number of steps required in a transfer from state ζ for column i to a state ξ for column $i+1$. More precisely, $m(\xi, \zeta)$ is the number of steps in the walk between the centers of columns i and $i+1$ when they are in states ζ and ξ, respectively. Then we define

$$n_\xi(i+1; t) \equiv \sum_{\zeta}^{m(\xi,\zeta)\neq 0} t^{m(\xi,\zeta)} n_\zeta(i; t) \tag{2.2}$$

Thus, with the choice

$$n_\zeta(1; t) \equiv t^{m(\zeta,0)} \tag{2.3}$$

where $m(\zeta, 0)$ is the number of steps required to initiate a walk with the first column in state ζ, we see that $n_\xi(x; 1)$ is the total number of x-column walks with the xth and last column in state ξ. Now letting $\mathbf{n}(i+1; t)$ denote the column vector with ξth component $n_\xi(i+1; t)$ and letting T_t denote the *transfer matrix* with (ξ, ζ)th element $t^{m(\xi,\zeta)}$ or 0, depending upon whether ξ can or cannot directly follow ζ, we see that (2.2) becomes

$$\mathbf{n}(i+1; t) = \mathsf{T}_t \mathbf{n}(i; t) \tag{2.4}$$

For example,

$$\mathsf{T}_t = \begin{bmatrix} t & 0 & t^2 & t^3 & t^3 \\ t^3 & t^3 & 0 & 0 & 0 \\ t^2 & 0 & t & t^2 & 0 \\ t^3 & t^3 & t^2 & t & 0 \\ 0 & 0 & 0 & t^3 & t^3 \end{bmatrix}, \quad 3 \times \infty \text{ strip} \tag{2.5}$$

and rather generally we have a familiar[6,7] type of transfer matrix problem.

[5] For a horizontal strip on a square planar lattice there is no more than one way to go from a given column state in column i to a second given state in column $i+1$. This is not necessarily true with cylinders or tubes, and in place of $t^{m(\xi,\zeta)}$ in (2.2) one then has $\sum_a t^{m_a(\xi,\zeta)}$, where $m_a(\xi, \zeta)$ is the number of steps in the ath way for going from ζ to ξ.

We have

$$\mathbf{n}(i+1; t) = \mathsf{T}_t^{\,i}\mathbf{n}(1; t) \tag{2.6}$$

and it becomes of interest to introduce the *generating function*

$$G_x(t) \equiv \sum_{\xi,\zeta} [\mathsf{T}_t^{x-1}]_{\xi\zeta} t^{m(0,\xi)+m(\zeta,0)} \tag{2.7}$$

where $m(0, \xi)$ is the number of steps to immediately terminate a chain with the last column state being ξ. Clearly $G_x(1)$ is just the total number of chains with $x - 1$ columns (and a span of x). Hence,

$$G_x(t) = \sum_l n(x, l)t^l \tag{2.8}$$

where $n(x, l)$ is the number of $x - 1$ column chains with length l. Then moments of chain length l at a fixed end-to-end separation x may be obtained via differentiation

$$\begin{aligned} \langle l \rangle_x &\equiv \frac{1}{G_x(1)} \sum_l n(x, l) = \left[\frac{1}{G_x(t)} \frac{\partial G_x(t)}{\partial t}\right]_{t=1} \\ \langle l^2 \rangle_x &\equiv \frac{1}{G_x(1)} \sum_l l^2 n(x, l) = \left[\frac{1}{G_x(t)} \frac{\partial t \partial G_x(t)}{\partial t^2}\right]_{t=1} \end{aligned} \tag{2.9}$$

Further, the matrix elements of $\mathsf{T}_t^{\,x}$ may, with some computational advantage, be exactly expanded in terms of eigenvectors and eigenvalues of T_t, whence all the x dependence appears as xth powers of eigenvalues (or possibly Jordan blocks).

3. ASYMPTOTICS FOR FIXED END-TO-END SEPARATION

In the asymptotic limit as the end-to-end separation x (and also the length l) approaches infinity, the eigenvalue of maximum magnitude dominates. Physically we expect (at $t = 1$) the corresponding eigenvector to necessarily have all components of like phase (whence it is nondegenerate) and the eigenvalue positive; mathematically this is guaranteed for $t > 0$ by the Frobenius–Perron theorem (e.g., Ref. 8). Thus,

$$G_x(t) \approx a_t \lambda_t^{x-1}, \qquad x \to \infty \tag{3.1}$$

where λ_t is the maximum eigenvalue and a_t is a proportionality constant. It is given as

$$a_t \equiv \sum_{\xi,\zeta} t^{m(0,\zeta)+m(\xi,0)} u_\xi(t) v_\zeta{}^*(t) \tag{3.2}$$

where $\mathbf{u}^{\dagger}(t)$ and $\mathbf{v}(t)$ are the left and right eigenvectors to T_t with a normalization such that

$$\sum_{\xi} u_{\xi}^{*}(t)v_{\xi}(t) = 1 \tag{3.3}$$

Now moments of (2.9) can be expressed in terms of derivatives of λ_t (and a_t) at $t = 1$, and these can in turn be evaluated via perturbation theory in terms of the $\mathbf{u}(t)$, $\mathbf{v}(t)$, and derivatives of T_t at $t = 1$. However, we take a different approach, which yields a complete[6] asymptotically accurate functional form for $n(x, l)$.

Let $n_{\xi}(x, l)$ be the number of x column walks of length l with the last column being in state ξ, and let E be the translation operator for chain length

$$E \equiv \exp(-\partial/\partial l) \tag{3.4}$$

Then in analogy to (2.2)–(2.4) we have

$$\begin{aligned} n_{\xi}(x+1, l) &= \sum_{\zeta}^{m(\xi,\zeta)\neq 0} n_{\zeta}[x, l - m(\xi, \zeta)] = \sum_{\zeta}^{m(\xi,\zeta)\neq 0} E^{m(\xi,\zeta)} n_{\zeta}(x, l) \\ n_{\xi}(1, l) &= \delta_{l,m(\xi,0)} \\ \mathbf{n}(x+1, l) &= \mathsf{T}_E \mathbf{n}(x, l) \end{aligned} \tag{3.5}$$

Further, for the asymptotic behavior, in analogy to (3.1), the number of x column chains of length l is given by

$$n(x, l) \approx \lambda_E^{x-1} a(l), \qquad x \to \infty \tag{3.6}$$

where λ_E is the eigenoperator[7] corresponding to λ_t and

$$a(l) \equiv \sum_{\xi,\zeta} E^{m(0,\zeta)+m(\xi,0)} u_{\xi}(E) v_{\zeta}^{*}(E)\, \delta_{l,m(\xi,0)} \tag{3.7}$$

[6] The solution is asymptotically complete in that the distribution we find correctly gives the leading nonvanishing terms in powers of x (and in the next section in powers of l). Moreover, there are several approaches to obtain the results of this section. One approach is given in Refs. 9 and 10, although the parameters (μ and Δ) of the asymptotic distribution are there characterized in a rather different way.

Another approach suggested by the referee is to consider the Fourier transform $\tilde{n}(x; \theta)$ of $n(x, l)$ and use (3.6) to obtain

$$\tilde{n}(x; \theta) \cong \int_0^{\infty} e^{il\theta} \lambda_E^{x-1} a(l)\, dl = \lambda_{e^{i\theta}}^{x-1} \tilde{a}(\theta)$$

The $\lambda_{e^{i\theta}}^{x-1}$ may be expanded, much as in (3.14), to give a Gaussian distribution for $\tilde{n}(x; \theta)$ and this Fourier-transformed back to give our result for $n(x, l)$. Alternatively, the formula for $\tilde{n}(x; \theta)$ above may be recognized to be like that for $x - 1$ independent random variables, so that the usual central limit theorem can be applied. It is to be noted, however, that the present variables [say the $m(\zeta, \xi)$] are not independent, and are, for instance, termed *chain-dependent* by Gnedenko.[11]

[7] Clearly if A_t and B_t are matrices with elements which are polynomials in t and $A_t B_t = C_t$, then $A_E B_E = C_E$. Hence if $\mathbf{v}_t$ and λ_t are functions of t such that $\mathsf{T}_t \mathbf{v}_t = \lambda_t \mathbf{v}_t$, then also $\mathsf{T}_E \mathbf{v}_E = \lambda_E \mathbf{v}_E$.

