THE LACE EXPANSION FOR SELF-AVOIDING WALK IN FIVE OR MORE DIMENSIONS

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Received 26 November 1991

This paper is a continuation of the companion paper [14], in which it was proved that the standard model of self-avoiding walk in five or more dimensions has the same critical behaviour as the simple random walk, assuming convergence of the lace expansion. In this paper we prove the convergence of the lace expansion, an upper and lower infrared bound, and a number of other estimates that were used in the companion paper. The proof requires a good upper bound on the critical point (or equivalently a lower bound on the connective constant). In an appendix, new upper bounds on the critical point in dimensions higher than two are obtained, using elementary methods which are independent of the lace expansion. The proof of convergence of the lace expansion is computer assisted. Numerical aspects of the proof, including methods for the numerical evaluation of simple random walk quantities such as the two-point function (or lattice Green function), are treated in an appendix.

Contents

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† Supported by NSERC grant A9351.

Reviews in Mathematical Physics Volume 4 No 2 (1992) 235–327

1. Introduction and Main Results

1.1. *The self-avoiding walk*

An n-step self-avoiding walk ω in the hypercubic lattice $\mathbf{Z}^d$ is an ordered set $\omega = (\omega(0), \omega(1), \ldots, \omega(n))$ in which $\omega(i) \in \mathbf{Z}^d$, $|\omega(i+1) - \omega(i)| = 1$ (Euclidean distance) and $\omega(i) \neq \omega(j)$ for $i \neq j$. Unless stated otherwise we take $\omega(0) = 0$. Thus a self-avoiding walk can be thought of as the path of a simple random walk starting at the origin, without any self-intersections. Let c_n denote the number of n-step self-avoiding walks, and let

$$\langle|\omega(n)|^2\rangle_n = \frac{1}{c_n} \sum_{\omega:|\omega|=n} |\omega(n)|^2 \tag{1.1}$$

denote the mean-square displacement. Here the sum over ω is the sum over all n-step self-avoiding walks. The mean-square displacement measures the average squared distance from the origin after n steps, with respect to the uniform probability measure on the set of all n-step self-avoiding walks.

It is a natural question, and one of significance in polymer chemistry and statistical physics, to ask for the asymptotic behaviour of c_n and the mean-square displacement as $n \to \infty$. The conjectured asymptotic behaviour is

$$c_n \sim A\mu^n n^{\gamma-1} \tag{1.2}$$

and

$$\langle|\omega(n)|^2\rangle_n \sim Dn^{2\nu}, \tag{1.3}$$

where $a_n \sim b_n$ means $\lim_{n\to\infty} a_n/b_n = 1$. The constants A, D are dimension dependent, and μ is a dimension dependent constant known as the *connective constant*. The critical exponent γ is believed to take the values 43/32 for $d = 2$, 1.162 ... for $d = 3$, and 1 for $d \geq 4$, with a logarithmic correction when $d = 4$. The conjectured values for ν are 3/4 for $d = 2$, 0.59 ... for $d = 3$, and 1/2 for $d \geq 4$, again with a logarithmic correction in four dimensions. These conjectures are based on nonrigorous renormalization group arguments [20, 21] and numerical work (see e.g. [9, 19] and references therein).

It is known that $\mu \equiv \lim_{n\to\infty} c_n^{1/n}$ exists and that $c_n \geq \mu^n$ [10]. The best general upper bounds on c_n are of the form $c_n \leq \mu^n \exp[O(n^{2/(d+2)} \log n)]$, with the $\log n$ not present for $d = 2$ [12, 15]. There is no general proof that $\nu \geq 1/2$ or that $\nu \leq 1 - \varepsilon$ for some $\varepsilon > 0$. In high dimensions, it has been proved that for $d \geq d_0$, for some undetermined dimension d_0, that (1.2) holds with $\gamma = 1$ [23] and (1.3) holds with $\nu = 1/2$ [22]. Progress is being made in the rigorous study of the weakly self-avoiding walk in four dimensions, using renormalization group methods [4, 1].

In the companion paper [14], which we will refer to as Part I, a number of results were established for the self-avoiding walk for $d \geq 5$, assuming convergence of an expansion known as the lace expansion and several related estimates. These results include (1.2) with $\gamma = 1$, (1.3) with $\nu = 1/2$, and related results including mean-field behaviour of the correlation length and the Gaussian nature of the scaling limit. In this paper we establish convergence of the lace expansion and prove the required estimates, thereby completing the proof of the results of Part I.

As one ingredient of the proof of convergence of the lace expansion, good lower bounds on the connective constant are required. In Corollary A.2 new lower bounds are obtained on the connective constant for $d > 2$. Equivalently these are upper bounds on the critical point $z_c \equiv \mu^{-1}$. Writing $\mu(d)$ to make the dimension dependence of the connective constant explicit, the new bounds for $d = 3, 4, 5$ are

$$\mu(3) \geq 4.43733$$

$$\mu(4) \geq 6.71800$$

$$\mu(5) \geq 8.82128.$$

These bounds are obtained using an elementary argument which is independent of the lace expansion. The above bound for $d = 3$ slightly improves the best previous rigorous bound 4.352 of [8].

The proof of convergence of the lace expansion is computer assisted. The computer calculations use precise numerical values for a number of simple random walk (Gaussian) quantities such as the lattice Green function. In Appendix B an effective method for the computation of Gaussian quantities is presented.

1.2. *The lace expansion*

In this section we give a brief description of the lace expansion, and state the principal results of this paper.

The lace expansion is a kind of cluster expansion [3], which can also be viewed as resulting from repeated application of the inclusion-exclusion relation [24]. It was first introduced by Brydges and Spencer [5] to analyze the *weakly* self-avoiding walk above four dimensions. In the weakly self-avoiding walk (or Domb-Joyce model), self-intersections are discouraged but not prohibited. Brydges and Spencer proved convergence of the lace expansion for $d > 4$, provided this discouragement of self-intersections is sufficiently weak.

In [22], convergence of the lace expansion was proved for the usual self-avoiding walk if the dimension d is sufficiently large. The small parameter responsible for convergence of the expansion was the critical bubble diagram. To define the bubble diagram, for $x \in \mathbf{Z}^d$ we denote by $c_n(x)$ the number of n-step self-avoiding walks for which $\omega(n) = x$, and set $c_0(x) = \delta_{0,x}$. If n and $\|x\|_1$ do not have the same parity then $c_n(x) = 0$. The two-point function is defined to be the generating function for the sequence $c_n(x)$, i.e.

$$G_z(x) = \sum_{n=0}^{\infty} c_n(x) z^n. \tag{1.4}$$

It is known [11] that for any nonzero x, $\lim_{n\to\infty} c_n(x)^{1/n} = \mu$ (provided the limit is taken through the sequence of n values having the same parity as $\|x\|_1$) and hence the above power series has radius of convergence z_c. The bubble diagram is then defined by

$$B_z(0) = \sum_{x \neq 0} G_z(x)^2, \tag{1.5}$$

and the critical bubble diagram is $B_{z_c}(0)$. The analogue of the critical two-point function for simple random walk is the Green function

$$C_z(x) = \sum_{n=0}^{\infty} p_n(x)(2dz)^n \tag{1.6}$$

evaluated at $z = (2d)^{-1}$, where $p_n(x)$ is the probability that a simple random walk starting at the origin ends at x after n steps. It can be shown (see e.g. [13]) that the simple random walk critical bubble diagram, defined by replacing $G_{z_c}(x)$ by $C_{1/2d}(x)$ in (1.5), is asymptotic to $(2d)^{-1}$ as $d \to \infty$. The proof of convergence of the lace expansion given in [22] was to a large degree based on the belief that the self-avoiding walk critical bubble diagram behaves similarly.

It follows from the fact that for $d > 2$ the Green function $C_{1/2d}(x)$ decays like $|x|^{2-d}$ for large x (see e.g. [17]), that the simple random walk critical bubble diagram is finite for $d > 4$ but diverges as $d \to 4^+$. For $d > 4$ it can be expected that the self-avoiding walk critical two-point function will have the same decay, and hence that the critical bubble diagram will be finite for $d > 4$ and diverge as $d \to 4^+$. This suggests that for d marginally larger than four the bubble diagram may not be effective as a small parameter. However, for $d = 5$ a numerical evaluation of the simple random walk critical bubble diagram gives the value 0.5979. In this paper we prove that for the self-avoiding walk the situation is somewhat better: $B_{z_c}(0) \le 0.493$. This value is not very small (in fact for a typical cluster expansion it would be extremely large for a small parameter), but it turns out to be small enough to prove convergence of the lace expansion. The convergence proof follows the general outline used in [22] to prove convergence of the lace expansion for very high dimensions. The proof here is however considerably more elaborate and technical, and the estimation of error terms must be handled with much more delicacy than was the case when the small parameter could be taken as small as desired.

Our proof is unnatural in its reliance on the fortuitous circumstance that in five dimensions the bubble is not too large. A more natural proof would have as its driving force the fact that the bubble is finite rather than small, and would reflect more directly the critical nature of four dimensions. Unfortunately such a proof has not materialized.

Before stating our results, we first repeat from Part I the definitions needed to state the lace expansion. For more details on the expansion the reader is referred to [5, 18].

Given an n-step simple random walk $\omega = (\omega(0), \omega(1), \ldots, \omega(n))$ and two integers s, $t \in [0, n]$, we define

$$\mathscr{U}_{st}(\omega) = \begin{cases} -1 & \text{if } \omega(s) = \omega(t) \\ 0 & \text{if } \omega(s) \neq \omega(t) \end{cases}. \tag{1.7}$$

The self-avoiding walk two-point function can then be written

$$G_z(x) = \sum_{\omega: 0 \to x} z^{|\omega|} \prod_{0 \le s < t \le |\omega|} (1 + \mathscr{U}_{st}(\omega)), \tag{1.8}$$

where the sum over ω is the sum over all simple random walks ending at x. The Fourier transform of (1.8) is given by

$$\hat{G}_z(k) = \sum_x G_z(x)e^{ik\cdot x} = \sum_\omega z^{|\omega|}e^{ik\cdot\omega(|\omega|)} \prod_{0\le s<t\le|\omega|} (1 + \mathscr{U}_{st}(\omega)). \tag{1.9}$$

Given an interval $I = [a,b]$ of positive integers, we refer to a pair st of elements of I, with $s < t$, as an *edge*. A set of edges is called a *graph*. A graph Γ is said to be *connected* if both a and b are endpoints of edges in Γ, and if in addition for any $c \in (a,b)$ there are $s,t \in [a,b]$ such that $s < c < t$ and $st \in \Gamma$. The set of all graphs on $[a,b]$ is denoted $\mathscr{B}[a,b]$, and the subset consisting of all connected graphs is denoted $\mathscr{G}[a,b]$. A *lace* is a minimally connected graph, i.e. a connected graph for which the removal of any edge would result in a disconnected graph. The set of laces on $[a,b]$ is denoted by $\mathscr{L}[a,b]$, and the set of laces on $[a,b]$ which consist of exactly N edges is denoted $\mathscr{L}_N[a,b]$.

The following prescription associates to each connected graph Γ a unique lace $\mathscr{L}_\Gamma$. The lace $\mathscr{L}_\Gamma$ consists of edges $s_1t_1, s_2t_2, \ldots$ where

$$s_1 = a, \qquad t_1 = \max\{t : at \in \Gamma\}$$

$$t_{i+1} = \max\{t : st \in \Gamma, s < t_i\}$$

$$s_i = \min\{s : st_i \in \Gamma\}.$$

Given a lace L, the set of all edges $st \notin L$ such that $\mathscr{L}_{L\cup\{st\}} = L$ is denoted $\mathscr{C}(L)$.

For $a < b$ we define

$$J_N[a,b] = \sum_{L\in\mathscr{L}_N[a,b]} \prod_{st\in L} \mathscr{U}_{st} \prod_{s't'\in\mathscr{C}(L)} (1 + \mathscr{U}_{s't'}) \tag{1.10}$$

and

$$J[a,b] = \sum_{N=1}^{\infty} J_N[a,b]. \tag{1.11}$$

The sum in (1.11) is a finite sum, since the sum in (1.10) is empty for $N > b - a$. We set $J[a,a] = 1$. We define

$$\Pi_z^{(N)}(x) = (-1)^N \sum_{\substack{\omega:0\to x\\ |\omega|\ge 2}} z^{|\omega|}J_N[0,|\omega|] \tag{1.12}$$

and

$$\Pi_z(x) = \sum_{N=1}^{\infty} (-1)^N \Pi_z^{(N)}(x) = \sum_{\substack{\omega:0\to x\\ |\omega|\ge 2}} z^{|\omega|}J[0,|\omega|] \tag{1.13}$$

for any z for which the right sides converge. This is the lace expansion. By definition, $\Pi_z^{(N)}(x) \geq 0$ for all nonnegative z.

Let

$$\hat{D}(k) = d^{-1} \sum_{\mu=1}^{d} \cos k_\mu . \tag{1.14}$$

Brydges and Spencer proved [5] that for any value of z for which $\sum_{|\omega| \geq 2} z^{|\omega|} J[0, |\omega|]$ and $\sum_x G_{|z|}(x)$ converge absolutely,

$$G_z(x) = \delta_{0,x} + z \sum_{y:|y|=1} G_z(x-y) + \sum_{v \in \mathbf{Z}^d} \Pi_z(v) G_z(x-v) \tag{1.15}$$

and

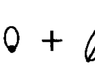
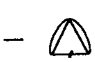
$$\hat{G}_z(k) = \frac{1}{1 - 2dz\hat{D}(k) - \hat{\Pi}_z(k)} . \tag{1.16}$$

In particular (1.16) gives a formula for the susceptibility $\chi(z) = \hat{G}_z(0)$.

Equation (1.16) gives an expression for the inverse of the propagator $\hat{G}_z(k)$. By definition,

$$\hat{\Pi}_z(k) = \sum_x \Pi_z(x) e^{ik\cdot x} = \sum_{N=1}^{\infty} \sum_{\omega:|\omega|\geq 2} e^{ik\cdot\omega(|\omega|)} z^{|\omega|} J_N[0, |\omega|] . \tag{1.17}$$

There is a useful diagrammatic interpretation for the terms in the above sum over N, arising from the fact that $J_N[0, |\omega|] \neq 0$ only for walks ω with a specific topology. This has been described in detail in [5], so we state this interpretation without detailed explanations here. The factor $\prod_{st \in L} \mathcal{U}_{st}$ in (1.10) is nonzero only if the walk intersects itself at times s and t, for each $st \in L$, while the factor $\prod_{st \in \mathscr{C}(L)} (1 + \mathcal{U}_{st})$ rules out many but in general not all other self-intersections. The walk decomposes in a natural way into $2N - 1$ strictly self-avoiding subwalks, corresponding to the time intervals intervening between the intersections required for $\prod_{st \in L} \mathcal{U}_{st} \neq 0$. We represent the Nth term $\hat{\Pi}_z^{(N)}(k)$ of (1.17) by an N-loop diagram, as follows:

$\hat{\Pi}_z(k) = -$ $+$  $-$  $+$  $- \cdots$ (1.18)

The subwalks which are not slashed in (1.18) must consist of at least one step, whereas the slashed subwalks can be of zero or more steps. The subwalks forming each loop of a diagram are mutually avoiding. Further mutual avoidance is also present.

To complete the proofs of the theorems stated in Part I, it remains to obtain a number of bounds on the two-point function and on $\hat{\Pi}_z(k)$. Specifically, the missing proofs from Part I are those of the bounds on the two-point function and $\hat{\Pi}_z(k)$ of Theorems I.2.5, I.2.6, I.2.7, I.2.8, and of the values of A and D of Theorem I.1.1, where the prefix I in theorem and equation numbers refers to part I. These are restated in the following theorem and corollary. The proof of the theorem constitutes the bulk of this paper.

It convenient to distinguish notationally between real and complex activity, and we use p to denote a nonnegative activity and z for a complex activity. An exception is the use of $z_c = \mu^{-1} \in \mathbf{R}$ to denote the critical point. For $x = (x_1, \ldots, x_d) \in \mathbf{Z}^d$, we write $|x| = [x_1^2 + \cdots + x_d^2]^{1/2}$. We write $\partial_\mu^u \equiv (\partial/\partial k_\mu)^u$, and $\nabla_k^2 \equiv \sum_{\mu=1}^d \partial_\mu^2$.

The following is a restatement of Theorems I.2.5–I.2.7 and an extension of Theorem I.2.8.

Theorem 1.1. *For $d \geq 5$ the lace expansion* (1.13) *converges absolutely for all $|z| \leq z_c$, and*

$$\hat{G}_z(k) = \frac{1}{1 - 2dz\hat{D}(k) - \hat{\Pi}_z(k)}. \tag{1.19}$$

The following numerical bounds are satisfied.

For $|z| \leq z_c$,

$$\| |x|^2 G_z(x) \|_\infty \leq 0.1425, \qquad \|G_z(x) - \delta_{0,x}\|_2^2 \equiv B_z(0) \leq 0.493. \tag{1.20}$$

For $|z| \leq z_c$, $k \in [-\pi, \pi]^d$, $u \in \{0, 1, 2\}$,

$$|\partial_\mu^u \hat{\Pi}_z(k)| \leq (0.09761)/d, \qquad |z\partial_z \hat{\Pi}_z(k)| \leq 1.517, \tag{1.21}$$

and thus for $\frac{1}{2d} \leq |z| \leq z_c$,

$$|\partial_z \hat{\Pi}_z(k)| \leq (1.517) \times (2d). \tag{1.22}$$

Moreover in (1.20)–(1.22) *the series on the left sides are bounded absolutely by the right sides. For $z = z_c e^{i\theta}$, $\theta \neq 0$,*

$$1 - 2dz - \hat{\Pi}_z(0) \neq 0. \tag{1.23}$$

There is a positive dimension-dependent ε_1 such that for $p \in [z_c - \varepsilon_1, z_c]$,

$$2d + \partial_p \hat{\Pi}_p(0) \geq (0.59) \times (2d). \tag{1.24}$$

For $p \in \left[\frac{1}{2d-1}, z_c\right]$,

$$2dp - \nabla_k^2 \hat{\Pi}_p(0) \geq \begin{cases} 1.087 & (d = 5) \\ 0.97 & (d \geq 6) \end{cases}, \tag{1.25}$$

and for $p \in [0, z_c]$,

$$-(0.02407)\{1 - \hat{D}(k)\} \leq \hat{\Pi}_p(0) - \hat{\Pi}_p(k) \leq (0.07355)\{1 - \hat{D}(k)\}. \qquad (1.26)$$

Remark. Since $\sum_x G_{|z|}(x) = \chi(|z|)$ converges for $|z| < z_c$, it can be concluded from the convergence of the lace expansion stated in the above theorem that (1.19) holds for $|z| < z_c$. Since $\hat{\Pi}_z(k)$ is absolutely convergent for $|z| \leq z_c$ and hence continuous on $|z| = z_c$, and since $\hat{G}_z(0)$ diverges to infinity as $z \nearrow z_c$, it follows that $1 - 2dz_c - \hat{\Pi}_{z_c}(0) = 0$. By (1.23), for $k = 0$ (1.19) also holds on the circle of convergence $|z| = z_c$, except at the critical point where both sides of (1.19) are undefined.

As a corollary of Theorem 1.1 we can prove the following two-sided infrared bound, which with (1.20) comes close to proving Theorem I.1.5.

Corollary 1.2. *For* $d \geq 5$ *and* $p \in \left[\frac{1}{2d-1}, z_c\right]$,

$$0 \leq \hat{G}_p(k) \leq \frac{C'}{1 - \hat{D}(k)}, \qquad (1.27)$$

and at $p = z_c$,

$$\frac{C}{1 - \hat{D}(k)} \leq \hat{G}_{z_c}(k) \leq \frac{C'}{1 - \hat{D}(k)}. \qquad (1.28)$$

In five dimensions we can take $C = 0.8283$, $C' = 0.9200$, *and for* $d \geq 6$ *we have* $C' \leq 1.025$.

Proof of Corollary 1.2, given Theorem 1.1. Both (1.27) and (1.28) follows from (1.19) and (1.26), since

$$\hat{G}_p(k)^{-1} = 1 - 2dp - \hat{\Pi}_p(0) + 2dp\{1 - \hat{D}(k)\} + \hat{\Pi}_p(0) - \hat{\Pi}_p(k) \qquad (1.29)$$

and

$$1 - 2dp - \hat{\Pi}_p(0) = \hat{G}_p(0)^{-1} \geq 0, \qquad (1.30)$$

with equality at $p = z_c$. For the numerical value of C we use the upper bound on z_c of Corollary A.2. □

1.3. *Reduction of Theorem 1.1 to basic numerical bounds*

In this section we essentially reduce the proof of Theorem 1.1 to establishing a number of numerical bounds on the two-point function, several "bubble" quantities, and $\hat{\Pi}_z(k)$. These bounds are given in Theorem 1.4. We restrict attention to the case of $d = 5$. Higher dimensions are less difficult, and are discussed briefly in Appendix C. At the end of the section the bounds stated in Part I for the amplitudes A and D of (1.2) and (1.3) are given.

We begin with several definitions. For $x \in \mathbf{Z}^d$, and $z \in \mathbf{C}$ we define the "bubble" quantities

$$B_z(x) \equiv \sum_{y \neq 0, x} G_z(y) G_z(x-y), \qquad B_z'(x) \equiv \sum_{y \neq x} G_z(y) G_z(x-y), \tag{1.31}$$

$$B_z''(x) \equiv \sum_{y} G_z(y) G_z(x-y), \qquad \tilde{B}_z(0) \equiv \sum_{y: |y| > 1} \{G_z(y)\}^2. \tag{1.32}$$

We denote the standard unit basis vectors of $\mathbf{Z}^5$ by $e_1, \ldots, e_5$. We also write

$$v_n = \sum_{\mu=1}^{n} e_\mu, \qquad n = 1, \ldots, 5. \tag{1.33}$$

We define two sets of sites:

$$\Lambda_1 \equiv \text{all } \mathbf{Z}^5 \text{ rotations and reflections of } \{v_1, v_2, v_3, v_4, v_5, 2e_1, 2e_1 + e_2\} \tag{1.34}$$

and

$$\Lambda_0 \equiv \Lambda_1 \cup \{0\}. \tag{1.35}$$

We define

$$\Pi_z^{(\mathrm{odd})}(x) = \sum_{k=0}^{\infty} \Pi_z^{(2k+1)}(x) \tag{1.36}$$

and

$$\Pi_z^{(\mathrm{even})}(x) = \sum_{k=1}^{\infty} \Pi_z^{(2k)}(x). \tag{1.37}$$

These are both nonnegative for all x when $0 \le z \le z_c$, and by (1.13)

$$\Pi_z(x) = -\Pi_z^{(\mathrm{odd})}(x) + \Pi_z^{(\mathrm{even})}(x). \tag{1.38}$$

We next define two sets of inequalities, which *a priori* may or may not be satisfied.

Definition 1.3. For $\alpha > 0$ and $z \in \mathbf{C}$, we define $P_z(\alpha)$ to be the following set of inequalities:

$$|B_z(0)| \le \alpha \cdot (0.493), \qquad |\tilde{B}_z(0)| \le \alpha \cdot (0.314), \qquad |G_z(e_1)| \le \alpha \cdot (0.1425) \tag{1.39}$$

$$\sup_{x \notin \Lambda_0} |x|^2 |G_z(x)| \leq \alpha \cdot (0.075) \tag{1.40}$$

$$|B_z'(e_1)| \leq \alpha \cdot (0.488), \qquad |B_z'(v_2)| \leq \alpha \cdot (0.356) \tag{1.41}$$

$$|B_z'(2e_1)| \leq \alpha \cdot (0.286), \qquad |B_z'(2e_1 + e_2)| \leq \alpha \cdot (0.24) \tag{1.42}$$

$$|B_z'(v_3)| \leq \alpha \cdot (0.289), \qquad |B_z'(v_4)| \leq \alpha \cdot (0.251) \tag{1.43}$$

$$|B_z'(v_5)| \leq \alpha \cdot (0.227), \qquad \sup_{x \notin \Lambda_0} |B_z'(x)| \leq \alpha \cdot (0.215). \tag{1.44}$$

For $z \in \mathbf{C}$, we define Q_z to be the following set of inequalities:

$$\sup_{x \in \mathbf{Z}^d} |x|^2 |G_z(x)| \leq 0.1425 \tag{1.45}$$

$$\sum_x |\Pi_z^{(\mathrm{odd})}(x)| \leq 0.173025 \tag{1.46}$$

$$\sum_x |\Pi_z^{(\mathrm{even})}(x)| \leq 0.0386478 \tag{1.47}$$

$$\sum_x |x|^2 |\Pi_z^{(\mathrm{odd})}(x)| \leq 0.0240623 \tag{1.48}$$

$$\sum_x |x|^2 |\Pi_z^{(\mathrm{even})}(x)| \leq 0.0735417 \tag{1.49}$$

$$|\hat{\Pi}_z^{(\mathrm{odd})}(0) - \hat{\Pi}_z^{(\mathrm{odd})}(k)| \leq (0.0240623)\{1 - \hat{D}(k)\} \tag{1.50}$$

$$|\hat{\Pi}_z^{(\mathrm{even})}(0) - \hat{\Pi}_z^{(\mathrm{even})}(k)| \leq (0.0735417)\{1 - \hat{D}(k)\} \tag{1.51}$$

$$\left| z\partial_z \sum_x \Pi_z^{(\mathrm{odd})}(x) \right| \leq 0.914078 \tag{1.52}$$

$$\left| z\partial_z \sum_x \Pi_z^{(\mathrm{even})}(x) \right| \leq 0.602171. \tag{1.53}$$

Remark. For $z = p \geq 0$, all absolute values in $P_p(\alpha)$ and Q_p can be removed since the corresponding quantities will be nonnegative by definition. Also, given any of the inequalities of (1.46)–(1.49) and (1.52), (1.53), we can easily obtain a corresponding inequality for the Fourier transform. For example, if (1.48) holds for $z = p \geq 0$, then we have

$$d |\partial_\mu^2 \hat{\Pi}_z^{(\mathrm{odd})}(k)| \leq 0.0240623. \tag{1.54}$$

In the remainder of this section we reduce the proof of Theorem 1.1 to the following three results.

Theorem 1.4. *For $d = 5$ and $p \in [0, z_c)$, the inequalities $P_p(0.999)$ and Q_p hold.*

We show below that the following corollary follows readily from Theorem 1.4.

Corollary 1.5. *For $d = 5$ and $|z| \le z_c$, the inequalities $P_z(0.999)$ and Q_z hold.*

Given Corollary 1.5, we prove the following result in Sec. 5.2.

Proposition 1.6. *For $d = 5$ and $z = z_c e^{i\theta}$, $\theta \neq 0$, we have*

$$1 - 2dz - \hat{\Pi}_z(0) \neq 0. \tag{1.55}$$

As we now show, Theorem 1.1 follows in a straightforward way from Theorem 1.4, Corollary 1.5 and Proposition 1.6.

Proof of Theorem 1.1, given Theorem 1.4, Corollary 1.5 and Proposition 1.6. By Theorem 1.4 and Corollary 1.5, all inequalities of $P_z(1)$ and Q_z hold for $|z| \le z_c$. In particular, the critical bubble diagram satisfies the inequality $B_{z_c}(0) \le 0.493$, and hence by Lemma I.2.4 the lace expansion for $\hat{\Pi}_z(k)$ converges absolutely. The inequalities of (1.20) are given by (1.45) and (1.39). The inequalities of (1.21) follow from (1.48), (1.49), (1.52), (1.53), and the fact that

$$\begin{aligned} |\partial_{k_\mu}^u \hat{\Pi}_z(k)| &\le d^{-1} \sum_x |x|^2 [\Pi_{|z|}^{(\mathrm{odd})}(x) + \Pi_{|z|}^{(\mathrm{even})}(x)] \\ |z\partial_z \hat{\Pi}_z(k)| &\le |z|\, \partial_z \sum_x [\Pi_z^{(\mathrm{odd})}(x) + \Pi_z^{(\mathrm{even})}(x)]\Big|_{z=|z|}. \end{aligned} \tag{1.56}$$

Proposition 1.6 gives (1.23). A lower bound weaker than (1.24) follows from (1.52), since fo $p \in \left[\frac{1}{2d-1}, z_c\right]$, we have $\partial_p \hat{\Pi}_p^{(\mathrm{even})} \ge 0$, $\partial_p \hat{\Pi}_p^{(\mathrm{odd})} \ge 0$, and hence

$$p(2d + \partial_p \hat{\Pi}_p(0)) \ge 2dp - p\partial_p \hat{\Pi}_p^{(\mathrm{odd})}(0) \ge \frac{10}{9} - 0.914078. \tag{1.57}$$

We improve this bound below. Similarly, (1.25) follows from (1.48). Finally, (1.26) follows from (1.50) and (1.51), because $-\{\hat{\Pi}_p^{(\mathrm{odd})}(0) - \hat{\Pi}_p^{(\mathrm{odd})}(k)\} \le \hat{\Pi}_p(0) - \hat{\Pi}_p(k) \le \hat{\Pi}_p^{(\mathrm{even})}(0) - \hat{\Pi}_p^{(\mathrm{even})}(k)$ for nonnegative p.

