

New Lower Bounds on the Self-Avoiding-Walk Connective Constant

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We give an elementary new method for obtaining rigorous lower bounds on the connective constant for self-avoiding walks on the hypercubic lattice \mathbb{Z}^d . The method is based on loop erasure and restoration, and does not require exact enumeration data. Our bounds are best for high d , and in fact agree with the first four terms of the $1/d$ expansion for the connective constant. The bounds are the best to date for dimensions $d \geq 3$, but do not produce good results in two dimensions. For $d = 3, 4, 5$, and 6 , respectively, our lower bound is within 2.4%, 0.43%, 0.12%, and 0.044% of the value estimated by series extrapolation.

KEY WORDS: Self-avoiding walk; connective constant; loop erasure; random walk; $1/d$ expansion.

1. INTRODUCTION

An n -step self-avoiding walk on the hypercubic lattice \mathbb{Z}^d is a sequence $\omega = (\omega(0), \omega(1), \dots, \omega(n))$ of points in \mathbb{Z}^d , with $\omega(i)$ and $\omega(i+1)$ separated by Euclidean distance one, subject to the constraint that $\omega(i) \neq \omega(j)$ for $i \neq j$. Unless otherwise stated, we take $\omega(0) = 0$. The self-avoiding walk provides a model of a polymer molecule with excluded volume. Also, its equivalence to the $N=0$ limit of the N -vector model has made it an important test case in the theory of critical phenomena.

Let c_n denote the number of n -step self-avoiding walks. It has been known for almost 40 years⁽¹⁾ that the limit $\mu = \lim_{n \rightarrow \infty} c_n^{1/n}$ exists and is

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finite and positive. Moreover, the subadditivity argument showing the existence of this limit also shows that $\mu = \inf_{n \geq 1} c_n^{1/n}$. This limit is known as the *connective constant*, and is the analogue of a critical temperature for the N -vector model. Roughly speaking, μ measures the number of sites available for the next step of a long self-avoiding walk. The connective constant is admittedly of lesser interest than the critical exponents, because it is lattice-dependent, while the critical exponents are universal. Nevertheless, much work has been done in finding rigorous upper and lower bounds for the connective constant, principally on two- and three-dimensional lattices. A review of work through 1982 is given by Guttmann.⁽²⁾

Recently, two of us^(3,4) proved that the critical exponents for self-avoiding walks in dimensions $d \geq 5$ take their mean-field values ($\gamma = 1$, $\nu = 1/2$, $\eta = 0$). One key ingredient in this proof was an accurate numerical lower bound on the connective constant μ . Unfortunately, we were unable to prove such a numerical bound with existing methods; in fact the previous methods give estimates which deteriorate as $d \rightarrow \infty$ (see Section 6). Therefore, we were led to develop a new method for obtaining lower bounds on μ , using loop erasure and restoration. This method (with the improvements presented here) provides bounds that agree with the first four terms of the $1/d$ expansion; for $d \geq 4$ they are within 0.43% of the best numerical estimate of μ , and even for $d = 3$ they are within 2.39% (greatly improving the best previous lower bounds). We therefore thought it worthwhile to develop these methods in detail; that is the goal of the present paper. The method presented here involves a conceptual simplification of the methods used in ref. 4, and also leads to better lower bounds. Remarkably, even the most elementary of our new methods leads to a better lower bound in $d = 3$ than has been obtained previously, including the enumeration bound 4.352 of ref. 2. Table I summarizes our best bounds and compares them to previously obtained bounds on μ .

Table I. Rigorous Lower and Upper Bounds on the Hypercubic-Lattice Connective Constant μ , Together with Estimates of Actual Values, for Dimensions 2, 3, 4, 5, 6^a

d	Previous bound	This work	Estimate	Upper bound
2	2.62002 ⁽⁵⁾	2.305766	2.6381585(10) ^(7,8)	2.69576 ⁽⁶⁾
3	4.43733 ⁽⁴⁾	4.572140	4.683907(22) ⁽⁹⁾	4.756 ⁽⁶⁾
4	6.71800 ⁽⁴⁾	6.742945	6.7720(5) ⁽¹⁰⁾	6.832 ⁽⁶⁾
5	8.82128 ⁽⁴⁾	8.828529	8.8386(8) ⁽¹¹⁾	8.881 ⁽⁶⁾
6	10.871199 ⁽⁴⁾	10.874038	10.8788(9) ⁽¹¹⁾	10.903 ⁽⁶⁾

^a Errors in the last digit(s) are shown in parentheses (numerals in superscript parentheses are reference numbers).

The evaluation of our bounds requires some numerical computation, for which we have obtained rigorous error estimates. All numerical values reported in this paper are accurate up to rounding of the last digit, except for lower bounds on μ , which have been truncated so as to provide true lower bounds.

Our methods can be applied to SAWs on any regular lattice. But for simplicity we restrict attention here to the hypercubic lattice \mathbb{Z}^d .

The plan of this paper is as follows: In Section 2 we describe the method of loop erasure and restoration, and systematize the lower bounds on μ that can be obtained from it. These bounds involve generating functions of random walks with taboo sets, and in Section 3 we show how these taboo generating functions can be computed in terms of the massless-free-field lattice propagator. In Section 4 we discuss some aspects of the lower bounds on μ obtained. In Section 5 we remark on a different method for proving lower bounds on μ , based on comparison with the Ising model. In Section 6 we show that our best bounds agree with the $1/d$ expansion for μ through order d^{-2} . In the Appendix we summarize our methods for the rigorous numerical calculation of quantities involving the free-field lattice propagator, and give $1/d$ expansions for various simple-random-walk quantities.

In a separate paper⁽¹²⁾ two of us give a rigorous $1/d$ expansion for μ through order d^{-3} , along with a similar expansion for the critical point of nearest-neighbor Bernoulli bond percolation.

2. LOOP ERASURE AND RESTORATION

2.1. Definitions

To describe our loop-erasure-and-restoration method, we need to introduce a number of generating functions. For this we need several definitions.

An n -step walk ($n \geq 0$) is an ordered sequence $\omega = (\omega(0), \dots, \omega(n))$ of points in \mathbb{Z}^d such that each point is a nearest neighbor of its predecessor, i.e., $|\omega(i) - \omega(i-1)| = 1$ for $1 \leq i \leq n$. We denote the number of steps in a walk ω by $|\omega|$. The walk ω is said to be a *memory- τ walk* if $\omega(i) \neq \omega(j)$ for all i, j satisfying $0 < |i - j| \leq \tau$. We denote by $\Omega_\tau(x, y)$ the union over all $n = 0, 1, 2, \dots$ of the set of memory- τ n -step walks from $\omega(0) = x$ to $\omega(n) = y$. Thus, $\Omega_0(x, y)$ is the set of all walks from x to y , $\Omega_2(x, y)$ is the set of all walks having no immediate reversals, $\Omega_4(x, y)$ is the set of all walks having neither immediate reversals nor elementary squares, and so on. The elements of Ω_0 are called *simple* (or *ordinary*) *random walks*. We denote by $\Omega(x, y) \equiv \bigcap_{\tau=0}^{\infty} \Omega_\tau(x, y)$ the set of all self-avoiding walks (of any number

of steps) which begin at x and end at y . Finally, we denote by $\Omega(x, \bullet) \equiv \bigcup_{y \in \mathbb{Z}^d} \Omega(x, y)$ the set of all self-avoiding walks (of any number of steps) which begin at x and end anywhere.

A walk $\omega = (\omega(0), \dots, \omega(n))$ is said to be a *loop* if $\omega(0) = \omega(n)$. We write $\mathcal{L}_\tau(x) = \Omega_\tau(x, x)$ for the set of memory- τ loops starting and ending at x . Note that such loops are allowed to pass through x many times, and that $\mathcal{L}_\tau(x)$ includes the zero-step walk $\omega = (x)$. Note also that the memory- τ constraint does *not* apply mod n : for example, $\omega(n-1)$ is permitted to equal $\omega(1)$.

Given a nonnegative real number β , we define the *generating function* (or *two-point function* or *Green function*) for memory- τ walks,

$$C_\tau(x, y; \beta) = \sum_{\omega \in \Omega_\tau(x, y)} \beta^{|\omega|} \tag{2.1}$$

and for self-avoiding walks,

$$G(x, y; \beta) = \sum_{\omega \in \Omega(x, y)} \beta^{|\omega|} \tag{2.2}$$

Denoting the number of n -step memory- τ walks (starting at the origin and ending anywhere) by $c_{n,\tau}$, we also define the susceptibilities

$$\chi_\tau(\beta) \equiv \sum_{x \in \mathbb{Z}^d} C_\tau(0, x; \beta) = \sum_{n=0}^\infty c_{n,\tau} \beta^n \tag{2.3}$$

and

$$\chi(\beta) \equiv \sum_{x \in \mathbb{Z}^d} G(0, x; \beta) = \sum_{n=0}^\infty c_n \beta^n \tag{2.4}$$

For $\beta \geq 0$ the sums (2.1)–(2.4) are always well defined, although they will be $+\infty$ for sufficiently large β . In fact, since $\lim_{n \rightarrow \infty} c_n^{1/n} = \mu$ and $c_n \geq \mu^n$, we have

$$(1 - \beta\mu)^{-1} \leq \chi(\beta) < \infty \quad \text{for } 0 \leq \beta < \mu^{-1} \tag{2.5a}$$

$$\chi(\beta) = \infty \quad \text{for } \beta \geq \mu^{-1} \tag{2.5b}$$

Similarly, the same subadditivity argument which implies existence of the limit defining μ can also be used to prove that

$$\mu_\tau \equiv \lim_{n \rightarrow \infty} c_{n,\tau}^{1/n} = \inf_{n \geq 1} c_{n,\tau}^{1/n} \tag{2.6}$$

for all $0 \leq \tau < \infty$. It follows from (2.6) that

$$(1 - \beta\mu_\tau)^{-1} \leq \chi_\tau(\beta) < \infty \quad \text{for } 0 \leq \beta < \mu_\tau^{-1} \tag{2.7a}$$

$$\chi_\tau(\beta) = \infty \quad \text{for } \beta \geq \mu_\tau^{-1} \tag{2.7b}$$

Clearly $\mu_0 \geq \mu_2 \geq \mu_4 \geq \dots \geq \mu$. A subadditivity argument can be used to show that $\lim_{\tau \rightarrow \infty} \mu_\tau = \mu$ (see, for example, Lemma 1.2.3 of ref. 13). Since $c_{n,0} = (2d)^n$ and $c_{n,2} = 2d(2d-1)^{n-1}$, we have $\mu_0 = 2d$ and $\mu_2 = 2d-1$. The value of μ_4 is shown in ref. 14 to be given by the unique positive root of the equation

$$x^3 - 2(d-1)x^2 - 2(d-1)x - 1 = 0 \tag{2.8}$$

Although methods are described in ref. 14 by which in principle μ_τ can be computed for $\tau \geq 6$, in practice these methods are difficult to carry out in general dimensions.

To compute our lower bounds on μ we will need the numerical values of $C_\tau(0, x; \mu_\tau^{-1})$ for a finite collection of sites x . For $\tau = 0$ this is given by the well-known Fourier integral (“free-field lattice propagator”)

$$C_0(0, x; \beta) = \int_{[-\pi, \pi]^d} \frac{d^d k}{(2\pi)^d} \frac{e^{ik \cdot x}}{1 - 2d\beta\hat{D}(k)} \tag{2.9}$$

where

$$\hat{D}(k) \equiv \frac{1}{d} \sum_{i=1}^d \cos k_i, \quad k = (k_1, \dots, k_d) \tag{2.10}$$

This expression is valid for $0 \leq \beta \leq 1/(2d)$. At the critical point $\beta = \mu_0^{-1} = 1/(2d)$, the integral (2.9) is finite for $d > 2$ but infinite for $d \leq 2$. An effective means for computing the numerical values of (2.9) to high precision for $d > 2$ is discussed in the Appendix.