Next, in order to utilize (3.6), we expand T_E and λ_E in terms of the differentiation operator,

$$\begin{aligned} \mathsf{T}_E &= \mathsf{T}_1 + \mathsf{T}_1^{(1)}(-\partial/\partial l) + \mathsf{T}_1^{(2)}(-\partial/\partial l)^2 + \cdots \\ \lambda_E &= \lambda_1 + \lambda_1^{(1)}(-\partial/\partial l) + \lambda_1^{(2)}(-\partial/\partial l)^2 + \cdots \end{aligned} \tag{3.8}$$

Then

$$[\mathsf{T}_t^{(1)}]_{\xi\zeta} = m(\xi,\zeta)t^{m(\xi,\zeta)}, \qquad [\mathsf{T}_t^{(2)}]_{\xi\zeta} = \tfrac{1}{2}\{m(\xi,\zeta)\}^2 t^{m(\xi,\zeta)} \tag{3.9}$$

and via perturbation theory for non-Hermitian operators[12]

$$\lambda_1^{(1)} = \mathbf{v}^\dagger(1)\mathsf{T}_1^{(1)}\mathbf{u}(1), \qquad \lambda_1^{(2)} = \mathbf{v}^\dagger(1)\left(\mathsf{T}_1^{(2)} + \mathsf{T}_1^{(1)}\frac{1}{\lambda_1\mathsf{1} - \mathsf{T}_1}\mathsf{T}_1^{(1)}\right)\mathbf{u}(1) \tag{3.10}$$

Thus, a power of λ_E as appears in (3.6) may be written

$$\lambda_E{}^x = \lambda_1{}^x\left(1 - \frac{\lambda_1^{(1)}}{\lambda_1}\frac{\partial}{\partial l} + \frac{\lambda_1^{(2)}}{\lambda_1}\frac{\partial^2}{\partial l^2} + \cdots\right)^x \tag{3.11}$$

Now for large x the chain lengths l are large, too, so that we might more appropriately consider $j = l/x$ as being finite while $x \to \infty$. Then

$$\lambda_1^{-x}\lambda_E{}^x = \left(1 - \frac{1}{x}\frac{\lambda_1^{(1)}}{\lambda_1}\frac{\partial}{\partial j} + \frac{1}{x^2}\frac{\lambda_1^{(2)}}{\lambda_1}\frac{\partial^2}{\partial j^2} + \cdots\right)^x = \exp\left(-\frac{\lambda_1^{(1)}}{\lambda_1}\frac{\partial}{\partial j}\right), \qquad x \to \infty \tag{3.12}$$

so that on a scale of lengths l comparable to x, the initial delta-function distribution asymptotically is just translated (a distance $\sim x\lambda_1^{(1)}/\lambda_1$) and grown in size (by a factor $\sim \lambda_1{}^x$). Hence

$$\langle l\rangle_x \approx (\lambda_1^{(1)}/\lambda_1)x, \qquad x \to \infty \tag{3.13}$$

and the higher (noncentral) moments are simple powers of $\langle l\rangle_x$, at least on a scale of lengths comparable to x.

Next, to look at the distribution in somewhat finer detail, we use (3.11) to write

$$\begin{aligned} \lambda_E{}^x &= \lambda_1{}^x \exp\left(-\frac{\lambda_1^{(1)}}{\lambda_1}x\frac{\partial}{\partial l}\right)\left\{\exp\left(\frac{\lambda_1^{(1)}}{\lambda_1}\frac{\partial}{\partial l}\right)\left[1 - \frac{\lambda_1^{(1)}}{\lambda_1}\frac{\partial}{\partial l} + \frac{\lambda_1^{(2)}}{\lambda_1}\frac{\partial^2}{\partial l^2} + \cdots\right]\right\}^x \\ &= \lambda_1{}^x \exp\left(-\mu x\frac{\partial}{\partial l}\right)\left\{1 + \frac{1}{2}\Delta\frac{\partial^2}{\partial l^2} + \cdots\right\}^x \end{aligned} \tag{3.14}$$

where the remaining terms in the curly brackets are third or higher degree in the differentiation operator, and

$$\mu \equiv \lambda_1^{(1)}/\lambda_1, \qquad \Delta \equiv 2\lambda_1^{(2)}/\lambda_1 - (\lambda_1^{(1)}/\lambda_1)^2 \tag{3.15}$$

Now considering values of l deviating from the average $\langle l\rangle_x$ by amounts finitely proportional to $\sqrt{x}$, we restrict $k \equiv (l - \langle l\rangle_x)/\sqrt{x}$ to be finite as $x \to \infty$. Then

$$\lambda_E{}^x \approx \lambda_1{}^x \exp(-\mu x\, \partial/\partial l) \exp(\tfrac{1}{2}\Delta\, \partial^2/\partial k^2), \qquad x \to \infty \tag{3.16}$$

and

$$n(x, l) = a_1 \lambda_1^{x-1}[\exp(-\mu x\, \partial/\partial l) \exp(\tfrac{1}{2}\Delta x\, \partial^2/\partial l^2)]\delta_{l,0}, \qquad x \to \infty \tag{3.17}$$

where we have replaced $a_E(l)$ by $a_1\delta_{l,0}$, as is allowable for asymptotic results since $a_E(l)$ is just a linear combination of a_1 delta functions all located within a few steps of $l = 0$. Next, as is well known,[13] $[\exp(\tfrac{1}{2}x\Delta\, \partial^2/\partial l^2)]f(l)$ is just the solution $F(x, l)$ to the diffusion equation

$$\frac{\partial}{\partial x} F(x, l) = \frac{\Delta}{2}\frac{\partial^2}{\partial l^2} F(x, l) \tag{3.18}$$

with the initial $x = 0$ value $F(0, l) = f(l)$, and if $f(l)$ is a delta function, this solution is well known to be a Gaussian. Thus

$$n(x, l) \approx \frac{a_1}{\lambda_1(2\pi\Delta)^{1/2}}\, \lambda_1{}^x \frac{1}{x^{1/2}} \exp\left[-\frac{(l - \langle l\rangle_x)^2}{2x\Delta}\right], \qquad x \to \infty \tag{3.19}$$

a distribution which will give the higher central moments $\langle (l - \langle l\rangle_x)^m\rangle_x$ asymptotically correct, on a scale of lengths comparable to $x^{1/2}$.

4. ASYMPTOTICS FOR FIXED LENGTH[8]

The distribution of (3.18) does not give asymptotically correct moments

$$\langle x^m\rangle_l \equiv \sum_x x^m n(x, l) \Big/ \sum_x n(x, l) \tag{4.1}$$

for end-to-end separations of chains with fixed length l, because the Gaussian of (3.18) is severely in error in its extreme tails. Although these extreme tails, where $(l - \langle l\rangle_x)/\sqrt{x} \to \infty$ as $x \to \infty$, do not contribute to the asymptotic $\langle l^m\rangle_x$ moments, they do contribute significantly to the $\langle x^m\rangle_l$ moments because of the weight factors $\lambda_1{}^x$, which are very large and rapidly varying in these extreme tails. Hence we seek a "connective constant" κ for these self-avoiding walks so that the remaining portion of the distribution will be

[8] The referee points out the results of this section can also be obtained in another way, by considering the discrete Fourier transform

$$n(\varphi; l) \equiv \sum_x n(x; l)e^{i\varphi x}$$

On showing that this behaves asymptotically as $(1/t_\varphi)^l$, where $\lambda_{t_\varphi} = e^{-i\varphi}$, and then proceeding as in the referee's suggestion for Section 3, one can obtain the results of Section 4.

more nearly normalized. Now κ is such that $t^l n(x, l)$ diverges to $+\infty$ or converges to 0,[14] both with exponential rates, for $t > 1/\kappa$ or $t < 1/\kappa$, respectively. In turn this implies that the generating function of (2.7) behaves as

$$G_x(t) \approx \begin{cases} 0, & t < 1/\kappa \\ \infty, & t > 1/\kappa \end{cases} \qquad x \to \infty \tag{4.2}$$

Hence, using the asymptotic formula of (3.1), we see that

$$\kappa = 1/t \qquad \lambda_t = 1 \tag{4.3}$$

and κ is determined simply by varying t in T_t till its maximum eigenvalue is 1.