We can improve (1.57) to (1.24) by using the bound

$$\frac{1}{1 + B_p(0)} - \frac{1}{\chi(p)} \le -z_c \partial_p [\chi(p)^{-1}] \le 1 - \frac{1}{\chi(p)} \tag{1.58}$$

of [2]. (In fact the form of the bound stated in [2] is slightly different; the above bound agrees with our conventions.) At $p = z_c$ this gives

$$z_c^{-1} \frac{1}{1 + B_{z_c}(0)} \leq -\partial_p[\chi(p)^{-1}]|_{p=z_c} \leq z_c^{-1}. \tag{1.59}$$

Recall that $\chi(p)^{-1} = 1 - 2dp - \hat{\Pi}_p(0)$. We bound z_c from above by the value 0.113363 of Corollary A.2, and use the upper bound $B_{z_c}(0) \leq 0.493$ of $P_p(1)$ to obtain

$$2d + \partial_p \hat{\Pi}_p(0)|_{p=z_c} \geq 5.9083. \tag{1.60}$$

Then (1.24) for $d = 5$ follows by continuity. For $d \geq 6$, we proceed similarly, now using $z_c \leq (1.08)/(2d - 1)$ and $B_{z_c}(0) \leq 0.26$. (See Appendix C for these bounds.) □

Proof of Corollary 1.5, given Theorem 1.4. The monotone convergence theorem can be used in a straightforward manner to extend the bounds of $P_p(0.999)$ and Q_p from $p \in [0, z_c)$ to $p = z_c$. These bounds then extend to $|z| \leq z_c$, since we are dealing with power series with nonnegative coefficients, which therefore give maximum absolute value for $z = z_c$. To see that (1.50) and (1.51) involve series with nonnegative coefficients, we use symmetry to write for example $\hat{\Pi}_z^{(\mathrm{odd})}(0) - \hat{\Pi}_z^{(\mathrm{odd})}(k) = \sum_x \{1 - \cos(k \cdot x)\} \Pi_z^{(\mathrm{odd})}(x)$. □

Proof of bounds on A and D. Since $A = (-z_c \partial_p[\chi(p)^{-1}]|_{p=z_c})^{-1}$ by (I.3.3), it follows immediately from (1.58) that $A \in [1, 1.493]$. For the diffusion constant, we have from (I.3.5) that $D = A[2dz_c + \sum_x |x|^2 \Pi_{z_c}(x)]$. We use the above bound on A together with (1.48) and (1.49). We also use the upper bound on z_c of Corollary A.2, and the fact that z_c is bounded below by the critical point of simple random walk with no loops of size four or less. This is shown in [7] to be the inverse of the largest root of $\lambda^3 - 2(d-1)\lambda^2 - 2(d-1)\lambda - 1 = 0$, which gives $z_c \geq (1.01)/9$. This leads to

$$D \in [1, 1.493] \cdot [2d(1.01)/9 - 0.0240623, 2d(0.113363) + 0.0735417] \subset [1.098, 1.803].$$

□

Our remaining task is to prove Theorem 1.4 and Proposition 1.6. The former is proven throughout Secs. 1.4–5.1, and the latter is proven in Sec. 5.2 relatively easily. Since Theorem 1.4 deals only with $p \in (0, z_c)$, we can restrict ourselves to this range of p until Sec. 5.2. In the next subsection we reduce the proof of Theorem 1.4 to several steps.

1.4. *Structure of the proof of Theorem 1.4*

The proof of Theorem 1.4 depends on the following three propositions and one lemma. To state the first of these results, we introduce

$$I_{n,0}(x) \equiv \int \frac{d^d k}{(2\pi)^d} \frac{e^{ik \cdot x}}{\{1 - \hat{D}(k)\}^n}. \tag{1.61}$$

In particular, $I_{1,0}(x)$ is the critical two-point function for simple random walk, or in other words the lattice Green function. Here, and throughout the paper, $\int \frac{d^dk}{(2\pi)^d}$ denotes integration over $[-\pi, \pi]^d$.

Proposition 1.7. *For $p \le p_0 \equiv \frac{6611}{9^5}$, we have*

$$G_p(x) \le \frac{713988}{812911} I_{1,0}(x), \tag{1.62}$$

and thus $P_p(0.999)$ holds.

Proof. The proof of (1.62) is given in Proposition A.3. Then it can be seen that $P_p(0.999)$ holds, using the bounds on $I_{1,0}(x)$ and $I_{2,0}(x)$ in Sec. B.2.3 and on $|x|^2 I_{1,0}(x)$ in Sec. B.2.5. For example, to obtain the desired bound on $B_p(0)$, we use the definition of $B_p(x)$ in (1.31) and the Parseval relation to obtain

$$B_p(0) = \sum_y [G_p(y) - \delta_{0,y}]^2 \le \int \frac{d^dk}{(2\pi)^d} \left[\frac{0.8784}{1 - \hat{D}(k)} - 1 \right]^2, \tag{1.63}$$

and then write the right side in terms of $I_{1,0}(0)$ and $I_{2,0}(0)$.

For (1.40), we multiply (1.62) by $|x|^2$ for small x and use Lemma B.12 for large x. □

Proposition 1.8. *All quantities appearing in the left side of the inequalities of $P_p(\alpha)$ are continuous in $p \in (0, z_c)$.*

Proof. The quantities on the left sides of $P_p(\alpha)$, except for $\sup |x|^2 G_p(x)$ and $\sup B'_p(x)$, are power series in p with radius of convergence z_c and hence are continuous for $p \in (0, z_c)$. For the same reason, the two exceptions are suprema of infinitely many continuous functions. To see that these suprema are continuous, we use the fact that the sub-critical two-point function decays exponentially. This can be seen by first observing that

$$G_p(x) \le \sum_{n \ge \|x\|_\infty} c_n(x) p^n. \tag{1.64}$$

Then by definition of μ, for $p < z_c$, $c_n(x)p^n \le c_n p^n$ can be bounded by a (p-dependent) multiple of θ^n, for some $\theta = \theta(p) < 1$, and hence G_p decays exponentially. Thus only finitely many values of x are relevant in the suprema over x, and the desired continuity follows from the fact that the supremum of finitely many continuous functions is continuous. □

Proposition 1.9. *For any fixed $p \in [p_0, z_c)$, if the set of inequalities $P_p(1)$ holds then in fact the stronger set of inequalities $P_p(0.999)$ must hold.*

This last proposition is the core of the proof, and is proved in Secs. 2–4. An overview of the proof is given in Sec. 1.5. In the course of the proof we obtain Lemmas 3.1 and 5.1, which together can be summarized as follows.

Lemma 1.10. *Given $P_p(1)$, the numerical bounds in Q_p hold.*

As we show below, these results are sufficient to prove Theorem 1.4, when combined with the following lemma.

Lemma 1.11. *Suppose that $f_1(p), f_2(p), \ldots, f_n(p)$ are nonnegative functions, and that there are $p_0 < p_1$ such that*

1. *$f_m(p_0) \leq 0.999$ for $1 \leq m \leq n$,*
2. *$f_m(p)$ is continuous in $p \in [p_0, p_1)$ for each $1 \leq m \leq n$,*
3. *for each fixed $p \in [p_0, p_1)$, the set of inequalities $f_m(p) \leq 1$ $(1 \leq m \leq n)$ implies the stronger set of inequalities $f_m(p) \leq 0.999$ $(1 \leq m \leq n)$.*

Then $f_m(p) \leq 0.999$ for all $p \in [p_0, p_1)$, $(1 \leq m \leq n)$.

Proof. Define $f_{\max}(p) \equiv \max_{1 \leq m \leq n} f_m(p)$. By Assumption 3, $f_{\max}(p) \notin (0.999, 1]$ for all $p \in [p_0, p_1)$. On the other hand, by the second assumption $f_{\max}(p)$ is continuous in $p \in [p_0, p_1)$. Since $f_{\max}(p_0) \leq 0.999$ by Assumption 1, the above two facts imply that the graph of $f_{\max}$ for $p \in [p_0, p_1)$ must remain below the forbidden interval $(0.999, 1]$ and hence $f_{\max}(p) \leq 0.999$ for all $p \in [p_0, p_1)$. □

Proof of Theorem 1.4, given Proposition 1.9 and Lemma 1.10. We first normalize the inequalities of $P_p(1)$ to give right sides equal to 1. The fact that $P_p(0.999)$ holds then follows immediately from Propositions 1.7–1.9, applying Lemma 1.11 with $p_1 = z_c$. Then Q_p follows immediately from Lemma 1.10. □

1.5. *Overview of the method and organization of the paper*

The basic strategy used to prove Proposition 1.9 is essentially the same as that used in [22]. In this section the driving force of the argument is described. We also comment briefly on the role of computer calculations in the analysis, and describe the organization of the remainder of the paper.

To prove Proposition 1.9, it must be shown that the set of inequalities $P_p(1)$ implies the stronger set of inequalities $P_p(0.999)$. To begin, we assume that $P_p(1)$ holds. It follows from (1.16) that

$$\begin{aligned} \hat{G}_z(k) &= \frac{1}{1 - 2dz\hat{D}(k) - \hat{\Pi}_z(k)} \\ &= \frac{1}{1 - 2dz - \hat{\Pi}_z(0) + 2dz\{1 - \hat{D}(k)\} + \hat{\Pi}_z(0) - \hat{\Pi}_z(k)}. \end{aligned} \tag{1.65}$$

The right side can be interpreted as the subcritical Gaussian quantity

$$\frac{1}{\chi(z)^{-1} + 2dz[1 - \hat{D}(k)]}, \tag{1.66}$$

perturbed by an amount $\hat{\Pi}_z(0) - \hat{\Pi}_z(k)$. This perturbation can be shown to be a small multiple of $1 - \hat{D}(k)$ by estimating $\partial_\mu^2 \hat{\Pi}_z(k)$ in terms of the quantities occurring in $P_p(1)$.

As a result, using the fact that $\chi^{-1} \geq 0$ it can be concluded that $\hat{G}_p(k)$ is bounded above by a multiple of $[1 - \hat{D}(k)]^{-1}$, as in Corollary 1.2.

On the other hand, all the quantities appearing in $P_p(0.999)$ can be calculated in terms of $\hat{G}_z(k)$, and hence estimated in terms of $[1 - \hat{D}(k)]^{-1}$. The upper bounds can be evaluated numerically, with the result that $P_p(0.999)$ holds.

This procedure was carried out in [22] for the self-avoiding walk in very high dimensions, where the above perturbation could be made as small as desired by taking d sufficiently large. For $d = 5$ the perturbation, although not terribly large, cannot be taken to be arbitrarily small. This has the effect that very little can be sacrificed in estimates. It is remarkable that the original bounds $P_p(1)$ can in fact be improved to $P_p(0.999)$ by this mechanism, but the values in $P_p(1)$ have been very carefully chosen so that this improvement is possible. Computer experimentation for finding good values for $P_p(1)$ proved to be very useful. Detailed numerical estimates were used for a number of quantities. The number of calculations involving precise numerical values is large, and to make it practical the entire calculation described in this paper was done by computer, using a FORTRAN program. Apart from making the calculation practical, the computer played a valuable role in the development of the proof, by allowing for convenient experimentation in comparing the effect of alternate or improved estimates. Our basic strategy was to push the estimates until they were sufficiently good to make the proof work, decreasing the dimension from $d = 10$ one by one. As the dimension decreased it became necessary to include additional quantities in $P_p(\alpha)$. Computer calculations were also used to evaluate precisely the simple random walk (Gaussian) Green function, at several thousand lattice sites. Rigorous error bounds were obtained for the computer calculations. A discussion of the error estimates and of the method of calculating Gaussian Green functions can be found in Appendix B.

The final numerical computations were performed with a VAX FORTRAN program on a VAX6440 at the Meson Science Laboratory of the Faculty of Science of the University of Tokyo, running the VAX/VMS operating system. The total computation time was approximately two hours. Of this, all but approximately one second was used to calculate the values of Gaussian quantities. The remaining second was used to perform the calculations in which $P_p(0.999)$ is concluded from $P_p(1)$. To make sure that there is no software (compiler) or hardware problems, we have run the same programs on a different machine (DECstation5400, running Ultrix 4.1), and have checked that they produce exactly the same results up to round-off errors. The FORTRAN source code is available from the authors upon request.

Many refinements need to be incorporated into the method used in [22] to treat $d = 5$. These refinements, and the organization of the paper, are summarized in the following.

It was stated above that given the estimates $P_p(1)$ on the bubble quantities and the two-point function, $\hat{\Pi}$ is then estimated in terms of these quantities. In fact we find it more efficient to estimate $\hat{\Pi}$ in terms of smaller repulsive bubble quantities, in which the two lines of the bubble diagram feel some mutual repulsion. A comparison of the repulsive and nonrepulsive bubbles is given in Sec. 2.1. We also find it useful to extract from $\hat{\Pi}$ some terms which can be evaluated explicitly. This is done in Sec. 3.1. Based on these preparations, Sec. 3 is concerned with refined diagrammatic estimates of $\hat{\Pi}$.

Detailed diagrammatic estimates are performed up to and including the eight loop diagram.

Next the quantities appearing in $P_p(0.999)$ are carefully estimated using the derived estimates on $\hat{\Pi}$ and (1.65). This step is carried out in Sec. 4.

The rest of the paper is somewhat anticlimactic. In Sec. 5, the proof of Proposition 1.6 is given. Upper bounds on the critical point, which prove the lower bounds on the connective constant stated at the end of Sec. 1.1 and also are needed to carry out the proof of Proposition 1.9, are obtained in Appendix A. Appendix A also contains proofs of upper and lower bounds on the two-point function in terms of the two-point function for simple random walk without immediate reversals. Numerical aspects of the proof are treated in Appendix B, in which values of various Gaussian quantities are also given. Finally Appendix C contains a brief discussion of dimensions above five; the paper otherwise deals primarily with $d = 5$, which is the most difficult case.

1.6. *Definitions and notation*

Throughout this paper, we denote upper and lower bounds on A by $\bar{A}$ and $\underline{A}$ respectively. Unless otherwise indicated, ω, ω_1, ω_2, ω'_1, ω'_2 are used to denote self-avoiding walks. We usually use e or f to denote a unit vector in $\mathbf{Z}^5$, and denote the usual basis of $\mathbf{Z}^5$ by $e_1, \dots, e_5$. We write $p_0 \equiv \frac{6611}{9^5}$, as in Proposition 1.7.

In addition to Λ_1 and Λ_0 introduced in (1.34), we define several subsets of $\mathbf{Z}^5$:

$$\Lambda_2 \equiv \{x \in \mathbf{Z}^5 : 0 < \|x\|_1 \leq 4\},$$

$$\Lambda'_2 \equiv \Lambda_2 \cup \{\mathbf{Z}^5 \text{ rotations and reflections of } (1,1,1,1,1)\}, \tag{1.67}$$

$$\Lambda_3 \equiv \Lambda'_2 \cup \{\mathbf{Z}^5 \text{ rotations and reflections of } (2,1,1,1,0)\}.$$

We also define the following "repulsive bubble" quantities:

$$R_p(x) \equiv \sum_{y \neq 0, x} \sum_{\omega_1 : 0 \to y} \sum_{\omega_2 : y \to x} p^{|\omega_1| + |\omega_2|} \mathrm{I}[\omega_1 \cap \omega_2 = \{y\}] \qquad (x \neq 0) \tag{1.68}$$

$$R_p(0) \equiv \sum_{y \neq 0} \sum_{\omega_1 : 0 \to y} \sum_{\omega_2 : y \to 0} p^{|\omega_1| + |\omega_2|} \mathrm{I}[\omega_1 \cap \omega_2 = \{0, y\}] \tag{1.69}$$

$$\tilde{R}_p(0) \equiv \sum_{y : |y| > 1} \sum_{\omega_1 : 0 \to y} \sum_{\omega_2 : y \to 0} p^{|\omega_1| + |\omega_2|} \mathrm{I}[\omega_1 \cap \omega_2 = \{0, y\}] \tag{1.70}$$

$$R'_p(x) \equiv \sum_{y \neq 0} \sum_{\omega_1 : 0 \to y} \sum_{\omega_2 : y \to x} p^{|\omega_1| + |\omega_2|} \mathrm{I}[\omega_1 \cap \omega_2 = \{y\}] \qquad (x \neq 0) \tag{1.71}$$

$$R''_p(x) \equiv \sum_{y} \sum_{\omega_1 : 0 \to y} \sum_{\omega_2 : y \to x} p^{|\omega_1| + |\omega_2|} \mathrm{I}[\omega_1 \cap \omega_2 = \{y\}] \qquad (x \neq 0). \tag{1.72}$$

We do not use $R'_p(x)$ or $R''_p(x)$ for $x = 0$.

We also introduce a number of Gaussian quantities. These are defined on $\mathbf{Z}^d$ for general d (provided the integrals converge), but we concentrate on $d = 5$. For $\varepsilon \geq 0$ we define

$$I_{n,m}^{(\varepsilon)}(x) \equiv \int \frac{d^d k}{(2\pi)^d} \frac{\hat{D}(k)^m}{\{\varepsilon + 1 - \hat{D}(k)\}^n} e^{ik \cdot x} \tag{1.73}$$

$$J_{n,m}^{(\varepsilon)} \equiv \int \frac{d^d k}{(2\pi)^d} \frac{|\hat{D}(k)|^m}{\{\varepsilon + 1 - \hat{D}(k)\}^n} \tag{1.74}$$

$$W_{n,m}^{(\varepsilon)} \equiv \int \frac{d^d k}{(2\pi)^d} \frac{\hat{D}(k)^m}{\{\varepsilon + 1 - \hat{D}(k)\}^n} \sum_{\mu=1}^{d} \left(\frac{\sin k_\mu}{d}\right)^2 \tag{1.75}$$

$$V_n^{(\varepsilon)} \equiv \int \frac{d^d k}{(2\pi)^d} \frac{1}{\{\varepsilon + 1 - \hat{D}(k)\}^n} \left[\sum_{\mu=1}^{d} \left(\frac{\sin k_\mu}{d}\right)^2\right]^2. \tag{1.76}$$

We also introduce

$$\hat{D}^{(x)}(k) \equiv \frac{1}{2^d} \cdot \frac{1}{d!} \sum_{\{\nu_1, \nu_2, \ldots, \nu_d\} \in \mathscr{P}_d} \sum_{\delta_1, \delta_2, \ldots, \delta_d = \pm 1} \exp\left[i \sum_{\mu=1}^{d} \delta_\mu k_{\nu_\mu} x_\mu\right] \tag{1.77}$$

where $\mathscr{P}_d$ is the set of all permutations of $\{1, 2, 3, \ldots, d\}$. Performing the sum over δ_μ gives cosines, so $\hat{D}^{(x)}(k)$ is real. Then we define

$$K_{n,m}^{(\varepsilon)}(x) \equiv \int \frac{d^d k}{(2\pi)^d} \frac{|\hat{D}(k)|^m}{\{\varepsilon + 1 - \hat{D}(k)\}^n} |\hat{D}^{(x)}(k)| \tag{1.78}$$

$$L_n^{(\varepsilon)}(x) \equiv \int \frac{d^d k}{(2\pi)^d} \frac{\hat{D}^{(x)}(k)^2}{\{\varepsilon + 1 - \hat{D}(k)\}^n} \tag{1.79}$$

$$U_n^{(\varepsilon)}(x) \equiv \int \frac{d^d k}{(2\pi)^d} \frac{|\hat{D}^{(x)}(k)|}{\{\varepsilon + 1 - \hat{D}(k)\}^n} \sum_{\mu=1}^{d} \left(\frac{\sin k_\mu}{d}\right)^2. \tag{1.80}$$

When $\varepsilon = 0$ we drop the superscript (ε).

Finally, regarding the display of numerical values, we use "..." to denote a result of round-off. For example, we write $x = 0.1234\ldots$ to denote $x \in [0.12335, 0.12345]$. Numbers without "..." represent exact values. We follow this convention unless stated otherwise. Also, care is required in interpreting intermediate values in a calculation. For example, Table I gives values of $R'(x)$, etc. The values in the table are truncated, but subsequent calculations are performed using the pre-truncation 16 digit precision. Furthermore, for ease of presentation we occasionally write for example $x \leq 0.1234\ldots$ as $x \leq 0.125$, which is true but may be less accurate than a more precise value used in subsequent calculations. Any possible discrepancy between our final

Table I. Upper bounds on $B'_p(x)$, $R'_p(x)$, $R_p(x)$, $G_p(x)$, $|x|^2 G_p(x)$ which follow from our starting assumption $P_p(1)$. "Others" means all nonzero x not explicitly given in the table.

x	$B'_p(x)$	$R'_p(x)$	$R_p(x)$	$G_p(x)$	$\|x\|^2 G_p(x)$
(1,0,0,0,0)	0.488	0.388213	0.257050	0.142500	0.142500
(1,1,0,0,0)	0.356	0.324548	0.286298	0.0456252	0.0912503
(2,0,0,0,0)	0.286	0.260733	0.238946	0.0273115	0.109246
(1,1,1,0,0)	0.289	0.263468	0.246297	0.0227560	0.0682681
(2,1,0,0,0)	0.240	0.218797	0.208297	0.0149322	0.0746609
(3,0,0,0,0)	0.215	0.196005	0.191112	0.00826689	0.0744020
(1,1,1,1,0)	0.251	0.228825	0.218961	0.0145000	0.0579999
(2,1,1,0,0)	0.215	0.196005	0.189597	0.0102381	0.0614286
(2,2,0,0,0)	0.215	0.196005	0.191710	0.00770495	0.0616396
(3,1,0,0,0)	0.215	0.196005	0.192737	0.00641781	0.0641781
(4,0,0,0,0)	0.215	0.196005	0.194516	0.00411651	0.0658642
(1,1,1,1,1)	0.227	0.206945	0.200398	0.0105934	0.0529672
others	0.215	0.196005	0.196005	0.00799278	0.0750000

results and results calculated from intermediate values in the text will be due to these two facts.

2. Some Preliminary Estimates

In this section, we derive several estimates which will be necessary in later sections. In particular, we derive the following lemma, which provides upper bounds on $B'_p(x)$, $R_p(x)$, $R'_p(x)$, $G_p(x)$, and $|x|^2 G_p(x)$, based on our starting assumption $P_p(1)$ of Definition 1.3. This lemma will be used in Sec. 3 to derive bounds on $\hat{\Pi}_z(k)$.

Lemma 2.1. *Let $p \in [p_0, z_c)$. Assuming $P_p(1)$ of Definition 1.3, we have*

$$R_p(0) \le 0.434636, \qquad \tilde{R}_p(0) \le 0.300905, \tag{2.1}$$

and the bounds tabulated in Table I.

The proof of Lemma 2.1 will be completed in Sec. 2.3, after we obtain a number of necessary estimates. We begin by using the inclusion-exclusion relation to derive (in Lemma 2.2) simple relations between $G_p(x)$ and $\sum_{|e|=1} G_p(x+e)$. Then partly using one of these relations, we derive (in Lemma 2.3) relations between the bubble quantities given in our starting assumption $P_p(1)$ and the repulsive bubble quantities of Sec. 1.6. The latter play an essential role in the diagrammatic estimates of Sec. 3. Finally, we describe a method (Lemma 2.4) to derive upper bounds on $G_p(x)$ in terms of $R'_p(x)$.

2.1. *Applications of the inclusion-exclusion relation*

In the next lemma, we apply the inclusion-exclusion relation to show that the two-point function at a point is bounded above and below by the average of the two-point function at its nearest neighbours, multiplied by a constant close to one.

Lemma 2.2. *For any $x \neq 0$, we have*

$$G_p(x) \geq \frac{2dp}{1 + 2dpG_p(e_1)} \cdot \frac{1}{2d} \sum_{|e|=1} G_p(x-e) \tag{2.2}$$

and

$$G_p(x) \leq 2dp \cdot \frac{1 + \{p + 2(2d-2)p^3\}G_p(e_1) + p^2 G_p(e_1+e_2)\{1 + 2dpG_p(e_1)\}}{1 + 2dp^2 + 2d(2d-2)p^4 + 2dp^4 G_p(e_1+e_2)} \cdot$$

$$\cdot \frac{1}{2d} \sum_{|e|=1} G_p(x-e). \tag{2.3}$$

Proof. We begin with a simple precursor of (2.3). Let $x \neq 0$. Extracting the first step of ω, and then using inclusion-exclusion, gives

$$\begin{aligned} G_p(x) &= \sum_{e \in \mathbf{Z}^d : |e|=1} p \sum_{\omega' : e \to x} p^{|\omega'|} \mathrm{I}[\omega' \not\ni 0] = p \sum_{|e|=1} \sum_{\omega : e \to x} p^{|\omega|}\{1 - \mathrm{I}[\omega \ni 0]\} \\ &= p \sum_{|e|=1} G_p(x-e) - p \sum_{|e|=1} \sum_{\omega_1 : e \to 0} p^{|\omega_1|} \sum_{\omega_2 : 0 \to x} p^{|\omega_2|} \mathrm{I}[\omega_1 \cap \omega_2 = \{0\}]. \end{aligned} \tag{2.4}$$

Discarding the second term, we immediately obtain

$$G_p(x) \leq 2dp \cdot \frac{1}{2d} \sum_{|e|=1} G_p(x-e). \tag{2.5}$$

If we now bound the indicator function of (2.4) using $\mathrm{I}[\omega_1 \cap \omega_2 = \{0\}] \leq 1$, we get the lower bound

$$G_p(x) \geq p \sum_{|e|=1} G_p(x-e) - p \sum_{|e|=1} G_p(e) G_p(x) \tag{2.6}$$

or (2.2).

To improve (2.5) to (2.3), we derive a lower bound on the second term of (2.4) by restricting the sum over ω_1 to $|\omega_1| = 1, 3$. For $|\omega_1| = 1$, the indicator becomes $\mathrm{I}[\omega_1 \cap \omega_2 = \{0\}] = \mathrm{I}[\omega_2 \not\ni e]$. For $|\omega_1| = 3$, denoting the two sites on ω_1 in addition to 0 and e by f and $f + e$ ($|f| = 1$), we have $\mathrm{I}[\omega_1 \cap \omega_2 = \{0\}] = \mathrm{I}[\omega_2 \not\ni e, f, e+f]$. Using the inclusion-exclusion relation we obtain

$$\sum_{\omega_1 : e \to 0} p^{|\omega_1|} \sum_{\omega_2 : 0 \to x} p^{|\omega_2|} \mathrm{I}[\omega_1 \cap \omega_2 = \{0\}]$$

$$\geq p \sum_{\omega_2 : 0 \to x} p^{|\omega_2|} \mathrm{I}[\omega_2 \not\ni e] + p^3 \sum_{f : |f|=1, f \neq \pm e} \sum_{\omega_2 : 0 \to x} p^{|\omega_2|} \mathrm{I}[\omega_2 \not\ni e, f, e+f]$$

$$\geq p\{G_p(x) - G_p(e)G_p(x-e)\}$$

$$+ p^3 \sum_{f:|f|=1, f\neq \pm e} \{G_p(x) - G_p(f)G_p(x-f) - G_p(e)G_p(x-e)$$

$$- G_p(f+e)G_p(x-e-f)\}$$

$$= \{p + (2d-2)p^3\}G_p(x) - \{p + (2d-2)p^3\}G_p(e_1)\cdot G_p(x-e)$$

$$- p^3 \sum_{f:|f|=1, f\neq \pm e} \{G_p(e_1)G_p(x-f) + G_p(e_1+e_2)G_p(x-e-f)\}, \tag{2.7}$$

and hence

$$G_p(x) \leq p[1 + \{p + 2(2d-2)p^3\}G_p(e_1)] \sum_{|e|=1} G_p(x-e)$$

$$- 2dp\{p + (2d-2)p^3\}G_p(x)$$

$$+ p^4 G_p(e_1+e_2) \sum_{|e|=|f|=1, e\neq \pm f} G_p(x-e-f). \tag{2.8}$$

Now note that

$$\sum_{e,f:|e|=|f|=1, e\neq \pm f} G_p(x-e-f) \leq \sum_{|e|=1} \sum_{|f|=1} G_p(\{x-e\}-f) - 2dG_p(x)$$

$$\leq \sum_{|e|=1} \frac{1 + 2dpG_p(e_1)}{p} G_p(x-e) - 2dG_p(x) \tag{2.9}$$

where in the last step we used (2.2) in the reverse direction. Using (2.9) in (2.8), we get (2.3). □

We now apply the inclusion-exclusion relation to obtain bounds on the repulsive bubble quantities in terms of the bubble quantities.