To study $d \leq 2$ (of course it is $d = 2$ which is of interest here), we introduce the *potential kernel*^(15,16)

$$\Delta_0(x; \beta) \equiv C_0(0, 0; \beta) - C_0(0, x; \beta) \tag{2.11}$$

which remains finite in all dimensions, as $\beta \uparrow 1/(2d)$. Indeed, it is an immediate consequence of the Lebesgue dominated convergence theorem that $\Delta_0(x) \equiv \lim_{\beta \uparrow 1/(2d)} \Delta_0(x; \beta)$ is given by the absolutely convergent Fourier integral

$$\Delta_0(x) = \int_{[-\pi, \pi]^d} \frac{d^d k}{(2\pi)^d} \frac{1 - \cos(k \cdot x)}{1 - \hat{D}(k)} \tag{2.12}$$

In dimension $d=1$, an easy calculation yields $\Delta_0(x) = |x|$. Remarkably, in dimension $d=2$ this integral can also be performed analytically for any x (ref. 15, Section 15): for example, $\Delta_0(e_1) = 1$, $\Delta_0(2e_1) = 4 - 8/\pi$, and $\Delta_0(e_1 + e_2) = 4/\pi$. (Here e_1, e_2 are the canonical unit vectors in \mathbb{Z}^2 .)

For $\tau = 2$ the two-point function can be evaluated using the identity

$$C_2(0, x; \beta) = \frac{1 - \beta^2}{1 + (2d - 1)\beta^2} C_0\left(0, x; \frac{\beta}{1 + (2d - 1)\beta^2}\right) \quad (2.13)$$

which was derived using convolution methods in ref. 17. At the critical point $\beta = \mu_2^{-1} = 1/(2d - 1)$, this reduces to

$$C_2\left(0, x; \frac{1}{2d - 1}\right) = \frac{2d - 2}{2d - 1} C_0\left(0, x; \frac{1}{2d}\right) \quad (2.14)$$

Unfortunately, we do not know how to compute the numerical values of $C_\tau(0, x; \mu_\tau^{-1})$ for $\tau \geq 4$; because of this we primarily restrict attention in what follows to $\tau = 0, 2$.

We remark that unlike the finite-memory case, it is believed that the self-avoiding-walk critical two-point function $G(0, x; \mu^{-1})$ is finite for all x in all dimensions, including $d = 1, 2$. This has been proven for $d \geq 5$ in refs. 3 and 4—and of course it is trivial in $d = 1$ —but it remains unproven in dimensions 2, 3, and 4. It has been known for some time that $G(0, x; \beta) = \infty$ for $\beta > \mu^{-1}$.⁽¹⁸⁾

2.2. Identities

We would like now to establish an inequality relating the two-point functions (2.1) and (2.2). For this, we recall the following loop-erasure algorithm, which has been studied in detail by Lawler.⁽¹⁶⁾ Given a walk $\omega \in \Omega_\tau(x, y)$, we can associate to it a (typically shorter) self-avoiding walk $\rho \in \Omega(x, y)$ by erasing loops in an appropriate sequence. We begin by finding the *last* time t_1 such that $\omega(t_1) = \omega(0) = x$, and then erase the sites $\omega(1), \omega(2), \dots, \omega(t_1)$ from ω , producing a walk which we call $\rho^{(1)}$. In other words, we have erased the largest possible loop at the site x , namely $L_0 = (\omega(0), \dots, \omega(t_1))$. (If ω does not visit x more than once, then we can think of having erased a trivial loop.) The walk $\rho^{(1)}$ does not visit x more than once, but it may visit the site $\rho^{(1)}(1)$ repeatedly. Let t_2 denote the *last* time that $\rho^{(1)}(t_2) = \rho^{(1)}(1)$, and erase the sites $\rho^{(1)}(2), \dots, \rho^{(1)}(t_2)$ as before. Note that the erased loop $L_1 = (\rho^{(1)}(1), \dots, \rho^{(1)}(t_2))$ cannot pass through $\omega(0) = x$. This procedure gives rise to a walk $\rho^{(2)}$, which does not visit $\rho^{(2)}(0)$ or $\rho^{(2)}(1)$ more than once. We repeat this procedure successively for

$\rho^{(2)}, \rho^{(3)}$, etc., until arriving at a result which is devoid of loops, or in other words, which is self-avoiding. For each τ , this defines a one-to-one mapping from $\Omega_\tau(x, y)$ into the set $\mathcal{R}_\tau(x, y)$ whose elements are of the form $(\rho, L_0, L_1, \dots, L_n)$, where $\rho \in \Omega(x, y)$ is an n -step self-avoiding walk (for some n) and each $L_i \in \mathcal{L}_\tau(\rho(i))$. We refer to ρ as the self-avoiding backbone of ω .

In fact it is not difficult to see precisely what the image of this mapping is, or in other words, to see exactly which elements of $\mathcal{R}_\tau(x, y)$ can be produced by this procedure, at least for $\tau = 0$ or 2 . One way to do so is to try to reverse the procedure, by beginning with an element of $\mathcal{R}_\tau(x, y)$ and associating to it the walk ω which is given by first following the steps of L_0 , then taking the first step of ρ , then taking the steps of L_1 , then taking the second step of ρ , and so on. For $\tau = 0$, each possible simple random walk from x to y can be obtained in precisely one way by this procedure, provided that the loop L_i attached at $\rho(i)$ does not intersect any of the previous sites $\rho(0), \dots, \rho(i - 1)$, for all $i = 1, \dots, |\rho|$. For $\tau = 2$ the situation is similar but slightly more involved: the attached loops must again avoid the previous sites as above, but in addition the *next-to-last* site of the loop L_i must avoid the *next* site $\rho(i + 1)$ of the backbone (except of course for $i = |\rho|$, when this constraint is vacuous). For memories $\tau \geq 4$ the situation is more complicated, due to the presence of interloop restrictions, and we refrain from entering into details.

The above discussion can be summarized with identities, which are stated below for $\tau = 0$ and $\tau = 2$. To state the identities we first define the *generating functions with taboo set A*:

$$C_\tau^A(x, y; \beta) = \sum_{\omega \in \Omega_\tau(x, y): \omega \cap A = \emptyset} \beta^{|\omega|} \tag{2.15}$$

$$\tilde{C}_\tau^{A,z}(x, y; \beta) = \sum_{\substack{\omega \in \Omega_\tau(x, y): \omega \cap A = \emptyset \\ \omega(|\omega| - 1) \neq z}} \beta^{|\omega|} \tag{2.16}$$

In both cases the sum is over walks which avoid the set of sites A ; in the latter case we impose the additional restriction that the next-to-last site of ω is not z . Clearly, $\tilde{C}_\tau^{A,z}(x, y; \beta) \leq C_\tau^A(x, y; \beta)$, and both quantities are decreasing functions of τ and of the set A . We also define $\rho[0, j)$ to be the set of sites $\{\rho(0), \dots, \rho(j - 1)\}$, for $j = 1, \dots, |\rho|$, and let $\rho[0, 0)$ be the empty set. We can then write the *identities*

$$C_0(x, y; \beta) = \sum_{\rho \in \Omega(x, y)} \beta^{|\rho|} \prod_{j=0}^{|\rho|} C_0^{\rho[0, j)}(\rho(j), \rho(j); \beta) \tag{2.17}$$

$$C_2(x, y; \beta) = \sum_{\rho \in \Omega(x, y)} \beta^{|\rho|} \prod_{j=0}^{|\rho|} \tilde{C}_2^{\rho[0, j), \rho(j+1)}(\rho(j), \rho(j); \beta) \tag{2.18}$$

where the $j = |\rho|$ term in this last equation should be interpreted as $C_2^{\rho[0,j]}$ [since the site $\rho(j+1)$ is nonexistent]. For higher memories it is less straightforward to write the analogous identities, because of the interloop constraints; but by dropping those constraints we have immediately the inequalities

$$C_\tau(x, y; \beta) \leq \sum_{\rho \in \Omega(x, y)} \beta^{|\rho|} \prod_{j=0}^{|\rho|} C_\tau^{\rho[0,j]}(\rho(j), \rho(j); \beta) \quad \text{for } \tau \geq 0 \quad (2.19)$$

$$C_\tau(x, y; \beta) \leq \sum_{\rho \in \Omega(x, y)} \beta^{|\rho|} \prod_{j=0}^{|\rho|} \tilde{C}_\tau^{\rho[0,j], \rho(j+1)}(\rho(j), \rho(j); \beta) \quad \text{for } \tau \geq 2 \quad (2.20)$$

2.3. Inequalities (First Version)

It is certainly difficult to analyze the right sides of (2.17)–(2.20) exactly, but we wish to do something less ambitious: we will obtain upper bounds by relaxing the avoidance constraints on the attached loops. In particular, we can obtain upper bounds by replacing the restriction that the loop attached at $\rho(j)$ avoid all of $\rho[0, j]$ by the weaker restriction that it avoid only the smaller set

$$\rho[j-k, j] \equiv \{\rho(j-k), \dots, \rho(j-1)\} \quad (2.21)$$

where k is a (small) fixed nonnegative integer. [For $k=0$, $\rho[j, j] = \emptyset$; and for $k > j$ we omit the nonexistent points $\rho(i)$ with $i < 0$.] Applying this to (2.17)/(2.19) leads to the inequality

$$C_\tau(x, y; \beta) \leq \sum_{\rho \in \Omega(x, y)} \beta^{|\rho|} \prod_{j=0}^{|\rho|} C_\tau^{\rho[j-k,j]}(\rho(j), \rho(j); \beta) \quad (2.22)$$

for any $\tau, k \geq 0$. Now the set of sites $\rho[j-k, j]$ is (for $j \geq k$) simply the range of a $(k-1)$ -step self-avoiding walk starting at a nearest neighbor of $\rho(j)$; so we can get a further upper bound by taking the maximum over all such sets. Taking into account translation invariance, this leads us to define

$$A_\tau(k; \beta) = \max_A C_\tau^A(0, 0; \beta) \quad (2.23)$$

where the maximum ranges over all k -element sets A which are the range of a $(k-1)$ -step self-avoiding walk starting at a nearest neighbor of the

origin. This maximum is obviously a nonincreasing function of τ and k . Clearly we have⁴

$$\begin{aligned}
 C_\tau(x, y; \beta) &\leq \sum_{\rho \in \Omega(x, y)} \beta^{|\rho|} A_\tau(0; \beta) A_\tau(1; \beta) \cdots A_\tau(k-1; \beta) A_\tau(k; \beta)^{|\rho|+1-k} \\
 &\equiv \alpha_{\tau, k}(\beta) G(x, y; \beta A_\tau(k; \beta))
 \end{aligned}
 \tag{2.24}$$

where

$$\alpha_{\tau, k}(\beta) \equiv \left[\prod_{i=0}^{k-1} A_\tau(i; \beta) \right] A_\tau(k; \beta)^{1-k}
 \tag{2.25}$$

Summing over $y \in \mathbb{Z}^d$, this gives

$$\frac{\chi_\tau(\beta)}{\alpha_{\tau, k}(\beta)} \leq \chi(\beta A_\tau(k; \beta))
 \tag{2.26}$$

This is our fundamental *loop-erasure-and-restoration inequality*, in its simplest form.

We shall argue below that

$$\lim_{\beta \uparrow \mu_\tau^{-1}} \frac{\chi_\tau(\beta)}{\alpha_{\tau, k}(\beta)} = \infty
 \tag{2.27}$$

for $\tau = 0, 2$, all $k \geq 0$, and all $d > 0$. We expect that (2.27) is true also for all $\tau \geq 4$, but we have not proved this, nor shall we make use of it. Given (2.27), it is now easy to obtain a lower bound on μ , in the following way. By (2.27) and (2.26), $\chi(\mu_\tau^{-1} A_\tau(k; \mu_\tau^{-1})) = +\infty$. But we know from (2.5a) that $\chi(x) < \infty$ for $x < 1/\mu$. We thus conclude that

$$\frac{A_\tau(k; \mu_\tau^{-1})}{\mu_\tau} \geq \frac{1}{\mu}
 \tag{2.28}$$

or in other words

$$\mu \geq \frac{\mu_\tau}{A_\tau(k; \mu_\tau^{-1})} \quad \text{for } \tau = 0, 2, \quad k \geq 0, \quad d > 0
 \tag{2.29}$$

The bound (2.29) would also follow for $\tau \geq 4$ if (2.27) were proven for such τ .

The claim (2.27) follows immediately from (2.7a) if $\alpha_{\tau, k}(\mu_\tau^{-1})$ is finite. And it follows easily from (2.25) that $\alpha_{\tau, k}(\mu_\tau^{-1})$ is finite precisely when

⁴ The terms with $|\rho| < k - 1$ here are being overcounted on the right-hand side, to simplify the form of the inequality.