It is of use to understand some features of how λ_t varies with t. The Frobenius–Perron theorem[8] applies to T_t for all $t > 0$, so that $\lambda_t > 0$ and all the components of the left and right eigenvectors for λ_t may be chosen to be positive. Then, also noting that all the elements of $\mathsf{T}_t^{(1)}$ are nonnegative for $t > 0$, we have

$$\partial\lambda_t/\partial t = \mathbf{v}^\dagger(t)\mathsf{T}_t^{(1)}\mathbf{u}(t) \geqslant 0, \qquad t > 0 \tag{4.4}$$

Thus, as t decreases from 1 to 0, the maximum eigenvalue λ_t decreases monotonically from $\lambda_1 > 1$ to $\lambda_0 = 0$, and there is exactly one value of t between 0 and 1 for which $\lambda_t = 1$. Hence, $t = 1/\kappa$ is the minimum positive value of t for which the determinant of $\mathsf{T}_t - \mathbb{1}$ is 0.

Now write

$$n(x, l) \equiv \kappa^l p(x, l), \qquad n_\xi(x, l) \equiv \kappa^l p_\xi(x, l) \tag{4.5}$$

with $p(x, l)$ and $p_\xi(x, l)$ at large x being normalized as nearly as is possible by such a simple factor. Then in analogy to Eq. (3.5) we have

$$\begin{aligned} p_\xi(x+1, l) &= \sum_{\zeta}^{m(\xi,\zeta)\neq 0} \{E/\kappa\}^{m(\xi,\zeta)} p_\xi(x, l) \\ p_\xi(1, l) &= \kappa^{-m(\xi,0)}\delta_{l,m(\xi,0)} \\ \mathbf{p}(x+1, l) &= \mathsf{T}_{E/\kappa}\mathbf{p}(x, l) \end{aligned} \tag{4.6}$$

In fact, the same type of asymptotic analysis as that of the previous section applies, so that

$$\begin{aligned} p(x, l) &\approx a_{1/\kappa} \exp\left(-\mu_\kappa x \frac{\partial}{\partial l}\right) \exp\left(\frac{1}{2}\Delta_\kappa x \frac{\partial}{\partial l^2}\right)\delta_{l,0} \\ &\approx \frac{a_{1/\kappa}}{(2\pi\Delta_\kappa)^{1/2}} \frac{1}{x^{1/2}} \exp\left[-\frac{(l-\mu_\kappa x)^2}{2x\Delta_\kappa}\right], \qquad x, l \to \infty \end{aligned} \tag{4.7}$$

which we expect to be valid for values deviating from the average $\langle x \rangle_l$ by amounts finitely proportional to $\sqrt{l}$. [Here μ_κ and Δ_κ are defined much as μ and Δ were in (3.15), except that λ_t and its perturbation coefficients are evaluated at $t = 1/\kappa$ now instead of at $t = 1$.] Next, substituting $x = \langle x \rangle_l + (x - \langle x \rangle_l)$ and restricting $(x - \langle x \rangle_l)/l \to 0$ as $l \to \infty$, we find

$$n(x, l) = \frac{a_{1/\kappa}}{(2\pi\Delta_\kappa)^{1/2}} \frac{1}{\langle x \rangle_l^{1/2}} \times \exp\left\{ -\frac{[(l - \mu_\kappa \langle x \rangle_l) + \mu_\kappa (x - \langle x \rangle_l)]^2}{2\langle x \rangle_l \Delta_\kappa} \right\}, \qquad l \to \infty \tag{4.8}$$

so that

$$\langle x \rangle_l = l/\mu_\kappa \tag{4.9}$$

Then, defining

$$\nu \equiv \frac{1}{\mu_\kappa} = \frac{\lambda_{1/\kappa}}{\lambda_{1/\kappa}^{(1)}}, \qquad \Gamma \equiv \frac{\Delta_\kappa}{{\mu_\kappa}^3} = 2\frac{(\lambda_{1/\kappa})^2 \lambda_{1/\kappa}^{(2)}}{(\lambda_{1/\kappa}^{(1)})^3} - \frac{\lambda_{1/\kappa}}{\lambda_{1/\kappa}^{(1)}} \tag{4.10}$$

we finally obtain

$$n(x, l) = \frac{\nu a_{1/\kappa}}{(2\pi\Gamma)^{1/2}} \frac{1}{l^{1/2}} \exp\left[-\frac{(x - \langle x \rangle_l)^2}{2l\Gamma} \right], \qquad l \to \infty \tag{4.11}$$

This then determines the central moments

$$\langle (x - \langle x \rangle_l)^m \rangle_l = \begin{cases} 0, & m \text{ odd} \\ \dfrac{m!}{(m/2)!} \left(\dfrac{\Gamma l}{2} \right)^{m/2}, & m \text{ even} \end{cases} \qquad l \to \infty \tag{4.12}$$

asymptotically correct.

5. SOME NUMERICAL RESULTS

The transfer matrix for the strip of width $M = 3$ has already been given in (2.5). But this 5×5 matrix may be block-diagonalized if we take into account the reflection symmetry through the horizontal line down the center of the strip. Indeed transformation to a basis composed from plus and minus, ξ^+ and ξ^-, combinations of reflection-related pairs, ξ and $\bar{\xi}$, yields

$$\mathsf{T}_t = \begin{bmatrix} t + t^3 & t^3 & t^2 & & \\ t^3 & t^3 & 0 & \mathbf{0} & \\ 2t^2 & 0 & t & & \\ & \mathbf{0} & & t - t^3 & -t^3 \\ & & & t^3 & t^3 \end{bmatrix}, \qquad 3 \times \infty \text{ strip} \tag{5.1}$$

Here we have ordered the basis as $\alpha^+, \beta^+, \gamma, \alpha^-, \beta^-$ so that the first 3×3 block corresponds to the symmetric part, while the second 2×2 part corresponds to the antisymmetric part. Since the maximum-eigenvalue eigenvector on the original basis was to have all components of like phase, this eigenvector must be symmetric and we may delete the antisymmetric block of T_t from consideration. The secular polynomial for the symmetric block is

$$\det(\hat{\mathsf{T}}_t - \lambda_t \mathsf{1}) = -\lambda_t^3 + (2t + 2t^3)\lambda_t^2 - (t^2 + t^4)\lambda_t + (t^5 - 2t^7) \quad (3 \times \infty \text{ strip}) \qquad (5.2)$$

whence setting $t = 1$ and solving for the maximum root gives λ_1, while setting $\lambda_t = 1$ and solving for the minimum positive root gives $t = 1/\kappa$. To find $\lambda_1^{(1)}$ and $\lambda_1^{(2)}$ one can now use (3.10); or alternatively the secular polynomial of (5.2) can simply be differentiated, the result set equal to 0, and the λ derivatives solved for. Hence

$$\begin{aligned} \lambda_1 &= \frac{3 + \sqrt{13}}{2} \\ \lambda_1^{(1)} &= \frac{8\lambda_1^2 - 6\lambda_1 - 9}{3\lambda_1^2 - 8\lambda_1 + 2} = \frac{18\lambda_1 - 1}{\lambda_1 + 5} = \frac{17 + 7\sqrt{13}}{6} \qquad (3 \times \infty \text{ strip}) \\ \lambda_1^{(2)} &= \frac{1}{2}\left(t^2 \frac{\partial^2 \lambda_t}{\partial t^2} + t \frac{\partial \lambda_t}{\partial t}\right)_{t=1} = \frac{4280\lambda_1 - 719}{2(\lambda_1 + 5)} \end{aligned} \qquad (5.3)$$

Numerical values for the parameters characterizing the distributions of Sections 3 and 4 are given for the $3 \times \infty$ strip in Table I. Results for several other pseudo-one-dimensional systems are also reported there. The values of κ and ν for the $2 \times \infty$ and $3 \times \infty$ strips agree with those previously given by Wall *et al.*[1]