Lemma 2.3. *For $x \neq 0$, we have*

$$R'_p(x) \leq [1 - 2dp^2 + 2pG_p(e_1)\{1 + 2dpG_p(e_1)\}]B'_p(x). \tag{2.10}$$

We also have

$$R_p(0) \leq \{1 - 4dp^2 + 4d^2p^4\}B_p(0) + 8dp^2G_p(e_1)B'_p(e_1)$$

$$+ 4dp^2\{G_p(e_1)^2 + dp^2\}, \tag{2.11}$$

$$\tilde{R}_p(0) \le \{1 - 4dp^2\}\tilde{B}_p(0) + 4d^2p^4B_p(0) + 8dp^2G_p(e_1)B'_p(e_1)$$
$$+ 4dp^2\{G_p(e_1)^2 + dp^2\}, \tag{2.12}$$

and

$$R'_p(e_1) = R_p(0)/(2dp). \tag{2.13}$$

Proof. By definition of $R'_p(x)$ $(x \neq 0)$,

$$R'_p(x) = \sum_{y \neq 0} \sum_{\substack{\omega_1 : y \to 0 \\ \omega_2 : y \to x}} p^{|\omega_1| + |\omega_2|} \mathrm{I}[\omega_1 \cap \omega_2 = \{y\}]$$
$$= B'_p(x) - \sum_{y \neq 0, x} \sum_{\substack{\omega_1 : y \to 0 \\ \omega_2 : y \to x}} p^{|\omega_1| + |\omega_2|} \mathrm{I}[\omega_1 \cap \omega_2 \neq \{y\}], \tag{2.14}$$

where in the last sum the $y = x$ term is automatically zero. To obtain a lower bound on the last sum, we restrict the summation to ω_1 and ω_2 having the same first step $(y, y + e)$. This gives

$$\sum_{\substack{\omega_1 : y \to 0 \\ \omega_2 : y \to x}} p^{|\omega_1| + |\omega_2|} \mathrm{I}[\omega_1 \cap \omega_2 \neq \{y\}] \ge \sum_{|e|=1} p^2 \sum_{\substack{\omega'_1 : y + e \to 0 \\ \omega'_2 : y + e \to x}} p^{|\omega'_1| + |\omega'_2|} \mathrm{I}[\omega'_1 \not\ni y, \omega'_2 \not\ni y]. \tag{2.15}$$

Now we again use inclusion-exclusion, in the form $\mathrm{I}[\omega'_1 \not\ni y, \omega'_2 \not\ni y] \ge 1 - \mathrm{I}[\omega'_1 \ni y] - \mathrm{I}[\omega'_2 \ni y]$, to obtain

$$R'_p(x) \le B'_p(x) - p^2 \sum_{|e|=1} \sum_{y \neq 0, x} G_p(y + e)G_p(x - y - e)$$
$$+ p^2 G_p(e_1) \sum_{|e|=1} \sum_{y \neq 0, x} \{G_p(y)G_p(x - y - e) + G_p(y + e)G_p(x - y)\}$$
$$= B'_p(x) - 2dp^2 B''_p(x) + 2p^2 G_p(e_1) \sum_{y \neq x} G_p(y) \sum_{|e|=1} G_p(x - y - e). \tag{2.16}$$

Then (2.10) follows, once we use (2.2) in the reverse direction to bound the sum over $|e| = 1$.

We proceed similarly for $R_p(0)$ and $\tilde{R}_p(0)$, but now restrict the summation to ω_1 and ω_2 having the same first or last step. For $R_p(0)$ we have

$$R_p(0) \le B_p(0) - \sum_{x \neq 0} \sum_{|e|=1 : e \neq x} p^2 \sum_{\substack{\omega'_1 : e \to x \\ \omega'_2 : e \to x}} p^{|\omega'_1| + |\omega'_2|} \mathrm{I}[\omega'_1 \not\ni 0, \omega'_2 \not\ni 0]$$
$$- \sum_{x \neq 0} \sum_{|f|=1 : f \neq x} p^2 \sum_{\substack{\omega'_1 : 0 \to x - f \\ \omega'_2 : 0 \to x - f}} p^{|\omega'_1| + |\omega'_2|} \mathrm{I}[\omega'_1 \not\ni x, \omega'_2 \not\ni x]$$

$$+ \sum_{x \neq 0} \sum_{\substack{|e|=1:e\neq x \\ |f|=1:f\neq x}} p^4 \sum_{\substack{\omega_1':e\to x-f \\ \omega_2':e\to x-f}} p^{|\omega_1'|+|\omega_2'|} \mathrm{I}[\omega_1' \not\ni 0,x; \omega_2' \not\ni 0,x]$$

$$\leq B_p(0) \sum_{x\neq 0} \sum_{|e|=1, e\neq x} p^2 G_p(x-e)^2 - \sum_{x\neq 0} \sum_{|f|=1:f\neq x} p^2 G_p(x-f)^2$$

$$+ 4 \sum_{x\neq 0} \sum_{|e|=1, e\neq x} p^2 G_p(e) G_p(x) G_p(x-e) + \sum_{x\neq 0} \sum_{\substack{|e|=1:e\neq x \\ |f|=1:f\neq x}} p^4 G_p(x-f-e)^2$$

$$\leq \{1 - 4dp^2 + 4d^2p^4\} B_p(0) + 8dp^2 G_p(e_1) B_p'(e_1) + 4dp^2 \{G_p(e_1)^2 + dp^2\}. \tag{2.17}$$

The bound (2.12) on $\tilde{R}_p(0)$ is obtained in the same way, subject to the additional condition $|x| > 1$.

Finally, extracting the first step of ω_1 gives

$$R_p(0) = \sum_{x\neq 0} \sum_{\substack{\omega_1:0\to x \\ \omega_2:0\to x}} p^{|\omega_1|+|\omega_2|} \mathrm{I}[\omega_1 \cap \omega_2 = \{0,x\}]$$

$$= \sum_{x\neq 0} p \sum_{|e|=1} \sum_{\substack{\omega_1':e\to x \\ \omega_2':0\to x}} p^{|\omega_1'|+|\omega_2|} \mathrm{I}[\omega_1' \cap \omega_2 = \{x\}]$$

$$= p \sum_{|e|=1} R_p'(e), \tag{2.18}$$

and hence (2.13). □

2.2. *Bound on the two-point function*

To prove Lemma 2.1 we must in particular provide bounds on $G_p(x)$ for $x \neq 0, e_1$, starting from our assumption $P_p(1)$. This is done using the following lemma.

Lemma 2.4. *For any $p \in (p_0, z_c)$,*

$$G_p(x) \leq G_{p_0}(x) + \frac{R_{p_0}'(x) + R_p'(x)}{2} \cdot \frac{z_c - p_0}{p_0}. \tag{2.19}$$

Proof. Differentiating the definition of $G_p(x)$, for any $x \neq 0$, gives

$$p \frac{d}{dp} G_p(x) = R_p'(x). \tag{2.20}$$

Let $p_1 \in (p_0, z_c)$. Integration of (2.19) gives

$$G_{p_1}(x) = G_{p_0}(x) + \int_{p_0}^{p_1} R_p'(x) \frac{dp}{p}. \tag{2.21}$$

For the second term, we note that all p-derivatives of $R'_p(x)$ are positive, so in particular $R'_p(x)$ is convex. But for any convex function f,

$$\int_{p_0}^{p_1} f(p)\frac{dp}{p} \leq \int_0^1 \{(1-t)f(p_0) + tf(p_1)\}\frac{(p_1 - p_0)\,dt}{(1-t)p_0 + tp_1}$$

$$= f(p_0)\ln(p_1/p_0) + \{f(p_1) - f(p_0)\}\left\{1 - \frac{p_0}{p_1 - p_0}\ln(p_1/p_0)\right\}. \quad (2.22)$$

This can be further simplified, using $y - y^2/2 \leq \ln(1+y) \leq y$ (for $y \geq 0$), to

$$\int_{p_0}^{p_1} f(p)\frac{dp}{p} \leq \frac{f(p_0) + f(p_1)}{2}\cdot\frac{p_1 - p_0}{p_0}. \quad (2.23)$$

Combining this with (2.21) gives (2.19). □

2.3. *Proof of Lemma 2.1*

We now use the results of Secs. 2.1 and 2.2 to prove Lemma 2.1.

For the bounds on $B'_p(x)$, we simply use the values from $P_p(1)$.

For $R'_p(x)$, we employ Lemma 2.3. More precisely, we first use (2.10) and $P_p(1)$ to bound $R'_p(x)$ for $|x| > 1$. We then use (2.11), (2.12) and $P_p(1)$ to bound $R_p(0)$ and $\tilde{R}_p(0)$, and finally use (2.13) to bound $R'_p(e_1)$.

Turning now to the bounds on $R_p(x)$, for $x \in \Lambda'_2$, we use

$$R_p(x) = R'_p(x) - G_p(x) \leq R'_p(x) - \underline{G_p(x)}, \quad (2.24)$$

and bound the last term on the right side using Corollary A.4. Specifically, since $p \geq p_0$ we can use

$$G_p(x) \geq (0.8758793)I^{(\varepsilon)}_{1,0}(x), \qquad \varepsilon = 0.0100504, \quad (2.25)$$

and the values of $I^{(\varepsilon)}_{1,0}(x)$ calculated from Proposition B.7. For the remaining x, we simply use

$$R_p(x) \leq R'_p(x). \quad (2.26)$$

The bounds on $G_p(x)$ of Lemma 2.1 are obtained using (2.19) as follows. For the quantities in (2.19) at $p_0 \equiv (6611)/(9^5)$, we first employ (1.62) to bound $G_{p_0}(x)$ and thus $B'_{p_0}(x)$, obtaining

$$G_{p_0}(x) \leq \frac{713988}{812911}I_{1,0}(x), \qquad B'_{p_0}(x) \leq \left(\frac{713988}{812911}\right)^2 I_{2,1}(x). \quad (2.27)$$

Values of the Gaussian quantities on the right side are given in Table V and Lemma

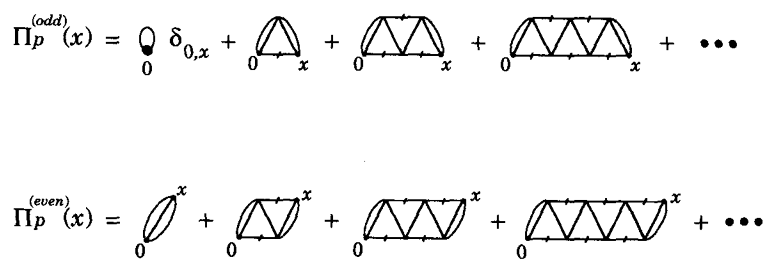


Fig. 1. Diagrams contributing to $\Pi_p^{(\mathrm{odd})}(x)$ and $\Pi_p^{(\mathrm{even})}(x)$. Slashed lines may correspond to zero-step subwalks, while other lines correspond to subwalks which take at least one step. There is some mutual avoidance present between subwalks, as prescribed by the lace expansion. In particular, the subwalks forming each elementary loop in the diagrams are mutually avoiding.

B.9. We then use (2.27) in conjunction with (2.10) to bound $R'_{p_0}(x)$. Then we use the bounds obtained above for $R'_p(x)$, and Corollary A.2 for z_c.

Finally, $|x|^2 G_p(x)$ is bounded by multiplying our bounds on $G_p(x)$ by $|x|^2$, for $x \in \Lambda'_2$, or simply from $P_1(p)$ for $x \notin \Lambda'_2$. $\square$

3. Diagrammatic Estimates

There are two main steps in the proof of Theorem 1.4. The first is to show that the bounds given in $P_p(1)$ yield bounds on $\hat{\Pi}_p(k)$, and the second is to use these bounds on $\hat{\Pi}_p(k)$ to obtain the improved bounds of $P_p(0.999)$. In this section we perform the first of these steps. To obtain adequate bounds on $\hat{\Pi}_p(k)$ for $d = 5$, very detailed estimates are required. Simple estimates similar to those used in [5] will be used to bound contributions from diagrams having nine or more loops, while more careful estimates will be used up to the eight-loop diagram.

Recall that $\Pi_p^{(\mathrm{odd})}(x)$ is the sum of diagrams contributing to $\Pi_p(x)$ having an odd number of loops, and $\Pi_p^{(\mathrm{even})}(x)$ the sum of diagrams having an even number of loops. Then $\Pi_p(x) = -\Pi_p^{(\mathrm{odd})}(x) + \Pi_p^{(\mathrm{even})}(x)$. The diagrams are illustrated in Fig. 1.

We wish to treat the self-avoiding walk as a small perturbation of simple random walk. In (1.19), roughly speaking $1 - 2dz\hat{D}(k)$ is the main term, and $\hat{\Pi}_z(k)$ is a perturbation. In the next section we absorb some contributions from $\hat{\Pi}_z(k)$ into the main term. This will be useful when we use the bounds of this section to conclude in Sec. 4 that $P_p(0.999)$ holds.

3.1. *Extraction of terms in the propagator*

The contribution to $\hat{\Pi}_p(k)$ from lattice points with $|x| = 1$ gives a multiple of $\hat{D}(k)$. Also, the contribution from $x = 0$ has no k-dependence, and merely shifts the critical value of p. We extract these two contributions from the one, two and three loop diagrams of $\hat{\Pi}_p(k)$.

For this purpose, we define

$$\pi_0 = \Pi_p^{(3)}(0), \qquad \pi_1 = \Pi_p^{(2)}(e_1) - \Pi_p^{(3)}(e_1). \tag{3.1}$$

For the one-loop diagram we note that

$$\Pi_p^{(1)}(0) = 2dpG_p(e_1). \tag{3.2}$$

Then we have

$$\hat{G}_p(k) = \frac{N_p}{A_p - \hat{D}(k) - \hat{\Phi}_p(k)} \tag{3.3}$$

where

$$N_p \equiv [2dp + 2d\pi_1]^{-1}, \qquad A_p \equiv [1 + 2dpG_p(e_1) + \pi_0]N_p \tag{3.4}$$

and

$$\hat{\Phi}_p(k) \equiv \sum_{n=2}^{\infty} (-1)^n \hat{\Phi}_p^{(n)}(k), \tag{3.5}$$

with

$$\hat{\Phi}_p^{(n)}(k) \equiv \begin{cases} N_p \sum_{|x| \neq 0, 1} \Pi_p^{(n)}(x) e^{ik \cdot x} & (n = 2, 3) \\ N_p \hat{\Pi}_p^{(n)}(k) & (n \geq 4) \end{cases}. \tag{3.6}$$

Adding and subtracting $N_p \chi(p)^{-1}$ in the denominator of (3.3) gives

$$\hat{G}_p(k) = \frac{N_p}{N_p \chi^{-1} + 1 - \hat{D}(k) + \hat{\Phi}_p(0) - \hat{\Phi}_p(k)}. \tag{3.7}$$

For later use we also define

$$X_p \equiv \frac{N_p}{A_p} = [1 + 2dpG_p(e_1) + \pi_0]^{-1}, \qquad Y_p \equiv \frac{X_p}{A_p}. \tag{3.8}$$

3.2. *Main estimates*

The main estimates on Φ and Π are given in the following lemma. This lemma will be proved by bounding Π and Φ (and their derivatives with respect to k and p) in terms of the basic bubble quantities, and then using Lemma 2.1. [In fact (3.9) follows immediately from Table I.]

Lemma 3.1. *Given $P_p(1)$ of Definition* 1.3, *we have*

$$\sup_x |x|^2 G_p(x) \leq 0.1425, \tag{3.9}$$

$$\begin{aligned} |\hat{\Phi}_p^{(\mathrm{odd})}(k)| &\leq \sum_x \Phi_p^{(\mathrm{odd})}(x) \leq 0.0054562605 \equiv c_1, \\ |\hat{\Phi}_p^{(\mathrm{even})}(k) &\leq \sum_x \Phi_p^{(\mathrm{even})}(x) \leq 0.0091636501 \equiv c_2, \end{aligned} \tag{3.10}$$

and for $u = 1, 2$,

$$d|\partial_\mu^u \hat{\Phi}_p^{(\mathrm{odd})}(k)| \le \sum_x |x|^2 \Phi_p^{(\mathrm{odd})}(x) \le 0.0205754616 \equiv c_3\,,$$
$$d|\partial_\mu^u \hat{\Phi}_p^{(\mathrm{even})}(k)| \le \sum_x |x|^2 \Phi_p^{(\mathrm{even})}(x) \le 0.0436887388 \equiv c_4\,. \tag{3.11}$$

For $u = 1$ we also have the k-dependent bound

$$|\partial_\mu \hat{\Phi}_p(k)| \le \frac{c_3 + c_4}{d}|\sin k_\mu|\,. \tag{3.12}$$

Also,

$$-c_3\{1 - \hat{D}(k)\} \le \hat{\Phi}_p(0) - \hat{\Phi}_p(k) \le c_4\{1 - \hat{D}(k)\}\,. \tag{3.13}$$

For bounds on $\hat{\Pi}_p$ we have

$$|\hat{\Pi}_p^{(\mathrm{odd})}(k)| \le \sum_x \Pi_p^{(\mathrm{odd})}(x) \le 0.1730244 \equiv c_1'\,,$$
$$|\hat{\Pi}_p^{(\mathrm{even})}(k)| \le \sum_x \Pi_p^{(\mathrm{even})}(x) \le 0.03864779 \equiv c_2'\,, \tag{3.14}$$

and for $u = 1, 2$

$$d|\partial_\mu^u \hat{\Pi}_p^{(\mathrm{odd})}(k)| \le \sum_x |x|^2 \Pi_p^{(\mathrm{odd})}(x) \le 0.02406226 \equiv c_3'\,,$$
$$d|\partial_\mu^u \hat{\Pi}_p^{(\mathrm{even})}(k)| \le \sum_x |x|^2 \Pi_p^{(\mathrm{even})}(x) \le 0.07354167 \equiv c_4'\,. \tag{3.15}$$

Finally,

$$-c_3'\{1 - \hat{D}(k)\} \le \hat{\Pi}_p(0) - \hat{\Pi}_p(k) \le c_4'\{1 - \hat{D}(k)\}\,. \tag{3.16}$$

We also prove the following lemma.

Lemma 3.2. *Given $P_p(1)$,*

$$N_p \le 0.877253586\,, \qquad X_p \equiv \frac{N_p}{A_p} \le 0.869945794\,, \tag{3.17}$$

$$A_p \ge 0.988764783\,, \qquad Y_p \equiv \frac{X_p}{A_p} \le 0.879830885\,. \tag{3.18}$$

These two lemmas will be proven throughout the remainder of Sec. 3.

3.3. *Estimates on some basic diagrams*

In [5], where there was a very small parameter, adequate diagrammatic estimates were obtained using the Hausdorff-Young inequality. For diagrams having eight loops or less, we will use the following inequality instead.

Lemma 3.3. *Suppose f and g are nonnegative functions on $\mathbf{Z}^d$, with given pointwise upper bounds $f(y) \le \overline{f(y)}$ and $g(y) \le \overline{g(y)}$, $y \in \mathbf{Z}^d$. Suppose also that $\sum_{y \in \mathbf{Z}^d} g(y) \le S_G$. Then for any nonnegative α,*

$$\sum_{y \in \mathbf{Z}^d} f(y)g(y) \le \alpha S_G + \sum_{y \in \mathbf{Z}^d} \max\{\overline{f(y)} - \alpha, 0\}\overline{g(y)}. \tag{3.19}$$

In particular, if for some subset $\mathrm{U} \subset \mathbf{Z}^d$ we take $\alpha \equiv \sup_{y \in \mathrm{U}^c} \overline{f(y)}$, then

$$\sum_{y \in \mathbf{Z}^d} f(y)g(y) \le \sup_{y \in \mathrm{U}^c} \overline{f(y)} \cdot S_G + \sum_{y \in \mathrm{U}} \max\left\{\overline{f(y)} - \sup_{y \in \mathrm{U}^c} \overline{f(y)}, 0\right\}\overline{g(y)}. \tag{3.20}$$

Remark. For $\mathrm{U} = \phi$, (3.20) is just the Hausdorff-Young inequality. For nonempty U, (3.20) gives an improvement by taking variations of f into account.

Proof. For any $\alpha \in \mathbf{R}$,

$$\sum_{y \in \mathbf{Z}^d} f(y)g(y) = \alpha \sum_{y \in \mathbf{Z}^d} g(y) + \sum_{y \in \mathbf{Z}^d} \{f(y) - \alpha\}g(y). \tag{3.21}$$

When α and $g(y)$ are both nonnegative, the right side is bounded above by

$$\alpha S_G + \sum_{y \in \mathbf{Z}^d} \{\overline{f(y)} - \alpha\}g(y) \le \alpha S_G + \sum_{y : \overline{f(y)} > \alpha} \{\overline{f(y)} - \alpha\}\overline{g(y)}. \tag{3.22}$$

Then (3.20) follows from the fact that all contributions from $y \notin \mathrm{U}$ are nonpositive in the second term of (3.20). $\square$

To simplify the notation, we introduce the following abbreviations for frequently encountered versions of the right side of (3.20). We will in fact encounter only sums of the form $\sum_{y \ne 0} f(y)g(y)$, or $\sum_{y \ne 0,x} f(y)g(x-y)$ with $x \ne 0$. With this in mind, given a subset U or V of $\mathbf{Z}^d$ ($\mathrm{U}, \mathrm{V} \ni 0$), nonnegative functions f and g, and $S = \sum_{y \ne 0} g(y)$, and given upper bounds for these, we define

$$U(S, g, f; \mathrm{U}) \equiv \sup_{y \in \mathrm{U}^c} \overline{f(y)} \cdot \bar{S} + \sum_{y \in \mathrm{U} : y \ne 0} \max\left\{\overline{f(y)} - \sup_{z \in \mathrm{U}^c} \overline{f(z)}, 0\right\}\overline{g(y)} \tag{3.23}$$

and

$$V(x; S, g, f; \mathrm{V}) \equiv \sup_{y \in \mathrm{V}^c} \overline{f(y)} \cdot \bar{S} + \sum_{y \in \mathrm{V} : y \ne 0, x} \max\left\{\overline{f(y)} - \sup_{z \in \mathrm{V}^c} \overline{f(z)}, 0\right\}\overline{g(x-y)}. \tag{3.24}$$

To apply (3.20), we need to make a choice of U. In practice, we evaluate the right side for nine sets U, each of which is given by the union of all $\mathbf{Z}^5$-rotations and reflections of each of the following nine sets:

$$\{0\}, \quad \{0, e_1\}, \quad \{0, e_1, v_2\}, \quad \{0, e_1, 2e_1\}, \quad \{0, e_1, v_2, v_3\}, \quad \{0, e_1, 2e_1, v_2, v_3\}$$

$$\{0, e_1, 2e_1, v_2, v_3, v_2 + e_1\}, \quad \{0, e_1, 2e_1, v_2, v_3, v_4\}, \quad \{0, e_1, 2e_1, v_2, v_3, v_4, v_2 + e_1\}. \tag{3.25}$$

We then take the minimum of $U(S, g, f; \mathrm{U})$ over these choices of U, and define

$$U(S, g, f) \equiv \min_{\mathrm{U}} U(S, g, f; \mathrm{U}). \tag{3.26}$$

To compute the right side of (3.26), individual upper bounds are required on $g(y)$ only for $\|y\|_1 \leq 4$. Similarly we define

$$V(x; S, g, f) \equiv \min_{\mathrm{V}} V(x; S, g, f; \mathrm{V}), \tag{3.27}$$

where now the minimum is taken over three, two or one set V, depending on x, as follows:

$$\begin{aligned} V &= \{0\}, \quad \{y \in \mathbf{Z}^5 : \|y\|_2 \leq 1\}, \quad \{y \in \mathbf{Z}^5 : \|y\|_2 \leq \sqrt{2}\} && \text{for } \|x\|_1 \leq 2 \\ V &= \{0\}, \quad \{y \in \mathbf{Z}^5 : \|y\|_2 \leq 1\}, && \text{for } \|x\|_1 = 3 \\ V &= \{0\} && \text{for } \|x\|_1 \geq 4. \end{aligned} \tag{3.28}$$

Then again to evaluate the right side, individual upper bounds are required on $g(y)$ only for $0 < \|y\|_1 \leq 4$.

Then by Lemma 3.3 we have

$$\sum_{y \neq 0} f(y) g(y) \leq U(S, g, f), \qquad \sum_{y \neq 0, x} f(y) g(x - y) \leq V(x; S, g, f). \tag{3.29}$$

In the following, we use the above lemma to derive efficient bounds on $\hat{\Pi}$, $\hat{\Phi}$, and their derivatives. We will encounter only the sum on the left side of (3.29), i.e. with the restrictions $y \neq 0$ or $y \neq 0$, x. The basic approach is to use the lemma in an iterative fashion to reduce a diagram to smaller units, which themselves can be bounded using the lemma.

We now define the six basic types of diagrams that will be used. We first define diagrams of type-$\mathscr{B}_*^{(n)}$ and $\mathscr{F}_*^{(n)}$ as in Fig. 2 (a) and (b). Here $*$ denotes one of a, b, c, d, and the superscript denotes the number of loops. Then we define

$$\mathscr{A}_*^{(n)} \equiv \sum_{y \neq 0} \mathscr{B}_*^{(n)}(y), \qquad \mathscr{D}_*^{(n)}(x) \equiv \sum_{y \neq 0, x} G(y) \mathscr{B}_*^{(n)}(x - y), \tag{3.30}$$

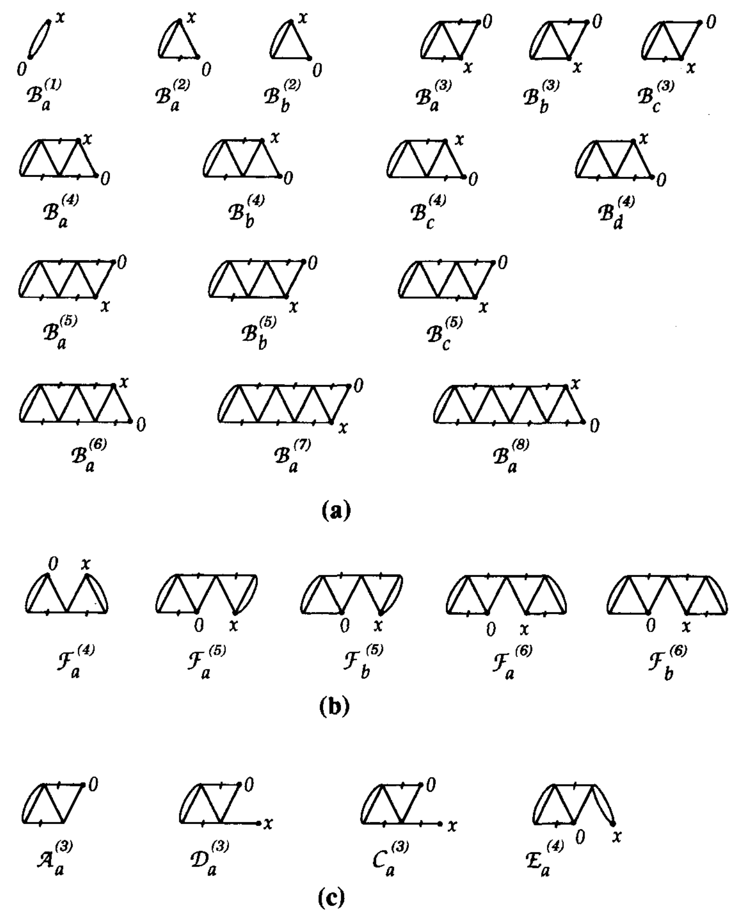


Fig. 2. Definitions of basic diagrams. (a) Diagrams $\mathscr{B}_*^{(n)}(x)$. (b) Diagrams $\mathscr{F}_*^{(n)}(x)$. (c) Examples of $\mathscr{A}_*^{(n)}$, $\mathscr{D}_*^{(n)}$, $\mathscr{C}_*^{(n)}$, $\mathscr{E}_*^{(n)}$. In each diagram it is implicit that all elementary loops in the diagram are self-avoiding, in the sense that no pair of lines in any loop has a common point other than the common endpoints explicitly indicated.

$$\mathscr{C}_*^{(n)}(x) \equiv \sum_{y \neq x} G(y)\mathscr{B}_*^{(n)}(x-y) = \mathscr{D}_*^{(n)}(x) + \mathscr{B}_*^{(n)}(x), \tag{3.31}$$

$$\mathscr{E}_*^{(n)}(x) \equiv \sum_{y \neq 0, x} \mathscr{B}_a^{(1)}(x-y)\mathscr{B}_*^{(n-1)}(y), \tag{3.32}$$

and $\mathscr{B}_*^{(n)}(0) \equiv \mathscr{C}_*^{(n)}(0) \equiv \mathscr{D}_*^{(n)}(0) \equiv 0$.