$A_\tau(0; \mu_\tau^{-1}) = C_\tau(0, 0; \mu_\tau^{-1})$ is finite [recall that $A_\tau(i; \beta) \leq A_\tau(0; \beta)$ and $A_\tau(k; \beta) \geq 1$]. For $\tau = 0$ or 2 the finiteness of $C_\tau(0, 0; \mu_\tau^{-1})$ in dimensions $d > 2$ follows immediately from (2.9) and (2.14). This proves the claim (2.27) for $d > 2$. For $d \leq 2$, consider first $\tau = 0$. We have trivially that $A_0(k; \beta) \geq 1$. Also, it is well-known (see Section 3.1) that $A_0(1; \beta) \equiv C_0^{\{e\}}(0, 0; \beta)$ is uniformly bounded for $\beta \leq 1/(2d)$, in all dimensions; hence the same is true for $A_0(i; 1/(2d))$ for all $i \geq 1$. Finally, for $i = 0$ we have

$$A_0(0; \beta) = C_0(0, 0; \beta) \sim \begin{cases} \text{const} \times (1 - 2d\beta)^{-(2-d)/2} & \text{for } d < 2 \\ \text{const} \times \log(1 - 2d\beta) & \text{for } d = 2 \\ \text{const} & \text{for } d > 2 \end{cases} \quad (2.30)$$

as $\beta \uparrow 1/(2d)$. Hence in any dimension $d > 0$ we see from (2.7a) and (2.30) that $A_0(0; \beta)$ diverges more slowly than $\chi_0(\beta)$ as $\beta \uparrow 1/(2d)$; therefore, $\lim_{\beta \uparrow 1/(2d)} \chi_0(\beta)/\alpha_{0,k}(\beta) = \infty$. The same argument can be used for $\tau = 2$, using also (2.13).

We remark that another possible approach to bounds on μ of this type, which we will not pursue further, would be to substitute some $\beta < \mu_\tau^{-1}$ in (2.26), rather than $\beta = \mu_\tau^{-1}$, and then to optimize over β . This surely gives an improvement when $d = 2$ and $k = 0$, but it requires some μ -dependent *a priori* upper bound on $\chi(\beta)$, and the only available such bound is the very weak Hammersley–Welsh bound^(19,20) (for which explicit constants would be required).

To see explicitly what the bounds (2.29) entail, let us consider first the case $\tau = 0$, for which $\mu_0 = 2d$. Taking $k = 0$ and $k = 1$ gives $A_0(0; 1/(2d)) = C_0(0, 0; 1/(2d))$ and $A_0(1; 1/(2d)) = C_0^{\{e\}}(0, 0; 1/(2d))$ (by symmetry, where e is any neighbor of the origin), so (2.29) becomes

$$\mu \geq \frac{2d}{C_0(0, 0; 1/(2d))} \quad [k = 0] \quad (2.31)$$

$$\mu \geq \frac{2d}{C_0^{\{e\}}(0, 0; 1/(2d))} \quad [k = 1] \quad (2.32)$$

For a discussion of the relation between (2.31) and some previously known results, see Section 5. The denominator on the right side of (2.31) is infinite in dimension $d \leq 2$, but this defect is remedied in (2.32): in Section 3.1 we shall prove the identity

$$C_0^{\{e\}}(0, 0; 1/(2d)) = 2 - \frac{1}{C_0(0, 0; 1/(2d))} \leq 2 \quad (2.33)$$

in all dimensions. This already improves the method used in ref. 4, where an infinite denominator was always encountered for $d \leq 2$. In the trivial case $d = 1$, (2.32) gives the exact answer $\mu \geq 1$. For $d = 2$, (2.32) gives the rather poor bound $\mu \geq 2$. For $d = 3$, (2.32) already does better than all previously known bounds, yielding $\mu \geq 4.475817\dots$ In Section 3.1 we show how to carry out the computations at least in principle for arbitrary values of k , and we give explicit numerical results for $k = 0, 1, 2, 3, 4$ in dimensions $d = 2, 3, 4, 5, 6$. The resulting lower bounds on μ are tabulated in Table II. In Section 6.3 we study the behavior of these bounds as $d \rightarrow \infty$.

Next let us evaluate the bound (2.29) with memory $\tau = 2$. Here $\mu_2 = 2d - 1$. For $k = 0$, we conclude from (2.14) that

$$\mu \geq \frac{2d - 1}{C_2(0, 0; 1/(2d - 1))} = \frac{(2d - 1)^2}{2d - 2} \frac{1}{C_0(0, 0; 1/(2d))} \tag{2.34}$$

This bound is nontrivial for $d > 2$, and is a factor

$$\frac{(2d - 1)^2}{2d(2d - 2)} = 1 + \frac{1}{2d(2d - 2)} \tag{2.35}$$

better than the corresponding bound (2.31) based on $\tau = 0$. For $k = 1$ the situation is less simple: we will show in Section 3.2 that $C_2^{\{e\}}(0, 0; 1/(2d - 1))$ can be obtained by solving a linear system of three equations in three unknowns. In Section 3.2 we show in fact how to carry out the computations at least in principle for arbitrary values of k , and we give explicit numerical results for $k = 0, 1, 2, 3, 4$ in dimensions $d = 2, 3, 4, 5, 6$. The resulting lower bounds on μ are tabulated in Table II. In Section 6.3 we study the behavior of these bounds as $d \rightarrow \infty$.

2.4. Inequalities (Second Version)

The foregoing inequalities are based on constraining the attached loops L_i to avoid the *preceding* k sites of the backbone ρ . For any memory $\tau \geq 2$, we can improve these results by using (2.18)/(2.20), i.e., by taking into account the further constraint that the next-to-last site of the loop avoid the *next* site of the backbone. The analysis given previously can be repeated almost verbatim in this case. We introduce

$$\tilde{\lambda}_\tau(k; \beta) = \max_{A, e} \tilde{C}_\tau^{A, e}(0, 0; \beta) \tag{2.36}$$

where the maximum ranges over all k -element sets A which are the range of a $(k - 1)$ -step self-avoiding walk starting at a nearest neighbor of the

origin, and over all nearest neighbors e of the origin satisfying $e \notin A$. The analogue of (2.24) becomes⁵

$$C_\tau(x, y; \beta) \leq \sum_{\rho \in \Omega(x, y)} \beta^{|\rho|} A_\tau(0; \beta) \cdots A_\tau(k-1; \beta) \tilde{A}_\tau(k; \beta)^{|\rho| - k} A_\tau(k; \beta) \equiv \tilde{\alpha}_{\tau, k}(\beta) G(x, y; \beta \tilde{A}_\tau(k; \beta)) \tag{2.37}$$

where

$$\tilde{\alpha}_{\tau, k}(\beta) = \left(\prod_{i=0}^k A_\tau(i; \beta) \right) \tilde{A}_\tau(k; \beta)^{-k} \tag{2.38}$$

Arguing as before, we have

$$\mu \geq \frac{\mu_\tau}{\tilde{A}_\tau(k; \mu_\tau^{-1})} \quad \text{for } \tau = 2, \quad k \geq 0, \quad d > 0 \tag{2.39}$$

(and again we expect, but have not proved, that this bound holds for all $\tau \geq 2$).

We will apply (2.39) with $\tau = 2$, which requires evaluation of $\tilde{C}_2^{A, e}(0, 0; \mu_2^{-1})$. In Section 3.2 we will prove the identity

$$\tilde{C}_2^{A, e}(0, 0; \beta) = \frac{1}{1 - \beta^2} [C_2^A(0, 0; \beta) - \beta C_2^A(0, e; \beta)] \tag{2.40}$$

from which the bound (2.39) can be computed once we know the values of $C_2^A(0, 0; \mu_2^{-1})$ and $C_2^A(0, e; \mu_2^{-1})$.

The use of (2.40) involves two improvements on our earlier method.⁽⁴⁾ The first improvement is conceptual, in that the derivation here of (2.40) is simpler and avoids the combinatorial niceties encountered in ref. 4. The second is that our earlier method used only $|A| = 1$, and moreover constrained loops to avoid the previous backbone site only with their first and next-to-last sites, rather than entirely as in the methods of this paper.

Our method for numerically evaluating the denominators $A_0(k; \beta)$, $A_2(k; \beta)$, and $\tilde{A}_2(k; \beta)$ which appear in the lower bounds on μ is described in Section 3. The numerical bounds resulting from (2.29) with $\tau = 0, 2$ and (2.39) with $\tau = 2$ are given in Table II as a function of the parameters τ and k . We have restricted attention to $\tau = 0$ and $\tau = 2$ due to our inability to compute the numerical values of $A_\tau(k; \beta)$ or $\tilde{A}_\tau(k; \beta)$ for higher memories.

In Section 2.5 we will show how to improve on the bounds obtained so far.

⁵ Here we are overcounting by neglecting the avoidance of the next backbone site, for the first k sites of the backbone, to allow for a unified treatment of $|\rho| \leq k - 1$ and $|\rho| \geq k$.

Table II. The Lower Bounds on μ of (2.29) for $\tau=0, 2$ and of (2.39) for $\tau=2$, for $k=1, 2, 3, 4$, and the Optimized Bounds Using the Method of Section 2.5, for Dimensions $d=2, 3, 4, 5, 6$ ^a

(τ, k)	$d=2$	$d=3$	$d=4$	$d=5$	$d=6$
(0, 0)	0	3.956775	6.454386	8.648213	10.743414
(0, 1)	2	4.475817	6.704650	8.809186	10.862525
(0, 2)	2.161367	4.492416	6.706478	8.809464	10.862584
(0, 3)	2.234696	4.499126	6.706931	8.809501	10.862588
(0, 4)	2.275515	4.502565	6.707091	8.809509	10.862588
(2, 0)	0	4.121641	6.588853	8.756316	10.832942
(2, 1)	1.712626	4.441266	6.696516	8.806308	10.861210
(2, 2)	1.917318	4.457137	6.698205	8.806565	10.861265
(2, 3)	2.019782	4.463834	6.698632	8.806599	10.861268
(2, 4)	2.079398	4.467350	6.698783	8.806607	10.861269
($\tilde{2}$, 0)	0	4.245957	6.637585	8.780089	10.846669
($\tilde{2}$, 1)	1.976372	4.539419	6.737460	8.827159	10.873577
($\tilde{2}$, 2)	2.153350	4.552467	6.738907	8.827387	10.873627
($\tilde{2}$, 3)	2.239265	4.557994	6.739273	8.827417	10.873630
($\tilde{2}$, 4)	2.286245	4.560903	6.739404	8.827424	10.873631
(0, 2) _{opt}	2.195201	4.518652	6.715924	8.813103	10.864240
(0, 3) _{opt}	2.267128	4.526286	6.716713	8.813204	10.864257
(0, 4) _{opt}	2.305766	4.530282	6.716982	8.813224	10.864259
(2, 2) _{opt}	1.936810	4.476092	6.704487	8.808707	10.862112
(2, 3) _{opt}	2.038216	4.483773	6.705232	8.808801	10.862128
(2, 4) _{opt}	2.092741	4.487869	6.705488	8.808820	10.862130
($\tilde{2}$, 2) _{opt}	2.165878	4.562269	6.742085	8.828430	10.874022
($\tilde{2}$, 3) _{opt}	2.248707	4.568677	6.742721	8.828512	10.874036
($\tilde{2}$, 4) _{opt}	2.290302	4.572140	6.742945	8.828529	10.874038

^a The numerical values have been truncated to give rigorous lower bounds. The lower line of the table provides the best lower bounds, except for $d=2$. Some discussion of the table entries is given in Section 4.

2.5. Optimized Bounds

Our method thus far has been based on taking the *maximum* over possible geometries for the incoming walk (i.e., the set A) in (2.23) or (2.36). This procedure is costly, because typically we expect that the incoming two steps of the backbone will be bent rather than straight, but the maximum for the small values of $|A|$ we are using corresponds to a straight backbone. In fact, given that there are on average about μ possible steps for a self-avoiding walk, the proportion of straight to bent steps should be

roughly one to $\mu - 1$. (This is not exactly right, because the straight and bent steps have different probabilities for respecting self-avoidance; but it does indicate the expected order of magnitude.) In this section we show a way of partially taking this into account to obtain an improved bound. For concreteness, we consider the case of memory $\tau = 0$, with $k \equiv |A| = 2$.