Table I. Parameters Characterizing Distributions of Self-Avoiding Walks

System	λ_1	μ	Δ	κ	ν	Γ
$2 \times \infty$ strip	2.0000	1.5000	0.2500	1.6180	0.7236	0.0894
$3 \times \infty$ strip	3.3028	2.1315	1.0363	1.9146	0.6244	0.1388
$4 \times \infty$ strip	5.4826	2.9650	1.6317	2.0873	0.5661	0.1785
$5 \times \infty$ strip	9.4103	3.818	1.703	2.1990	0.526	0.213
$6 \times \infty$ strip	16.355	4.622	1.793	2.276	0.495	0.246
$2 \times \infty$ diagonal strip	3.3830	1.6953	0.2376	2.1265	0.6466	0.0405
$2 \times \infty$ strip from a triangular lattice	3.3830	1.6344	0.2993	2.2056	0.6911	0.0761
$4 \times \infty$ cylinder, $2 \times 2 \times \infty$ tube	9.4956	3.1424	1.0698	2.4090	0.5090	0.1510

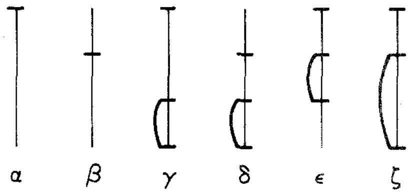

Fig. 3. Six of the column states for a strip of width $D = 4$. In addition there are six states obtained via reflection about the center of the column.

In the remainder of this section we indicate how the symmetry-reduced transfer matrices for the other systems of Table I are set up. For the $2 \times \infty$ and $4 \times \infty$ strips the procedure is quite similar to that already carried out for the $3 \times \infty$ strip; one obtains

$$\hat{\mathsf{T}}_t = t^2 + t, \qquad 2 \times \infty \text{ strip}$$

$$\hat{\mathsf{T}}_t = \begin{bmatrix} t + t^4 & t^2 + t^3 & t^4 & t^3 & t^4 & t^3 \\ t^2 + t^3 & t + t^2 & 0 & 0 & t^3 & t^4 \\ t^3 & t^4 & t^3 & t^4 & 0 & t^4 \\ t^4 & t^3 & t^4 & t^3 & 0 & 0 \\ t^3 & 0 & 0 & 0 & t^3 & t^4 \\ t^4 & 0 & t^4 & 0 & t^4 & t^3 \end{bmatrix}, \qquad 4 \times \infty \text{ strip} \tag{5.4}$$

where the states for the $4 \times \infty$ strip are indicated in Fig. 3. The $4 \times \infty$ cylinder may also be termed a $4 \times \infty$ strip with cyclic boundary conditions (in the transverse direction), and as such is labeled by the same states as for the $4 \times \infty$ strip, although there are now just three symmetry-nonequivalent states (say α,

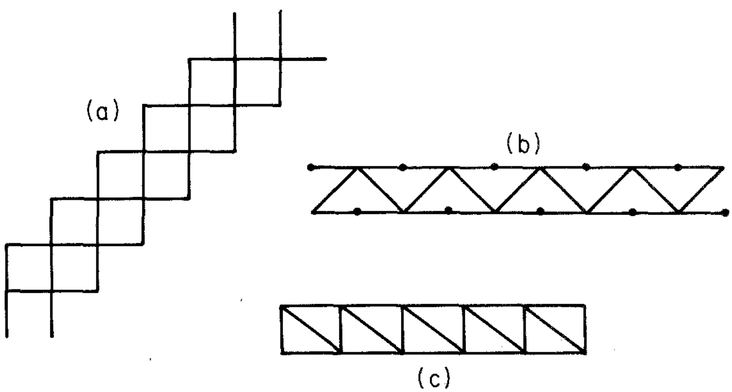

Fig. 4. Three views of a $2 \times \infty$ diagonal strip.

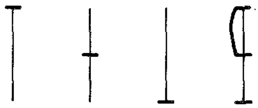

Fig. 5. The four column states associated with the $2 \times \infty$ diagonal strip (of Fig. 4c).

γ, and ζ of Fig. 3). The resulting symmetry-reduced transfer matrix is found to be

$$\hat{\mathsf{T}}_t = \begin{bmatrix} t + 2t^2 + 2t^3 + 2t^4 & t^3 + t^4 + t^5 & 2t^3 \\ 2t^3 + 2t^4 & t^3 + t^4 & 2t^4 \\ t^4 & t^4 & t^3 \end{bmatrix}, \qquad 4 \times \infty \text{ cylinder} \tag{5.5}$$

where we note that the same state may arise from a given predecessor in several ways. Of course the $2 \times 2 \times \infty$ tube is the same as the $4 \times \infty$ cylinder.

The $2 \times \infty$ diagonal strip is a section from a square planar lattice as indicated in Fig. 4a. We, however, distort it so as to appear as in Fig. 4b. Then we may delete the "isolated" sites of valence two, as in Fig. 4c, if we remember to count a single horizontal step with a weight factor of $t^{\sqrt{2}} \equiv \tau^4$ instead of τ^2 as for the diagonal and vertical steps. (Here we take the x axis along the diagonal direction of Fig. 4a.) The four states for the system are given in Fig. 5, and the resulting transfer matrix is

$$\mathsf{T}_t = \begin{bmatrix} \tau^4 & \tau^5 & \tau^6 & \tau^7 \\ \tau^3 & \tau^4 & \tau^5 & \tau^6 \\ \tau^6 & \tau^3 & \tau^4 & 0 \\ 0 & \tau^6 & \tau^7 & 0 \end{bmatrix}, \qquad 2 \times \infty \text{ diagonal strip} \tag{5.6}$$

For a $2 \times \infty$ strip from a triangular lattice the situation is fairly similar, except that now a horizontal step has just weight t, and

$$\mathsf{T}_t = \begin{bmatrix} t & t^2 & t^2 & t^2 \\ t & t^2 & t^2 & t^2 \\ t^2 & t & t & 0 \\ 0 & t^2 & t^2 & 0 \end{bmatrix}, \qquad 2 \times \infty \text{ strip of a triangular lattice} \tag{5.7}$$

Clearly, the present transfer matrix technique applies to a wide variety of pseudo-one-dimensional systems.

6. SELF-AVOIDING CYCLES

Self-avoiding cyclic paths on strips, tubes, and cylinders may be treated in a similar manner. Column states can be identified much as was done for walks

Fig. 6. The three column states for self-avoiding cycles on a strip of width $D = 3$.

in Section 2, so that, for example, the $3 \times \infty$ strip gives rise to the three column states depicted in Fig. 6. Here there is no dangling end. Further, we may similarly construct a transfer matrix T_t', an example of which is

$$\mathsf{T}_t' = \begin{bmatrix} t^2 & t^3 & 0 \\ t^3 & t^2 & t^3 \\ 0 & t^2 & t^2 \end{bmatrix}, \qquad 3 \times \infty \text{ strip} \tag{6.1}$$

In analogy to Eq. (2.7), the generating function for self-avoiding cycles, with a left-to-right span of x, is

$$G_x'(t) = \sum_{\xi,\zeta} [\mathsf{T}_t^{x-1}]_{\xi\zeta} t^{m'(0,\xi) + m'(\zeta,0)} \tag{6.2}$$

where now $m'(0, \xi)$ is the number of steps to immediately terminate a cycle with the last column state being ξ. Then

$$G_x'(t) = \sum_l n'(x, l) t^l \tag{6.3}$$

where $n'(x, l)$ is the number of length-l cycles with a span of x. Arguments parallel to those of Sections 3 and 4 still apply, and finally give asymptotic expressions

$$\begin{aligned} n'(x, l) &\approx \frac{a_1'}{\lambda_1'(2\pi\Delta')^{1/2}} (\lambda_1')^x \frac{1}{x^{1/2}} \exp\left[-\frac{(l - \langle l \rangle_x)^2}{2x\Delta'} \right], \qquad x \to \infty \\ n'(x, l) &= \frac{a'_{1'\kappa'} \nu'}{(2\pi\Gamma')^{1/2}} \frac{2}{l^{1/2}} \exp\left[-\frac{(x - \langle x \rangle_l)^2}{2l\Gamma'} \right], \qquad l \to \infty \end{aligned} \tag{6.4}$$

in analogy to Eqs. (3.19) and (4.11), respectively. Here

$$\langle x \rangle_l = \mu' x, \qquad \langle x \rangle_l = \nu' l \tag{6.5}$$

and μ', Δ', ν', Γ' are defined analogously to μ, Δ, ν, Γ of Eqs. (3.15) and (4.10) but now in terms of the eigenvalues λ_1', $\lambda'_{1/\kappa'}$, and their perturbation expansion coefficients.