We first establish bounds on diagrams of type $\mathscr{A}, \mathscr{B}, \mathscr{C}, \mathscr{D}$. Then bounds on diagrams of type $\mathscr{E}$ and $\mathscr{F}$ follow rather easily.

3.3.1. *One loop diagrams*

There are four types of one-loop diagram. By definition,

$$\mathscr{A}_a^{(1)} = R(0), \qquad \mathscr{B}_a^{(1)}(x) \leq G(x)^2. \tag{3.33}$$

To bound $\mathscr{D}_a^{(1)}$, we use (3.29) to obtain

$$\mathscr{D}_a^{(1)}(x) = \sum_{y \neq 0, x} G(y)\mathscr{B}_a^{(1)}(x - y) \leq V(x; \mathscr{A}_a^{(1)}, \mathscr{B}_a^{(1)}, G), \tag{3.34}$$

and then use (3.33) and the results of Lemma 2.1 for the upper bounds on $\mathscr{A}_a^{(1)}$, $\mathscr{B}_a^{(1)}(x)$ and $G(x)$ in the definition of $V(x; \mathscr{A}_a^{(1)}, \mathscr{B}_a^{(1)}, G)$. Finally, by definition

$$\mathscr{C}_a^{(1)}(x) = \mathscr{D}_a^{(1)}(x) + \mathscr{B}_a^{(1)}(x). \tag{3.35}$$

3.3.2. *Higher loop diagrams*

Diagrams with a higher number of loops are bounded similarly. To demonstrate the method, we now bound the two-loop diagrams of type a. The method is the same for type b.

Beginning with $\mathscr{A}_a^{(2)}$, we use $\sum_{y \neq 0} \mathscr{B}_a^{(1)}(y) = \mathscr{A}_a^{(1)}$ and apply (3.29) to obtain

$$\mathscr{A}_a^{(2)} = \sum_{y \neq 0} R'(y)\mathscr{B}_a^{(1)}(y) \leq U(\mathscr{A}_a^{(1)}, \mathscr{B}_a^{(1)}, R'). \tag{3.36}$$

Next, $\mathscr{B}_a^{(2)}$ is simply the product of $\mathscr{C}_a^{(1)}$ and G with repulsion. Ignoring the repulsion gives the upper bound

$$\mathscr{B}_a^{(2)}(x) \leq \mathscr{C}_a^{(1)}(x)G(x). \tag{3.37}$$

Then $\mathscr{D}_a^{(2)}$ is estimated using (3.29) as for $\mathscr{D}_a^{(1)}$, to obtain

$$\mathscr{D}_a^{(2)}(x) = \sum_{y \neq 0, x} G(y)\mathscr{B}_a^{(2)}(x - y) \leq V(x; \mathscr{A}_a^{(2)}, \mathscr{B}_a^{(2)}, G). \tag{3.38}$$

Finally, by definition of $\mathscr{C}_a^{(2)}$, we have

$$\mathscr{C}_a^{(2)}(x) = \mathscr{D}_a^{(2)}(x) + \mathscr{B}_a^{(2)}(x). \tag{3.39}$$

Diagrams with more loops are estimated similarly, yielding the results summarized below. In these bounds all one-loop diagrams are estimated first, then their upper bounds are used in the estimates of the two-loop diagrams, and so on.

Type $\mathscr{A}$ and $\mathscr{B}$

$$\mathscr{A}_a^{(2)} \leq U(\mathscr{A}_a^{(1)}, \mathscr{B}_a^{(1)}, R'), \qquad \mathscr{A}_b^{(2)} \leq U(\mathscr{A}_a^{(1)}, \mathscr{B}_a^{(1)}, R),$$

$$\mathscr{B}_a^{(2)}(x) \leq \mathscr{C}_a^{(1)}(x) \cdot G(x), \qquad \mathscr{B}_b^{(2)}(x) \leq \mathscr{D}_a^{(1)}(x) \cdot G(x),$$

$$\mathscr{A}_a^{(3)} \leq U(\mathscr{A}_a^{(2)}, \mathscr{B}_a^{(2)}, R'), \qquad \mathscr{A}_b^{(3)} \leq U(\mathscr{A}_b^{(2)}, \mathscr{B}_b^{(2)}, R'), \qquad \mathscr{A}_c^{(3)} \leq U(\mathscr{A}_a^{(2)}, \mathscr{B}_a^{(2)}, R),$$

$$\mathscr{B}_a^{(3)}(x) \leq \mathscr{C}_a^{(2)}(x) \cdot G(x), \qquad \mathscr{B}_b^{(3)}(x) \leq \mathscr{C}_b^{(2)}(x) \cdot G(x), \qquad \mathscr{B}_c^{(3)}(x) \leq \mathscr{D}_a^{(2)}(x) \cdot G(x),$$

$$\mathscr{A}_a^{(4)} \le U(\mathscr{A}_a^{(3)}, \mathscr{B}_a^{(3)}, R'), \qquad \mathscr{A}_b^{(4)} \le U(\mathscr{A}_a^{(3)}, \mathscr{B}_a^{(3)}, R),$$

$$\mathscr{A}_c^{(4)} \le U(\mathscr{A}_b^{(3)}, \mathscr{B}_b^{(3)}, R'), \qquad \mathscr{A}_d^{(4)} \le U(\mathscr{A}_c^{(3)}, \mathscr{B}_c^{(3)}, R'),$$

$$\mathscr{B}_a^{(4)}(x) \le \mathscr{C}_a^{(3)}(x) \cdot G(x), \qquad \mathscr{B}_b^{(4)}(x) \le \mathscr{D}_a^{(3)}(x) \cdot G(x),$$

$$\mathscr{B}_c^{(4)}(x) \le \mathscr{C}_b^{(3)}(x) \cdot G(x), \qquad \mathscr{B}_d^{(4)}(x) \le \mathscr{C}_c^{(3)}(x) \cdot G(x),$$

$$\mathscr{A}_a^{(5)} \le U(\mathscr{A}_a^{(4)}, \mathscr{B}_a^{(4)}, R'), \qquad \mathscr{A}_b^{(5)} \le U(\mathscr{A}_b^{(4)}, \mathscr{B}_b^{(4)}, R'), \qquad \mathscr{A}_c^{(5)} \le U(\mathscr{A}_c^{(4)}, \mathscr{B}_c^{(4)}, R'),$$

$$\mathscr{B}_a^{(5)}(x) \le \mathscr{C}_a^{(4)}(x) \cdot G(x), \qquad \mathscr{B}_b^{(5)}(x) \le \mathscr{C}_b^{(4)}(x) \cdot G(x), \qquad \mathscr{B}_c^{(5)}(x) \le \mathscr{C}_c^{(4)}(x) \cdot G(x),$$

$$\mathscr{A}_a^{(6)} \le U(\mathscr{A}_a^{(5)}, \mathscr{B}_a^{(5)}, R'), \qquad \mathscr{B}_a^{(6)}(x) \le \mathscr{C}_a^{(5)}(x) \cdot G(x),$$

$$\mathscr{A}_a^{(7)} \le U(\mathscr{A}_a^{(6)}, \mathscr{B}_a^{(6)}, R'), \qquad \mathscr{B}_a^{(7)}(x) \le \mathscr{C}_a^{(6)}(x) \cdot G(x),$$

$$\mathscr{A}_a^{(8)} \le U(\mathscr{A}_a^{(7)}, \mathscr{B}_a^{(7)}, R').$$

Type $\mathscr{C}$ and $\mathscr{D}$

$$\mathscr{D}_*^{(n)}(x) \le V(x; \mathscr{A}_*^{(n)}, \mathscr{B}_*^{(n)}, G), \qquad \mathscr{C}_*^{(n)}(x) = \mathscr{D}_*^{(n)}(x) + \mathscr{B}_*^{(n)}(x). \tag{3.40}$$

Type $\mathscr{E}$

$$\mathscr{E}_*^{(n+1)}(x) \le V(x; \mathscr{A}_*^{(n)}, \mathscr{B}_*^{(n)}, G^2). \tag{3.41}$$

Type $\mathscr{F}$

To simplify notation, we temporarily write

$$G \equiv \sup_{x \ne 0} G(x), \qquad R' \equiv \sup_{x \ne 0} R'(x), \qquad R \equiv \sup_{x \ne 0} R(x).$$

$$\mathscr{F}_a^{(4)}(x) = G^2 \cdot (R')^2 \cdot R(x),$$

$$\mathscr{F}_a^{(5)}(x) = G^2 \cdot (R')^3 \cdot R(x), \qquad \mathscr{F}_b^{(5)}(x) = G^2 \cdot R \cdot (R')^2 \cdot R(x),$$

$$\mathscr{F}_a^{(6)}(x) = G^2 \cdot (R')^4 \cdot R(x), \qquad \mathscr{F}_b^{(6)}(x) = G^2 \cdot R \cdot (R')^3 \cdot R(x).$$

3.4. *Bounds on* $\sum_x \Pi^{(n)}(x)$, $\sum_x |x|^2 \Pi^{(n)}(x)$, $\sum_x \Phi^{(n)}(x)$ and $\sum_x |x|^2 \Phi^{(n)}(x)$

In this section we use the results of the previous section to derive bounds on $\sum_x \Psi^{(n)}(x)$ and $\sum_x |x|^2 \Psi^{(n)}(x)$, where here and in the following Ψ denotes either Π or Φ.

3.4.1. *Bounds on* $\sum_x \Psi^{(n)}(x)$

Bounds are obtained for $\sum_x \Psi^{(n)}(x)$ $(n \leq 8)$ using Lemma 3.3 as follows. Defining

$$\tilde{\mathscr{B}}_a^{(1)}(x) \equiv \begin{cases} 0 & (|x| = 0, 1) \\ \mathscr{B}_a^{(1)}(x) & (\text{otherwise}) \end{cases}, \tag{3.42}$$

we have

$$N_p^{-1} \sum_x \Phi^{(2)}(x) \leq U(\tilde{R}(0), \tilde{\mathscr{B}}_a^{(1)}, G), \tag{3.43}$$

$$\sum_x \Pi^{(2)}(x) \leq U(R(0), \mathscr{B}_a^{(1)}, G). \tag{3.44}$$

Similarly, defining

$$\tilde{\mathscr{E}}_a^{(2)}(x) \equiv \begin{cases} 0 & (|x| = 0, 1) \\ \mathscr{E}_a^{(2)}(x) & (\text{otherwise}) \end{cases}, \tag{3.45}$$

we have

$$N_p^{-1} \sum_x \Phi^{(3)}(x) \leq U(\{\mathscr{A}_a^{(1)}\}^2, \tilde{\mathscr{E}}_a^{(2)}, G) \tag{3.46}$$

and

$$\sum_x \Pi^{(3)}(x) \leq U(\mathscr{A}_a^{(2)}, \mathscr{B}_a^{(2)}, G). \tag{3.47}$$

For $4 \leq n \leq 8$,

$$N_p^{-1} \sum_x \Phi^{(n)}(x) = \sum_x \Pi^{(n)}(x) \leq U(\mathscr{A}_a^{(n-1)}, \mathscr{B}_a^{(n-1)}, G). \tag{3.48}$$

For $n \geq 9$, we simply bound

$$N_p^{-1} \sum_x \Phi^{(n)}(x) = \sum_x \Pi^{(n)}(x) \leq \mathscr{A}_a^{(8)} \cdot \sup_{z \neq 0} G(z) \cdot \left[\sup_{y \neq 0} R'(y) \right]^{n-9}. \tag{3.49}$$

3.4.2. *Bounds on* $\sum_x |x|^2 \Psi^{(n)}(x)$

We now obtain bounds for $\sum_x |x|^2 \Pi^{(n)}(x)$ and $\sum_x |x|^2 \Phi^{(n)}(x)$. Let

$$\bar{\bar{G}}(x) \equiv |x|^2 G(x). \tag{3.50}$$

Arguing as when no factor $|x|^2$ was present, we have

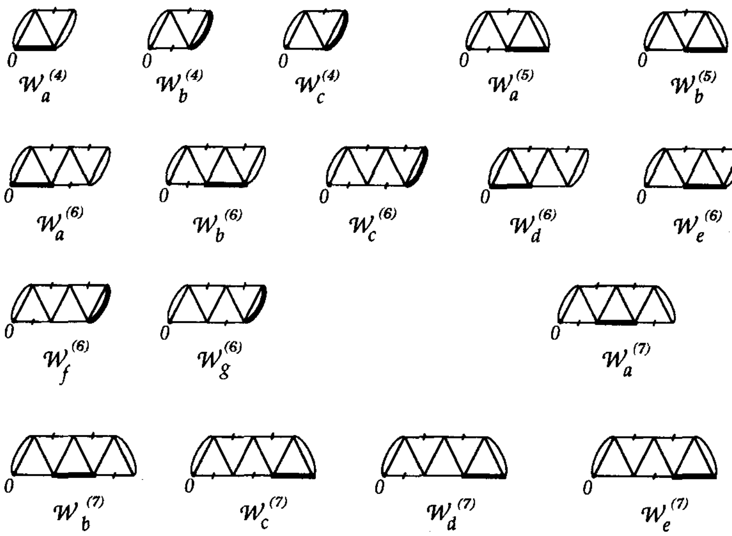


Fig. 3. Diagrams used to estimate $\sum_x |x|^2 \Psi^{(n)}(x)$.

$$N_p^{-1} \sum_x |x|^2 \Phi^2(x) \le U(\tilde{R}(0), \tilde{\mathscr{B}}_a^{(1)}, \bar{\bar{G}}), \tag{3.51}$$

$$\sum_x |x|^2 \Pi^{(2)}(x) \le U(R(0), \mathscr{B}_a^{(1)}, \bar{\bar{G}}), \tag{3.52}$$

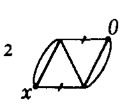
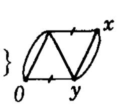
and

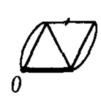
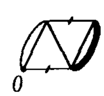
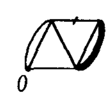
$$N_p^{-1} \sum_x |x|^2 \Phi^{(3)}(x) \le U(\{\mathscr{A}_a^{(1)}\}^2, \tilde{\mathscr{E}}_a^{(2)}, \bar{\bar{G}}), \tag{3.53}$$

$$\sum_x |x|^2 \Pi^{(3)}(x) \le U(\{\mathscr{A}_a^{(1)}\}^2, \mathscr{E}_a^{(2)}, \bar{\bar{G}}). \tag{3.54}$$

To deal with higher orders, we define several diagrams in Fig. 3. In these diagrams, bold lines represent lines weighted with a factor $|x|^2$. Note that for $n \ge 4$, $N_p^{-1}\Phi^{(n)}(x) = \Pi^{(n)}(x)$.

Then for example, to estimate the four-loop diagram we use

$$\sum_x |x|^2$$  $$= \sum_{x,y} \{|y|^2 + |x-y|^2 + 2y \cdot (x-y)\}$$ 

$$\le 2$$  $$+$$  $$+$$  (3.55)

In the last step, we used $2(x-y)\cdot y \le |x-y|^2 + |y|^2$ and took into account the fact that this gives rise to a diagram with the constraint $y \ne 0$, i.e. $\mathscr{W}_c^{(4)}$. Then we bound the diagrams $\mathscr{W}_*^{(4)}$ as in Sec. 3.4.1, obtaining

$$\mathscr{W}_a^{(4)} \le U(\mathscr{A}_a^{(1)}\mathscr{A}_a^{(2)}, \mathscr{E}_a^{(3)}, \bar{\bar{G}}), \qquad \mathscr{W}_b^{(4)} \le U(\mathscr{A}_a^{(3)}, \mathscr{B}_a^{(3)}, \bar{\bar{G}}),$$
$$\mathscr{W}_c^{(4)} \le U(\mathscr{A}_b^{(3)}, \mathscr{B}_b^{(3)}, \bar{\bar{G}}). \tag{3.56}$$

Thus we have

$$N_p{}^{-1} \sum_x |x|^2 \Phi^{(4)}(x) = \sum_x |x|^2 \Pi^{(4)}(x) \le 2\mathscr{W}_a^{(4)} + \mathscr{W}_b^{(4)} + \mathscr{W}_c^{(4)}. \tag{3.57}$$

Similarly, using the triangle inequality and keeping track of non-zero lines, we obtain

$$N_p{}^{-1} \sum_x |x|^2 \Phi^{(5)}(x) = \sum_x |x|^2 \Pi^{(5)}(x) \le 2\mathscr{W}_a^{(5)} + 2\mathscr{W}_b^{(5)}, \tag{3.58}$$

with

$$\mathscr{W}_a^{(5)} \le U(\mathscr{A}_a^{(1)}\mathscr{A}_a^{(3)}, \mathscr{E}_a^{(4)}, \bar{\bar{G}}), \qquad \mathscr{W}_b^{(5)} \le U(\mathscr{A}_a^{(1)}\mathscr{A}_b^{(3)}, \mathscr{E}_b^{(4)}, \bar{\bar{G}}). \tag{3.59}$$

Also

$$\sum_x |x|^2 \Pi^{(6)}(x) \le 2\mathscr{W}_a^{(6)} + 2\mathscr{W}_b^{(6)} + \mathscr{W}_c^{(6)} + \mathscr{W}_d^{(6)} + \mathscr{W}_e^{(6)} + \mathscr{W}_f^{(6)} + \mathscr{W}_g^{(6)}, \tag{3.60}$$

with

$$\mathscr{W}_a^{(6)} \le U(\mathscr{A}_a^{(1)}\mathscr{A}_a^{(4)}, \mathscr{E}_a^{(5)}, \bar{\bar{G}}), \qquad \mathscr{W}_b^{(6)} \le U(\mathscr{A}_a^{(2)}\mathscr{A}_a^{(3)}, \mathscr{F}_a^{(5)}, \bar{\bar{G}}),$$
$$\mathscr{W}_c^{(6)} \le U(\mathscr{A}_a^{(5)}, \mathscr{B}_a^{(5)}, \bar{\bar{G}}), \qquad \mathscr{W}_d^{(6)} \le U(\mathscr{A}_a^{(1)}\mathscr{A}_d^{(4)}, \mathscr{E}_d^{(5)}, \bar{\bar{G}}),$$
$$\mathscr{W}_e^{(6)} \le U(\mathscr{A}_a^{(2)}\mathscr{A}_b^{(3)}, \mathscr{F}_b^{(5)}, \bar{\bar{G}}), \qquad \mathscr{W}_f^{(6)} \le U(\mathscr{A}_b^{(5)}, \mathscr{B}_b^{(5)}, \bar{\bar{G}}),$$
$$\mathscr{W}_g^{(6)} \le U(\mathscr{A}_c^{(5)}, \mathscr{B}_c^{(5)}, \bar{\bar{G}}). \tag{3.61}$$

For the seven-loop diagram we have

$$\sum_x |x|^2 \Pi^{(7)}(x) \le \mathscr{W}_a^{(7)} + 2(\mathscr{W}_b^{(7)} + \mathscr{W}_c^{(7)} + \mathscr{W}_d^{(7)} + \mathscr{W}_e^{(7)}), \tag{3.62}$$

with

$$\mathscr{W}_a^{(7)} \le U(\mathscr{A}_a^{(3)}\mathscr{A}_a^{(3)}, \mathscr{F}_a^{(6)}, \bar{\bar{G}}), \qquad \mathscr{W}_b^{(7)} \le U(\mathscr{A}_a^{(3)}\mathscr{A}_b^{(3)}, \mathscr{F}_b^{(6)}, \bar{\bar{G}}),$$
$$\mathscr{W}_c^{(7)} \le U(\mathscr{A}_a^{(1)}\mathscr{A}_a^{(5)}, \mathscr{E}_a^{(6)}, \bar{\bar{G}}), \qquad \mathscr{W}_d^{(7)} \le U(\mathscr{A}_a^{(1)}\mathscr{A}_b^{(5)}, \mathscr{E}_b^{(6)}, \bar{\bar{G}}), \tag{3.63}$$
$$\mathscr{W}_e^{(7)} \le U(\mathscr{A}_a^{(1)}\mathscr{A}_c^{(5)}, \mathscr{E}_c^{(6)}, \bar{\bar{G}}).$$

For $n = 8, 9$, we have

$$\sum_x |x|^2 \Pi^{(8)}(x) \le \sup_x \bar{\bar{G}}(x) \cdot \{4\mathscr{A}_a^{(1)}\mathscr{A}_a^{(6)} + 4\mathscr{A}_a^{(7)} + \mathscr{A}_a^{(2)}(2\mathscr{A}_a^{(5)} + \mathscr{A}_b^{(5)} + \mathscr{A}_c^{(5)})$$

$$+ \mathscr{A}_a^{(4)}(2\mathscr{A}_a^{(3)} + \mathscr{A}_b^{(3)}) + \mathscr{A}_a^{(3)}\mathscr{A}_d^{(4)}\}, \tag{3.64}$$

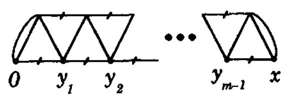
$$\sum_x |x|^2 \Pi^{(9)}(x) \le \sup_x \bar{\bar{G}}(x) \cdot \{8\mathscr{A}_a^{(1)}\mathscr{A}_a^{(7)} + 8\mathscr{A}_a^{(3)}\mathscr{A}_a^{(5)}\}. \tag{3.65}$$

For $n \ge 10$, we use less careful estimates. To simplify the notation, we temporarily write

$$M \equiv \sup_x |x|^2 G_p(x), \qquad r \equiv R_p(0), \qquad R' \equiv \sup_{x \ne 0} R_p'(x). \tag{3.66}$$

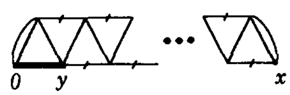
We begin with n odd, and write $n = 2m + 1$. To bound

$$\sum_{y_1, y_2, \ldots, y_{m-1}, x} |x|^2 \tag{3.67}$$

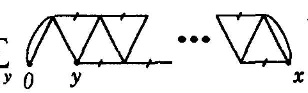


we first use the inequality $|x|^2 \le m \sum_{i=1}^m |y_i - y_{i-1}|^2$ and then bound each term of the resulting expression. For example,

$$\sum_{y,x}$$



$$\le \left(\sup_y |y|^2 G_p(y)\right)\left(\sum_{x,y}\right.$$



$$\left.\right)$$

$$\le Mr^2(R')^{2m-2}. \tag{3.68}$$

All other contributions are bounded in the same way, with the result that

$$\sum_x |x|^2 \Pi^{(2m+1)}(x) \le m^2 M r^2 (R')^{2m-2}. \tag{3.69}$$

For $n = 2m$ even we similarly have

$$\sum_x |x|^2 \Pi^{(2m)}(x) \le mMr\{R' + (m-1)r\}(R')^{2m-3}. \tag{3.70}$$

The numerical bounds on $\sum_x \Psi(x)$ and $\sum_x |x|^2 \Psi(x)$ stated in Lemma 3.1 then follow, once the results of this section are combined with those of Sec. 3.3. The bounds of Lemma 3.1 on the Fourier transforms are then obtained as explained in the next subsection.

3.4.3. *Bounds on* $\hat{\Psi}(k)$

The bounds of Lemma 3.1 on $\partial_\mu^u \hat{\Psi}$ $(u = 0, 1, 2)$ now follow easily from the bounds on $\sum_x \Psi(x)$ and $\sum_x |x|^2 \Psi(x)$. For $u = 0$ we simply use

$$|\hat{\Psi}(k)| \leq \sum_{n=1}^{\infty} \sum_{x} \Psi^{(n)}(x). \tag{3.71}$$

Similarly, for $u = 1, 2$ we use $|x_\mu| \leq x_\mu^2$ and symmetry to obtain

$$|\partial_\mu^u \hat{\Psi}(k)| \leq \frac{1}{d} \sum_{n=1}^{\infty} \sum_{x} |x|^2 \Psi^{(n)}(x). \tag{3.72}$$

To prove (3.12), we first use symmetry to write

$$\partial_\mu \hat{\Phi}_p(k) = i \sum_{x} x_\mu \Phi_p(x) e^{ik \cdot x} = -\sum_{x} x_\mu \sin(k_\mu x_\mu) \prod_{\nu \neq \mu} \cos(k_\nu x_\nu) \Phi_p(x). \tag{3.73}$$

Thus we have

$$|\partial_\mu \hat{\Phi}_p(k)| \leq \sum_{x} |x_\mu \sin k_\mu x_\mu| |\Phi_p(x)|. \tag{3.74}$$

Since $|\sin nt| \leq n |\sin t|$ for any nonnegative integer n, this gives

$$|\partial_\mu \hat{\Phi}_p(k)| \leq |\sin k_\mu| \sum_{x} x_\mu^2 |\Phi_p(x)| \leq \frac{c_3 + c_4}{d} |\sin k_\mu|. \tag{3.75}$$

We next observe that

$$\begin{aligned} \hat{\Psi}(0) - \hat{\Psi}(k) &= \sum_{n=1}^{\infty} (-1)^n \sum_{x} \{1 - \cos(k \cdot x)\} \Psi^{(n)}(x) \\ &\geq - \sum_{n=3:\mathrm{odd}}^{\infty} \sum_{x} \{1 - \cos(k \cdot x)\} \Psi^{(n)}(x). \end{aligned} \tag{3.76}$$

To bound the right side we proceed as follows. First we use symmetry to replace the cosine by an exponential, and then use a telescoping sum:

$$1 - e^{ik \cdot x} = 1 - e^{ik_1 x_1} + e^{ik_1 x_1}(1 - e^{ik_2 x_2}) + \cdots + e^{ik_1 x_1 + \cdots + ik_{d-1} x_{d-1}}(1 - e^{ik_d x_d}).$$

By symmetry all these exponentials can be replaced by cosines. Then using the fact that $1 - \cos nt \leq n^2(1 - \cos t)$ for every integer n, we obtain

$$\begin{aligned} \hat{\Psi}(0) - \hat{\Psi}(k) &\geq - \sum_{n=3:\mathrm{odd}}^{\infty} \sum_{\mu=1}^{d} \sum_{x} x_\mu^2 \{1 - \cos k_\mu\} \Psi^{(n)}(x) \\ &= -\{1 - \hat{D}(k)\} \sum_{n=3:\mathrm{odd}}^{\infty} \sum_{x} |x|^2 \Psi^{(n)}(x). \end{aligned} \tag{3.77}$$

Similarly,

$$\hat{\Psi}(0) - \hat{\Psi}(k) \le \sum_{n=2:\text{even}}^{\infty} \sum_{x} \{1 - \cos(k \cdot x)\} \Psi^{(n)}(x)$$

$$\le \{1 - \hat{D}(k)\} \sum_{n=2:\text{even}}^{\infty} \sum_{x} |x|^2 \Psi^{(n)}(x). \tag{3.78}$$

This completes the proof of Lemma 3.1.

3.5. *Proof of Lemma 3.2*

To prove Lemma 3.2, we require upper bounds on N_p, $X_p \equiv N_p/A_p$, and $Y_p \equiv X_p/A_p$. We obtain these with upper bounds on N_p and X_p, and a lower bound on A_p. By definition, these quantities are given by

$$N_p^{-1} = 2dp + 2d\pi_1, \qquad X_p^{-1} = 1 + 2dpG_p(e_1) + \pi_0 \tag{3.79}$$

and

$$A_p = \frac{1 + 2dpG_p(e_1) + \pi_0}{2dp + 2d\pi_1}. \tag{3.80}$$

Thus we need lower bounds on p, $G_p(e_1)$, π_0 and π_1, and upper bounds on π_1 and p. To bound p we simply use $p_0 \le p < z_c$, and bound z_c using Corollary A.2.

Lower bounds on π_0 and π_1 are obtained using

$$\pi_0 = \Pi^{(3)}(0) \ge 2d[p^4 + 4(\underline{G_p(e_1) - p})p^3] \tag{3.81}$$

and

$$\pi_1 = \Pi^{(2)}(e_1) - \Pi^{(3)}(e_1)$$

$$\ge p^3 + 3(\underline{G_p(e_1) - p})p^2 + 3(2d-2)(2d-3)p^7 - G_p(e_1)\mathscr{E}_a^{(2)}(e_1). \tag{3.82}$$

For an upper bound on π_1, we discard the contribution from the three-loop diagram to obtain

$$\pi_1 \le G_p(e_1)^3. \tag{3.83}$$

The right side of (3.83) and the last term on the right side of (3.82) are bounded using Lemma 2.1 and (3.41).