Summing the identity (2.17) over $y \in \mathbb{Z}^d$, we have

$$\chi_0(\beta) = \sum_{\rho \in \Omega(0, \bullet)} \beta^{|\rho|} \prod_{j=0}^{|\rho|} C_0^{\rho^{[0,j]}}(\rho(j), \rho(j); \beta) \tag{2.41}$$

Relaxing the avoidance constraints on the attached loops, to $k = 2$, we obtain

$$\chi_0(\beta) \leq \sum_{\rho \in \Omega(0, \bullet)} \beta^{|\rho|} \prod_{j=0}^{|\rho|} C_0^{\rho^{[j-2,j]}}(\rho(j), \rho(j); \beta) \tag{2.42}$$

Our previous approach was to replace the quantities $C_0^{\rho^{[j-2,j]}}$ by the corresponding upper bounds based on using the *worst* two-element set A in place of $\rho^{[j-2, j]}$ [cf. (2.23)/(2.24)]. Now let us try instead to distinguish the two possible cases,

$A = \text{straight (i.e., congruent to } \{e_1, 2e_1\})$

$A = \text{bent (i.e., congruent to } \{e_1, e_1 + e_2\})$

Correspondingly, let us define

$$a \equiv C_0^{\{e_1, 2e_1\}}(0, 0; 1/(2d)) \tag{2.43a}$$

$$b \equiv C_0^{\{e_1, e_1 + e_2\}}(0, 0; 1/(2d)) \tag{2.43b}$$

We only consider the case of

$$0 < b < a < 2d \tag{2.44}$$

which is shown to be valid for our applications by numerical computation. It follows that⁶

$$\chi_0(\beta) \leq \sum_{\rho \in \Omega(0, \bullet)} \beta^{|\rho|} A_0(0; \beta) A_0(1; \beta) a^{l(\rho)} b^{|\rho| - 1 - l(\rho)} \tag{2.45}$$

where l denotes the number of straight vertices among $\rho(1), \dots, \rho(n - 1)$ (here $n \equiv |\rho|$). Defining

$$c_n(l) \equiv \#\{\rho \in \Omega(0, \bullet) : |\rho| = n, \#(\text{straight vertices in } \rho) = l\} \tag{2.46}$$

⁶ The terms with $|\rho| = 0, 1$ are here being overcounted on the right-hand side.

we can rewrite this as

$$\begin{aligned} \chi_0(\beta) &\leq A_0(0; \beta) A_0(1; \beta) \sum_{n=0}^{\infty} \sum_{l=0}^{n-1} c_n(l) \beta^n a^l b^{n-1-l} \\ &\equiv A_0(0; \beta) A_0(1; \beta) \sum_{n=0}^{\infty} \beta^n S(n; a, b) \end{aligned} \tag{2.47}$$

where

$$S(n; a, b) \equiv \sum_{l=0}^{n-1} c_n(l) a^l b^{n-1-l} \tag{2.48}$$

As in the preceding subsections, we will let $\beta \uparrow 1/(2d)$, and use the fact that

$$\lim_{\beta \uparrow 1/(2d)} \frac{\chi_0(\beta)}{A_0(0; \beta) A_0(1; \beta)} = +\infty \tag{2.49}$$

This together with (2.47) implies that

$$\limsup_{n \rightarrow \infty} S(n; a, b)^{1/n} \geq 2d \tag{2.50}$$

Therefore, if we can get upper bounds on $S(n; a, b)$ in terms of the $\{c_n\}$, then we will be able to deduce lower bounds on μ .

Example 1. Since $a > b > 0$, we have trivially

$$S(n; a, b) \leq c_n a^{n-1} \tag{2.51}$$

and hence

$$\limsup_{n \rightarrow \infty} S(n; a, b)^{1/n} \leq \mu a \tag{2.52}$$

Combining this with (2.50), we obtain $\mu \geq 2d/a$. This is, of course, our old bound (2.29) with $\tau = 0$, $k = 2$, based on using the *worst* set A .

Example 2. We claim that

$$c_n(l) \leq 2d \binom{n-1}{l} 1^l (2d-2)^{n-1-l} \tag{2.53}$$

Indeed, there are $\binom{n-1}{l}$ ways of distributing l straight vertices among the $n-1$ internal vertices of an n -step walk; and at each straight (resp. bent)

vertex there are at most 1 (resp. $2d - 2$) choices for the next step. The first step of the walk has, of course, $2d$ choices. [We remark that summing (2.53) over l gives $c_n \leq 2d(2d - 1)^{n-1}$, which is the trivial bound on c_n in terms of memory-2 walks.] Inserting this bound into (2.48) and performing the sum, we conclude that

$$S(n; a, b) \leq 2d[a + (2d - 2)b]^{n-1} \tag{2.54}$$

and hence

$$\limsup_{n \rightarrow \infty} S(n; a, b)^{1/n} \leq a + (2d - 2)b \tag{2.55}$$

Combining this with (2.50), we learn that

$$a + (2d - 2)b \geq 2d \tag{2.56}$$

which is an interesting fact, but one which unfortunately teaches us nothing about μ .

Our approach now will be to *combine*, in an optimal way, these two ways of bounding $S(n; a, b)$. We shall use the first bound for $l \leq \lambda n$ and the second bound for $l > \lambda n$, with a suitable choice of λ . That is, we shall split $S = S_1 + S_2$, with

$$S_1(n; a, b) \equiv \sum_{l=0}^{\lfloor \lambda n \rfloor} c_n(l) a^l b^{n-1-l} \tag{2.57a}$$

$$S_2(n; a, b) \equiv \sum_{l=\lfloor \lambda n \rfloor + 1}^{n-1} c_n(l) a^l b^{n-1-l} \tag{2.57b}$$

Since $a > b > 0$, we have trivially

$$S_1(n; a, b) \leq c_n a^{\lfloor \lambda n \rfloor} b^{n-1-\lfloor \lambda n \rfloor} \tag{2.58}$$

and hence

$$\limsup_{n \rightarrow \infty} S_1(n; a, b)^{1/n} \leq \mu a^\lambda b^{1-\lambda} \tag{2.59}$$

On the other hand, from (2.53) we have

$$S_2(n; a, b) \leq 2d \sum_{l=\lfloor \lambda n \rfloor + 1}^{n-1} \binom{n-1}{l} a^l [(2d - 2)b]^{n-1-l} \tag{2.60}$$

Using Stirling's formula, we find that the summand achieves its maximum at

$$\frac{l}{n} \approx \lambda_0 \equiv \frac{a}{a + (2d - 2)b} \tag{2.61}$$

and is decreasing thereafter. So let us take $\lambda \in [\lambda_0, 1]$; then easy estimates show that

$$\limsup_{n \rightarrow \infty} S_2(n; a, b)^{1/n} \leq \left(\frac{a}{\lambda}\right)^\lambda \left(\frac{(2d-2)b}{1-\lambda}\right)^{1-\lambda} \tag{2.62}$$

Combining (2.50) with (2.59) and (2.62), we conclude that

$$\max \left[\mu a^\lambda b^{1-\lambda}, \left(\frac{a}{\lambda}\right)^\lambda \left(\frac{(2d-2)b}{1-\lambda}\right)^{1-\lambda} \right] \geq 2d \tag{2.63}$$

for all $\lambda \in [\lambda_0, 1]$. We will choose $\lambda \in [\lambda_0, 1]$ such that the second expression is just barely less than $2d$; then we can conclude that the first expression is $\geq 2d$. Now, the second expression equals $a + (2d-2)b \geq 2d$ [the inequality due to (2.56)] when $\lambda = \lambda_0$, and equals $a < 2d$ [the inequality due to our assumption (2.44)] when $\lambda = 1$, and is a continuous and strictly decreasing function of λ in the interval $[\lambda_0, 1]$. Therefore, there is a unique $\lambda^* \in [\lambda_0, 1]$ such that

$$\left(\frac{a}{\lambda^*}\right)^{\lambda^*} \left(\frac{(2d-2)b}{1-\lambda^*}\right)^{1-\lambda^*} = 2d \tag{2.64}$$

We then have the bound

$$\mu \geq \frac{2d}{a^{\lambda^*} b^{1-\lambda^*}} = \left(\frac{2d-2}{1-\lambda^*}\right)^{1-\lambda^*} \left(\frac{1}{\lambda^*}\right)^{\lambda^*} \tag{2.65}$$

The above inequality can be used to improve on our previous bounds. For $|A| = 2$, it can be applied directly. To apply it when $|A| > 2$, we classify A according to its first two steps, and distinguish the two possibilities by defining now [we write $A \equiv (a_1, a_2, a_3, \dots)$]

$$\begin{aligned} a &\equiv \max_{A: a_1 = e_1, a_2 = 2e_1} C_0^A(0, 0; 1/(2d)) \\ b &\equiv \max_{A: a_1 = e_1, a_2 = e_1 + e_2} C_0^A(0, 0; 1/(2d)) \end{aligned} \tag{2.66a}$$

Then (2.45) still holds for these a and b , and we can proceed in exactly the same way as for the $|A| = 2$ case. The bounds for memory-2 and memory- $\tilde{2}$ can be optimized in the same way. The resulting bounds are given in Table II.

3. EVALUATION OF LOOP GENERATING FUNCTIONS

3.1. Simple Random Walk

In this section we shall reduce the computation of $A_0(k; \beta)$ to the evaluation of the simple-random-walk two-point function $C_0(0, x; \beta)$ at a suitable finite set of sites x . In particular, for computing the numerical bounds in Table II we need only the critical case $\beta = 1/(2d)$. Methods for obtaining the values of the critical two-point function are discussed in detail in Appendix B of ref. 4, and a brief summary is given in the Appendix below. Of course the critical simple-random-walk two-point function is infinite in dimensions $d = 1, 2$; we briefly indicate the modifications needed to treat $d \leq 2$ at the end of this section.

We begin by deriving a recursion relation which relates the generating functions $C_0^A(y, x; \beta)$ and $C_0^{A \cup \{b\}}(y, x; \beta)$, where b is a single site and A is a finite set of sites which does not contain b . Applying inclusion-exclusion gives

$$C_0^{A \cup \{b\}}(y, x; \beta) = C_0^A(y, x; \beta) - \sum_{\substack{\omega \in \Omega_0(y, x) \\ \omega \ni b, \omega \cap A = \emptyset}} \beta^{|\omega|} \tag{3.1}$$

Given a walk ω contributing to the sum on the right side, we break the walk into two pieces at its first visit to b . The generating function for walks which go from y to b , which hit b only once (namely at their last step), and which avoid the set A is equal to $C_0^A(y, b; \beta)/C_0^A(b, b; \beta)$. Therefore

$$C_0^{A \cup \{b\}}(y, x; \beta) = C_0^A(y, x; \beta) - \frac{C_0^A(y, b; \beta) C_0^A(b, x; \beta)}{C_0^A(b, b; \beta)} \tag{3.2}$$

When A is the empty set, the right side can be computed in terms of the ordinary two-point function C_0 , and then by iteration we can compute $C_0^A(y, x; \beta)$ for any finite set A .

An amusing special case is $y = x = 0$ and $A = \{e\}$, where e is a nearest neighbor of the origin. Using the identity

$$C_0(0, 0; \beta) = 1 + 2d\beta C_0(0, e; \beta) \tag{3.3}$$

together with (3.2), we find

$$C_0^{\{e\}}(0, 0; \beta) = \left(1 - \frac{1}{(2d\beta)^2}\right) C_0(0, 0; \beta) + \frac{2}{(2d\beta)^2} - \frac{1}{(2d\beta)^2 C_0(0, 0; \beta)} \tag{3.4}$$

This is finite as $\beta \uparrow 1/(2d)$ in all dimensions $d > 0$ [since $C_0(0, 0; \beta)$ diverges as $\beta \uparrow 1/(2d)$ more slowly than $(1 - 2d\beta)^{-1}$] and yields

$$C_0^{\{e\}}\left(0, 0; \frac{1}{2d}\right) = 2 - \frac{1}{C_0(0, 0; 1/(2d))} \leq 2 \tag{3.5}$$

In particular, we conclude that $A_0(i; \beta) \leq A_0(1; \beta) = C_0^{\{e\}}(0, 0; \beta) \leq 2$ for all $i \geq 1$ and all $\beta \leq 1/(2d)$, in all dimensions.

The computation of $A_0(k; \beta)$ for any chosen β is now reduced to a finite amount of labor. We simply list all the allowable sets A of the given cardinality k , exploiting the obvious lattice symmetries, and then compute $C_0^A(0, 0; \beta)$ for each such A by iterating (3.2). For $|A| = 1$, we have only one choice, $A = \{e\}$. For $|A| = 2$, we compute the maximum over the two choices $A = \{e_1, 2e_1\}$ and $A = \{e_1, e_1 + e_2\}$, where e_i are the canonical unit vectors. And so forth. Values for $C_0^A(0, 0; \beta)$ are tabulated in Table V in the Appendix, and the resulting lower bounds on μ are given in Table II.