Treatment of the transfer matrices T_t' can be done much as in Section 5 for the T_t. Numerical results for some of the narrower systems are given in Table II. The cases for the three types of diagonal strips of Table I are omitted from the present table, since their present transfer matrices are trivial, being

Table II. Parameters Characterizing Distributions of Self-Avoiding Cycles

System	λ_1'	μ'	Δ'	κ'	ν'	Γ'
$3 \times \infty$ strip	2.4142	2.5858	0.2419	1.4142	0.4000	0.0160
$4 \times \infty$ strip	4.7535	3.1663	0.6763	1.6818	0.3520	0.0246
$5 \times \infty$ strip	8.5972	3.8487	1.3064	1.8631	0.3218	0.0318
$6 \times \infty$ strip	15.1712	4.617	1.800	1.9924	0.300	0.038
$4 \times \infty$ cylinder, $2 \times 2 \times \infty$ tube	6.5877	3.3063	0.5786	1.8268	0.3388	0.0224

essentially 1×1 with a single power of t. Although Hammersly[15] has shown that the connective constants for walks and cycles on extended square planar or cubic lattices are the same, his proof does not apply for walks and cycles on strips, cylinders, or tubes. Indeed, on comparing Tables I and II, we see that

$$\kappa' < \kappa \tag{6.6}$$

Further noting that λ_t and λ_t' decrease monotonically as t decreases, we infer that

$$\lambda_t' < \lambda_t, \qquad \text{for } 1/\kappa \leqslant t \leqslant 1/\kappa' \tag{6.7}$$

an observation of use in the following section.

7. CHAINS WITH FREE ENDS

In this section we consider self-avoiding walks with free ends, not necessarily located at the left and right extremes of the walk. We identify three regions: first, the region extending from the left extreme walk boundary to the leftmost end of the walk; second, the region extending from the leftmost end to the rightmost end; and third, the region extending from the rightmost end to the right extreme walk boundary. We let the horizontal widths of these regions be x_{I}, x_{II}, and x_{III}. Thus the chains of Sections 2–5 have $x_{\mathrm{I}} = 0$, $x_{\mathrm{III}} = 0$. Now column states can be identified in region I without a dangling end off to the left just as for the column states of Section 6. Further, the transfer matrix $\mathsf{T}_t^{\mathrm{I}}$ for region I is exactly the same as that for the cyclic case of Section 6.

For region II there are some additional column states which could not arise for the fixed-end situation previously considered. These additional column states have the dangling end between a pair of occupied links which are connected, a case of which is illustrated in Fig. 7. Again we may construct a region II transfer matrix, which generally takes the block form

$$\mathsf{T}_t^{\mathrm{II}} = \begin{pmatrix} \mathsf{T}_t & \mathsf{R}_t \\ \mathbf{0} & \mathsf{S}_t \end{pmatrix} \tag{7.1}$$

Fig. 7. The additional (region II) column state which arises on a strip of width $D = 3$ when the walk is allowed to have free ends rather than fixed.

Here T_t is as in Section 2 and a zero matrix occurs in the lower left block because none of the additional region II states can follow those already considered in Section 2. Here

$$\mathsf{R}_t = \begin{bmatrix} t^3 \\ 0 \\ 0 \\ t^3 \\ 0 \end{bmatrix} \quad \text{and } \mathsf{S}_t = (t^3), \qquad 3 \times \infty \text{ strip} \tag{7.2}$$

as an example.

For region III we choose to specify a column state in terms of whether a pair of occupied links are connected by a sequence of states to the right of the column under consideration. Then the possible column states for region III are in one-to-one correspondence with those of region I, the correspondence being effected by a reflection in the vertical plane of the column. Then the transfer matrix for region III,

$$\mathsf{T}_t^{\mathrm{III}} = \tilde{\mathsf{T}}_t^{\mathrm{I}} \tag{7.3}$$

is the transpose of that for region I.

In addition to these transfer matrices applying within each region, there are also *connection* (or interregion transfer) matrices between pairs of regions. The manner of their construction is similar to that of the intraregion transfer matrices, though the connection matrices are in general rectangular rather than square. For example,

$$\mathsf{C}_t^{\mathrm{II,I}} = \begin{bmatrix} t^{3/2} & t^{3/2} & t^{5/2} \\ 0 & 0 & t^{5/2} \\ t^{3/2} & 2t^{5/2} & t^{3/2} \\ t^{5/2} & t^{3/2} & t^{3/2} \\ t^{5/2} & 0 & 0 \\ 0 & t^{5/2} & 0 \end{bmatrix}$$

$$\mathsf{C}_t^{\mathrm{III,II}} = \begin{bmatrix} t^{3/2} & t^{3/2} & t^{3/2} & t^{5/2} & 0 & t^{5/2} \\ t^{3/2} & t^{3/2} & 2t^{5/2} & t^{3/2} & t^{3/2} & 0 \\ t^{5/2} & 0 & t^{3/2} & t^{3/2} & t^{3/2} & t^{5/2} \end{bmatrix} \qquad 3 \times \infty \text{ strip} \tag{7.4}$$

Connection matrices (or vectors) are needed for going from the empty region (region 0) preceding I to region I or for going from region III to the empty region following. Finally, should x_{I}, x_{II}, or x_{III} be 0, connection matrices between otherwise nonadjacent regions are required. All are constructed in a similar manner, and examples for $\mathsf{C}_t^{0,\mathrm{II}}$ and $\mathsf{C}_t^{\mathrm{II},0}$ are given in Section 2 (for the special case that the initial and final steps of the walk are horizontal).

Once all the transfer and connection matrices are available, the generating function for walks with widths x_{I}, x_{II}, x_{III} for the various regions is given as

$$\begin{aligned}
\mathscr{G}_{x_{\mathrm{I}},x_{\mathrm{II}},x_{\mathrm{III}}}(t) &\equiv \mathsf{C}_t^{0,\mathrm{III}}(\mathsf{T}_t^{\mathrm{III}})^{x_{\mathrm{III}}-1}\mathsf{C}_t^{\mathrm{III},\mathrm{II}}(\mathsf{T}_t^{\mathrm{II}})^{x_{\mathrm{II}}-1}\mathsf{C}_t^{\mathrm{II},\mathrm{I}}(\mathsf{T}_t^{\mathrm{I}})^{x_{\mathrm{I}}-1}\mathsf{C}_t^{\mathrm{I},0}, \qquad x_{\mathrm{I}}x_{\mathrm{II}}x_{\mathrm{III}} \neq 0\\
&\equiv \mathsf{C}_t^{0,\mathrm{III}}(\mathsf{T}_t^{\mathrm{III}})^{x_{\mathrm{III}}-1}\mathsf{C}_t^{\mathrm{III},\mathrm{II}}(\mathsf{T}_t^{\mathrm{II}})^{x_{\mathrm{II}}-1}\mathsf{C}_t^{\mathrm{II},0}, \qquad x_{\mathrm{I}} = 0, \qquad x_{\mathrm{II}}x_{\mathrm{III}} \neq 0\\
&\equiv \mathsf{C}_t^{0,\mathrm{III}}(\mathsf{T}_t^{\mathrm{III}})^{x_{\mathrm{III}}-1}\mathsf{C}_t^{\mathrm{III},\mathrm{I}}(\mathsf{T}_t^{\mathrm{I}})^{x_{\mathrm{I}}-1}\mathsf{C}_t^{\mathrm{II},0}, \qquad x_{\mathrm{II}} = 0, \qquad x_{\mathrm{I}}x_{\mathrm{II}} \neq 0\\
&\equiv \mathsf{C}_t^{0,\mathrm{II}}(\mathsf{T}_t^{\mathrm{II}})^{x_{\mathrm{II}}-1}\mathsf{C}_t^{\mathrm{II},\mathrm{I}}(\mathsf{T}_t^{\mathrm{I}})^{x_{\mathrm{I}}-1}\mathsf{C}_t^{\mathrm{I},0}, \qquad x_{\mathrm{III}} = 0, \qquad X_{\mathrm{I}}x_{\mathrm{III}} \neq 0\\
&\equiv \mathsf{C}_t^{0,\mathrm{III}}(\mathsf{T}_t^{\mathrm{III}})^{x_{\mathrm{III}}-1}\mathsf{C}_t^{\mathrm{III},0}, \qquad x_{\mathrm{I}} = x_{\mathrm{II}} = 0\\
&\equiv \mathsf{C}_t^{0,\mathrm{II}}(\mathsf{T}_t^{\mathrm{II}})^{x_{\mathrm{II}}-1}\mathsf{C}_t^{\mathrm{II},0}, \qquad x_{\mathrm{I}} = x_{\mathrm{III}} = 0\\
&\equiv \mathsf{C}_t^{0,\mathrm{I}}(\mathsf{T}_t^{\mathrm{I}})^{x_{\mathrm{I}}-1}\mathsf{C}_t^{\mathrm{I},0}, \qquad x_{\mathrm{II}} = x_{\mathrm{III}} = 0
\end{aligned} \tag{7.5}$$