It remains to obtain a lower bound on $G_p(e_1)$. This we do by first noting that a lower bound is obtained when $p = p_0$, and this is then bounded below using (2.25). Similarly we use $\underline{G_p(e_1) - p} \ge G_{p_0}(e_1) - p_0$.

These bounds give the upper and lower bounds on N_p, X_p, and A_p stated in Lemma 3.2. □

4. Proof of $P_p(0.999)$

In this section we prove $P_p(0.999)$, given $P_p(1)$, and thereby complete the proof of Proposition 1.9. The basic strategy is to write the various quantities of $P_p(\alpha)$ in k-space, and then to use the results of Secs. 2 and 3 to obtain an upper bound. The upper bounds will be in terms of the Gaussian quantities introduced in Sec. 1.6.

We analyze separately the three kinds of bubble quantities, $G_p(e_1)$, and $\sup_{x \notin \Lambda_0} |x|^2 G_p(x)$. To simplify the notation, we write $\varepsilon \equiv N_p \chi(p)^{-1} > 0$ and $\varepsilon' \equiv \varepsilon/(1 - c_3)$ without further mention, and often drop subscripts p.

4.1. *Bubble quantities*

Here we derive bounds on the three types of bubble quantities appearing in $P_p(0.999)$.

4.1.1. *Bound on $B_p(0)$*

We first observe that $1 = G(0) = \int \frac{d^d k}{(2\pi)^d} \hat{G}(k)$. By the Parseval relation, for any $X \in \mathbf{R}$

$$B_p(0) = \sum_{x \neq 0} G(x)^2 = \int \frac{d^d k}{(2\pi)^d} \{\hat{G}(k)^2 - 1\} = \int \frac{d^d k}{(2\pi)^d} \{\hat{G}(k) - X\}^2 - (1 - X)^2. \quad (4.1)$$

Now we take $X = X_p = N_p/A_p$. Then from (3.3) and (3.7),

$$\hat{G}(k) - X_p = X_p \frac{\hat{D}(k) + \hat{\Phi}(k)}{A_p - \hat{D}(k) - \hat{\Phi}(k)} = X_p \frac{\hat{D}(k) + \hat{\Phi}(k)}{\varepsilon + 1 - \hat{D}(k) + \hat{\Phi}(0) - \hat{\Phi}(k)}, \quad (4.2)$$

and hence

$$B_p(0) = X_p^{\,2} \int \frac{d^d k}{(2\pi)^d} \left(\frac{\hat{D}(k) + \hat{\Phi}(k)}{\varepsilon + 1 - \hat{D}(k) + \hat{\Phi}(0) - \hat{\Phi}(k)} \right)^2 - (1 - X_p)^2. \quad (4.3)$$

Next we expand the square in the numerator of the integrand, and estimate each of the resulting terms. The first term can be bounded above, using (3.13) and the fact that $\varepsilon' > 0$, by

$$\frac{X_p^{\,2}}{(1 - c_3)^2} I_{2,2}^{(\varepsilon')} \le \frac{X_p^{\,2}}{(1 - c_3)^2} I_{2,2}. \quad (4.4)$$

For the cross term, we first rewrite it as

$$2X_p{}^2 \int \frac{d^dk}{(2\pi)^d} \frac{\hat{D}(k)\hat{\Phi}(k)}{\{\varepsilon + 1 - \hat{D}(k) + \hat{\Phi}(0) - \hat{\Phi}(k)\}^2} = \frac{2X_p{}^2}{N_p{}^2} \int \frac{d^dk}{(2\pi)^d} \hat{G}(k)^2 \hat{D}(k)\hat{\Phi}(k)$$

$$= \frac{2X_p{}^2}{N_p{}^2}(G * G * D * \Phi)(0), \tag{4.5}$$

where $*$ denotes convolution in x-space. Because G and D are nonnegative in x-space, we can bound the above convolution by neglecting the negative part of Φ, i.e. contributions from an odd number of loops. Returning then to k-space and using (3.7), (3.13), (3.10), we can bound (4.5) above by

$$\frac{2X_p{}^2}{N_p{}^2} \int \frac{d^dk}{(2\pi)^d} \hat{G}(k)^2 \hat{D}(k) \hat{\Phi}^{(\text{even})}(k) \leq \frac{2X_p{}^2 c_2}{(1-c_3)^2} J_{2,1}^{(\varepsilon')}. \tag{4.6}$$

For the third term, we now have $\Phi * \Phi$ instead of $D * \Phi$. Proceeding as for the cross term, we obtain

$$B_p(0) \leq \frac{X_p{}^2}{(1-c_3)^2} \cdot \{I_{2,2} + 2c_2 J_{2,1} + (c_1^2 + c_2^2) I_{2,0}\} - (1 - X_p)^2. \tag{4.7}$$

Now we use the bound on X_p of Lemma 3.2 and the Gaussian bounds of Lemma B.8 to conclude that $B_p(0) \leq 0.49012$, and hence the bound of $P_p(0.999)$ is satisfied.

4.1.2. *Bound on $\tilde{B}_p(0)$*

Using the fact that $\int \frac{d^dk}{(2\pi)^d} \hat{D}(k)^2 = \frac{1}{2d}$, for any X, $Y \in \mathbf{R}$ we have

$$\tilde{B}_p(0) = \sum_{|x|>1} G_p(x)^2 = \int \frac{d^dk}{(2\pi)^d} \{\hat{G}(k)^2 - 1 - 2dG_p(e_1)^2\}$$

$$= \int \frac{d^dk}{(2\pi)^d} \{\hat{G}(k) - X - Y\hat{D}(k)\}^2 - (1-X)^2 - 2d\{G_p(e_1) - Y/(2d)\}^2. \tag{4.8}$$

Taking $X = X_p \equiv N_p/A_p$ and $Y = Y_p \equiv N_p/A_p{}^2$ gives

$$\hat{G}(k) - X_p - Y_p\hat{D}(k) = \frac{X_p\hat{\Phi}(k) + Y_p\hat{D}(k)^2 + Y_p\hat{\Phi}(k)\hat{D}(k)}{A_p - \hat{D}(k) - \hat{\Phi}(k)}. \tag{4.9}$$

Inserting (4.9) into (4.8), performing the square, and then bounding the resulting expression term by term gives

$$\tilde{B}_p(0) \le \frac{1}{(1-c_3)^2}\{Y_p{}^2 I_{2,4} + 2c_2(Y_p{}^2 J_{2,3} + X_p Y_p I_{2,2})$$

$$+ (c_1^2 + c_2^2)(Y_p{}^2 I_{2,2} + X_p{}^2 I_{2,0} + 2X_p Y_p J_{2,1})\}$$

$$- (1 - X_p)^2 - 2d\{G_p(e_1) - Y_p/(2d)\}^2. \tag{4.10}$$

Now we use the bound on Y_p of Lemma 3.2, the Gaussian bounds of Lemma B.8, and the lower bound on $G_p(e_1)$ of (2.25) to conclude that $\tilde{B}_p(0) \le 0.3121$, which satisfies the bound of $P_p(0.999)$.

4.1.3. *Bounds on $B'_p(x)$*

To bound $B'_p(x)$, we will write it as a perturbation of a Gaussian quantity which decays nicely with $|x|$. To begin, we proceed as above and write, for any $x \in \mathbf{Z}^d$,

$$B'_p(x) = \int \frac{d^d k}{(2\pi)^d} \hat{G}(k)\{\hat{G}(k) - X_p + X_p - 1\}e^{ik\cdot x}$$

$$= N_p X_p \int \frac{d^d k}{(2\pi)^d} \frac{\{\hat{D}(k)e^{ik\cdot x} + \hat{\Phi}(k)\hat{D}^{(x)}(k)\}}{\{A_p - \hat{D}(k) - \hat{\Phi}(k)\}^2} - (1 - X_p)G_p(x), \tag{4.11}$$

where we have used symmetry to replace $e^{ik\cdot x}$ by $\hat{D}^{(x)}(k)$ of (1.77). In the last term we use Lemma 3.2 to bound $1 - X_p$, and the lower bound on $G_p(x)$ of Corollary A.4. For the second term in the integrand, we argue exactly as in Sec. 4.1.1, using (3.10) and (3.13) to bound it by

$$\frac{N_p X_p c_2}{(1 - c_3)^2} K_{2,0}(x). \tag{4.12}$$

Now for the first term in the integral, we extract the Gaussian contribution by writing

$$\frac{1}{A_p - \hat{D}(k) - \hat{\Phi}(k)} = \frac{1}{\varepsilon + 1 - \hat{D}(k) + \hat{\Phi}(0) - \hat{\Phi}(k)} = \frac{1 - f(k)}{\varepsilon + 1 - \hat{D}(k)}, \tag{4.13}$$

with

$$f(k) \equiv \frac{\hat{\Phi}(0) - \hat{\Phi}(k)}{\varepsilon + 1 - \hat{D}(k) + \hat{\Phi}(0) - \hat{\Phi}(k)}. \tag{4.14}$$

By (3.13), we have $-c_3/(1 - c_3) \le f(k) \le c_4/(1 + c_4)$. [For the upper bound, we used the fact that $x/(1 + x)$ is monotone increasing for small x.] Now, if $f(k)$ were constant then the first term in the integral of (4.11) would be proportional to $I^{(\varepsilon)}_{2,1}(x)$, which decays rather rapidly with $|x|$. In order to profit from this decay, we first introduce

$$f_0 \equiv \frac{1}{2}\left(\frac{c^4}{1+c_4} - \frac{c_3}{1-c_3}\right), \qquad f_1(k) \equiv f(k) - f_0. \tag{4.15}$$

Then

$$|f_1(k)| \le \frac{1}{2}\left(\frac{c_4}{1+c_4} + \frac{c_3}{1-c_3}\right) \equiv f_2. \tag{4.16}$$

Next we rewrite the first term of the integral of (4.11), using (4.13) and (4.15), as

$$\begin{aligned}
&\int \frac{d^dk}{(2\pi)^d} \frac{\{1-f(k)\}^2 \hat{D}(k) e^{ik\cdot x}}{\{\varepsilon + 1 - \hat{D}(k)\}^2} \\
&= \int \frac{d^dk}{(2\pi)^d} \frac{\{1 - f_0 - f_1(k)\}^2 \hat{D}(k)\hat{D}^{(x)}(k)}{\{\varepsilon + 1 - \hat{D}(k)\}^2} \\
&= (1-f_0)^2 \int \frac{d^dk}{(2\pi)^d} \frac{\hat{D}(k)\hat{D}^{(x)}(k)}{(\varepsilon + 1 - \hat{D}(k))^2} - 2(1-f_0) \int \frac{d^dk}{(2\pi)^d} \frac{f_1(k)\hat{D}(k)\hat{D}^{(x)}(k)}{(\varepsilon + 1 - \hat{D}(k))^2} \\
&\quad + \int \frac{d^dk}{(2\pi)^d} \frac{f_1(k)^2 \hat{D}(k)\hat{D}^{(x)}(k)}{(\varepsilon + 1 - \hat{D}(k))^2}.
\end{aligned} \tag{4.17}$$

The first term is equal to $(1-f_0)^2 I^{(\varepsilon)}_{2,1}(x)$, which is bounded above by $(1-f_0)^2 I_{2,1}(x)$. The second term is bounded by

$$2(1-f_0)f_2 \int \frac{d^dk}{(2\pi)^d} \frac{|\hat{D}(k)| \cdot |\hat{D}^{(x)}(k)|}{(1-\hat{D}(k))^2} = 2(1-f_0)f_2 K_{2,1}(x). \tag{4.18}$$

Similarly, the third term is bounded by $f_2^2 K_{2,1}(x)$.

Combining the above bounds, we obtain

$$\begin{aligned}
B_p'(x) \le{}& N_p X_p \{(1-f_0)^2 I_{2,1}(x) + 2(1-f_0)f_2 K_{2,1}(x) + f_2^2 K_{2,1}(x)\} \\
&+ \frac{N_p X_p c_2}{(1-c_3)^2} K_{2,0}(x) - (1-X_p)G_p(x).
\end{aligned} \tag{4.19}$$

For $x \in \Lambda_1$, we use this bound together with the bounds on N_p and X_p of Lemma 3.2, the Gaussian bounds of Lemma B.8 [bounding $K_{2,0}$ and $K_{2,1}$ as in (B.26) and (B.27)], and the lower bound on $G_p(x)$ of (2.25), to conclude the required bounds on $B_p'(x)$ from $P_p(0.999)$, for $x \in \Lambda_1$.

For $\sup_{x \notin \Lambda_0} B_p'(x)$ we proceed as above, using the Gaussian bounds of Lemma B.8

to conclude that $\sup_{x \in \Lambda_3 \setminus \Lambda_1} B'_p(x) \leq 0.2129$, and those of Lemma B.9 to conclude that $\sup_{x \notin \Lambda_3, x \neq 0} B'_p(x) \leq 0.191$. These bounds clear those of $P_p(0.999)$.

4.2. *Bound on $G_p(e_1)$*

To obtain the bound on $G_p(e_1)$ of $P_p(0.999)$, we use Lemma 2.4. This requires upper bounds on $G_{p_0}(e_1)$, $R'_{p_0}(e_1)$, $R'_p(e_1)$ and z_c. For $G_{p_0}(e_1)$ we use Proposition 1.7, and for z_c we use Corollary A.2. For $R'_{p_0}(e_1)$ we use Lemma 2.3, bounding $B'_{p_0}(e_1)$ via Proposition 1.7. For $R'_p(e_1)$ we use the entry in Table I. Substitution of these values into (2.19) gives $G_p(e_1) \leq 0.142021$, which satisfies the corresponding bound of $P_p(0.999)$.

4.3. *Bounds on $|x|^2 G(x)$*

In this section we complete the proof of $P_p(0.999)$ by showing that $\sup_{x \notin \Lambda_0} |x|^2 G_p(x) \leq 0.0747$. The limitations of our approach are most apparent at this point.

We mainly use two kinds of bounds. The first is to simply multiply the bound on $G_p(x)$ of Lemma 2.4 by $|x|^2$. This gives a good result for small $|x|$, but for large x any overestimate of $G_p(x)$ is severely magnified and results in an inadequate bound. The second and main approach is to go to k-space and use our bounds on $\hat{\Phi}$. In this process the factor $|x|^2$ is transformed to a second derivative with respect to k. Taking the derivative explicitly gives rise to several terms. In extracting from these the corresponding Gaussian quantity $N_p |x|^2 I^{(e)}_{1,0}(x)$, we are left with a large number of error terms and little room for comfort below the required bound 0.0749.

We divide $\mathbf{Z}^5$ into four distinct regions, and employ a different method to bound $|x|^2 G_p(x)$ in each of these regions. The regions are: $\{\|x\|_\infty \leq 6\}$, $\{\|x\|_\infty \geq 7$ and $\mathrm{dist}(x, \mathrm{axes}) > 0\}$, $\{\|x\|_\infty = 7,\ 8$ and $\mathrm{dist}(x, \mathrm{axes}) = 0\}$, and $\{\|x\|_\infty \geq 9$ and $\mathrm{dist}(x, \mathrm{axes}) = 0\}$. Here $\mathrm{dist}(x, \mathrm{axes})$ denotes the Euclidean distance from x to the coordinate axes of $\mathbf{Z}^5$. The Gaussian quantities appearing in the upper bounds decay least rapidly along coordinate axes, and this is why we consider separately the case of x on an axis. For x on an axis, we use an iterative averaging process employing Lemma 2.2 to bound $G_p(x)$ in terms of its primarily smaller neighbouring values. We also use monotonicity of upper bounds to bound $|x|^2 G_p(x)$ for large $\|x\|_\infty$ in terms of its values for smaller $\|x\|_\infty$.

We now proceed through the four regions in sequence.

4.3.1. *Bounds for $\|x\|_\infty \leq 6$*

We bound $|x|^2 G_p(x)$ using two methods, and take the minimum.

The first method is to multiply (2.19) by $|x|^2$ to obtain

$$|x|^2 G_p(x) \leq |x|^2 \left\{ G_{p_0}(x) + \frac{z_c - p_0}{p_0} \frac{R'_{p_0}(x) + R'_p(x)}{2} \right\}. \tag{4.20}$$

As in Sec. 2.3, $p_0 \equiv (6611)/9^5$. To bound $G_{p_0}(x)$ and $R'_{p_0}(x)$ in terms of gaussian quantities, we use (1.62). For an upper bound on $R'_p(x)$, we use (4.19) to calculate an upper bound on $B_p'(x)$, and then bound $R_p'(x)$ according to (2.10). An upper bound on z_c is given in Corollary A.2. This method is effective for small $\|x\|_\infty$.

We now turn to the second method, which involves going to k-space. We have

$$
\begin{aligned}
|x|^2 G(x) &= -\sum_{\mu=1}^{d} \int \frac{d^d k}{(2\pi)^d} e^{ik\cdot x} \partial_\mu^2 \hat{G}(k) \\
&= N_p \int \frac{d^d k}{(2\pi)^d} \frac{\hat{D}(k) - \sum_\mu \partial_\mu^2 \hat{\Phi}(k)}{\{A_p - \hat{D}(k) - \hat{\Phi}(k)\}^2} e^{ik\cdot x} \\
&\quad - 2N_p \int \frac{d^d k}{(2\pi)^d} \frac{\sum_\mu \{(\sin k_\mu)/d - \partial_\mu \hat{\Phi}(k)\}^2}{\{A_p - \hat{D}(k) - \hat{\Phi}(k)\}^3} e^{ik\cdot x}.
\end{aligned}
\tag{4.21}
$$

We perform the square in the numerator of the second term on the right side. No further manipulation is required of the second term of the first integral or the second and third terms of the second integral. For the first terms of each integral, we rewrite the denominator using (4.13) and (4.15). The resulting terms are

$$
\frac{\hat{D}}{\{\varepsilon + 1 - \hat{D}\}^2}(1 - f_0 - f_1)^2 - 2\frac{\sum_\mu (\partial_\mu \hat{D})^2}{\{\varepsilon + 1 - \hat{D}\}^3}(1 - f_0 - f_1)^3. \tag{4.22}
$$

We then extract $(1 - f_0)^3 |x|^2 I_{1,0}(x)$ from the resulting expression. The result is

$$
\begin{aligned}
|x|^2 G(x) &= N_p (1 - f_0)^3 |x|^2 I_{1,0}^{(\varepsilon)}(x) + N_p (1 - f_0)^2 f_0 I_{2,1}^{(\varepsilon)}(x) \\
&\quad + 2N_p (1 - f_0) \int \frac{d^d k}{(2\pi)^d} \frac{\beta^{(\varepsilon)}(k) f_1(k) e^{ik\cdot x}}{\{\varepsilon + 1 - \hat{D}(k)\}^2} - N_p \int \frac{d^d k}{(2\pi)^d} \frac{\gamma^{(\varepsilon)}(k) f_1(k)^2 e^{ik\cdot x}}{\{\varepsilon + 1 - \hat{D}(k)\}^2} \\
&\quad + 2N_p \int \frac{d^d k}{(2\pi)^d} \frac{f_1(k)^3}{\{\varepsilon + 1 - \hat{D}(k)\}^3} \sum_\mu \left(\frac{\sin k_\mu}{d}\right)^2 e^{ik\cdot x} \\
&\quad + N_p \int \frac{d^d k}{(2\pi)^d} \frac{-\sum_\mu \partial_\mu^2 \hat{\Phi}(k)}{\{A_p - \hat{D}(k) - \hat{\Phi}(k)\}^2} e^{ik\cdot x} \\
&\quad + 4N_p \int \frac{d^d k}{(2\pi)^d} \frac{\sum_\mu (\sin k_\mu)/d \cdot \partial_\mu \hat{\Phi}(k)}{\{A_p - \hat{D}(k) - \hat{\Phi}(k)\}^3} e^{ik\cdot x} \\
&\quad - 2N_p \int \frac{d^d k}{(2\pi)^d} \frac{\sum_\mu \{\partial_\mu \hat{\Phi}(k)\}^2}{\{A_p - \hat{D}(k) - \hat{\Phi}(k)\}^3} e^{ik\cdot x},
\end{aligned}
\tag{4.23}
$$

where

$$
\beta^{(\varepsilon)}(k) \equiv 3\frac{1 - f_0}{\varepsilon + 1 - \hat{D}(k)} \sum_\mu \left(\frac{\sin k_\mu}{d}\right)^2 - \hat{D}(k) \tag{4.24}
$$

and

$$\gamma^{(\varepsilon)}(k) \equiv 6\frac{1-f_0}{\varepsilon+1-\hat{D}(k)}\sum_{\mu}\left(\frac{\sin k_\mu}{d}\right)^2 - \hat{D}(k). \tag{4.25}$$

Now the rest is routine. We bound each term above by using convolution methods as for the bubble quantities, and also simple applications of the Schwarz inequality. We also use (3.12) for the last two terms in (4.23). The result is

$$\begin{aligned}|x|^2G(x) \le\ & N_p(1-f_0)^3|x|^2I_{1,0}^{(\varepsilon)}(x) + N_p(1-f_0)^2f_0I_{2,1}^{(\varepsilon)}(x)\\ &+ 2N_p(1-f_0)f_2[I_\beta^{(\varepsilon)}L_2^{(\varepsilon)}(x)]^{1/2} + N_pf_2^2[I_\gamma^{(\varepsilon)}L_2^{(\varepsilon)}(x)]^{1/2} + 2N_pf_2^3U_3^{(\varepsilon)}(x)\\ &+ \frac{N_pc_4}{(1-c_3)^2}K_{2,0}^{(\varepsilon')}(x) + 4\frac{N_p(c_3+c_4)}{(1-c_3)^3}U_3^{(\varepsilon')}(x) + 2\frac{N_p(c_3+c_4)^2}{(1-c_3)^3}U_3^{(\varepsilon')}(x),\end{aligned} \tag{4.26}$$

where we have introduced

$$I_\beta^{(\varepsilon)} \equiv \int\frac{d^dk}{(2\pi)^d}\frac{\beta^{(\varepsilon)}(k)^2}{\{\varepsilon+1-\hat{D}(k)\}^2}, \qquad I_\gamma^{(\varepsilon)} \equiv \int\frac{d^dk}{(2\pi)^d}\frac{\gamma^{(\varepsilon)}(k)^2}{\{\varepsilon+1-\hat{D}(k)\}^2}. \tag{4.27}$$

For later convenience we further bound the above in terms of Gaussian quantities which are monotone in each $|x_\mu|$. We proceed as follows. We remove all the ε,ε'-dependence of the bounds except for that of $I_\beta^{(\varepsilon)}$ and $I_\gamma^{(\varepsilon)}$ by setting ε, $\varepsilon' = 0$. This gives an upper bound by Lemma B.2. Then, making use of the bounds (B.24)–(B.28), we bound all terms except for the first one in (4.26) using

$$\begin{aligned}H_0(x) \equiv\ & (1-f_0)^2f_0I_{2,0}(x) + 2(1-f_0)f_2[I_\beta^{(\varepsilon)}L_2(x)]^{1/2} + f_2^2[I_\gamma^{(\varepsilon)}L_2(x)]^{1/2}\\ &+ \frac{c_4}{(1-c_3)^2}\cdot\min\{[I_{2,0}\cdot L_2(x)]^{1/2}, [I_{1,0}(0)L_1(x)]^{1/2} + [I_{1,4}\cdot L_1(x)]^{1/2}\\ &+ [I_{2,4}\cdot L_2(x)]^{1/2}\} + \left\{2f_2^3 + 4\frac{(c_3+c_4)}{(1-c_3)^3} + 2\frac{(c_3+c_4)^2}{(1-c_3)^3}\right\}\left\{\frac{V_4\cdot L_2(x)}{2}\right\}^{1/2}.\end{aligned} \tag{4.28}$$

This gives

$$|x|^2G_p(x) \le N_p\{(1-f_0)^3|x|^2I_{1,0}(x) + H_0(x)\}. \tag{4.29}$$

To calculate concrete values from the above equations, bounds are needed for $I_\beta^{(\varepsilon)}$ and $I_\gamma^{(\varepsilon)}$. We employ Lemma B.11, but this needs an upper bound on ε. For this we first note that $p\dfrac{d}{dp}\chi(p) \le \chi(p)^2$, or

$$-\frac{d}{d(\ln p)}\chi(p)^{-1} \leq 1. \tag{4.30}$$

Integrating (4.30) from z_c down to p_0 gives, for any $p \in [p_0, z_c]$,

$$\chi^{-1}(p) \leq \chi^{-1}(p_0) \leq \ln\left(\frac{z_c}{p_0}\right). \tag{4.31}$$

Using Lemma 3.2 to bound N_p and Corollary A.2 for z_c then gives, for any $p \in [p_0, z_c]$,

$$\varepsilon \equiv N_p \chi(p)^{-1} \leq 0.0109388. \tag{4.32}$$

This bound on ε, together with Lemma B.11, gives

$$I_\beta^{(\varepsilon)} \leq 0.270562, \qquad I_\gamma^{(\varepsilon)} \leq 1.653224. \tag{4.33}$$

Now we can calculate concrete values from (4.29), employing the above bounds on $I_\beta^{(\varepsilon)}$ and $I_\gamma^{(\varepsilon)}$. Taking the minimum of (4.20) and (4.29), for $\|x\|_\infty \leq 6$, gives

$$|x|^2 G(x) \leq \begin{cases} 0.142\,021 & (x = e_1) \\ 0.091\,251 & (x = e_1 + e_2) \\ 0.109\,247 & (x = 2e_1) \\ 0.074\,661 & (\|x\|_1 > 2, \|x\|_\infty \leq 6) \end{cases}, \tag{4.34}$$

which satisfies the bound of $P_p(0.999)$, for $\|x\|_\infty \leq 6$.

4.3.2. *Bounds for* $\{\|x\|_\infty \geq 7$ *and dist*$(x, \text{axes}) > 0\}$

To get the desired bound for $\{\|x\|_\infty \geq 7$ and $\text{dist}(x, \text{axes}) > 0\}$, we employ the Fourier bound (4.29) and monotonicity of $I_{n,0}(x)$ and $L_n(x)$.

That is, Lemmas B.10 and B.12 state that for x with $\|x\|_\infty \geq 7$ and $\text{dist}(x, \text{axes}) > 0$,

$$|x|^2 I_{1,0}(x) \leq 0.019163, \qquad I_{1,0}(x) \leq 0.00037697, \qquad I_{2,0}(x) \leq 0.090467, \tag{4.35}$$

$$L_1(x) \leq 0.036151, \qquad L_2(x) \leq 0.12102. \tag{4.36}$$

Using Lemma B.11 and these values, with (4.28) and (4.29), yields $|x|^2 G_p(x) \leq 0.07383$ for all x under consideration. This satisfies the bound of $P_p(0.999)$ for these values of x.

4.3.3. *Bounds for* $\{x = ne_\mu : n = 7, 8\}$

In this section, we bound $|x|^2 G(x)$ for $x = ne_\mu$ with $n = 7, 8$. By symmetry, it is only necessary to consider $x = ne_1$. The bounds obtained in the previous subsection are inadequate for these values of x. We improve them by an iterative averaging procedure, which employs Lemma 2.2 to bound $G_p(x)$ essentially by the average of its primarily smaller values at neighbours of x.

The basic averaging estimate (2.3) states that

$$G_p(x) \leq \frac{C}{2d} \sum_{|e|=1} G_p(x-e), \tag{4.37}$$

where by Lemma 2.1, the upper bound on z_c of Lemma A.2, and the lower bound on $G_p(x)$ of (2.25), we can take

$$C = 1.0127. \tag{4.38}$$

To prepare for the iterative application of (4.37), we define $H_m(x)$, for $m \geq 1$, recursively by

$$H_{m+1}(x) \equiv \min\left\{H_m(x), \frac{C}{2d} \sum_{|e|=1} \frac{|x|^2}{|x-e|^2} \cdot H_m(x-e)\right\} \tag{4.39}$$

starting from $H_0(x)$. When there is insufficient information to evaluate the second quantity on the right side, e.g. when the value of $H_m(x-e)$ is unknown but $H_m(x)$ is known, then we define $H_{m+1}(x)$ to be $H_m(x)$.