In dimension $d > 2$, we can perform these computations directly at the critical point $\beta = 1/(2d)$: all quantities are finite. However, in dimension $d \leq 2$ the two-point function $C_0(0, x; 1/(2d))$ is infinite for all x . Nevertheless we can show that $C_0^A(0, x; 1/(2d))$ is finite whenever $A \neq \emptyset$, by working first at $\beta < 1/(2d)$ and then letting $\beta \uparrow 1/(2d)$. Note first that by the monotone convergence theorem we have

$$C_0^A\left(0, x; \frac{1}{2d}\right) = \lim_{\beta \uparrow 1/(2d)} C_0^A(0, x; \beta) \tag{3.6}$$

Now the trick is to rewrite the case $A = \emptyset$ of (3.2), which is certainly valid for $\beta < 1/(2d)$, in terms of a quantity that (unlike C_0) stays finite as $\beta \uparrow 1/(2d)$. Such a quantity is the potential kernel $A_0(x; \beta) \equiv C_0(0, 0; \beta) - C_0(0, x; \beta)$ discussed in Section 2.1. Rewriting (3.2) with $A = \emptyset$ in terms of the potential kernel gives

$$C_0^{\{b\}}(y, x; \beta) = -A_0(x - y; \beta) + A_0(b - y; \beta) + A_0(x - b; \beta) - \frac{A_0(b - y; \beta) A_0(x - b; \beta)}{C_0(0, 0; \beta)} \tag{3.7}$$

which in the limit $\beta \uparrow 1/(2d)$ in dimension $d \leq 2$ reduces to the result of Proposition 11.6 of ref. 15:

$$C_0^{\{b\}}\left(y, x; \frac{1}{2d}\right) = -A_0(x - y) + A_0(b - y) + A_0(x - b) \tag{3.8}$$

In particular, this shows that $C_0^A(y, x; 1/(2d)) < \infty$ whenever $A \neq \emptyset$. Thus, once we have handled the step from C_0 to $C_0^{\{b\}}$ using (3.8), we can then advance to larger values of $|A|$ using (3.2) directly at $\beta = 1/(2d)$, just as in higher dimensions. (An alternate method of computation is given in Theorem 14.11 of ref. 15, but we have found the recursion easier to implement numerically.)

3.2. Memory-2 Walk

The computation of our memory-2 lower bounds on μ has now been reduced to the evaluation of the generating functions $C_2^A(0, 0; \mu_2^{-1})$ and $C_2^A(0, e; \mu_2^{-1})$ for finitely many finite sets A , just as was described in Section 3.1. The basic idea for the evaluation of these quantities is the same here as for the simple random walk, but the recursion relation requires more care. Suppose that $b \notin A$. If $b = y$, we just have

$$C_2^{A \cup \{b\}}(y, x; \beta) = 0 \tag{3.9}$$

If $b \neq y$, we begin as for a simple random walk by writing

$$C_2^{A \cup \{b\}}(y, x; \beta) = C_2^A(y, x, \beta) - \sum_{\substack{\omega \in \Omega_2(y, x) \\ \omega \ni b, \omega \cap A = \emptyset}} \beta^{|\omega|} \tag{3.10}$$

To deal with the sum on the right side, we again want to cut the walk at the first time it hits b , but now the two pieces of the walk are no longer independent because of the memory-2 constraint. The sum on the right side is equal to

$$\begin{aligned} & \sum_{\substack{\omega_1 \in \Omega_2(y, b), \omega_2 \in \Omega_2(b, x) \\ \omega_1 \cup \omega_2 \cap A = \emptyset}} \beta^{|\omega_1| + |\omega_2|} I[\omega_1(j) \neq b \text{ for } j < |\omega_1|] I[\omega_1 \circ \omega_2 \in \Omega_2(y, x)] \\ &= \sum_{f: |f|=1} \beta \sum_{\substack{\omega'_1 \in \Omega_2(y, b+f) \\ \omega'_1 \cap A = \emptyset}} \beta^{|\omega'_1|} I[\omega'_1 \not\ni b] \sum_{\substack{\omega_2 \in \Omega_2(b, x) \\ \omega_2 \cap A = \emptyset}} \beta^{|\omega_2|} I[\omega_2(1) \neq b + f] \end{aligned} \tag{3.11}$$

where $\omega_1 \circ \omega_2$ denotes the concatenation of the two walks. The sum over ω'_1 exactly gives

$$C_2^{A \cup \{b\}}(y, b + f; \beta)$$

For the sum over ω_2 , we use repeated inclusion-exclusion to remove the constraint that $\omega_2(1) \neq b + f$, to obtain

$$\begin{aligned}
 \sum_{\substack{\omega_2 \in \Omega_2(b, x) \\ \omega_2 \cap A = \emptyset}} \beta^{|\omega_2|} I[\omega_2(1) \neq b + f] &= C_2^A(b, x; \beta) - \beta C_2^A(b + f, x; \beta) \\
 &+ \beta^2 C_2^A(b, x; \beta) - \beta^3 C_2^A(b + f, x; \beta) + \dots \\
 &= \frac{1}{1 - \beta^2} [C_2^A(b, x; \beta) - \beta C_2^A(b + f, x; \beta)]
 \end{aligned}
 \tag{3.12}$$

The result is

$$\begin{aligned}
 C_2^{A \cup \{b\}}(y, x; \beta) &= C_2^A(y, x; \beta) - \frac{\beta}{1 - \beta^2} \sum_{f: |f|=1} C_2^{A \cup \{b\}}(y, b + f; \beta) \\
 &\times [C_2^A(b, x; \beta) - \beta C_2^A(b + f, x; \beta)]
 \end{aligned}
 \tag{3.13}$$

The above unfortunately is not a closed-form expression for the left side, because of the occurrence of similar quantities on the right side. However, for a fixed y , (3.13) provides a system of $2d$ linear equations for $2d$ unknowns, namely $\{C_2^{A \cup \{b\}}(y, b + f; \beta)\}_{|f|=1}$. Once we know these $2d$ quantities by solving the equations, then everything on the right-hand side of (3.13) is known, and $C_2^{A \cup \{b\}}(y, x; \beta)$ can then be computed for general x . Fortunately, the number of unknowns is often reduced by symmetry. For example, for $y=0, A = \emptyset$, and $b = e_1$, there are three inequivalent values of $b + f$, namely $0, 2e_1$, and $e_1 + e_2$. Thus we can first solve the system of three equations in three unknowns which results by taking x to be each of the three values $0, 2e_1$, and $e_1 + e_2$, and once this system has been solved we can then compute the left side directly for any other value of x . Concretely, for $d=3$, we get

$$C_2^{\{e_1\}}(0, 0; \frac{1}{3}) \approx 1.125805 \tag{3.14a}$$

$$C_2^{\{e_1\}}(0, 2e_1; \frac{1}{3}) \approx 0.074441 \tag{3.14b}$$

$$C_2^{\{e_1\}}(0, e_1 + e_2; \frac{1}{3}) \approx 0.138449 \tag{3.14c}$$

For $|A| \geq 1$ we can proceed similarly; results are given in Table VI in the Appendix.

The right side of (3.13) can be used directly at the critical point in more than two dimensions, but it contains infinities for $d=2$ when A is the empty set. In two dimensions a limiting argument is first used to deal with $A = \emptyset$, and then for $|A| \geq 1$ the recursion can be used directly as above. Surprisingly, the resulting bounds are worse than those obtained using

simple random walk, and so we do not give the details of the limiting argument, but instead give only the result: for $b \neq y$,

$$C_2^{\{b\}}(y, x; \frac{1}{3}) = \frac{1}{3} + \frac{2}{3} [\Delta_0(b-y) - \Delta_0(x-y)] + \Delta_0(x-b) - \frac{1}{12} \sum_{f:|f|=1} C_2^{\{b\}}(y, b+f; \frac{1}{3}) \Delta_0(x-b-f) \quad (3.15)$$

Results are discussed in Section 4.2.

Finally, let us derive the identity (2.40), which shows how the evaluation of $\tilde{C}_2^{A,e}(0, 0; \beta)$ can be reduced to the evaluation of $C_2^A(0, 0; \beta)$ and $C_2^A(0, e; \beta)$. In fact, (2.40) is just the special case $b = x = 0$ of (3.12), once one takes into account the symmetry between the two endpoints of the walk.

4. DISCUSSION OF RESULTS

4.1. Three or More Dimensions

From Table II it can be seen that for $d \geq 3$ the $\tau = 2$ bound does better than $\tau = 0$ when $k = 0$, as was already shown at the end of Section 2.3. Perhaps surprisingly, for $k \geq 1$ this situation is reversed: higher memory means a more “sophisticated” bound, but it does not necessarily mean a *better* bound! In any case, the bounds with memory- $\tilde{2}$ do better than the corresponding memory-0 bounds.

In all cases with memory-0 or memory-2 in Table II, the set A giving the maximum of $C_0^A(0, 0; 1/(2d))$ is the straight line segment, as can be expected intuitively for small $|A|$. However, for large $|A|$ in general it is not to be expected that the straight segment is optimal, and an example of an optimal A which is not straight is given below for $d = 2$. (We thank Greg Lawler and Alain Sznitman for discussions on the nonoptimality of straight A for large $|A|$.) In Table II it is also the case that straight A gives the maximum for the memory- $\tilde{2}$ bounds, although *a priori* there seems to be no compelling reason to expect this to be the case: in (2.40) straight A will give the maximum individually for each of $C_2^A(0, 0; \beta)$ and $C_2^A(0, e; \beta)$, but possibly not for the difference.

4.2. Two Dimensions

Unfortunately, for $d = 2$ our methods do not produce good bounds on μ , as can be seen from Table II. For example, with $|A| = 4$ and $\tau = 0$ we have only $\mu \geq 2.275515$. To get a measure of the inherent limitation of the method in two dimensions, and in view of the relatively slow convergence

of the bounds as k increases, we computed the value of $2d/C_0^{L_k}(0, 0; 1/(2d))$ with L_k the collinear set of k sites joining $(-1, 0)$ to $(-k, 0)$. For large k we do not expect that $C_0^A(0, 0; 1/(2d))$ is maximized over sets A with $|A|=k$ by $C_0^{L_k}(0, 0; 1/(2d))$, and in fact already for $k=5$ and $A = \{(-1, 0), (-2, 0), (-3, 0), (-4, 0), (-4, 1)\}$ we have

$$C_0^A\left(0, 0; \frac{1}{2d}\right) \approx 1.739044 > 1.738131 \approx C_0^{L_5}\left(0, 0; \frac{1}{2d}\right)$$

Nevertheless $2d/C_0^{L_k}(0, 0; 1/(2d))$ does provide an *upper bound* on the best possible $\tau=(0, k)$ lower bound on μ . For $k=60$ we found $2d/C_0^{L_{60}}(0, 0; 1/(2d)) = 2.404210$, and by extrapolating the sequence for $k \leq 60$ to $k \rightarrow \infty$, we found a limiting value less than 2.42. Substantially better lower bounds on μ can be obtained by other methods.^(2,5)

The situation for $\tau=2$ is only slightly better. Solving the system (3.15) of three equations in three unknowns gives

$$C_2^{\{e_1\}}(0, 0; \frac{1}{3}) \approx 1.751695 \tag{4.1a}$$

$$C_2^{\{e_1\}}(0, 2e_1; \frac{1}{3}) \approx 0.649131 \tag{4.1b}$$

$$C_2^{\{e_1\}}(0, e_1 + e_2; \frac{1}{3}) \approx 0.799587 \tag{4.1c}$$

This gives the very weak bound $\mu \geq 3/1.751695 \geq 1.712626$. By imposing the additional restriction that there should be no direct returns at the end of the loop [the memory- $\tilde{2}$ bound of inequality (2.39)], this is improved to $\mu \geq 1.976372$, which is comparable to the result obtained with memory-0.

Again for memory-2 and memory- $\tilde{2}$ we computed the bounds arising from $A = L_k$ for large k , to obtain an idea of the inherent limitation of the method. For memory-2 and $k=58$ we found a bound of 2.268661, while for memory- $\tilde{2}$ and $k=58$ we found a bound of 2.443124. Only marginally higher values result when these are extrapolated to $k \rightarrow \infty$. Since straight A in general will not be optimal, the best possible bound on μ using memory-2 or memory- $\tilde{2}$ may in fact do worse than these values. In particular, for the memory- $\tilde{2}$ bounds straight A already fails to provide a maximum when $k=4$, where the optimal A is the bent set $A = \{(-1, 0), (-2, 0), (-3, 0), (-3, 1)\}$.