The total generating function for walks with a total span of x is

$$\mathscr{G}_x(t) \equiv \sum_{a=0}^{x} \sum_{b=0}^{x-a} \mathscr{G}_{a,b,x-a-b}(t) \tag{7.6}$$

Now $\mathscr{G}_x(t)$ can in principle be manipulated much as $G_x(t)$ of Section 2 might be, so as to yield exact moments and enumerations.

For asymptotic results, the same type of arguments as given in Section 3 apply, and

$$\mathscr{G}_x(t) \approx A_t \sum_{a,b,c}^{a+b+c=x} (\lambda_t^{\mathrm{I}})^a(\lambda_t^{\mathrm{II}})^b(\lambda_t^{\mathrm{III}})^c, \qquad x \to \infty \tag{7.7}$$

where λ_t^{I}, λ_t^{II}, and λ_t^{III} are the maximum eigenvalues to $\mathsf{T}_t^{\mathrm{I}}$, $\mathsf{T}_t^{\mathrm{II}}$, and $\mathsf{T}_t^{\mathrm{III}}$. Because of the blocked form in (7.1), λ_t^{II} is equal to the maximum eigenvalue λ_t of Sections 2–5 (unless the maximum eigenvalue of $\mathsf{T}_t^{\mathrm{II}}$ arises from S_t). Also, because of (6.4), $\lambda_t^{\mathrm{I}} = \lambda_t^{\mathrm{III}} = \lambda_t'$. Now in the case that $\lambda_t > \lambda_t'$, we have

$$\mathscr{G}_x(t) \approx \frac{A_t}{1 - \lambda_t'/\lambda_t} (\lambda_t)^x, \qquad x \to \infty \tag{7.8}$$

and the evaluation of distributions proceeds as in Sections 3 and 4, and the asymptotic moments are the same. The case that $\lambda_t < \lambda_t'$ cannot occur at $t = 1/\kappa$ because this would imply that $\langle x \rangle_l / l \to 0$ as $l \to \infty$, contrary to what has elsewhere[9] been rigorously proved. The case with $\lambda_t = \lambda_t'$ at $t = 1/\kappa$ is not forbidden by these earlier rigorous results. Nevertheless, it is found that $\lambda_t > \lambda_t'$ at $t = 1/\kappa$ and $t = 1/\kappa'$. Hence it seems likely that in general for these pseudo-one-dimensional systems the fixed-end and free-end self-avoiding walks exhibit the same asymptotic behavior.

8. VARIATIONS WITH STRIP WIDTH

The numerical results of the preceding sections for self-avoiding walks and cycles on strips provide evidence as to the behavior of their distributions as a function of strip width D. Thus the dependence on D of the parameters characterizing the various asymptotic distributions is now explicitly noted, e.g., by writing $\kappa(D)$ and $\nu(D)$ for κ and ν.

First, since λ_1 represents some sort of an average number of ways for a very long walk to proceed one unit to the right along a strip, $\lambda_1(D)$ should increase rapidly with D. Indeed, as proved in Appendix C, $\lambda_1(D)$ increases exponentially with D, and the numerical values of $[\ln \lambda_1(D)]/D$ appear to converge to a value near 0.5. Also it is proved in Appendix C that $[\ln \lambda_1'(D)]/D$ should converge to the same value as does $[\ln \lambda_1(D)]/D$, and this is observed numerically. Indeed it is argued in Appendix C that $\lambda_1(D)$ and $\lambda_1'(D)$ should behave rather similarly for larger D, and numerically it appears that

$$\lambda_1'(D)/\lambda_1(D) \to 1.0 \qquad \text{as } D \to \infty \tag{8.1}$$

Further, Appendix C establishes that $\kappa(D)$ and $\kappa'(D)$ should approach one another for larger D, and numerically it appears that

$$\kappa'(D)/\kappa(D) \to 1.00 \qquad \text{as } D \to \infty \tag{8.2}$$

Further, the difference between $\kappa'(D)$ and $\kappa(D)$ seems to fall off as $D^{-\phi}$ with ϕ of the order of magnitude of 1.

The scaling arguments of Daoud and de Gennes[4] predict that for large D the compressional free energy (per unit length) is of the form[2]

$$\ln \kappa(\infty) - \ln \kappa(D) \approx c_1 D^{-\phi}, \qquad \phi \approx 4/3 \tag{8.3}$$

and that for large D the mean end-to-end separation is of the form[2,3]

$$\nu(D) \approx c_2 D^{-\theta}, \qquad \theta \approx 1/3 \tag{8.4}$$

where c_1 and c_2 are proportionality constants. To test these functional forms

[9] The theorem is given in Ref. 16 and a correction to the proof is given in Ref. 17. It should be noted that the correction (as it stands) applies only to strips, although intuitively one also expects it to apply to cylinders and tubes.

Table III. Estimates for Scaling Exponents

	θ_D			ϕ_D		
D	Numerically exact	Extrapolation[a]	Monte Carlo[b]	Numerically exact	Extrapolation[a]	Monte Carlo[c]
2	0.467	—	—	0.988	—	—
3	0.364	—	—	1.041	—	—
4	0.341	0.370	0.341	1.091	0.997	1.096
5	0.329	0.330	0.338	1.128	1.04	1.121
6	0.334	0.343	0.303	1.15	0.99	1.164
7	—	—	—	—	0.96	—
8	—	—	0.32[d]	—	—	1.22[d]

[a] Data from Ref. 2 (incorporating exact result for $D = 3$).
[b] Data from Ref. 3 (incorporating exact result for $D = 3$).
[c] Data (provided by W. A. Seitz and incorporating the exact result for $D = 3$) as computed in conjunction with Ref. 2, but not reported there.
[d] Data calculated using equations as in (8.5) with the arguments $D - 1$ replaced by $D - 2$.

one may calculate the quantities

$$\begin{aligned} \phi_D &\equiv \frac{\ln[\ln \kappa(\infty)/\kappa(D)] - \ln[\ln \kappa(\infty)/\kappa(D-1)]}{\ln[(D-1)/D]} \\ \theta_D &\equiv \frac{\ln[\nu(D)/\nu(D-1)]}{\ln[(D-1)/D]} \end{aligned} \tag{8.5}$$

for a sequence of values of D. This is done in Table III, where $\kappa(\infty)$ is assumed to take the same value as for the extended plane and is estimated[18] as $\kappa(\infty) = 2.6385$. Estimates from exact finite-chain enumerations and from Monte Carlo studies are also given in the table. As noted previously,[2,3] θ_D appears to approach the expected scaling value of 1/3 very rapidly. The sequence of values for ϕ_D converges sufficiently slowly that it is unclear whether the value of 4/3 expected from scaling theory will be achieved; however, the value of 4/3 appears to be a possibility, while the value of 1, previously considered[2] as possible, now appears unlikely.