Multiplying (4.37) by $|x|^2$ gives

$$|x|^2 G_p(x) \leq \frac{C}{2d} \sum_{|e|=1} \frac{|x|^2}{|x-e|^2} \cdot |x-e|^2 G_p(x-e). \tag{4.40}$$

Now we use (4.29) to estimate the right side, noting that for $x \neq 0$ the simple random walk two-point function satisfies $I_{1,0}(x) = \frac{1}{2d} \sum_{e:|e|=1} I_{1,0}(x-e)$. This gives

$$|x|^2 G_p(x) \leq N_p \left\{C(1-f_0)^3 |x|^2 I_{1,0}(x) + \frac{C}{2d} \sum_{|e|=1} \frac{|x|^2}{|x-e|^2} \cdot H_0(x-e)\right\}. \tag{4.41}$$

Since $C > 1$, it follows trivially from (4.29) that

$$|x|^2 G_p(x) \leq N_p \{C(1-f_0)^3 |x|^2 I_{1,0}(x) + H_0(x)\}. \tag{4.42}$$

Taking the minimum of the above two bounds gives

$$|x|^2 G_p(x) \leq N_p \{C(1-f_0)^3 |x|^2 I_{1,0}(x) + H_1(x)\}. \tag{4.43}$$

Now we iterate, i.e. we substitute (4.43) into the right side of (4.40) and get a new bound on $|x|^2 G_p(x)$, and then substitute the result into (4.40) again, and so on. The result, after m iterations, is

$$|x|^2 G_p(x) \le N_p\{C^m(1-f_0)^3|x|^2 I_{1,0}(x) + H_m(x)\}. \tag{4.44}$$

To use (4.44), we first calculate $H_0(y)$ from (4.28), for all y with $\|y - ne_1\|_1 \le 2, n = 7$, 8. Then $H_m(y)$ is calculated using (4.39), for $1 \le m \le 2$. [This iteration will of course only improve the value of $H_0(y)$ for y with $\|y - ne_1\|_1 \le 1$.] As a result, for $n = 7$, 8 we have

$$H_2(ne_1) \le H_2(7e_1) \le 0.06357. \tag{4.45}$$

Now (4.44) for $x = ne_1$, together with the bound $|x|^2 I_{1,0}(x) \le 0.01917$ for $\|x\|_\infty \ge 7$ of Lemma B.12, gives

$$|x|^2 G_p(x) \le 0.07303 \quad (x = ne_1; n = 7, 8) \tag{4.46}$$

which satisfies $P_p(0.999)$.

4.3.4. *Bounds for* $\{x = ne_\mu : n \ge 9\}$

We now obtain bounds on $|x|^2 G_p(x)$ for $x = ne_1$, with $n \ge 9$. The method uses the averaging procedure employed in the last subsection to handle $n = 9$, and then appeals to the monotonicity of Gaussian quantities appearing in (4.28) to deal with larger n.

We first calculate $H_0(9e_1 + w)$ for $\|w\|_1 \le 1$. By symmetry, there are four distinct values of w to consider. The corresponding values are

$$H_0(9e_1 + w) = \begin{cases} 0.09193 & (w = 0) \\ 0.09306 & (w = -e_1) \\ 0.09102 & (w = e_1) \\ 0.05936 & (w = e_2) \end{cases}. \tag{4.47}$$

The basic monotonicity result needed is stated in the following lemma.

Lemma 4.1. *The bounds $H_0(ne_1 + w) \le H_0(9e_1 + w)$ hold for $\|w\|_1 \le 1$ and $n \ge 9$.*

Proof. We fix $n > 9$, and compare $H_0(ne_1 + w)$ and $H_0(9e_1 + w)$. Defining $z = (n-9)e_1$, the two arguments of H_0 are related by $ne_1 + w = (9e_1 + w) + z$. Therefore,

$$I_{m,0}(ne_1 + w) \le I_{m,0}(9e_1 + w), \qquad L_m(ne_1 + w) \le L_m(9e_1 + w), \tag{4.48}$$

by Lemma B.3 and Lemma B.4. The lemma then follows from the definition of H_0 in (4.28). □

We now perform averaging once to improve the large on-axis values of (4.47). The definition of $H_m(ne_1 + w)$ in (4.39) involves the factor $|ne_1 + w|^2/|ne_1 + w - e|^2$ with $|e| = 1$. For $n \geq 9$ and $w = 0$, this factor can be bounded using

$$\frac{n^2}{|ne_1 - e|^2} = \begin{cases} n^2/(n+1)^2 \leq 1 & (e = -e_1) \\ n^2/(n-1)^2 \leq (9/8)^2 & (e = e_1) \\ n^2/(n^2+1) \leq 1 & (e \neq \pm e_1) \end{cases} . \tag{4.49}$$

Using Lemma 4.1 and these bounds in the right side of (4.39) then gives, for $n \geq 9$,

$$H_1(ne_1) \leq 0.06833. \tag{4.50}$$

This bound, together with the bound of Lemma B.12 (i.e. $|x|^2 I_{1,0}(x) \leq 0.01455$ for $x = ne_1$ for $n \geq 9$) and (4.44), gives

$$|x|^2 G_p(x) \leq 0.0729, \tag{4.51}$$

which satisfies the bound of $P_p(0.999)$.

5. Bounds on $\partial_p \Pi$, and the Circle of Convergence

We begin this section by completing the proof of Lemma 1.10, by establishing the bounds (1.52) and (1.53) on $\partial_p \Pi_p$. We then prove Proposition 1.6.

5.1. *Bounds on $\partial_p \Pi$*

Here we prove the remaining two bounds of Lemma 1.10, on $p\partial_p \Pi_p$ for $p \in [p_0, z_c)$.

Lemma 5.1. *For $p \in [p_0, z_c)$,*

$$p\frac{\partial}{\partial p}\hat{\Pi}_p^{(\mathrm{odd})}(0) \leq 0.914078, \qquad p\frac{\partial}{\partial p}\hat{\Pi}_p^{(\mathrm{even})}(0) \leq 0.602171. \tag{5.1}$$

Proof. The proof makes use of the diagrams introduced in Fig. 4, and also the diagrams $\mathscr{K}_a^{(n)}$ defined by

$$\mathscr{K}_a^{(n)} = \sum_{x \neq 0} \mathscr{L}_a^{(n)}(x) \qquad (n = 3, 4). \tag{5.2}$$

In the definition of $\mathscr{L}_a^{(n)}$, contrary to our usual convention the square is not repulsive. Explicitly,

$$\mathscr{L}_a^{(3)}(x) = \mathscr{C}_a^{(1)}(x) \cdot \mathscr{C}_a^{(1)}(x), \qquad \mathscr{L}_a^{(4)}(x) = \mathscr{C}_a^{(1)}(x) \cdot \mathscr{C}_a^{(2)}(x). \tag{5.3}$$

The right side of (5.3) can now be estimated using the existing estimates from Sec. 3.

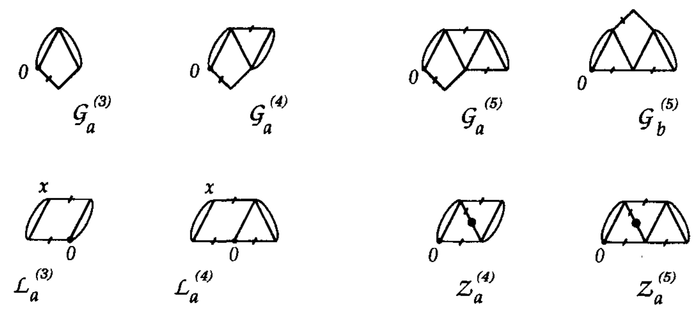
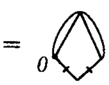


Fig. 4. Diagrams $\mathscr{G}_*^{(n)}$, $\mathscr{L}_a^{(n)}$, $\mathscr{Z}_a^{(n)}$.

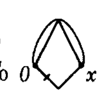
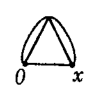
The diagrams $\mathscr{G}_*^{(n)}$ can be bounded using the methods of Sec. 3, to obtain

$$\begin{aligned} &\mathscr{G}_a^{(3)} \le U(\mathscr{A}_a^{(1)}\mathscr{A}_a^{(1)}, \mathscr{E}_a^{(2)}, R'), \qquad \mathscr{G}_a^{(4)} \le U(\mathscr{A}_a^{(1)}\mathscr{A}_a^{(2)}, \mathscr{E}_a^{(3)}, R'), \\ &\mathscr{G}_a^{(5)} \le U(\mathscr{A}_a^{(1)}\mathscr{A}_a^{(3)}, \mathscr{E}_a^{(4)}, R'), \qquad \mathscr{G}_b^{(5)} \le U(\mathscr{A}_a^{(2)}\mathscr{A}_a^{(2)}, \mathscr{F}_a^{(4)}, R'). \end{aligned} \tag{5.4}$$

For $\mathscr{K}_a^{(n)}$, we have

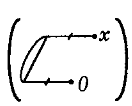
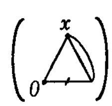
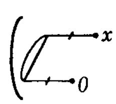
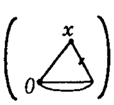
$$\mathscr{K}_a^{(3)} = (\mathscr{B}_a^{(1)} * G * \mathscr{B}_a^{(1)} * G)(0) = (\mathscr{B}_a^{(1)} * \mathscr{B}_a^{(1)} * G * G)(0) =$$  $.$ (5.5)

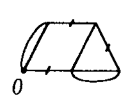
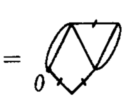
Considering separately the case where the second slashed line does or does not have zero length, and also the case where the right and left vertices are equal or not, gives

$$\mathscr{K}_a^{(3)} = \sum_{x \neq 0}$$  $$+ \sum_{x \neq 0}$$  $$+$$ 

$$\begin{aligned} &\le U(\mathscr{A}_a^{(1)}\mathscr{A}_a^{(1)}, \mathscr{E}_a^{(2)}, B') + \\ &\quad + U(\mathscr{A}_a^{(1)}\mathscr{A}_a^{(1)}, \mathscr{E}_a^{(2)}, G) + [1 + B(0)]\, U(\mathscr{A}_a^{(1)}, \mathscr{B}_a^{(1)}, G^2). \end{aligned} \tag{5.6}$$

Using the fact that $\mathscr{B}_a^{(2)}(x) = \mathscr{B}_a^{(2)}(-x)$ by symmetry, a similar manipulation of convolutions gives

$$\mathscr{K}_a^{(4)} = \sum_x$$   $$= \sum_x$$  

$$=$$  $$=$$ 

$$\leq U(\mathscr{A}_a^{(1)}\mathscr{A}_a^{(2)}, \mathscr{E}_a^{(3)}, B') + U(\mathscr{A}_a^{(1)}\mathscr{A}_a^{(2)}, \mathscr{E}_a^{(3)}, G)$$

$$+ [1 + B(0)]\left\{\sup_{x\neq 0} G_p(x)\right\}^2 \mathscr{A}_a^{(2)}. \tag{5.7}$$

We next observe that $p\partial_p\Pi_p(x)$ can be estimated in terms of the diagrams defined above. In fact, application of the operation $p\partial_p$ to a diagram produces a sum of similar diagrams, with each term given by the original diagram with a new vertex on one line. For example,

$$p\frac{\partial}{\partial p}G_p(x) = R'_p(x), \tag{5.8}$$

and

$$p\partial_p\hat{\Pi}_p^{(1)}(0) = p\partial_p[2dpG_p(e_1)] = 2dp\{G_p(e_1) + R'_p(e_1)\} = \mathscr{A}_a^{(1)} + 2dpG_p(e_1). \tag{5.9}$$

Similarly,

$$\begin{aligned}
&p\partial_p\hat{\Pi}_p^{(2)}(0) \leq 3\mathscr{A}_a^{(2)}\\
&p\partial_p\hat{\Pi}_p^{(3)}(0) \leq 4\mathscr{A}_a^{(3)} + \mathscr{G}_a^{(3)}\\
&p\partial_p\hat{\Pi}_p^{(4)}(0) \leq 4\mathscr{A}_a^{(4)} + 2\mathscr{G}_a^{(4)} + \mathscr{Z}_a^{(4)}\\
&p\partial_p\hat{\Pi}_p^{(5)}(0) \leq 4\mathscr{A}_a^{(5)} + 2\mathscr{G}_a^{(5)} + \mathscr{G}_b^{(5)} + 2\mathscr{Z}_a^{(5)}.
\end{aligned} \tag{5.10}$$

To estimate the right sides we use

$$\mathscr{Z}_a^{(4)} \leq U(\mathscr{K}_a^{(3)}, \mathscr{L}_a^{(3)}, R'), \qquad \mathscr{Z}_a^{(5)} \leq U(\mathscr{K}_a^{(4)}, \mathscr{L}_a^{(4)}, R'). \tag{5.11}$$

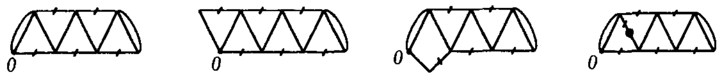
In the above we have inequalities rather than equalities, because although we obtain diagrams which appear identical to $\mathscr{A}_a^{(2)}$ etc., the left side has additional repulsive restrictions.

Diagrams with six or more loops are estimated less carefully. To illustrate the method, we consider in detail only the seven-loop diagram. To simplify the notation, we temporarily use

$$G \equiv \sup_{x\neq 0} G_p(x), \qquad r \equiv R_p(0), \qquad R' \equiv \sup_{x\neq 0} R'_p(x), \tag{5.12}$$

and

$$b \equiv B_p(0), \qquad B' \equiv \sup_{x\neq 0} B'_p(x). \tag{5.13}$$



(a) (b) (c) (d)

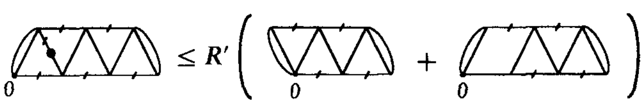
Fig. 5. Diagrams used to estimate $p\partial_p \hat{\Pi}_p^{(7)}(0)$.

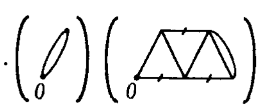
Differentiating the diagram of Fig. 5(a), which represents $\hat{\Pi}^{(7)}(0)$, gives 13 new diagrams which can be divided into three types:

1. A new vertex appears on a line in the bubble at the beginning or end of the diagram, as in Fig. 5(b). There are four diagrams of this type, each of which is bounded above by $\mathscr{A}_a^{(7)} \le r(R')^{7-1}$.

2. A new vertex appears on a horizontal line, as in Fig. 5(c). There are $5 = 7 - 2$ such diagrams, each of which is simply bounded by $r^2(R')^{7-2}$.

3. A new vertex appears on a diagonal line, as in Fig. 5(d). There are $4 = 7 - 3$ such diagrams, each of which can be bounded in the same manner. We illustrate this bound with the diagram of Fig. 5(d):



$\le R'GB'(R')^{7-4}r + R'\max\{b, B'\}\cdot$ 

$$\le (R')^{7-3}[GrB' + r^2 \max\{b, B'\}]. \tag{5.14}$$

Proceeding in a similar fashion, for any $n \ge 6$

$$p\frac{\partial}{\partial p}\hat{\Pi}_p^{(n)}(0) \le 4r(R')^{n-1} + (n-2)r^2(R')^{n-2} + (n-3)r^2 \max\{b, B'\}(R')^{n-3}. \tag{5.15}$$

Summing the estimates over even and odd n and using the numerical bounds from the previous sections then completes the proof. □

5.2. *The circle of convergence*

In this section we prove Proposition 1.6, which states that $1 - 2dz - \hat{\Pi}_z(0)$ is nonzero on the circle of convergence $|z| = z_c$, apart from $z = z_c$. In the course of the proof, we employ the following elementary lemma whose proof is deferred to the end of the section.

Lemma 5.2. *For all $\theta \in [0, 2\pi]$ and $n = 1, 2, 3, \ldots$, the quantity $\gamma_n(\theta)$ defined by*

$$\gamma_n(\theta) = \frac{1}{n}\operatorname{Re}\frac{1 - e^{in\theta}}{1 - e^{i\theta}} \tag{5.16}$$

satisfies the sharp upper and lower bounds

$$-0.217233628\ldots = -\frac{1}{\sqrt{1 + a^2}} \leq \gamma_n(\theta) \leq 1, \tag{5.17}$$

where $a = 4.49340946\ldots$ *is the root of* $\tan x = x$ *in* $(\pi, 3\pi/2)$.

Proof of Proposition 1.6, given Lemma 5.2. We first use the fact that $1 - 2dz_c - \hat{\Pi}_{z_c}(0) = 0$ to write

$$1 - 2dz - \hat{\Pi}_z(0) = (z_c - z)\left[2d + \frac{\hat{\Pi}_{z_c}(0) - \hat{\Pi}_z(0)}{z_c - z}\right] \equiv (z_c - z)A(z). \tag{5.18}$$

It suffices to show that the real part of $A(z)$ is nonzero for $z = z_c e^{i\theta}$, $\theta \neq 0$. Introducing the temporary notation π_n for the coefficient of z^n in $\hat{\Pi}_z(0)$, direct calculation gives

$$\operatorname{Re} A(z) = 2d + \sum_{n\geq 2} n\gamma_n(\theta)\pi_n z_c^{n-1}, \tag{5.19}$$

with $\gamma_n(\theta)$ given by (5.16).

We further introduce $\pi_n^{(\text{even})}$ and $\pi_n^{(\text{odd})}$ to denote the coefficient of z^n in $\hat{\Pi}_z^{(\text{even})}$ and $\hat{\Pi}_z^{(\text{odd})}$. Then from (5.19) we obtain

$$z_c \operatorname{Re} A(z) = 2dz_c + \sum_{n\geq 2} n\gamma_n(\theta)\pi_n^{(\text{even})} z_c^n - \sum_{n\geq 2} n\gamma_n(\theta)\pi_n^{(\text{odd})} z_c^n. \tag{5.20}$$

Now we employ Lemma 5.2 to bound the right side from below. The result is

$$\begin{aligned} z_c \operatorname{Re} A(z) &\geq 2dz_c + (-0.218)\sum_{n\geq 2} n\pi_n^{(\text{even})} z_c^n - \sum_{n\geq 2} n\pi_n^{(\text{odd})} z_c^n \\ &= 2dz_c - (0.218)p\partial_p \hat{\Pi}_p^{(\text{even})}(0)|_{p=z_c} - p\partial_p \hat{\Pi}_p^{(\text{odd})}(0)|_{p=z_c}. \end{aligned} \tag{5.21}$$

To bound the right side, we apply the numerical estimates on p-derivatives of Proposition 1.5. The critical point is bounded below by the inverse of the connective constant for memory-4 walks. This connective constant is shown in [7] to be the largest root of the cubic equation $\lambda^3 - 2(d-1)\lambda^2 - 2(d-1)\lambda - 1 = 0$, from which we conclude that $z_c \geq (1.01)/9$. The result is

$$z_c \operatorname{Re} A(z) \geq 10(1.01/9) - 0.91408 - (0.218)(0.60218) > 0.076866 > 0. \tag{5.22}$$

□

Proof of Lemma 5.2. The upper bound on γ_n follows immediately from the observation

$$|\gamma_n(\theta)| \leq \left| \frac{1}{n} \sum_{m=0}^{n-1} e^{im\theta} \right| \leq 1, \tag{5.23}$$

and is attained at $\theta = 0$. It remains to prove the lower bound. Since $\gamma_n(\theta) = \gamma_n(2\pi - \theta)$ we need only consider $\theta \in [0, \pi]$, and since the lower bound is obvious for $\theta = 0$ or π, we can restrict attention to $\theta \in (0, \pi)$.

We rewrite $\gamma_n(\theta)$ as

$$\gamma_n(\theta) = \frac{1}{2n}\left[1 - \cos n\theta + \frac{\sin n\theta \sin\theta}{1 - \cos\theta}\right]. \tag{5.24}$$

Introducing the temporary notation $x = 2n$ and $\phi = \theta/2$ and applying a trigonometric identity gives

$$\gamma_n(\theta) = \frac{1}{x}[1 - \cos x\phi] + f_\phi(x) \tag{5.25}$$

with

$$f_\phi(x) = \cot\phi \frac{\sin x\phi}{x}. \tag{5.26}$$

Since $f_\phi(1) = \cos\phi > 0$ and $f_\phi(\infty) = 0$, and since f_ϕ does take on negative values, there is an $x_\phi \in (1, \infty)$ at which $f_\phi(x)$ takes on its (negative) global minimum. At x_ϕ, we have $\sin x_\phi\phi < 0$ and $f'_\phi(x_\phi) = 0$, i.e. $\tan\beta = \beta$ where $\beta = x_\phi\phi$. Thus also $\cos\beta < 0$, and from $\tan\beta = \beta$ we obtain

$$\cos\beta = -\frac{1}{\sqrt{1 + \beta^2}}. \tag{5.27}$$

We therefore have

$$f_\phi(x) \geq f_\phi(x_\phi) = \phi\cot\phi\cos x_\phi\phi = -\phi\cot\phi\frac{1}{\sqrt{1 + \beta^2}}. \tag{5.28}$$

In fact whenever x satisfies $\tan x\phi = x\phi$ and $\sin x\phi < 0$, we have the equality $f_\phi(x) = -\phi\cot\phi[1 + (x\phi)^2]^{-1/2}$, and hence in particular

$$f_\phi(a/\phi) = -\frac{\phi\cot\phi}{\sqrt{1 + a^2}}. \tag{5.29}$$

Substituting (5.28) into (5.25) gives

$$\gamma_n(\theta) \geq \frac{1}{x}[1 - \cos x\phi] - \frac{\phi \cot \phi}{\sqrt{1 + \beta^2}}. \tag{5.30}$$

Now by definition of β, $\beta \geq a$, and hence

$$\gamma_n(\theta) \geq -\frac{1}{\sqrt{1 + a^2}}, \tag{5.31}$$

where we have used the fact that $\phi \cot \phi < 1$ for $\phi \in (0, \pi/2)$. To see that (5.31) is sharp, we take $x = a/\phi$ and use (5.29) to observe that

$$\gamma_{a/2\phi}(2\phi) = \frac{\phi}{a}[1 - \cos a] - \frac{\phi \cot \phi}{\sqrt{1 + a^2}}. \tag{5.32}$$

As $\phi \to 0$, the right side becomes arbitrarily close to $-[1 + a^2]^{-1/2}$. $\square$

A. Bounds on the Two-Point Function

In this appendix, we derive upper and lower bounds on the self-avoiding walk two-point function in terms of the two-point function of simple random walk. A special case of the upper bound has already been stated explicitly in Proposition 1.7, and the lower bound has already been used in (2.25). As a consequence of the lower bound, we will obtain new upper bounds on the critical point (or lower bounds on the connective constant) which are valid in three or more dimensions. The methods of this appendix are elementary, and are independent of the rest of the paper. We do however use the numerical values of certain simple random walk quantities which are computed in Appendix B.

Before stating the results, we need some definitions. For any $\tau \in [0, \infty]$ let Ω_τ be the set of all memory-τ walks, i.e. simple random walks starting at the origin, of arbitrary length (including zero), which contain no closed loops of length τ or less. Evidently $\tau = 0$ corresponds to simple random walk, while $\tau = \infty$ is the self-avoiding walk. We denote by $\Omega_\tau(x, y)$ the set of all memory-τ walks from x to y. For simplicity, we write $\Omega = \Omega_\infty$ and $\Omega(x, y) = \Omega_\infty(x, y)$. For $\tau < \infty$ we define $\mathscr{L}_\tau(x) = \Omega_\tau(x, x)$, the set of memory-$\tau$ loops at x. It is worth noting that elements of $\mathscr{L}_\tau(x)$ may return several times to x, and that the empty loop is contained in $\mathscr{L}_\tau(x)$.

We denote the two-point function for the self-avoiding walk as usual by $G_p(x)$, and for $\tau < \infty$ denote the memory-τ two-point function by

$$C_{p,\tau}(x) = \sum_{\omega \in \Omega_\tau(0,x)} p^{|\omega|}. \tag{A.1}$$

For the simple random walk two-point function we write simply $C_p(x)$. The memory-2 two-point function can be readily shown [18] to be given by the following expression, which can be used for numerical calculations:

$$C_{p,2}(x) = \gamma_p I_{1,0}^{(\varepsilon_p)}(x), \tag{A.2}$$

where

$$I_{1,0}^{(\varepsilon)}(x) = \int \frac{d^dk}{(2\pi)^d} \frac{e^{ik\cdot x}}{\varepsilon + 1 - \hat{D}(k)} \tag{A.3}$$

and

$$\gamma_p = \frac{1 - p^2}{2dp}, \qquad \varepsilon_p = \frac{1 + (2d-1)p^2}{2dp} - 1. \tag{A.4}$$

The memory-2 critical point occurs at $p = 1/(2d-1)$.

The lower bound on the two-point function can now be stated as follows.

Proposition A.1. *The inequality*

$$C_{p,2}(x) \le \alpha_p G_{p'}(x) \tag{A.5}$$

holds whenever both sides are defined, where

$$\alpha_p = \left(1 + \frac{2d-1}{2d}[C_{p,2}(0) - 1]\right)\left(1 + \frac{1}{2d}[C_{p,2}(0) - 1]\right) \tag{A.6}$$

and

$$p' = [1 + \delta(p)]p \tag{A.7}$$

with

$$\delta(p) = \frac{[(2d-2) + 2dp^2](2d-3) + 1}{2d(2d-2)}[C_{p,2}(0) - 1] + \frac{2d-3}{2d-2}p^2[C_{p,2}(2e_1) - p^2]. \tag{A.8}$$

As an immediate corollary we obtain upper bounds on the critical point for $d > 2$.

Corollary A.2. *For $d > 2$, the critical point z_c is bounded above by the value of* (A.7) *at $p = 1/(2d-1)$. Explicitly, writing $z_c(d)$ for the critical point for $\mathbf{Z}^d$, we have*

$$z_c(3) \le 0.22536066 \qquad z_c(4) \le 0.14885372 \qquad z_c(5) \le 0.11336221. \tag{A.9}$$

Taking reciprocals gives

$$\mu(3) \ge 4.43733 \qquad \mu(4) \ge 6.71800 \qquad \mu(5) \ge 8.82128. \tag{A.10}$$

Proof of Corollary A.2, given Proposition A.1. At $p = 1/(2d-1)$ the left side of (A.5) does not decay exponentially, and α_p is finite. Since the subcritical self-avoiding walk two-point function decays exponentially, we must have $p' \geq z_c$. Evaluation of δ_p at $p = 1/(2d-1)$ using (A.2) and Lemma B.8 then gives the numerical bounds quoted. (For $d = 2$, $\delta_p = \infty$ at $p = 1/3$ and the resulting bound is $z_c(2) \leq \infty$.) $\square$

As another consequence of Proposition A.1, we will obtain an explicit numerical lower bound on $G_{p_0}(x)$, for a particular choice of p_0. As the choice we make for p_0 is influenced by an upper bound on the two-point function, we postpone the precise numerical lower bound until after stating the upper bound.

Proposition A.3. *Whenever both sides make sense,*

$$C_{p,2}(x) \geq \beta_p G_{p_1}(x), \tag{A.11}$$

where

$$p_1 = p[1 + \{(2d-3)^2 + 1\}p^4] \tag{A.12}$$

and

$$\beta_p = \frac{[1 + (2d-1)(2d-2)p^4]\cdot[1 + \{(2d-2)(2d-3) + 1\}p^4]}{1 + \{(2d-3)^2 + 1\}p^4}. \tag{A.13}$$

Specializing now to $d = 5$, defining p_0 to be the value of p_1 corresponding to $p = 1/9$, i.e.

$$p_0 = \frac{6611}{9^5} \tag{A.14}$$

gives

$$G_{p_0}(x) \leq \frac{713988}{812911} I_{1,0}(x). \tag{A.15}$$

Remark. From Proposition A.3 it can be concluded as in the proof of Corollary A.2 that for $d = 5$, $z_c \geq (1.00762)/9$. This is not as good as the lower bound $(1.01)/9$ obtained from the memory-4 critical point using the cubic polynomial derived in [7].

For $d = 5$, a numerical lower bound on the two point function at p_0 is given by the following corollary to Proposition A.1.

Corollary A.4. *For $d = 5$,*

$$G_{p_0}(x) \geq \frac{\gamma}{\alpha} I^{(\varepsilon)}_{1,0}(x) \tag{A.16}$$

with

$$\gamma = 0.900\,315\,651\,, \qquad \alpha = 1.027\,899\,148\,, \qquad \varepsilon = 0.010\,050\,309\,8\,. \tag{A.17}$$

Proof. By (A.5),

$$G_{p_0}(x) \geq \frac{1}{\alpha_p} C_{p,2}(x), \tag{A.18}$$

where p is given by $p(1 + \delta(p)) = p_0$. Since $\delta(p)$ is increasing in p and infinite for $p > 1/9$, we have $p \leq 1/9$. Hence a lower bound on p is given by $p \geq p_0/(1 + \delta(1/9)) \equiv p_2 = 0.109\ 734\ 658\ 4\ldots$. Since α_p is increasing, we decrease the right side of (A.18) by replacing α_p by its value at $p = 1/9$, an upper bound for which is given by the value of α stated in the corollary. Since the memory-2 two-point function is also increasing in p, we bound it below by its value at p_2. Then we rewrite the memory-2 two-point function using (A.2) and calculate γ_{p_2} and ε_{p_2} explicitly, to obtain the corollary. □

The remainder of this appendix is devoted to the proofs of Propositions A.1 and A.3.