Because of the poor results for $d=2$ we have not done a rigorous error analysis of these $d=2$ computations, but we do expect that they are correct to the given accuracy.

5. COMPARISON TO THE ISING MODEL AND THE INFRARED BOUND

Our simplest (and worst) bound

$$\mu \geq \frac{2d}{C_0(0, 0; 1/(2d))} \quad (5.1)$$

is in fact not new, as it is an immediate consequence of earlier results of Fisher⁽²¹⁾ and Fröhlich *et al.*⁽²²⁾ Also, this bound was proven by Lawler⁽²³⁾ for dimensions $d > 4$, via a different perspective on loop erasure.

Fisher's result is that the two-point spin correlation function $\langle \sigma_x \sigma_y \rangle_J$ of the nearest-neighbor ferromagnetic Ising model with inverse temperature J (and zero external field) obeys the inequality

$$\langle \sigma_x \sigma_y \rangle_J \leq G(x, y; \tanh J) \quad (5.2)$$

from which he concluded that

$$\mu \geq \coth J_{c, \text{Ising}} \quad (5.3)$$

where $J_{c, \text{Ising}}$ is the critical inverse temperature of the Ising model. The infrared bound of ref. 22 gives

$$J_{c, \text{Ising}} \leq \frac{C_0(0, 0; 1/(2d))}{2d} \quad (5.4)$$

Combining these two inequalities yields

$$\mu \geq \coth \left(\frac{C_0(0, 0; 1/(2d))}{2d} \right) \quad (5.5)$$

This bound is an improvement on (5.1), and yields (5.1) when combined with the inequality $\coth x \geq x^{-1}$ (for positive x).

Table III gives the value of $\coth J_{c, \text{Ising}}$, using numerical estimates of $J_{c, \text{Ising}}$, and compares it with the bounds (5.1) and (5.5) as well as with the best rigorous lower bounds on μ . Values of $J_{c, \text{Ising}}$ are taken from the exact solution $J_{c, \text{Ising}} = \frac{1}{2} \log(1 + \sqrt{2})$ for $d=2$, from the Monte Carlo study⁽²⁴⁾ for $d=3$, and from the series extrapolation results of ref. 25 for $d=4$ and ref. 11 for $d=5, 6$. If we accept the (nonrigorous for $d \geq 3$) numerical values of $J_{c, \text{Ising}}$, then our best lower bounds are better than the best possible bound that can arise from (5.3) for $d \geq 4$, but not for $d=2, 3$. However, for $d=2$ the enumeration bound of Conway and Guttmann⁽⁵⁾ does better than the Ising-model bound. The fact that our best bounds do better in high

Table III. Comparison of the Ising-Model Lower Bound $J_{c, \text{Ising}}$ with the Best Lower Bounds on μ^a

d	2	3	4	5	6
$J_{c, \text{Ising}}$	0.440687	0.2216595(26)	0.149663(34)	0.113917(7)	0.092294(7)
$2d/C_0(0, 0; 1/(2d))$	0	3.956776	6.454386	8.648214	10.743415
$\text{coth}[(1/2d) C_0(0, 0; 1/(2d))]$	1	4.040663	6.505948	8.686723	10.774424
$\text{coth } J_{c, \text{Ising}}$	2.414213	4.58507(5)	6.7315(15)	8.8162(6)	10.8657(9)
Our best bound on μ	2.305766	4.572140	6.742945	8.828529	10.874038
Best bound on μ	2.62002	4.572140	6.742945	8.828529	10.874038

^a The values of $J_{c, \text{Ising}}$ are nonrigorous numerical estimates for $d=3, 4, 5, 6$; errors in the last digit(s) are shown in parentheses. Other quantities are rounded to six digits, except for the lower bounds in the last two lines, which have been truncated.

dimensions than (5.3) can be explained by the fact that our best bounds capture more terms of the $1/d$ expansion for μ than does the right side of (5.3); see Section 6.

6. HIGH- d BEHAVIOR OF THE LOWER BOUNDS

The lace expansion has been used⁽¹²⁾ to give a rigorous proof that as $d \rightarrow \infty$,

$$\mu = 2d - 1 - \frac{1}{2d} - \frac{3}{(2d)^2} - \frac{16}{(2d)^3} + O(d^{-4}) \tag{6.1}$$

The next term has been given in refs. 26 and 27,

$$\mu = 2d - 1 - \frac{1}{2d-1} - \frac{2}{(2d-1)^2} - \frac{11}{(2d-1)^3} - \frac{62}{(2d-1)^4} + \dots \tag{6.2a}$$

$$= 2d - 1 - \frac{1}{2d} - \frac{3}{(2d)^2} - \frac{16}{(2d)^3} - \frac{102}{(2d)^4} + \dots \tag{6.2b}$$

but with no rigorous bound on the error. In this section we study the $1/d$ expansion for our (and other people's) lower bounds on μ , and show that our best bound agrees with (6.1) up to and including the term of order d^{-2} .

In Section 6.1 we analyze briefly the d -dependence of some older lower bounds on μ . It turns out that most of these methods have very poor behavior as $d \rightarrow \infty$; this was, in fact, the original motivation for us to develop the loop-erasure-and-restoration method. In Section 6.2 we com-

ment briefly on some results of Kesten,⁽²⁰⁾ which are based on a precursor of our method. In Section 6.3 we analyze the high- d behavior of the loop-erasure-and-restoration bounds, and show that they capture the first few terms of the $1/d$ expansion of μ . An interesting structure emerges from the comparison of how many terms are captured for different pairs (τ, k) . In Section 6.4 we carry out an analogous analysis for the bounds based on comparison to the Ising model.

6.1. High- d Behavior of the Older Lower-Bound Methods

We assume in this subsection that the reader is acquainted with the definition and fundamental properties of *bridges* and *irreducible bridges*; see, e.g., refs. 2 and 13.

Let b_n (resp. i_n) be the number of n -step bridges (resp. n -step irreducible bridges) starting at the origin and ending anywhere. By convention, $b_0 = 1$ and $i_0 = 0$. These counts satisfy the renewal equation

$$b_n = \delta_{n,0} + \sum_{k=1}^n i_k b_{n-k} \tag{6.3}$$

We define for $\beta \geq 0$ the generating functions

$$B(\beta) = \sum_{n=0}^{\infty} b_n \beta^n \tag{6.4}$$

$$I(\beta) = \sum_{n=0}^{\infty} i_n \beta^n \tag{6.5}$$

Now $0 \leq i_n \leq b_n \leq \mu^n$, and hence it follows from (6.3) that

$$B(\beta) = \frac{1}{1 - I(\beta)} \quad \text{for } \beta \leq \mu^{-1} \tag{6.6}$$

Also, it is known that

$$B(\beta) \begin{cases} \leq (1 - \beta\mu)^{-1} < \infty & \text{for } 0 \leq \beta < \mu^{-1} \\ \rightarrow +\infty & \text{for } \beta \uparrow \mu^{-1} \\ = +\infty & \text{for } \beta > \mu^{-1} \end{cases} \tag{6.7}$$

$$I(\beta) \begin{cases} \leq \beta\mu < 1 & \text{for } 0 \leq \beta < \mu^{-1} \\ = 1 & \text{for } \beta = \mu^{-1} \\ = +\infty & \text{for } \beta > \mu^{-1} \end{cases} \tag{6.8}$$

Now suppose that we have enumerated i_1, \dots, i_N . (In practice one does this by enumerating b_1, \dots, b_N and solving (6.3).⁽²⁾) Then, defining

$$I_N(\beta) \equiv \sum_{n=1}^N i_n \beta^n \tag{6.9}$$

we have $I_N(\beta) \leq I(\beta) < 1$ for $\beta < \mu^{-1}$. It follows that

$$\mu \geq \mu_{*,N} \equiv \frac{1}{\beta_{*,N}} \tag{6.10}$$

where $\beta_{*,N}$ is the unique positive solution of the polynomial equation $I_N(\beta) = 1$.

How does the bound (6.10) behave as $d \rightarrow \infty$ for fixed N ? We are unable to give the precise asymptotic behavior, but we can give an upper bound as follows: Trivially we have $i_n \leq b_n \leq (2d-1)^{n-1}$, because the first step of a bridge must be in the $+e_1$ direction, and for the remaining steps there are at most $2d-1$ choices each. Therefore,

$$I_N(\beta) \leq \sum_{n=1}^N (2d-1)^{n-1} \beta^n \tag{6.11}$$

In particular, the solution $\beta_{*,N}$ of $I_N(\beta_{*,N}) = 1$ must be greater than or equal to the solution $\beta_{**,N}$ of $\sum_{n=1}^N (2d-1)^{n-1} \beta_{**,N}^n = 1$. Now, it is easy to see that for each fixed N , as $d \rightarrow \infty$ we have

$$\beta_{**,N} = (2d-1)^{-(N-1)/N} [1 - O(d^{-1/N})] \tag{6.12}$$

so that

$$\mu_{*,N} \equiv \frac{1}{\beta_{*,N}} \leq \frac{1}{\beta_{**,N}} = (2d-1)^{(N-1)/N} [1 + O(d^{-1/N})] \tag{6.13}$$

So this method, for any fixed N , can never get even the correct leading asymptotic order (namely $\mu \sim d$) as $d \rightarrow \infty$.

In practice, this method gives the best currently available bounds for $d=2$,^(2,5) but it is inferior to the loop-erasure-and-restoration method for $d \geq 3$.

Other early lower bounds on μ are those of Rennie,⁽²⁸⁾

$$\mu \geq 2d - \log d - 3 + \sqrt{2} + \log 2 - \sum_{j=3}^{\infty} \frac{\log(j+1)}{j[j - \log(j+1)]} \tag{6.14}$$

and Hammersley,⁽²⁹⁾

$$\mu \geq 2d - \log(2d-1) - 1 \tag{6.15}$$

These bounds get the correct first term in the large- d expansion, but numerically they are rather poor.

Some other methods for proving lower bounds on μ in $d=2, 3$ are given in ref. 14; but they do not appear to behave well as $d \rightarrow \infty$.

6.2. Kesten's Bounds

A precursor of our method was used by Kesten⁽²⁰⁾ to prove that

$$\mu \geq \mu_{2r} - O(d^{-r}) \tag{6.16}$$

for all $r \geq 0$. Kesten's method involves loop erasure and restoration at the level of *counts* rather than generating functions. Since trivially $\mu \leq \mu_{2r}$, (6.16) implies that the $1/d$ expansion of μ_{2r} agrees with the first $r + 1$ terms of the $1/d$ expansion for μ . Unfortunately, from the point of view of numerical estimates on μ , (6.16) is not very helpful, since it is difficult to get good constants in the error term. Nor is it easy to compute the $1/d$ expansion of μ_{2r} for $r \geq 3$, so as to obtain the $1/d$ expansion for μ beyond three terms. However, using $r = 2$ in (6.16) together with (2.8), one obtains

$$\mu \geq 2d - 1 - \frac{1}{2d} + O(d^{-2}) \tag{6.17}$$

which gives a bound agreeing with the first three terms of the $1/d$ expansion for μ , albeit without good control of the error term.

6.3. $1/d$ Expansion for the Loop-Erasure-and-Restoration Lower Bounds

We now turn to the computation of the $1/d$ expansions for some of our lower bounds on μ . We use the shorthand $s = 1/(2d)$. The standard of comparison for all our bounds is the series (6.2),

$$\mu = s^{-1} - 1 - s - 3s^2 - 16s^3 - 102s^4 + \dots \tag{6.18}$$

which is provably correct through order s^3 and presumably correct also at order s^4 . As always, we classify our bounds according to the memory they use ($\tau = 0, 2$, or $\tilde{2}$) and how far back on the backbone they enforce avoidance of the attached loops ($k = 0, 1, 2, 3, \dots$). We introduce the notation $\mu^{(\tau, k)}$ to denote the bound obtained by considering (τ, k) -quantities.