Scaling arguments similar to those leading to Eqs. (8.3) and (8.4) should also apply to $\kappa'(D)$ and $\nu'(D)$ for cycles. Since one expects the span of self-avoiding cycles in the extended plane to scale in the same way as the end-to-end separation for self-avoiding walks, the values for the exponents ϕ' and θ' are expected to be the same as for ϕ and θ. Rather than utilize analogs of Eqs. (8.5) to report estimates[10] for ϕ' and θ', we simply note the behavior of the ratios $\kappa'(D)/\kappa(D)$ and $\nu'(D)/\nu(D)$. That the difference $\kappa(D) - \kappa'(D)$ converges to zero as $D^{-\varphi}$ with a value of $\varphi = 4/3$ not being excluded by the

[10] Such estimates seem to exhibit slower convergence than for the case of self-avoiding walks.

numerical data indicates that these data are not inconsistent with the scaling value of $\phi' = 4/3$ for the exponent in the compressional free energy. Since it appears that

$$v'(D)/v(D) \to 0.60 \qquad \text{as } D \to \infty \tag{8.6}$$

from the numerical data, the scaling theory result of $\theta' = 1/3$ is indicated to hold.

Further we note that our data suggest that

$$\mu'(D)/\mu(D) \to 1.000, \qquad \Gamma'(D)/\Gamma(D) \to 0.18, \qquad \Delta'(D)/\Delta(D) \to 1.0 \tag{8.7}$$

Thus the behavior of the self-avoiding cycles on strips appears to be, in the large, simply related to that for self-avoiding walks.

9. CONCLUSION

An exact approach for self-avoiding walks with fixed or free ends, as well as self-avoiding cycles, has been developed. The distributions $n(x, l)$ and $p(x, l)$, for spans x and lengths l, have been shown to be asymptotically Gaussian for pseudo-one-dimensional systems. Numerically exact results have been given for a number of systems, particularly the narrower strips.

The scaling theory arguments, a few exact results, and numerical evidence all referred to in Section 8 suggest how the distributions vary with strip width D. Further numerical evidence for wider strips would be of use in clarifying this picture. Such a picture would not only be of interest in itself, but also by scaling up to $D \sim l^{3/4}$ information about distributions on a full two-dimensional lattice might be obtained. The transfer matrices for tubes appear to become large rather rapidly, as a function of tube diameter. Thus a parallel program concerning distributions in tubes might most readily be implemented if a Monte Carlo procedure for finding the maximum eigenvalue of the (nonnegative) transfer matrices T_t were developed.

APPENDIX A. THE NUMBER OF COLUMN STATES FOR A STRIP

The figures of Section 2 labeling column states for a strip of width D are similar to the drawings representing valence-bond spin pairings of electrons (see, e.g., Ref. 19). Indeed these column state drawings are in one-to-one correspondence with Rumer's linearly independent covalent doublet valence-bond states involving an odd number of electrons assigned to a subset of D independent spin-free orbitals. The number of such valence-bond states when a given set of $2m + 1$ spin-free orbitals is occupied is well known to be

$$f^{(1/2, 2m+1)} = \frac{(2m + 1)!\, 2}{m!\, (m + 2)!} \tag{A1}$$

and the number of such sets of $2m + 1$ spin-free orbitals is the binomial coefficient $\binom{D}{2m+1}$. Hence the number of column states is

$$n_D = \sum_{m=0}^{[(D-1)/2]} \frac{D!\,2}{(D-2m-1)!\,m!\,(m+2)!} \tag{A2}$$

where $[A]$ denotes the greatest integer not exceeding A. By a similar argument involving singlet valence-bond states the case of self-avoiding cycles on a strip may also be treated; in this case the number of column states is

$$n_D' = \sum_{m=1}^{[D/2]} \frac{D!}{(D-2m)!\,m!\,(m+1)!} \tag{A3}$$

Utilizing these formulas, one obtains, for the narrower strips

$$\begin{aligned} n_D &= 2,\ 5,\ 12,\ 30,\ 76,\ 196,\ 512,\ 1332,\ 3610 \\ n_D' &= 1,\ 3,\ 8,\ 20,\ 50,\ 126,\ 322,\ 834,\ 2187 \\ D &= 2,\ 3,\ 4,\ 5,\ 6,\ 7,\ 8,\ 9,\ 10 \end{aligned} \tag{A4}$$

Hence numerical results through at least $D = 7$ are feasible by machine. Taking into account the reflection symmetry of strips, the T_t matrix can be advantageously blocked into two approximately equal pieces (in fact, for the case of a walk and D even, the two pieces are each exactly $n_D/2$ by $n_D/2$, while for the case of a cycle and D odd, the two pieces are exactly $n_D'/2$ by $n_D'/2$). Further, since the fraction of nonzero matrix elements in T_t for walks is found to be 0.600, 0.417, 0.274, and 0.180 for $D = 3, 4, 5$, and 6, it appears that these matrices may be rather sparse for larger D. Then, utilizing special techniques for sparse matrices, strips through widths of about $D = 9$ might be treated.

APPENDIX B. INEQUALITIES ON EIGENVALUES

In this appendix we establish some relations among the maximum eigenvalues $\lambda_t(D)$ and $\lambda_t'(D)$ for strips of various widths D. The generating functions of (2.8) and (6.3) are written, with their width dependence explicitly indicated,

$$G_x(t, D) = \sum_w^D t^{l(w)}, \qquad G_x'(t, D) = \sum_c^D t^{l(c)} \tag{B1}$$

Further, we shall presume that $0 \leqslant t \leqslant 1$. Here the w sum is over fixed-end walks with a horizontal span of x and a length of $l(w)$, while the c sum is over cycles with a span of x and $l(c)$ steps. Now two fixed-end walks w_a and w_b, each of the same span x but on strips of widths D_a and D_b, may be combined together to give a single self-avoiding cycle c_{ab} of span $x + 2$ on a strip of width

$D_a + D_b$ as follows: first, place the horizontal strips one above the other with w_a directly over w_b; second, extend the beginning of each walk one step to the left and the ending of each one step to the right; and third, join these new beginnings by a series of vertical steps and similarly join the new endings. This resulting cycle c_{ab} has a length greater than the sum of the walk lengths for w_a and w_b; however,

$$l(c_{ab}) \leqslant l(w_a) + l(w_b) + 2(D_a + D_b + 1) \tag{B2}$$

so that

$$t^{l(c_{ab})} \geqslant t^{l(w_a)} + l(w_b) + 2(D_a + D_b + 1) \tag{B3}$$

Then, also noting that each distinct pair of walks gives a distinct cycle c_{ab}, we have

$$t^{2(D_a+D_b+1)}G_x(t, D_a)G_x(t, D_b) \leqslant \sum_{c_{ab}} t^{l(c_{ab})} \leqslant G'_{x+2}(t, D_a + D_b) \tag{B4}$$

Now these generating functions approach their asymptotic forms to within a factor approaching unity as $x \to \infty$. Thus factors close to 1 (and satisfying $f_a < 1, f_b < 1, f > 1$) can be found such that

$$\begin{aligned} G_x(t, D_a) &> f_a a_t(D_a)\{\lambda_t(D_a)\}^x \\ G_x(t, D_b) &> f_b a_t(D_b)\{\lambda_t(D_b)\}^x \\ G_x'(t, D_a + D_b) &< f a_t'(D_a + D_b)\{\lambda_t'(D_a + D_b)\}^x \end{aligned} \tag{B5}$$

for x sufficiently large, say $x > x_f$. Then

$$\begin{aligned} \left\{\frac{\lambda_t(D_a)\lambda_b(D_b)}{\lambda_t'(D_a + D_b)}\right\}^x &\leqslant t^{-2(D_a+D_b+1)} \frac{a_t'(D_a + D_b)}{a_t(D_a)a_t(D_b)} \frac{f}{f_a f_b} \\ &\quad \times \{\lambda_t'(D_a + D_b)\}^2, \qquad x > x_f \end{aligned} \tag{B6}$$

But the ratio of λ's raised to the xth power must be no greater than 1, for otherwise a sufficiently large power x could be found such that the left-hand side of (B6) would exceed the x-independent right-hand side. Therefore

$$\lambda_t(D_a)\lambda_t(D_b) \leqslant \lambda_t'(D_a + D_b) \tag{B7}$$

which is one of the desired relations.