A.1 *Lower bound on the two-point function*

In this section we prove Proposition A.1.

A.1.1. *Step 1: Loop erasure*

A basic notion in the proof of Proposition A.1 is that to each simple random walk there can be associated a unique self-avoiding walk, by applying chronological loop erasure as in [16]. This provides a many-to-one correspondence between $\Omega_0(0, x)$ and $\Omega(0, x)$.

The sum

$$\sum_{\omega \in \Omega(0,x)} p^{|\omega|} \prod_{l=0}^{|\omega|} \sum_{L \in \mathscr{L}_0(\omega(l))} p^{|L|} \tag{A.19}$$

can thus be interpreted in two ways. First, if we sum over loops first then each sum over L is independent of the base point $\omega(l)$ and is equal to $C_p(0)$. Therefore (A.19) is equal to

$$\sum_{\omega \in \Omega(0,x)} \{p \cdot C_p(0)\}^{|\omega|} \cdot C_p(0) = C_p(0) \cdot G_{p_1}(x) \tag{A.20}$$

with

$$p_1 = pC(0). \tag{A.21}$$

Second, we note that because of the correspondence between Ω_0 and Ω mentioned above, (A.19) is greater than or equal to $C_p(x)$. As a result, we have

$$C_p(x) \le C_p(0) \cdot G_{p_1}(x) \tag{A.22}$$

with p and p_1 related by (A.21). The inequality clearly holds whenever both sides have meaning.

This bound can be improved if instead of adding all loops at each vertex as in (A.19) we add only the memory-2 loops $\mathscr{L}_2$. Then by the same argument we obtain

$$C_{p,2}(x) \le C_{p,2}(0) G_{p_2}(x), \tag{A.23}$$

where now

$$p_2 = p C_{p,2}(0). \tag{A.24}$$

A.1.2. *Step 2: Removal of loops giving immediate reversals*

One source of overcounting on the right side of (A.23) is due to the fact that in adding memory-2 loops at each vertex we have included loops which give rise to an immediate reversal, for which there is no counterpart on the left side. For example, consider a site a on a self-avoiding walk ω, with incoming step $(a - e, a)$ and outgoing step $(a, a + f)$ ($|e| = |f| = 1$). Then there is no need to add a loop at a with initial step $(a, a - e)$ or final step $(a + f, a)$, as this would produce an immediate reversal.

To proceed systematically to avoid this sort of overcounting, we classify memory-2 loops according to their first and last steps. Using e_μ, ($\mu = \pm 1, \pm 2, \ldots, \pm d$) to denote a unit vector in the positive or negative μ^{th} direction, a loop is said to *have endings* (μ, ν) if its first step is e_μ and its last step is e_ν. Similarly, we say that a given site a on a self-avoiding walk ω *has steps* (μ, ν) if the incoming step is $(a - e_\mu, a)$ and the outgoing step is $(a, a + e_\nu)$.

We further classify loops and sites according to the relative position of μ and ν. A (nonempty) loop which has endings $(\mu, -\mu)$ is said to be of *type-I*. Loops and sites with endings or steps (μ, μ) are said to be of *type-II*, and those with (μ, ν) with $|\mu| \neq |\nu|$ are said to be of *type-III*. These definitions are illustrated in Fig. 6. Note that there can be no site of type-I on a self-avoiding walk.

We can then avoid the introduction of immediate reversals by observing the following three rules. If we add memory-2 loops according to these rules then we will generate exactly the set of all memory-2 walks (with some walks generated more than once—see Step 3).

Rule 1. At the initial point of a walk with first step e_λ, either add the empty loop, or add a loop with endings (μ, ν), $\nu \neq -\lambda$.

Rule 2. At a site with steps (λ, ρ), add either the empty loop, or a loop with endings (μ, ν), with $\mu \neq -\lambda$ and $\nu \neq -\rho$.

Rule 3. At the final point of a walk with last step e_λ, either add the empty loop or a loop with endings (μ, ν), $\mu \neq -\lambda$.

We now compute the fraction of loops which will be accepted on the basis of these

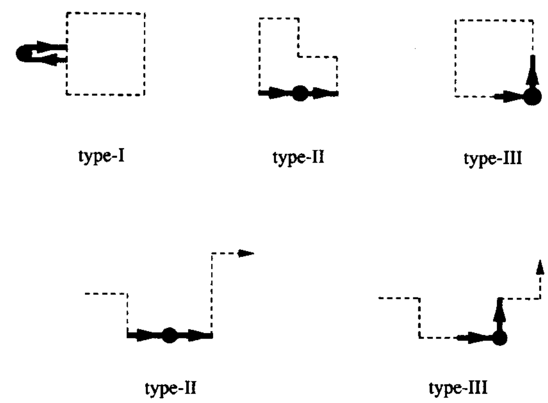


Fig. 6. Types of loops and sites.

three rules. For a site of type-II, with steps (λ, λ), Rule 2 prohibits loops with endings (μ, ν) if $\mu = -\lambda$ or $\nu = -\lambda$. This means that of $2d$ possible endings of loops of type-I, only $2d - 2$ of them are allowed; of $2d$ endings of loops of type-II, only $2d - 1$ of them are allowed; and of $2d(2d - 2)$ endings of loops of type-III, only $(2d - 2)(2d - 3) + 1(2d - 2) = (2d - 2)^2$ of them are allowed. Continuing in a similar fashion for the case of type-III sites, and for the walk's endpoints, gives the result summarized in Table II.

Taking the above into account, we now consider the sum

$$\sum_{\omega \in \Omega(0,x)} p^{|\omega|} \sum_{L_0 \in \mathscr{L}'_2(0)} p^{|L_0|} \left(\prod_{l=1}^{|\omega|-1} \sum_{L_l \in \mathscr{L}'_2(\omega(l))} p^{|L_l|} \right) \sum_{L_{|\omega|} \in \mathscr{L}'_2(\omega(|\omega|))} p^{|L_{|\omega|}|}. \tag{A.25}$$

Here $\mathscr{L}'_2(\omega(l))$ denotes the set of memory-2 loops which start and end at $\omega(l)$ and satisfy Rules 1–3. This set depends on ω. Now we proceed along the lines of Step 1.

First, by symmetry the sum $\sum_{L_l \in \mathscr{L}'_2(\omega(l))} p^{|L_l|}$ depends only on whether $\omega(l)$ is of type-II or type-III. We denote its maximum by $1 + \delta_1$. We also write

$$1 + \delta_2 \equiv \sum_{L_0 \in \mathscr{L}'_2(0)} p^{|L_0|} = \sum_{L_{|\omega|} \in \mathscr{L}'_2(\omega(|\omega|))} p^{|L_{|\omega|}|} = 1 + \frac{2d-1}{2d}[C_{p,2}(0) - 1]. \tag{A.26}$$

Then (A.25) is bounded above by

Table II. Ratios of accepted loops in Step 2. Column headings label loop types and row headings label site types.

	type-I	type-II	type-III
II	$(2d-2)/2d$	$(2d-1)/2d$	$(2d-2)^2/\{2d(2d-2)\}$
III	$(2d-2)/2d$	$(2d-1)/2d$	$\{(2d-2)^2+1\}/\{2d(2d-2)\}$
beginning	$(2d-1)/2d$	$(2d-1)/2d$	$(2d-1)/2d$
ending	$(2d-1)/2d$	$(2d-1)/2d$	$(2d-1)/2d$

$$\sum_{\omega \in \Omega(0,x)} p^{|\omega|}(1+\delta_2)(1+\delta_1)^{|\omega|-1}(1+\delta_2) = \frac{(1+\delta_2)^2}{(1+\delta_1)} G_{p_3}(x) \tag{A.27}$$

with

$$p_3 = (1+\delta_1)p. \tag{A.28}$$

On the other hand, (A.25) involves a sum over all memory-2 walks (with some overcounting), and hence is greater than or equal to $C_{p,2}(x)$. Therefore,

$$C_{p,2}(x) \le \frac{(1+\delta_2)^2}{(1+\delta_1)} G_{p_3}(x). \tag{A.29}$$

To get a concrete value for δ_1, we denote by I (resp. II, III) the total contribution to $C_{p,2}(0) - 1$ $(=\sum_{\omega \in \mathscr{L}_2(0),\, |\omega| \neq 0} p^{|\omega|})$ from type-I (resp. II, III) memory-2 loops. Then from Table II, if $\omega(l)$ is of type-II we have

$$\sum_{L_l \in \mathscr{L}_2'(\omega(l))} p^{|L_l|} = 1 + \frac{2d-2}{2d}(I) + \frac{2d-1}{2d}(II) + \frac{2d-2}{2d}(III), \tag{A.30}$$

while if $\omega(l)$ is of type-III,

$$\sum_{L_l \in \mathscr{L}_2'(\omega(l))} p^{|L_l|} = 1 + \frac{2d-2}{2d}(I) + \frac{2d-1}{2d}(II) + \frac{(2d-2)^2+1}{2d(2d-2)}(III). \tag{A.31}$$

Thus $1+\delta_1$ is the right side of (A.31).

A.1.3. *Step 3: Removal of some redundant overlapping loops*

We can further improve the above by reducing the overcounting in Step 2. An example of this overcounting is given in Fig. 7. In this example, the addition of two loops at neighbouring sites gives rise to the same memory-2 walk, even though the two additions both satisfy Rules 1–3. We will remove the overcounting corresponding to overlapping loops of this type which are added at neighbouring sites on a self-avoiding walk, and leave all other overcounting intact.

When a loop with endings (μ, ν) is added to a site with steps (λ, ρ), overcounting of

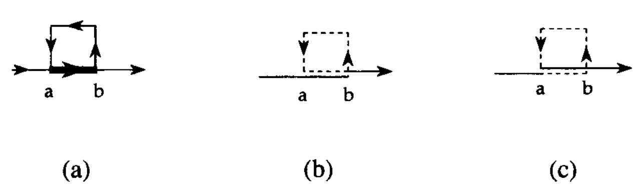


Fig. 7. An example of overcounting: The walk (a), in which the thick line at the bottom is traversed twice, can be constructed by adding a loop either as in (b), or as in (c).

Table III. Ratios of accepted loops in Step 3. Column headings label loop types and row headings label site types.

	type-I	type-II	type-III
II	$(2d-2)/2d$	$(2d-2)/2d$	$(2d-2)(2d-3)/\{2d(2d-2)\}$
III	$(2d-2)/2d$	$(2d-3)/2d$	$\{(2d-2)(2d-3)+1\}/\{2d(2d-2)\}$
beginning	$(2d-1)/2d$	$(2d-1)/2d$	$(2d-1)/2d$
ending	$(2d-1)/2d$	$(2d-2)/2d$	$(2d-2)/2d$

the above type occurs when $\mu = \rho$ or $\nu = \lambda$. We can avoid this overcounting by employing a rule that we do not add loops when $\nu = \lambda$, and still construct all memory-2 walks. The loop will thus be considered to be attached at the earlier of the two neighbouring sites on the self-avoiding walk. We incorporate this new restriction by augmenting Rules 1–3 with the following two rules:

Rule 4. At a site with steps (λ, ρ), either add the empty loop, or a loop with endings (μ, ν) with $\nu \neq \lambda$.

Rule 5. At the endpoint of ω with last step e_λ, either add the empty loop or add a loop with endings (μ, ν) with $\nu \neq \lambda$.

Taking Rules 1–5 into account, the acceptance ratio of added loops can be calculated as in Step 2. The result is summarized in Table III.

Arguing as in Step 2, we obtain

$$C_{p,2}(x) \leq \frac{(1+\delta_2)(1+\delta_4)}{1+\delta_3} G_{p_4}(x), \tag{A.32}$$

with $p_4 = [1 + \delta_3]p$ and

$$\delta_3 = \frac{2d-2}{2d}(I + II) + \frac{(2d-2)(2d-3)+1}{2d(2d-2)}(III),$$

$$\delta_2 = \frac{2d-1}{2d}\{C_{p,2}(0) - 1\},$$

$$\delta_4 = \frac{2d-1}{2d}(I) + \frac{2d-2}{2d}(II) + \frac{2d-2}{2d}(III). \tag{A.33}$$

To obtain concrete values for I, II, III, we first note that by definition

$$I + II + III = C_{p,2}(0) - 1. \tag{A.34}$$

Also, it can be seen from Fig. 6 that

$$I \leq 2dp^2\{C_{p,2}(0) - 1\}, \qquad II \leq 2dp^2\{C_{p,2}(2e_1) - p^2\}. \tag{A.35}$$

This gives

$$\begin{aligned}
\delta_3 &= \frac{d-1}{d}(I + II) + \frac{(2d-2)(2d-3)+1}{2d(2d-2)}(III) \\
&= \frac{(2d-2)(2d-3)+1}{2d(2d-2)}(I + II + III) + \frac{2d-3}{2d(2d-2)}(I + II) \\
&\leq \frac{(2d-2)(2d-3)+1}{2d(2d-2)}\{C_{p,2}(0) - 1\} \\
&\quad + \frac{2d-3}{2d(2d-2)}(2dp^2\{C_{p,2}(0) - 1\} + 2dp^2\{C_{p,2}(2e_1) - p^2\}) \\
&\equiv \delta(p).
\end{aligned} \tag{A.36}$$

Letting $p' = [1 + \delta(p)]p$, we thus obtain

$$C_{p,2}(x) \leq \frac{(1 + \delta_2)(1 + \delta_4)}{1 + \delta_3} G_{p'}(x).$$

Let $S = I + II + III$. The value of α_p given in Proposition A.1 then comes from the fact that

$$\frac{1 + \delta_4}{1 + \delta_3} \leq \frac{1 + \frac{2d-3}{2d}S + \frac{I}{2d} + \frac{S}{2d}}{1 + \frac{2d-3}{2d}S + \frac{I}{2d}} \leq 1 + \frac{S}{2d}. \tag{A.37}$$

□

A.2. *Upper bound on the two-point function*

For the lower bound on the two-point function obtained in the previous section, we added loops to self-avoiding walks to obtain all possible memory-2 walks, with some overcounting. To obtain the upper bound on the two-point function of Proposition A.3, we will now add loops to self-avoiding walks in such a way as to produce a subset of all memory-2 walks, with no overcounting. To simplify the prevention of overcounting, we will add at each site only the smallest loops, namely the *4-loops* consisting of exactly four steps.

In the addition of 4-loops, it must be ensured that (1) the resulting walk is in $\Omega_2(0, x)$, and (2) distinct ways of adding 4-loops to self-avoiding walks lead to distinct memory-2 walks. The first requirement will be satisfied for 4-loop additions which satisfy Rules 1–3 of the previous section. The second requirement, which prevents overcounting, requires more attention. Rules 4 and 5 have already been used to partially reduce

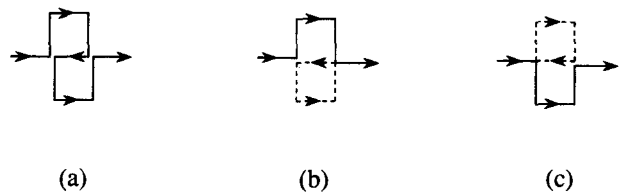


Fig. 8. A memory-2 walk (a) which can be constructed either as in (b) or (c).

overcounting. However these rules do not prevent all overcounting, as illustrated in the example of Fig. 8. In the figure, the memory-2 walk (a) can be constructed by adding a 4-loop to a self-avoiding walk either as in (b) or (c), and both of these constructions satisfy Rules 1–5.

To prevent this overcounting, we supplement Rules 1–5 with the following new rule.

Rule 6. Considering loops to be added sequentially from the initial point to the final point of a self-avoiding walk ω, suppose that loops have been added up to but not including the site a on ω, and let ω' denote the walk formed by ω up to and including a together with all loops added before a. Suppose that the three steps of ω' leading into a are e_α, e_β, e_γ. Then if $\gamma = -\alpha$, any 4-loop may be added at a except those with endings $(-\beta, v)$, for any v. If $\gamma \neq -\alpha$ or fewer than three steps precede a in ω', then there is no restriction beyond Rules 1–5.

For example, Rule 6 disallows (b) in Fig. 8, so that the memory-2 walk (a) can be constructed only as in (c). Addition of 4-loops according to Rules 1–6 always produces a memory-2 walk. The following lemma shows that a memory-2 walk can be constructed in at most one way by adding 4-loops to self-avoiding walks following Rules 1–6.

Lemma A.5. *A memory-2 walk which can be constructed by adding at most one 4-loop at each site of a self-avoiding walk from 0 to x, obeying Rules 1–6, can be constructed in one and only one way.*

Proof. Let $\hat{\Omega}(0,x)$ denote the subset of $\Omega_2(0,x)$ consisting of walks which are constructed by adding at most one 4-loop at each site of a self-avoiding walk from 0 to x. Suppose that $\omega \in \hat{\Omega}(0,x)$ can be constructed in more than one way. We will show that any construction of ω must violate one of the Rules 4–6.

Of all possible constructions of ω, with different underlying self-avoiding walks or "backbones" $\beta_1, \ldots, \beta_n \in \Omega(0,x)$, consider the first site a along the backbones after which two of the constructions differ. Let ω' denote the portion of ω up to and including the step in the backbone which leads to a. Now since ω can have different constructions beyond a, it must have a loop at a. By definition of a, ω could have been formed either by adding a 4-loop L at a, or by not adding L at a but rather adding a 4-loop M at a later backbone site b. If both of these constructions are to lead to the same element of $\hat{\Omega}(0,x)$, b can be at most 3 sites along a backbone from a.

Now if ω is formed by not adding L at a but rather M at b, at least one of the steps in M must be identical to a step in L (considered as steps in ω). There are three possibilities: either one or two or three steps in M are identical to steps in L. The four steps in M cannot be identical to those of L, because in that case L and M would both be added to the backbone at site a. We consider each of these possibilities in turn, and show that the addition of M rather than L leads to a violation of Rules 4–6.

First, suppose that three steps of M are identical to steps in L. This corresponds to the situation where the first steps of ω leading out of a after ω' are topologically (abbreviations are for cardinal directions) ENWSE. Here M would be the last four steps, but this possibility is disallowed by Rules 4 or 5.

Second, suppose that exactly two steps of M are identical to steps in L. Then the steps leading out of a as above are topologically ENWSEN, and M consists of the last four of these steps. (The middle four steps have three steps in common with L, not two.) This possibility is disallowed by Rules 4 or 5.

Third, suppose that exactly one step of M is identical to a step in L. The only possible topology here is that of Fig. 8, i.e. the steps leading out of a are topologically NESWSEN, with M given by the last four steps. But this possibility is the one explicitly disallowed by Rule 6.

Therefore any construction of ω violates one of Rules 1–6, and the lemma is proved. $\square$

Now we consider

$$\sum_{\omega \in \Omega(0,x)} p^{|x|} \sum_{L_0 \in \mathscr{L}'_2(0)} p^{|L_0|} \left(\prod_{l=1}^{|\omega|-1} \sum_{L_l \in \mathscr{L}'_2(\omega(l))} p^{|L_l|} \right) \sum_{L_{|\omega|} \in \mathscr{L}'_2(\omega(|\omega|))} p^{|L_{|\omega|}|}, \tag{A.38}$$

where the $\mathscr{L}'_2$ are mutually and ω-dependent and denote the set of all 4-loops satisfying Rules 1–6. The sum (A.38) can be considered as a sum over a subset of $\Omega_2(0,x)$, and hence is bounded above by $C_{p,2}(x)$. On the other hand it can be bounded below by the self-avoiding walk two-point function at a modified activity. For this we want to minimize the sums over loops which appear in (A.38). Let $1 + \delta_m$ denote a lower bound on $\sum_{L_l \in \mathscr{L}'_2(\omega(l))} p^{|L_l|}$, let $(1 + \delta_i)$ denote a lower bound on $\sum_{L_0 \in \mathscr{L}'_2(0)} p^{|L_0|}$, and let $(1 + \delta_f)$ denote a lower bound on $\sum_{L_{|\omega|} \in \mathscr{L}'_2(\omega(|\omega|))} p^{|L_{|\omega|}|}$. Then (A.38) is bounded below by

$$\sum_{\omega \in \Omega(0,x)} p^{|\omega|}(1 + \delta_i)(1 + \delta_m)^{|\omega|-1}(1 + \delta_f) = \frac{(1 + \delta_i)(1 + \delta_f)}{1 + \delta_m} G_{p_1}(x) \tag{A.39}$$

with

$$p_1 = (1 + \delta_m)p. \tag{A.40}$$

To obtain concrete lower bounds for δ_i, δ_m, δ_f, we need only decrease the numbers of accepted loops found in Table III by an amount prescribed by Rule 6. The only change will be in the case where there are three steps leading into the site of the form

Table IV. The number of 4-loops to be added at a site with incoming steps e_α, e_β, e_γ and outgoing step e_δ, to satisfy Rules 1–6.

	$\alpha \neq -\gamma$	$\alpha = -\gamma$
$\delta = \gamma$	$(2d-2)(2d-3)$	$(2d-3)^2+1$
$\lvert\delta\rvert \neq \lvert\gamma\rvert, \lvert\beta\rvert = \lvert\delta\rvert$	$(2d-2)(2d-3)+1$	$(2d-3)^2+1$
$\lvert\delta\rvert \neq \lvert\gamma\rvert, \lvert\beta\rvert$	$(2d-2)(2d-3)+1$	$(2d-3)^2+2$
endpoint	$(2d-2)^2$	$(2d-3)(2d-2)+1$

initial site	$(2d-1)(2d-2)$

e_α, e_β, e_γ with $\gamma = -\alpha$, and in this case the reduction in the number of allowed 4-loops will depend on the backbone step e_δ following e_γ. For $\delta = \gamma$ an additional $(2d-4)$ 4-loops can be disallowed; for $|\delta| \neq |\gamma|, |\beta| = |\delta|$ an additional $(2d-3)$ 4-loops can be disallowed; for $|\delta| \neq |\gamma|, |\beta|$ an additional $(2d-4)$ 4-loops can be disallowed. The initial site is not affected by Rule 6. The result is summarized in Table IV.

From Table IV we obtain

$$\delta_i = (2d-1)(2d-2)p^4, \tag{A.41}$$

$$\delta_f = [(2d-3)(2d-2)+1]p^4, \tag{A.42}$$

$$\delta_m = [(2d-3)^2+1]p^4, \tag{A.43}$$

and hence

$$C_{p,2}(x) \geq \frac{[1+(2d-1)(2d-2)p^4][1+\{(2d-3)(2d-2)+1\}p^4]}{1+[(2d-3)^2+1]p^4} G_{p_1}(x) \tag{A.44}$$

with

$$p_1 = p[1+\{(2d-3)^2+1\}p^4]. \tag{A.45}$$

This completes the proof of Proposition A.3.

B. Numerical Estimation of Simple Random Walk Quantities

This appendix consists of three subsections. The first discusses relations between the various Gaussian (simple random walk) quantities introduced in Sec. 1.6 and encountered throughout the paper, and derives formulas for Gaussian quantities involving integrals of modified Bessel functions. The second subsection describes the method we use to obtain numerical estimates, with controlled errors, of the Gaussian quantities. The final subsection discusses the control of round-off errors in the numerical calculations of the Gaussian quantities and in the computations involved in the proof that $P_p(1)$ implies $P_p(0.999)$.

B.1. *General properties of simple random walk quantities*

It will be shown below that all the Gaussian quantities used in this paper can be calculated or bounded in terms of

$$I_{n,m}^{(\varepsilon)}(x) = \int \frac{d^d k}{(2\pi)^d} \frac{\hat{D}(k)^m}{\{\varepsilon + 1 - \hat{D}(k)\}^n} e^{ik\cdot x}, \tag{B.1}$$

with $n = 1, 2$, $m = 0$ and $\varepsilon \geq 0$. In fact only three values of ε are required for $d = 5$: $\varepsilon = 0$ for Lemma B.8, $\varepsilon = 0.0100504$ for (2.25), $\varepsilon = 0.0109388$ for Lemma B.11. The right side of (B.1) can be written in terms of the modified Bessel functions $I_N(z)$, or more precisely in terms of

$$f_N(z) \equiv e^{-z} I_N(z) \equiv \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{-z(1-\cos\theta)} \cos N\theta, \tag{B.2}$$

if we use the identity

$$A^{-n} = \frac{1}{(n-1)!} \int_0^\infty dt\, e^{-At} t^{n-1}$$

with $A = \varepsilon + 1 - \hat{D}(k)$. This leads to

$$I_{n,0}^{(\varepsilon)}(x) = \frac{d^n}{(n-1)!} \int_0^\infty dt\, e^{-d\varepsilon t} t^{n-1} \prod_{\mu=1}^{d} f_{|x_\mu|}(t). \tag{B.3}$$

To analyze the right side of (B.3), the properties of f_N summarized in the next proposition will be useful. Alternate expressions for f_N are provided by the following standard integral representation and Taylor expansion for I_N, for nonnegative integers N:

$$I_N(z) = \frac{z^N}{(2N-1)!!} \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{z\cos\theta} (\sin\theta)^{2N}, \tag{B.4}$$

$$I_N(z) = \left(\frac{z}{2}\right)^N \sum_{m=0}^{\infty} \frac{(z^2/4)^m}{m!(m+N)!} \tag{B.5}$$

Proposition B.1. (a)

$$f_N(z) = \frac{z^N}{(2N-1)!!} \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{-z(1-\cos\theta)} (\sin\theta)^{2N} \tag{B.6}$$

(b) *For* $t \geq 0$,

$$f_N(t) \geq \max\left\{0, \frac{1}{\sqrt{2\pi t}}\left(1 - \frac{N^2 + \delta_{N,1}}{2t} - 2^{N+1}e^{-t}\right)\right\}. \tag{B.7}$$

(c) *For* $z \in \mathbf{C}$ *with* $\operatorname{Re} z \geq 0$,

$$|f_N(z)| \leq \min\left\{1, \left(\frac{\pi}{8\operatorname{Re} z}\right)^{1/2}, \frac{|z|^N}{(2N-1)!!}\right\}. \tag{B.8}$$

(d) *For* $t > 0$, $I_N(t)$ *and* $f_N(t)$ *are strictly decreasing in* N. *For* $t = 0$, $I_N(0) = f_N(0) = \delta_{N,0}$.

Proof. (a) This is an immediate consequence of (B.4).

(b) The fact that $f_N(t)$ is nonnegative follows immediately from (a). To prove the second bound, we begin by making the change of variable $s = t(1 - \cos\theta)$ in (B.6) to obtain

$$f_N(t) = \frac{2^N}{\pi\sqrt{2t}(2N-1)!!}\int_0^{2t} ds\, e^{-s}s^{N-1/2}\left(1 - \frac{s}{2t}\right)^{N-1/2}. \tag{B.9}$$

Consider first $N \geq 2$. Using $(1-y)^\nu \geq 1 - \nu y$, which is valid when $\nu \geq 1$ and $0 \leq y \leq 1$, we obtain

$$f_N(t) \geq \frac{2^N}{\pi\sqrt{2t}(2N-1)!!}\int_0^{2t} ds\, e^{-s}s^{N-1/2}\left(1 - \frac{(N-1/2)s}{2t}\right). \tag{B.10}$$

The second integral is bounded above by extending the domain of integration to $(0, \infty)$. To obtain a lower bound on the first integral, we use

$$\int_0^{2t} ds\, e^{-s}s^\nu = \Gamma(\nu + 1) - \int_{2t}^\infty ds\, e^{-s}s^\nu \tag{B.11}$$

and bound the second integral above using the fact that for any $0 < \alpha < 1$,

$$\begin{aligned}\int_{2t}^\infty ds\, e^{-s}s^\nu &= \int_{2t}^\infty ds\, e^{-\alpha s}s^\nu e^{-(1-\alpha)s} \\ &\leq e^{-2t(1-\alpha)}\int_0^\infty ds\, e^{-\alpha s}s^\nu = \Gamma(\nu+1)\alpha^{-\nu-1}e^{-2(1-\alpha)t}.\end{aligned} \tag{B.12}$$

For a concrete bound we take $\alpha = 1/2$.

For $N = 0$ we use $(1-y)^{-1/2} \geq 1$ and for $N = 1$ we use $(1-y)^{1/2} \geq 1 - y$, and proceed similarly. This gives the bound stated in (b).

(c) By (B.2),

$$|f_N(z)| \leq \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{-\mathrm{Re}\, z(1-\cos\theta)}. \tag{B.13}$$

Using $e^{-\mathrm{Re}\, z(1-\cos\theta)} \leq 1$ gives the first bound of (c), and using $e^{-\mathrm{Re}\, z(1-\cos\theta)} \leq \exp(-2\,\mathrm{Re}\, z\theta^2/\pi^2)$ and extending the integration domain to the whole real line gives the second bound. The third bound follows immediately from (a).