Our most basic bound (2.31) is based on $\tau = 0, k = 0$; using (A.17), its $1/d$ expansion is

$$\mu^{(0,0)} = \frac{2d}{C_0(0, 0; 1/(2d))} = s^{-1} - 1 - 2s - 7s^2 - 35s^3 - 215s^4 + O(s^5) \tag{6.19}$$

This gets the first two terms correct, but misses the term of order s . The next simplest bound (2.32) is based on $\tau = 0, k = 1$; using (A.17) and (2.33), we obtain

$$\mu^{(0,1)} = \frac{2d}{C_0^{\{e\}}(0, 0; 1/(2d))} = s^{-1} - 1 - s - 4s^2 - 22s^3 - 143s^4 + O(s^5) \quad (6.20)$$

This gets the first three terms correct, and just barely misses the term of order s^2 . As can be seen from Table VIII in the Appendix, taking $k = 2$ or 3 does not improve on (6.20).

Next let us consider the bounds based on the memory-2 loop. The simplest such bound (2.34) is based on $\tau = 2, k = 0$; using (2.14) and (A.17), it becomes

$$\mu^{(2,0)} = \frac{2d-1}{C_2(0, 0; 1/(2d-1))} = s^{-1} - 1 - s - 6s^2 - 35s^3 - 222s^4 + O(s^5) \quad (6.21)$$

This gets the first three terms correct. The bound is further improved if we go to $k = 1$: making use of Table IX, we have

$$\mu^{(2,1)} = \frac{2d-1}{C_2^{\{e\}}(0, 0; 1/(2d-1))} = s^{-1} - 1 - s - 4s^2 - 23s^3 - 150s^4 + O(s^5) \quad (6.22)$$

The term of order s^2 is improved compared to (6.21), but the coefficient is still not correct. This bound based on $\tau = 2, k = 1$ is inferior (at order s^3) to the simpler bound based on $\tau = 0, k = 1$, as was the case for the numerical values of Table II. Using Table IX, we can see that the expansion for $\mu^{(2,2)}$ is identical to (6.22).

Better memory-2 bounds can be obtained by insisting that the attached loops avoid also the next site on the backbone (Section 2.4). The simplest such bound is

$$\mu^{(2,0)} = \frac{2d-1}{\tilde{C}_2^{\emptyset,e}(0, 0; 1/(2d-1))} = s^{-1} - 1 - s - 5s^2 - 29s^3 - 188s^4 + O(s^5) \quad (6.23)$$

where we have used Table X. This gets the first three terms correct, and does better at order s^2 than (6.21), but still has not yet got the correct coefficient -3 . This coefficient is, however, captured correctly if we combine the constraints involving the previous and next steps on the backbone, i.e., if we go to $\tau = \tilde{2}, k = 1$. To see this, consider the loop generating functions $\tilde{C}_2^{\{e_1\}, -e_1}(0, 0; 1/(2d-1))$ and $\tilde{C}_2^{\{e_1\}, e_2}(0, 0; 1/(2d-1))$, which by symmetry

are the only two geometries to be considered. Intuitively, the second should be greater than the first, since a walk which must avoid e_1 will prefer to return to the origin from $-e_1$, so the constraint is greater when this possibility is disallowed. In fact this intuition is borne out by the numerical results, and, as can be seen from Table X, it is also evident from the $1/d$ expansion. From Table X we have

$$\mu^{(2,1)} = \frac{2d-1}{\tilde{C}_2^{(e_1),e_2}(0,0;1/(2d-1))} = s^{-1} - 1 - s - 3s^2 - 18s^3 - 124s^4 + O(s^5) \tag{6.24}$$

which has the correct coefficient of order s^2 , and as a bonus only misses the correct coefficient of order s^3 by 2. It is also clear from Table X that the expansion for $\mu^{(2,2)}$ is identical to that of $\mu^{(2,1)}$, through the order shown in (6.24).

The optimized bounds of Section 2.5 do not improve substantially on (6.24): we find that for the optimized bound using $k=2$ and $\tau=2$ the terms up to and including order s^3 are as in (6.24), while the coefficient of s^4 is improved slightly from -124 to -122 .

In general we do not expect that there will be improvements below order s^5 when k is increased beyond 1, for a given memory. For example, for $k=2$ the number of hexagons which pass through a specific next-nearest neighbor of the origin is only $O(d)$, and hence when multiplied by β^6 is an order- s^5 effect. This can be viewed as a partial explanation of the small size of the improvements observed in the numerical bounds as $|A|$ increases beyond 1.

6.4. $1/d$ Expansion for the Ising-Model Lower Bounds

Let us first look at the bound (5.5) obtained by using comparison to the Ising model together with the infrared bound on $J_{c, \text{Ising}}$. This improves our basic $\tau=0, k=0$ bound by virtue of the coth, and yields

$$\mu \geq s^{-1} - 1 - \frac{5}{3}s - \frac{20}{3}s^2 - \frac{1531}{45}s^3 + O(s^4) \tag{6.25}$$

We see that the coth makes only a slight improvement in the term of order s , and does *not* achieve the correct coefficient -1 .

The method based on comparison to the Ising model is potentially more powerful than this, if one could get a better bound on $J_{c, \text{Ising}}$. The best possible result is obtained by inserting the exact (nonrigorous) expansion

$$J_{c, \text{Ising}} = \left(s^{-1} - 1 - \frac{4}{3}s - \frac{13}{3}s^2 - \frac{979}{45}s^3 - \frac{2009}{15}s^4 + \dots \right)^{-1} \tag{6.26}$$

derived by Fisher and Gaunt⁽²⁶⁾ into (5.3); the result is

$$\mu \geq \coth(J_{c, \text{Ising}}) = s^{-1} - 1 - s - 4s^2 - 21s^3 - \frac{394}{3}s^4 + \dots \quad (6.27)$$

This achieves the correct first three terms, but does not do as well as (6.24) on the term of order s^2 . Of course, it is a highly nontrivial open problem to prove rigorously such good bounds on $J_{c, \text{Ising}}$.

APPENDIX. SIMPLE RANDOM WALK

A.1. Numerical Evaluation of the Two-Point Function

To evaluate our lower bounds on μ numerically, it is necessary to know the numerical values of the critical simple-random-walk two-point function $C_0(0, x; 1/(2d))$ for various values of x . An effective method of evaluating this quantity (as well as the subcritical two-point function) numerically to high precision, with rigorous error bounds, has been described in considerable detail in Appendix B of ref. 4. We now summarize briefly how the calculation goes in the critical case.

We begin with the integral formula

$$C_0\left(0, x; \frac{1}{2d}\right) = \int_{[-\pi, \pi]^d} \frac{d^d k}{(2\pi)^d} \frac{e^{ik \cdot x}}{1 - \hat{D}(k)} \quad (A.1)$$

where

$$\hat{D}(k) = \frac{1}{d} \sum_{i=1}^d \cos k_i \quad (A.2)$$

We then apply the identity

$$\frac{1}{A} = \int_0^\infty e^{-At} dt \quad (A.3)$$

which is valid for $A > 0$, with $A = 1 - \hat{D}(k)$. This factorizes the integrals over k_1, \dots, k_d , which can then be performed to give

$$C_0\left(0, x; \frac{1}{2d}\right) = d \int_0^\infty \prod_{i=1}^d f_{|x_i|}(t) dt \quad (A.4)$$

where

$$f_N(z) \equiv e^{-z} I_N(z) \equiv \frac{1}{2\pi} \int_{-\pi}^\pi e^{-z(1 - \cos \theta)} \cos N\theta d\theta \quad (A.5)$$

and $I_N(z)$ is the modified Bessel function. This transforms the d -dimensional integral (A.1) into a one-dimensional integral over a semi-infinite interval.

The integrand in (A.4) decays as $t \rightarrow \infty$ only as a power. We speed up the decay by making the change of variables $t = e^u$, obtaining

$$C_0\left(0, x; \frac{1}{2d}\right) = d \int_{-\infty}^{\infty} F(u) du \tag{A.6}$$

where

$$F(u) = e^u \prod_{i=1}^d f_{|x_i|}(e^u) \tag{A.7}$$

We then use standard methods to bound the difference between the integral (A.6) and an infinite Riemann sum, truncate the Riemann sum with bounds

Table IV. Numerical Values of $\Delta_0(x)$ for $d=2$, and of $C_0(0, x; 1/(2d))$ for $d=3, 4, 5, 6$, for the Values of x Needed to Compute the Lower Bounds on μ^a

x	$\Delta_0(x)$	$C_0(0, x; 1/(2d))$			
	$d=2$	$d=3$	$d=4$	$d=5$	$d=6$
(0)	0	1.5163860744	1.2394671218	1.1563081248	1.1169633732
(1)	1	0.5163860744	0.2394671218	0.1563081248	0.1169633732
(1, 1)	1.2732395447	0.3311486174	0.1017176302	0.0474085960	0.0271774706
(1, 1, 1)	—	0.2614701416	0.0618723811	0.0222517907	0.0100651251
(1, 1, 1, 1)	—	—	0.0447274307	0.0133523237	0.0049990827
(1, 1, 1, 1, 1)	—	—	—	0.0092253734	0.0029872751
(2)	1.4535209105	0.2573359025	0.0659640719	0.0275043553	0.0148223998
(2, 1)	1.5464790895	0.2155896361	0.0436586366	0.0139794831	0.0058409498
(2, 1, 1)	—	0.1917916659	0.0334570990	0.0089609415	0.0030848645
(2, 1, 1, 1)	—	—	0.0275824802	0.0065163319	0.0019448478
(2, 2)	1.6976527263	0.1683310508	0.0259898362	0.0062387819	0.0019599801
(2, 2, 1)	—	0.1569524280	0.0221867673	0.0047601264	0.0013047592
(3)	1.7211254632	0.1652707962	0.0262936339	0.0068995628	0.0024959268
(3, 1)	1.7615031763	0.1531389140	0.0217691587	0.0048774493	0.0014526312
(3, 1, 1)	—	0.1441957255	0.0189286425	0.0038130772	0.0009927439
(3, 2)	1.8488263632	0.1324510884	0.0159271735	0.0029340473	0.0006998942
(4)	1.9079745896	0.1217332189	0.0137700477	0.0024716782	0.0006024105
(4, 1)	1.9295817894	0.1171305125	0.0125592552	0.0020829365	0.0004528519
(5)	2.0516093163	0.0966064672	0.0085112166	0.0011537265	0.0002044795

^a The values are rounded to ten digits after the decimal point. Final components of x which are not shown are equal to zero.

Table V. Numerical Values of $C_0^A(0, 0; 1/(2d))$ for $d=2, 3, 4, 5, 6$, for Various Choices of A^a

A	$d=2$	$d=3$	$d=4$	$d=5$	$d=6$
\emptyset	∞	1.516386	1.239467	1.156308	1.116963
$\{e_1\}$	2	1.340537	1.193202	1.135179	1.104715
$\{e_1, 2e_1\}$	1.850680	1.335584	1.192876	1.135143	1.104709
$\{e_1, e_1 + e_2\}$	1.735910	1.322546	1.190625	1.134570	1.104514
$\{e_1, 2e_1, 3e_1\}$	1.789955	1.333592	1.192796	1.135138	1.104709
$\{e_1, 2e_1, 2e_1 + e_2\}$	1.767994	1.330950	1.192528	1.135103	1.104703
$\{e_1, e_1 + e_2, 2e_1 + e_2\}$	1.695733	1.320170	1.190465	1.134555	1.104512
$\{e_1, e_1 + e_2, e_1 + 2e_2\}$	1.658351	1.317957	1.190277	1.134530	1.104507
$\{e_1, e_1 + e_2, e_1 + e_2 + e_3\}$	—	1.314688	1.189764	1.134435	1.104485
$\{e_1, e_1 + e_2, e_2\}$	1.357421	1.226256	1.153726	1.115672	1.093040

^a The values are rounded to six digits after the decimal point.

on the omitted tails, and evaluate the resulting finite Riemann sum, using the large- z asymptotic expansion for the modified Bessel function to deal with large t and a truncated Taylor series for the modified Bessel function to deal with the remaining t . We also take into account possible roundoff errors in the numerical computations. The result is that we obtain the values in Table IV. The values of $A_0(x)$ for $d=2$, which are known exactly, have been computed using the algorithm described in Section 15 of ref. 15.