A second relation is obtained if we note that a walk w_a and a cycle c_b, each with equal spans x but on strips of widths D_a and D_b, may be combined to give a single walk w_{ab} on a strip of width $D_a + D_b$. The combining process is as follows: first, place the walk directly above the cycle; second, delete a vertical step at the left extreme of the cycle and replace it by two horizontal steps each extending to the left from the pair of sites between which the vertical step was removed; third, extend the left end of the walk one step to the left; and fourth, join the new left end of the walk on the upper strip with the upper left end on the lower strip, by adding a series of vertical bonds. Following a procedure similar to that which led to (B7), we find

$$\lambda_t(D_a)\lambda_t'(D_b) \leqslant \lambda_t(D_a + D_b) \tag{B8}$$

Our third relation uses a process where cycles c_a and c_b of the same span on strips of widths D_a and D_b are combined to give a single cycle on a strip of width $D_a + D_b$. In this process two vertical bonds, one each from the left extremes of the cycles c_a and c_b are removed, to give at this intermediate stage two walks; the top and bottom ends are extended two steps to the left and joined together by a sequence of vertical bonds, while the two central ends are extended one step to the left and joined together. This process ultimately leads to

$$\lambda_t'(D_a)\lambda_t'(D_b) \leqslant \lambda_t'(D_a + D_b), \qquad 0 \leqslant t \leqslant 1 \tag{B9}$$

Clearly (B7)–(B9) are provable not only for rather general strips, but for cylinders and tubes as well.

A final type of relation considered in this appendix concerns bounds for $G_x(1, D)$ and $G_x'(1, D)$, the numbers of walks and cycles with span x. Letting z be the maximum coordination number of a site, we see that there are no more than $z(z - 1)/2$ ways in which two different links attached to a site can be occupied. Further, the number of ways in which zero or two occupied links can be independently assigned to each site within a span of x is

$$[1 + \tfrac{1}{2}z(z - 1)]^{xD} \equiv \xi^{xD} \tag{B10}$$

But to generate a walk or cycle the assignment for each site is not independent, so that

$$G_x(1, D) \leqslant \xi^{xD}, \qquad G_x'(1, D) \leqslant \xi^{xD} \tag{B11}$$

Finally considering the large-x behavior of these generating functions, we are led to

$$\lambda_t(D) \leqslant \lambda_1(D) \leqslant \xi^D, \qquad \lambda_t'(D) \leqslant \lambda_1'(D) \leqslant \xi^D \tag{B12}$$

Although these rather crude bounds of (B12) can rather easily be improved upon, it is sufficient for our present purposes that ξ is simply independent of the strip width D.

APPENDIX C. THEOREMS FOR THE $D \to \infty$ LIMIT

In this appendix we use the various bounds of (B7)–(B9) and (B12) to establish some theorems concerning changes with strip width D. Throughout the discussion here we presume that $0 \leqslant t \leqslant 1$.

First we utilize (B9) and (B12) to obtain

$$\begin{gathered} \ln[\xi^D/\lambda_t'(D)] \geqslant 0 \\ \ln[\xi^{D_a}/\lambda_t'(D_a)] + \ln[\xi^{D_b}/\lambda_t'(D_b)] \geqslant \ln[\xi^{D_a+D_b}/\lambda_t(D_a + D_b)] \end{gathered} \tag{C1}$$

Thus $\ln[\xi^D/\lambda_t'(D)]$ satisfies the conditions of being a nonnegative subadditive function of D (see, e.g., Ref. 20), and for such functions it is well known that the limit

$$\lim_{D\to\infty} \frac{1}{D} \ln \frac{\xi^D}{\lambda_t'(D)} \tag{C2}$$

exists. Hence the limit

$$\lim_{D\to\infty} \frac{1}{D} \ln \lambda_t'(D) \equiv \omega_t' \tag{C3}$$

also exists.

Now utilizing (B8), then (B7), we obtain

$$\lambda_t(D_a + D_b + 1) \geqslant \lambda_t(D_a)\lambda_t'(D_b + 1) \geqslant \lambda_t(D_a)\lambda_t(D_b)\lambda_t(1) \tag{C4}$$

In addition, noting $\lambda_t(1) = t$ and using (B12), we obtain

$$\ln \frac{\xi^{D-1}}{t\lambda_t(D)} \geqslant 0, \qquad \ln \frac{\xi^{D_a-1}}{t\lambda_t(D_a)} + \ln \frac{\xi^{D_b-1}}{t\lambda_t(D_b)} \geqslant \ln \frac{\xi^{D_a+D_b-2}}{t\lambda_t(D_a + D_b + 1)} \tag{C5}$$

so that $\ln[\xi^D/t\lambda_t(D + 1)]$ is a nonnegative subadditive function of D. Hence the limit

$$\lim_{D\to\infty} \frac{1}{D} \ln \frac{\xi^D}{t\lambda_t(D + 1)} \tag{C6}$$

exists, which in turn implies that the limit

$$\lim_{D\to\infty} \frac{1}{D} \ln \lambda_t(D) \equiv \omega_t \tag{C7}$$

exists, too.

Next let us note that (B7), with $D_a = 1$ and $D_b = D$, may be written as

$$\frac{\ln t}{D} + \frac{\ln \lambda_t(D)}{D} \leqslant \frac{\ln \lambda_t'(D + 1)}{D} \tag{C8}$$

Hence, taking the limit of large D yields $\omega_t \leqslant \omega_t'$. But similarly considering (B8) with $D_a = 1$ and $D_b = D$ leads us to $\omega_t' \leqslant \omega_t$. Thus

$$\omega_t' = \omega_t \tag{C9}$$

That ω_t and ω_t' take the same value, even at $t = 1/\kappa(\infty)$ or $t = 1/\kappa'(\infty)$, suggests that $\kappa(D)$ and $\kappa'(D)$ might both approach the same limit for large D.

To show that this is in fact the case, we first note that since $\{\kappa(D)\}^l$ essentially counts walks of length l, $\kappa(D)$ must monotonically increase as D increases and must be bounded by the coordination number z. Thus the limit $\kappa(\infty)$ exists, and similarly the limit $\kappa'(\infty)$ exists. Now taking $t = 1/\kappa(\infty)$ and taking the limit of large $D = D_a = D_b$ in Eqs. (B7) and (B8) leads to $1 \leqslant \lambda'_{1/\kappa(\infty)}(\infty)$ and $\lambda'_{1/\kappa(\infty)}(\infty) \leqslant 1$, respectively. Thus $\lambda'_{1/\kappa(\infty)}(\infty) = 1$, which implies

$$\kappa'(\infty) = \kappa(\infty) \tag{C10}$$

This result is similar to that of Hammersly,[15] although the present result applies on a variety of types of lattices and is established in a rather different manner. In addition, the connective constants $\kappa(\infty)$ and $\kappa'(\infty)$ technically differ from Hammersly's in that the limits as strip width $D \to \infty$ and length $l \to \infty$ are taken in the opposite order.

The existence of the limits for ω_t and $\omega_{t'}$ along with their equality and (C10) constitute the major results of this appendix. These results suggest that $\lambda_t(D)$ and $\lambda_t'(D)$ behave similarly for large D, but in fact the similarity is stronger than these results indicate. For, suppose

$$\lambda_t(D) \approx cD^{\gamma_t}\omega_t^{\,D}, \qquad \lambda_t'(D) \approx c'D^{\gamma_t'}\omega_t^{\,D} \tag{C11}$$

Then (C7) and (C8) with $D_a = 1$ and $D_b = D$ lead to

$$D^{\gamma_t - \gamma_t'} \lesssim \frac{c'}{ct}\left(\frac{D+1}{D}\right)^{\gamma_t'} \omega_t, \qquad D^{\gamma_t' - \gamma_t} \lesssim \frac{c}{c't}\left(\frac{D+1}{D}\right)^{\gamma_t} \omega_t \tag{C12}$$

Considering the behavior of these equations for large D, we then find $\gamma_t - \gamma_t' \leqslant 0$ and $\gamma_t' - \gamma_t \leqslant 0$, so that

$$\gamma_t = \gamma_t' \tag{C13}$$

Thus the behavior of $\lambda_t(D)$ and $\lambda_t'(D)$ should converge together rather rapidly as D increases. This then further suggests that their derivatives with respect to t should behave similarly for large D, and hence also $\mu(D)$ and $\mu'(D)$ as well as $\nu(D)$ and $\nu'(D)$.

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