Table V gives numerical values of $C_0^A(0, 0; 1/(2d))$, computed as described in Section 3.1. Table VI gives the values of $C_2^A(0, 0; 1/(2d-1))$,

Table VI. Numerical Values of $C_2^A(0, 0; 1/(2d-1))$ for $d=2, 3, 4, 5, 6$, for Various Choices of A^a

A	$d=2$	$d=3$	$d=4$	$d=5$	$d=6$
\emptyset	∞	1.213109	1.062400	1.027829	1.015421
$\{e_1\}$	1.751695	1.125805	1.045320	1.021995	1.012778
$\{e_1, 2e_1\}$	1.564686	1.121796	1.045056	1.021965	1.012773
$\{e_1, e_1 + e_2\}$	1.481256	1.113713	1.043739	1.021661	1.012681
$\{e_1, 2e_1, 3e_1\}$	1.485308	1.120113	1.044989	1.021961	1.012773
$\{e_1, 2e_1, 2e_1 + e_2\}$	1.465260	1.118079	1.044790	1.021935	1.012769
$\{e_1, e_1 + e_2, 2e_1 + e_2\}$	1.423896	1.111657	1.043606	1.021649	1.012680
$\{e_1, e_1 + e_2, e_1 + 2e_2\}$	1.388210	1.110045	1.043471	1.021631	1.012677
$\{e_1, e_1 + e_2, e_1 + e_2 + e_3\}$	—	1.107650	1.043096	1.021561	1.012660
$\{e_1, e_1 + e_2, e_2\}$	1.211771	1.071615	1.031850	1.017013	1.010433

^a The values are rounded to six digits after the decimal point.

Table VII. Numerical Values of $\tilde{C}_2^{A,e}(0, 0; 1/(2d-1))$ for $d=2, 3, 4, 5, 6$, for Various Choices of A, e^a

A, e	$d=2$	$d=3$	$d=4$	$d=5$	$d=6$
\emptyset, e	∞	1.177591	1.054600	1.025047	1.014136
$\{e_1\}, -e_1$	1.304467	1.097370	1.038115	1.019313	1.011519
$\{e_1\}, e_2$	1.349274	1.101462	1.038967	1.019581	1.011627
$\{e_1, 2e_1\}, -e_1$	1.193791	1.093963	1.037871	1.019285	1.011514
$\{e_1, 2e_1\}, e_2$	1.238380	1.098305	1.038744	1.019554	1.011622
$\{e_1, e_1+e_2\}, -e_1$	1.140666	1.086889	1.036639	1.018992	1.011424
$\{e_1, e_1+e_2\}, e_2$	1.210882	1.094439	1.038093	1.019408	1.011579
$\{e_1, e_1+e_2\}, -e_2$	1.170686	1.090659	1.037469	1.019256	1.011531
$\{e_1, e_1+e_2\}, e_3$	—	1.091432	1.037558	1.019272	1.011535

^aThe values are rounded to six digits after the decimal point.

computed using the method of Section 3.2. Table VII gives numerical values for $\tilde{C}_2^{A,e}(0, 0; 1/(2d-1))$, computed using the method of Section 3.2.

A.2. 1/d Expansions

This section contains 1/d expansions for several relevant quantities. As before, we use the shorthand $s = 1/(2d)$. First, the following are obtained by directly integrating powers of cosines:

$$\int_{[-\pi, \pi]^d} \frac{d^d k}{(2\pi)^d} \hat{D}(k)^n = \begin{cases} s & (n=2) \\ 3s^2 - 3s^3 & (n=4) \\ 15s^3 - 45s^4 + 40s^5 & (n=6) \\ 105s^4 - 630s^5 + 1435s^6 - 1155s^7 & (n=8) \\ 945s^5 + O(s^6) & (n=10) \\ O(s^6) & (n \geq 12) \end{cases} \tag{A.8}$$

$$\int_{[-\pi, \pi]^d} \frac{d^d k}{(2\pi)^d} \hat{D}(k)^n \cos 2k_1 = \begin{cases} s^2 & (n=2) \\ 6s^3 - 8s^4 & (n=4) \\ 45s^4 - 165s^5 + 165s^6 & (n=6) \\ 420s^5 + O(s^6) & (n=8) \\ O(s^6) & (n \geq 10) \end{cases} \tag{A.9}$$

$$\int_{[-\pi, \pi]^d} \frac{d^d k}{(2\pi)^d} \hat{D}(k)^n \cos k_1 \cos k_2 = \begin{cases} 2s^2 & (n=2) \\ 12s^3 - 24s^4 & (n=4) \\ 90s^4 - 450s^5 + 660s^6 & (n=6) \\ 840s^5 + O(s^6) & (n=8) \\ O(s^6) & (n \geq 10) \end{cases} \tag{A.10}$$

$$\int_{[-\pi, \pi]^d} \frac{d^d k}{(2\pi)^d} \hat{D}(k)^n \cos 3k_1 = \begin{cases} s^3 & (n=3) \\ 10s^4 - 15s^5 & (n=5) \\ 105s^5 + O(s^6) & (n=7) \\ O(s^6) & (n \geq 9) \end{cases} \tag{A.11}$$

$$\int_{[-\pi, \pi]^d} \frac{d^d k}{(2\pi)^d} \hat{D}(k)^n \cos 2k_1 \cos k_2 = \begin{cases} 3s^3 & (n=3) \\ 30s^4 - 70s^5 & (n=5) \\ 315s^5 + O(s^6) & (n=7) \\ O(s^6) & (n \geq 9) \end{cases} \tag{A.12}$$

$$\int_{[-\pi, \pi]^d} \frac{d^d k}{(2\pi)^d} \hat{D}(k)^n \cos k_1 \cos k_2 \cos k_3 = \begin{cases} 6s^3 & (n=3) \\ 60s^4 - 180s^5 & (n=5) \\ 630s^5 + O(s^6) & (n=7) \\ O(s^6) & (n \geq 9) \end{cases} \tag{A.13}$$

The above, combined with the expansion

$$\frac{1}{1 - \hat{D}} = \sum_{m=0}^n \hat{D}^m + \frac{\hat{D}^{n+1}}{1 - \hat{D}} \quad (n \geq 0) \tag{A.14}$$

and estimates on errors using Lemma B.1 of ref. 30, i.e.,

$$\int_{[-\pi, \pi]^d} \frac{d^d k}{(2\pi)^d} \frac{|\hat{D}(k)|^m}{[1 - \hat{D}(k)]^n} = O(s^{m/2}) \quad (d > 2n, \quad m \geq 0) \tag{A.15}$$

leads to expansions for the integrals

$$I_{n,m}(x) = \int_{[-\pi, \pi]^d} \frac{d^d k}{(2\pi)^d} \frac{\hat{D}(k)^m e^{ik \cdot x}}{[1 - \hat{D}(k)]^n} \tag{A.16}$$

In particular for $C_0(0, x; 1/(2d)) = I_{1,0}(x)$, we have

$$I_{10}(0) = 1 + s + 3s^2 + 12s^3 + 60s^4 + 355s^5 + O(s^6) \tag{A.17}$$

$$I_{10}(e_1) = s + 3s^2 + 12s^3 + 60s^4 + 355s^5 + O(s^6) \tag{A.18}$$

Table VIII. $1/d$ Expansions for $C_0^A(0, 0; 1/(2d))$ for Various Choices of A

A	$C_0^A(0, 0; 1/(2d))$
\emptyset	$1 + s + 3s^2 + 12s^3 + 60s^4 + 355s^5 + O(s^6)$
$\{e_1\}$	$1 + s + 2s^2 + 7s^3 + 35s^4 + 215s^5 + O(s^6)$
$\{e_1, 2e_1\}$	$1 + s + 2s^2 + 7s^3 + 35s^4 + 215s^5 + O(s^6)$
$\{e_1, e_1 + e_2\}$	$1 + s + 2s^2 + 7s^3 + 34s^4 + 202s^5 + O(s^6)$
$\{e_1, 2e_1, 3e_1\}$	$1 + s + 2s^2 + 7s^3 + 35s^4 + 215s^5 + O(s^6)$
$\{e_1, 2e_1, 2e_1 + e_2\}$	$1 + s + 2s^2 + 7s^3 + 35s^4 + 215s^5 + O(s^6)$
$\{e_1, e_1 + e_2, 2e_1 + e_2\}$	$1 + s + 2s^2 + 7s^3 + 34s^4 + 202s^5 + O(s^6)$
$\{e_1, e_1 + e_2, e_1 + 2e_2\}$	$1 + s + 2s^2 + 7s^3 + 34s^4 + 202s^5 + O(s^6)$
$\{e_1, e_1 + e_2, e_1 + e_2 + e_3\}$	$1 + s + 2s^2 + 7s^3 + 34s^4 + 202s^5 + O(s^6)$
$\{e_1, e_1 + e_2, e_2\}$	$1 + s + s^2 + 2s^3 + 14s^4 + 115s^5 + O(s^6)$

$$I_{10}(2e_1) = s^2 + 6s^3 + 37s^4 + 255s^5 + O(s^6) \tag{A.19}$$

$$I_{10}(e_1 + e_2) = 2s^2 + 12s^3 + 66s^4 + 390s^5 + O(s^6) \tag{A.20}$$

$$I_{10}(3e_1) = s^3 + 10s^4 + 90s^5 + O(s^6) \tag{A.21}$$

$$I_{10}(2e_1 + e_2) = 3s^3 + 30s^4 + 245s^5 + O(s^6) \tag{A.22}$$

$$I_{10}(e_1 + e_2 + e_3) = 6s^3 + 60s^4 + 450s^5 + O(s^6) \tag{A.23}$$

It can also be shown that

$$\sup_{|x| > 3} I_{10}(x) = O(s^4). \tag{A.24}$$

Analogous expansions for higher $I_{n,m}$ will be given and used in ref. 12.

Finally, we turn to the $1/d$ expansions for loop-generating functions with taboo set. Beginning with the $1/d$ expansions for $C_0(y, x; 1/(2d)) = I_{10}(x - y)$ given above, and then using the recursion (3.1), we obtain the $1/d$ expansions for $C_0^A(0, 0; 1/(2d))$ given in Table VIII. The $1/d$ expansions

Table IX. $1/d$ Expansions for $C_2^A(0, 0; 1/(2d - 1))$ for Various Choices of A

A	$C_2^A(0, 0; 1/(2d - 1))$
\emptyset	$1 + s^2 + 7s^3 + 43s^4 + 278s^5 + O(s^6)$
$\{e_1\}$	$1 + s^2 + 5s^3 + 29s^4 + 188s^5 + O(s^6)$
$\{e_1, 2e_1\}$	$1 + s^2 + 5s^3 + 29s^4 + 188s^5 + O(s^6)$
$\{e_1, e_1 + e_2\}$	$1 + s^2 + 5s^3 + 29s^4 + 182s^5 + O(s^6)$

Table X. $1/d$ Expansions for $\tilde{C}_2^{A,e}(0, 0; 1/(2d-1))$ for Various Choices of A, e

A, e	$\tilde{C}_2^{A,e}(0, 0; 1/(2d-1))$
\emptyset, e	$1 + s^2 + 6s^3 + 36s^4 + 235s^5 + O(s^6)$
$\{e_1\}, -e_1$	$1 + s^2 + 4s^3 + 22s^4 + 146s^5 + O(s^6)$
$\{e_1\}, e_2$	$1 + s^2 + 4s^3 + 23s^4 + 154s^5 + O(s^6)$
$\{e_1, 2e_1\}, -e_1$	$1 + s^2 + 4s^3 + 22s^4 + 146s^5 + O(s^6)$
$\{e_1, 2e_1\}, e_2$	$1 + s^2 + 4s^3 + 23s^4 + 154s^5 + O(s^6)$
$\{e_1, e_1 + e_2\}, -e_1$	$1 + s^2 + 4s^3 + 22s^4 + 140s^5 + O(s^6)$
$\{e_1, e_1 + e_2\}, e_2$	$1 + s^2 + 4s^3 + 23s^4 + 152s^5 + O(s^6)$
$\{e_1, e_1 + e_2\}, -e_2$	$1 + s^2 + 4s^3 + 23s^4 + 148s^5 + O(s^6)$
$\{e_1, e_1 + e_2\}, e_3$	$1 + s^2 + 4s^3 + 23s^4 + 148s^5 + O(s^6)$

for memory-2 quantities are more difficult to handle. As described under (3.13), we first solve (3.13) for $\{C_2^{A \cup \{b\}}(y, b + f)\}_{|f|=1}$, for fixed y . At this stage, special care is needed to make full use of symmetry, since naively (3.13) is a system of equations for $2d$ unknowns (and here $d \nearrow \infty$). By symmetry, we can reduce (3.13) to a system of equations for a number of unknowns which is uniformly bounded in d (at least for small $|A|$ and $|y|, |x|$), and obtain the results in Table IX. Then, using (2.40), we compute the $1/d$ expansions for $\tilde{C}_2^{A,e}(0, 0)$ given in Table X.

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