(d) The statement for $t = 0$ follows immediately from (B.2). For $t > 0$, integration by parts in the expression for f_{N+1} given in (B.6), using

$$e^{t\cos\theta} = \frac{-1}{t\sin\theta} \cdot \frac{d}{d\theta} e^{t\cos\theta},$$

gives

$$f_{N+1}(t) = \frac{t^N}{(2N-1)!!} \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{-t(1-\cos\theta)} (\sin\theta)^{2N} \cdot \cos\theta. \tag{B.14}$$

The right side differs from (B.6) for f_N only by the presence of $\cos\theta \leq 1$. □

We now show that the Gaussian quantities can be calculated in terms of $I_{n,0}^{(\varepsilon)}(x)$, with $n = 1, 2$. See Sec. 1.6 for the definitions of the various Gaussian quantities. Beginning with $I_{2,1}^{(\varepsilon)}(x)$, rewriting $\hat{D}(k) = 1 + \varepsilon - \{1 + \varepsilon - \hat{D}(k)\}$ in the numerator gives

$$I_{2,1}^{(\varepsilon)}(x) = \int \frac{d^d k}{(2\pi)^d} \frac{\hat{D}(k) e^{ik\cdot x}}{\{\varepsilon + 1 - \hat{D}(k)\}^2} = (1+\varepsilon) I_{2,0}^{(\varepsilon)}(x) - I_{1,0}^{(\varepsilon)}(x). \tag{B.15}$$

Arguing in a similar fashion, we obtain

$$I_{2,2}^{(\varepsilon)}(x) = (1+\varepsilon)^2 I_{2,0}^{(\varepsilon)}(x) - 2(1+\varepsilon) I_{1,0}^{(\varepsilon)}(x) + \delta_{x,0}, \tag{B.16}$$

and at $x = 0$,

$$I_{1,1}^{(\varepsilon)}(0) = (1+\varepsilon) I_{1,0}^{(\varepsilon)}(0) - 1, \qquad I_{1,2}(0) = I_{1,0}(0) - 1,$$

$$I_{1,4}(0) = I_{1,0}(0) - 1 - 1/(2d), \tag{B.17}$$

$$I_{2,4}(0) = I_{2,0}(0) - 4I_{1,0}(0) + 3 + 1/(2d). \tag{B.18}$$

Explicit computation of the derivative followed by setting $x = 0$ in

$$|x|^2 I_{1,0}^{(\varepsilon)} = -\sum_{\mu=1}^{d} \int \frac{d^d k}{(2\pi)^d} e^{ik\cdot x} \frac{\partial^2}{\partial k_\mu^2} \left(\frac{1}{\varepsilon + 1 - \hat{D}(k)} \right) \tag{B.19}$$

gives

$$W_{3,0}^{(\varepsilon)} = \{(1+\varepsilon)I_{2,0}^{(\varepsilon)}(0) - I_{1,0}^{(\varepsilon)}(0)\}/2. \tag{B.20}$$

Also, by the definition of $\hat{D}^{(x)}(k)$ in (1.77),

$$\begin{aligned} L_n^{(\varepsilon)}(x) &= \int \frac{d^dk}{(2\pi)^d} \frac{\hat{D}^{(x)}(k)^2}{\{\varepsilon + 1 - \hat{D}(k)\}^n} \\ &= \frac{1}{2^d d!} \sum_{\{\nu_1,\nu_2,\ldots,\nu_d\} \in \mathscr{P}_d} \sum_{\delta_1,\delta_2,\ldots,\delta_d = \pm 1} I_{n,0}^{(\varepsilon)}(x + p(x;\nu,\delta)), \end{aligned} \tag{B.21}$$

where in the right side $p(x;\nu,\delta)$ denotes the site with coordinates $p(x;\nu,\delta)_\mu = \delta_\mu x_{\nu_\mu}$.

Before estimating the remaining Gaussian quantities in terms of $I_{n,0}^{(\varepsilon)}(x)$, we observe that they are all positive and decreasing in ε.

Lemma B.2. *For any fixed $x \in \mathbf{Z}^d$, $I_{n,m}^{(\varepsilon)}(x)$, $L_n^{(\varepsilon)}(x)$, $J_{n,m}^{(\varepsilon)}$, $W_{n,0}^{(\varepsilon)}$, $V_n^{(\varepsilon)}$, $U_n^{(\varepsilon)}(x)$, and $K_{n,m}^{(\varepsilon)}(x)$ are all positive and decreasing in $\varepsilon \geq 0$ (in dimensions where they are well-defined).*

Proof. Positivity and monotonicity in ε of these quantities, except $I_{n,m}^{(\varepsilon)}(x)$, follow immediately from definitions as integrals in (1.74)–(1.80). To deal with $I_{n,m}^{(\varepsilon)}(x)$, we begin with $n = 1$, $m = 0$. Positivity of $I_{1,0}^{(\varepsilon)}(x)$ follows from the fact that

$$I_{1,0}^{(\varepsilon)}(x) = 2dp \int \frac{d^dk}{(2\pi)^d} \frac{e^{ik\cdot x}}{1 - 2dp\hat{D}(k)} = 2dp \sum_{\omega : 0 \to x} p^{|\omega|} > 0 \tag{B.22}$$

where the sum is over all simple random walks from 0 to x, and $2dp \equiv (1+\varepsilon)^{-1}$. Positivity of $I_{n,0}^{(\varepsilon)}(x)$ then follows from the fact that $I_{n,0}^{(\varepsilon)} = I_{1,0}^{(\varepsilon)} * I_{1,0}^{(\varepsilon)} * \cdots * I_{1,0}^{(\varepsilon)}$, where $*$ denotes convolution in x-space, and there are n factors. Monotonicity in ε of $I_{n,0}^{(\varepsilon)}(x)$ then follows from positivity of $I_{n+1,0}^{(\varepsilon)}(x)$ and the fact that

$$\frac{\partial}{\partial\varepsilon} I_{n,0}^{(\varepsilon)}(x) = -nI_{n+1,0}^{(\varepsilon)}(x) < 0. \tag{B.23}$$

For $m > 0$, we observe that $I_{n,m}^{(\varepsilon)}(x)$ can be expressed as a linear combination of $I_{n,0}^{(\varepsilon)}(x)$, with positive coefficients, since $\hat{D}(k) = \frac{1}{2d}\sum_{|f|=1} e^{ik\cdot f}$. Then positivity and monotonicity of $I_{n,m}^{(\varepsilon)}(x)$ follow from the corresponding properties of $I_{n,0}^{(\varepsilon)}(x)$. □

The remaining Gaussian quantities we need can be estimated in terms of $I_{n,m}(0)$ [and hence in terms of $I_{n,0}(0)$ by the identities obtained above] using the Schwarz inequality, with the following result (V_4 is treated in Lemma B.11):

$$J_{n,m}^{(\varepsilon)} \leq J_{n,m} \begin{cases} = I_{n,m}(0) & m \text{ even} \\ \leq [I_{n,m-1}(0) I_{n,m+1}(0)]^{1/2} & m \text{ odd} \end{cases} \tag{B.24}$$

$$K_{1,0}^{(\varepsilon)}(x) \le K_{1,0}(x) \le [I_{1,0}(0) L_1(x)]^{1/2} \tag{B.25}$$

$$\begin{aligned} K_{2,0}^{(\varepsilon)}(x) &\le K_{2,0}(x) \\ &\le \min\{[I_{2,0}(0) L_2(x)]^{1/2}, K_{1,0}(x) + [I_{1,4}(0) L_1(x)]^{1/2} + [I_{2,4}(0) \cdot L_2(x)]^{1/2}\} \end{aligned} \tag{B.26}$$

$$K_{2,1}^{(\varepsilon)}(x) \le K_{2,1}(x) \le [I_{2,2}(0) \cdot L_2(x)]^{1/2} \tag{B.27}$$

$$U_3^{(\varepsilon)}(x) \le U_3(x) \le [V_4 \cdot L_2(x)]^{1/2}. \tag{B.28}$$

We end this section with two lemmas concerning monotonicity of $I_{n,0}(x)$ and $L_n(x)$ in x. These lemmas will be used to bound these quantities for large x in terms of their values at smaller x.

Lemma B.3. *For any positive integer n and any $\varepsilon \ge 0$, $I_{n,0}^{(\varepsilon)}(x)$ is monotone decreasing in each $|x_\mu|$ ($\mu = 1, 2, \ldots, d$).*

Proof. Monotonicity follows immediately from the integral representation of $I_{n,0}^{(\varepsilon)}(x)$ in (B.3) and the monotonicity of modified Bessel functions from Proposition B.1(d). □

Lemma B.4. *Let n be a positive integer, let $\varepsilon \ge 0$, and consider $x, z \in \mathbf{Z}^d$ with $x_1 \ge x_2 \ge \cdots \ge x_d \ge 0$ and $z_1 \ge z_2 \ge \cdots \ge z_d \ge 0$. Then*

$$L_n^{(\varepsilon)}(x) \ge L_n^{(\varepsilon)}(x + z). \tag{B.29}$$

Moreover if $\|x\|_\infty$ is strictly greater than some nonnegative integer J, then $L_n^{(\varepsilon)}(x) \le \max_{\|y\|_\infty = J} L_n^{(\varepsilon)}(y)$.

Proof. By (B.21) and Lemma B.3, it suffices to show that

$$|x_\mu + p(x; \nu, \delta)_\mu| \le |x_\mu + z_\mu + p(x + z; \nu, \delta)_\mu| \tag{B.30}$$

for each μ and for every x, z as in the statement of the lemma. To obtain (B.30), we first observe that by definition of $p(x; \nu, \delta)$,

$$\begin{aligned} |x_\mu + p(x; \nu, \delta)_\mu| &= |x_\mu + \delta_\mu x_{\nu_\mu}|, \\ |x_\mu + z_\mu + p(x + z; \nu, \delta)_\mu| &= |(x_\mu + z_\mu) + \delta_\mu (x_{\nu_\mu} + z_{\nu_\mu})|. \end{aligned} \tag{B.31}$$

If $\delta_\mu = 1$ then the absolute values can be removed in (B.31), and (B.30) is trivially satisfied. For $\delta_\mu = -1$, we must show that

$$|x_\mu - x_{\nu_\mu}| \le |(x_\mu + z_\mu) - (x_{\nu_\mu} + z_{\nu_\mu})| \tag{B.32}$$

whenever x and z satisfy the conditions of the lemma. To dispense with the absolute value signs we consider separately two cases:

1. If $\mu \le \nu_\mu$ then (B.32) becomes $x_\mu - x_{\nu_\mu} \le (x_\mu + z_\mu) - (x_{\nu_\mu} + z_{\nu_\mu})$, which is true since $z_1 \ge z_2 \ge \cdots \ge z_d \ge 0$.
2. If $\mu \ge \nu_\mu$ then (B.32) becomes $x_{\nu_\mu} - x_\mu \le (x_{\nu_\mu} + z_{\nu_\mu}) - (x_\mu + z_\mu)$, which is again true for the same reason.

Thus (B.32) holds and the proof of (B.29) is complete.

To prove the last statement in the lemma, we proceed as follows. Given a site x with $\|x\|_\infty > J$, we first make use of symmetry to replace x by a site x' with $\|x'\|_\infty = \|x\|_\infty$, $x_1' \ge x_2' \ge \cdots \ge 0$, and $L_n^{(\varepsilon)}(x) = L_n^{(\varepsilon)}(x')$. Next we define a site z by $z_\mu = \max\{x_\mu' - J, 0\}$, and let $y = x' - z$. Then both y and z have nonincreasing nonnegative components, and hence by (B.29) $L_n^{(\varepsilon)}(y) \ge L_n^{(\varepsilon)}(x')$. The result then follows, since by construction $\|y\|_\infty = J$. □

B.2. *Numerical estimation of Gaussian quantities*

We begin this section by describing the method used to evaluate $f_N(t)$, and then discuss the evaluation of $I_{n,0}(x)$ using (B.3). Finally we obtain the concrete numerical estimates on Gaussian quantities that are used in the paper.

Although the methods apply in greater generality, all numerical values given in this section are for $d = 5$. Also we restrict attention in the calculation of $f_N(x)$ to $N \le 54$, which is sufficient for our needs.

Bounds on the round-off errors involved in the computer calculations are discussed separately in Sec. B.3.

B.2.1. *Numerical estimation of $f_N(t)$*

We require numerical values of $f_N(t)$ for nonnegative t and for integer $0 \le N \le 54$. In this section we describe methods for obtaining these values with relative error less than 10^{-16}.

We begin by introducing

$$T(t; N, M) = e^{-t}\left(\frac{t}{2}\right)^N \sum_{m=0}^{M} \frac{(t^2/4)^m}{m!(m+N)!}, \tag{B.33}$$

which is an approximation of $f_N(t)$ obtained by approximating $I_N(t)$ by its truncated Taylor series. For large t we will use the truncated asymptotic series

$$A(t; N, M) = \frac{1}{\sqrt{2\pi t}} \sum_{l=0}^{M} \frac{(-1)^l (N, l)}{(2t)^l} \tag{B.34}$$

to approximate $f_N(t)$. Here

$$(N, l) \equiv \begin{cases} 1 & (l = 0) \\ \dfrac{(4N^2 - 1^2)(4N^2 - 3^2)(4N^2 - 5^2)\cdots(4N^2 - (2l-1)^2)}{4^l l!} & (l = 1, 2, \ldots) \end{cases}. \tag{B.35}$$

We will primarily be interested in relative, rather than absolute, approximation errors. The *relative error* in the approximation of A by B is defined to be $|(A - B)/A|$.

The following proposition gives values of M which guarantee that (B.33) or (B.34) provides an approximation to $f_N(t)$ with relative error less than 10^{-16}.

Proposition B.5. (a) *For any nonnegative integer N, the relative error in the approximation of $f_N(t)$ by $T(t; N, M)$ is less than 10^{-16} if*

$$M = \begin{cases} 30 & (0 \le t \le 10) \\ 60 & (10 \le t \le 30) \\ \lfloor 2t \rfloor + 1 & (30 \le t) \end{cases}. \tag{B.36}$$

(b) *For $t \ge 2000$ and $N \le 54$, the relative error in the approximation of $f_N(t)$ by $A(t; N, M)$ is less than 10^{-16} if*

$$M = \begin{cases} 9 & (0 \le N \le 10) \\ N - 1 & (10 \le N \le 54) \end{cases}. \tag{B.37}$$

Proof. (a) Let

$$S_{M,N}(t) \equiv \sum_{m=0}^{M} \frac{(t^2/4)^m}{m!(m+N)!}, \qquad R_{M+1,N}(t) \equiv \sum_{m=M+1}^{\infty} \frac{(t^2/4)^m}{m!(m+N)!}. \tag{B.38}$$

For $M \ge 0$, $S_{M,N}(t) \ge 1/N!$. For $t \le M/2$,

$$\begin{aligned} R_{M+1,N}(t) &\le \frac{(t^2/4)^{M+1}}{(M+1)!(N+M+1)!} \sum_{m'=0}^{\infty} \left(\frac{t^2}{4M^2}\right)^{m'} \\ &\le \frac{16}{15} \frac{(t^2/4)^{M+1}}{(M+1)!(N+M+1)!}. \end{aligned} \tag{B.39}$$

Thus the relative error satisfies

$$\begin{aligned} \frac{R_{M+1,N}(t)}{S_{M,N}(t) + R_{M+1,N}(t)} &\le \frac{R_{M+1,N}(t)}{S_{M,N}(t)} \\ &\le \frac{16}{15} \frac{(t^2/4)^{M+1} N!}{(M+1)!(N+M+1)!} \le \frac{16}{15} \left(\frac{(t/2)^{M+1}}{(M+1)!}\right)^2. \end{aligned} \tag{B.40}$$

The desired result then follows, since the right side is less than 10^{-16} when $t = 10$, $M = 30$ or $t = 30$, $M = 60$ or $t \geq 30$, $M = \lfloor 2t \rfloor + 1$, using the inequality form of Stirling's formula in the last case.

(b) We start from the integral representation (B.9). The asymptotic expansion for $f_N(t)$ can be obtained by extending the domain of integration to $(0, \infty)$ and expanding $\left(1 - \frac{s}{2t}\right)^{N-1/2}$. To bound the errors involved in the asymptotic expansion, we proceed as follows. Define $r_\nu^{(M+1)}(y)$ by

$$(1 - y)^\nu = \sum_{l=0}^{M} \frac{\nu(\nu-1)\dots(\nu-l+1)}{l!}(-y)^l + r_\nu^{(M+1)}(y). \tag{B.41}$$

For $0 \leq y \leq 1$,

$$|r_\nu^{(M+1)}(y)| \leq \frac{|\nu(\nu-1)\dots(\nu-M)|}{(M+1)!} y^{M+1}. \tag{B.42}$$

We rewrite (B.9) as

$$\begin{aligned} f_N(t) = {} & \frac{2^N}{\pi\sqrt{2t}(2N-1)!!} \sum_{l=0}^{M} \frac{(N-\frac{1}{2})(N-\frac{3}{2})\dots(N-l+\frac{1}{2})}{l!(-2t)^l} \\ & \times \left[\int_0^\infty ds\, s^{l+N-1/2} e^{-s} - \int_{2t}^\infty ds\, s^{l+N-1/2} e^{-s} \right] \\ & + \frac{2^N}{\pi\sqrt{2t}(2N-1)!!} \int_0^{2t} ds\, e^{-s} s^{N-1/2} r_{N-1/2}^{(M+1)}(s/2t). \end{aligned} \tag{B.43}$$

The first term on the right side is $A(t; f_N, M)$. For the last term, we use (B.42) to obtain

$$\begin{aligned} & \left| \frac{2^N}{\pi\sqrt{2t}(2N-1)!!} \int_0^{2t} ds e^{-s} s^{N-1/2} r_{N-1/2}^{(M+1)}(s/2t) \right| \\ & \quad \leq \frac{2^N}{\pi\sqrt{2t}(2N-1)!!} \int_0^\infty ds e^{-s} s^{N-1/2} \frac{|(N-\frac{1}{2})(N-\frac{3}{2})\dots(N-M-\frac{1}{2})|}{(M+1)!} \frac{s^{M+1}}{(2t)^{M+1}} \\ & \quad \leq \frac{|(N, M+1)|}{\sqrt{2\pi t}(2t)^{M+1}}. \end{aligned} \tag{B.44}$$

For the second term, we use (B.12) with $\alpha = 1/2$ to obtain

$$\int_{2t}^\infty ds\, e^{-s} s^{N+l-1/2} \leq (2\pi)^{1/2} (2N + 2l - 1)!! e^{-t}. \tag{B.45}$$

Combining the above, for $t \geq 0$ and nonnegative integers N, M, we have

$$f_N(t) = \frac{1}{\sqrt{2\pi t}}\left[\sum_{l=0}^{M} \frac{(-1)^l (N,l)}{(2t)^l} + \mathscr{E}_N^{(M+1)}(t)\right] \tag{B.46}$$

with

$$|\mathscr{E}_N^{(M+1)}(t)| \leq 2^{N+1/2} e^{-t} \sum_{l=0}^{M} \frac{|(N,l)|}{t^l} + \frac{|(N,M+1)|}{(2t)^{M+1}}. \tag{B.47}$$

We then use the fact that $|(N,l)| \leq N^{2l}/l!$ if $l \leq N$ to see that

$$|f_N(t) - A(t;N,M)| \leq \frac{1.7 \times 10^{-21}}{\sqrt{2\pi t}} \tag{B.48}$$

if $M = 9$, $N \leq 10$ or $M = N - 1$, $11 \leq N \leq 54$. Combining this with the lower bound (B.7), which states that $f_N(t) \geq (0.27)/\sqrt{2\pi t}$ for $t \geq 2000$ and $N \leq 54$, yields the required bound on the relative error. $\square$

B.2.2. *Numerical estimation of $I_{1,0}^{(\varepsilon)}(x)$ and $I_{2,0}^{(\varepsilon)}(x)$*

In this section we discuss the method used to obtain numerical estimates for $I_{n,0}^{(\varepsilon)}(x)$ of (B.3). In the paper, these quantities are required only for the three values $\varepsilon = 0$, $\varepsilon = 0.0100504$, and $\varepsilon = 0.0109388$. When $\varepsilon > 0$, the integrand of (B.3) enjoys exponential decay, while for $\varepsilon = 0$ it decays like a power. We speed up the decay to simplify the estimation of error terms, by making the change of variables $t = e^u$ in (B.3). This gives

$$I_{n,0}^{(\varepsilon)}(x) = \int_{-\infty}^{\infty} du\, F_n^{(\varepsilon)}(u), \tag{B.49}$$

where

$$F_n^{(\varepsilon)}(u) = \frac{d^n}{(n-1)!} \exp(-d\varepsilon e^u) e^{nu} \prod_{\mu=1}^{d} f_{|x_\mu|}(e^u). \tag{B.50}$$

We will use the following lemma (see e.g. [6]) to estimate the error involved in the numerical evaluation of (B.49).

Lemma B.6. *Suppose that F is analytic on the strip $0 \leq \operatorname{Im} z \leq s$ for some $s > 0$, that $F(x)$ is real for real x, and that $F(z) \to 0$ uniformly as $|\operatorname{Re} z| \to \infty$ in the strip. Then for any $h > 0$,*

$$\int_{-\infty}^{\infty} du\, F(u) - h \sum_{m=-\infty}^{\infty} F(mh) = \operatorname{Re} \int_{-\infty+is}^{\infty+is} F(z)[1 - i\cot(\pi z/h)]\, dz.$$

Consequently,

$$\left| \int_{-\infty}^{\infty} du\, F(u) - h \sum_{m=-\infty}^{\infty} F(mh) \right| \le \frac{2}{\exp(2\pi s/h) - 1} \int_{-\infty+is}^{\infty+is} |F(z)|\, dz.$$

Here the integrations on the right sides are performed along the horizontal line through $z = is$.

Using $h = 45/256$ and $M = 256$, we will approximate $I_{n,0}^{(\varepsilon)}(x)$ for $d = 5$, $n = 1, 2$ and $\|x\|_\infty \le 54$ by

$$A_n(x; h, M) = d^n h \sum_{m=-M}^{M} e^{nmh} \prod_{\mu=1}^{d} f_{|x_\mu|}(e^{mh}) + \frac{d^n}{(2\pi)^{d/2}} \frac{h \exp\{-(M+1)(d/2 - n)h\}}{1 - \exp\{-(d/2 - n)h\}} \tag{B.51}$$

for $\varepsilon = 0$, and by

$$B_n(x, \varepsilon; h, M) = d^n h \sum_{m=-M}^{M} \exp(-d\varepsilon e^{mh}) e^{nmh} \prod_{\mu=1}^{d} f_{|x_\mu|}(e^{mh}) \tag{B.52}$$

for $\varepsilon > 0$. Bounds on the absolute errors involved in these approximations are given in the following proposition.

Proposition B.7. *For $d = 5$, $h = 45/256$, $M = 256$ and $\|x\|_\infty \le 54$,*

$$|I_{1,0}(x) - A_1(x; h, M)| \le \begin{cases} 1.312 \times 10^{-19} & (x = 0) \\ 2.625 \times 10^{-22} & (x \ne 0) \end{cases} \tag{B.53}$$

and

$$|I_{2,0}(x) - A_2(x; h, M)| \le 1.882 \times 10^{-20}. \tag{B.54}$$

Also, for $\varepsilon \ge 0.001$,

$$|I_{1,0}^{(\varepsilon)}(x) - B_1(x, \varepsilon; h, M)| \le \begin{cases} 1.312 \times 10^{-19} & (x = 0) \\ 2.625 \times 10^{-22} & (x \ne 0) \end{cases} \tag{B.55}$$

and

$$|I_{2,0}^{(\varepsilon)}(x) - B_2(x, \varepsilon; h, M)| \le 1.882 \times 10^{-20}. \tag{B.56}$$

Proof. We divide the summation involved in the discretization of the integral (B.49) into three parts, and for $n = 1, 2$ define

$$S_{n,a}^{(\varepsilon)}(x; h, M) = h \sum_{m=-\infty}^{-(M+1)} F_n^{(\varepsilon)}(mh), \tag{B.57}$$

$$S_{n,b}^{(\varepsilon)}(x;h,M) = h \sum_{m=-M}^{M} F_n^{(\varepsilon)}(mh), \tag{B.58}$$

$$S_{n,c}^{(\varepsilon)}(x;h,M) = h \sum_{m=M+1}^{\infty} F_n^{(\varepsilon)}(mh). \tag{B.59}$$

As usual we will drop the superscript (0) when $\varepsilon = 0$. The error involved in this discretization is given by

$$\mathscr{E}_n^{(\varepsilon)}(x;h) = I_{n,0}^{(\varepsilon)}(x) - S_{n,a}^{(\varepsilon)}(x;h,M) - S_{n,b}^{(\varepsilon)}(x;h,M) - S_{n,c}^{(\varepsilon)}(x;h,M). \tag{B.60}$$

Writing $S_{n,b}^{(\varepsilon)}(x;h,M)$ in terms of A_n or B_n, we obtain

$$\begin{aligned} I_{n,0}(x) &= A_n(x;h,M) + \mathscr{E}_n(x;h) + S_{n,a}(x;h,M) \\ &\quad + \left(S_{n,c}(x;h,M) - \frac{d^n}{(2\pi)^{d/2}} \frac{h\exp\{-(M+1)(d/2-n)h\}}{1-\exp\{-(d/2-n)h\}} \right) \end{aligned} \tag{B.61}$$

and

$$I_{n,0}^{(\varepsilon)}(x) = B_n(x,\varepsilon;h,M) + \mathscr{E}_n^{(\varepsilon)}(x;h) + S_{n,a}^{(\varepsilon)}(x;h,M) + S_{n,c}^{(\varepsilon)}(x;h,M). \tag{B.62}$$

The last three terms on each side are error terms, which we now proceed to estimate.

We first consider the case $\varepsilon = 0$. We bound

$$\mathscr{E}_n(x;h) = \int_{-\infty}^{\infty} du\, F_n(u) - h \sum_{m=-\infty}^{\infty} F_n(mh) \tag{B.63}$$

using Lemma B.6 and the upper bound on $f_N(z)$ of Proposition B.1. The result, for $0 < s < \pi/2$, is

$$\begin{aligned} |\mathscr{E}_1(x;h)| &\le \frac{2d}{\exp(2\pi s/h) - 1} \int_{-\infty}^{\infty} du\, e^u \left[\min\left\{1, \left(\frac{\pi}{8\cos s}\right)^{1/2} e^{-u/2}\right\}\right]^d \\ &= \frac{2d^2}{d-2}\left(\frac{\pi}{8\cos s}\right) \frac{1}{\exp(2\pi s/h) - 1} \end{aligned} \tag{B.64}$$

and

$$|\mathscr{E}_2(x;h)| \le \frac{d^3}{d-4}\left(\frac{\pi}{8\cos s}\right)^2 \frac{1}{\exp(2\pi s/h) - 1}. \tag{B.65}$$

Taking $s = \arctan(2\pi/h)$ for $I_{1,0}$ and $s = \arctan(\pi/h)$ for $I_{2,0}$, this gives

$$|\mathscr{E}_1(x;45/256)| \le 2.625 \times 10^{-22}, \qquad |\mathscr{E}_2(x;45/256)| \le 1.880 \times 10^{-20}. \tag{B.66}$$

For $S_{n,a}(x; h, M)$, it follows from (B.8) that

$$\prod_{\mu=1}^{d} f_{|x_\mu|}(e^{mh}) \le \exp(mh\|x\|_1), \tag{B.67}$$

and thus for $M = 256$, $h = 45/256$ and $d = 5$,

$$S_{1,a}(x; h, M) \le dh \frac{\exp\{-(M+1)(\|x\|_1 + 1)h\}}{1 - \exp\{-(\|x\|_1 + 1)h\}} \le \begin{cases} 1.3092 \times 10^{-19} & (x = 0) \\ 1.7095 \times 10^{-39} & (x \ne 0) \end{cases} \tag{B.68}$$

and

$$S_{2,a}(x; h, M) \le d^2 h \frac{\exp\{-(M+1)(\|x\|_1 + 2)h\}}{1 - \exp\{-(\|x\|_1 + 2)h\}} \le 8.55 \times 10^{-39}. \tag{B.69}$$

Finally we consider the last term of (B.61). It is the estimation of this term which places a restriction on the size of $\|x\|_\infty$. The last term of (B.61) can be rewritten, for $n = 1$, as

$$dh \sum_{m=M+1}^{\infty} e^{mh} \left[\prod_{\mu=1}^{d} f_{|x_\mu|}(e^m h) - (2\pi e^{mh})^{-d/2} \right]. \tag{B.70}$$

By (B.46) and (B.47) with $M = 0$, we have for $N \le 54$ (in fact for much larger N),

$$\left| f_N(e^{mh}) - \frac{1}{\sqrt{2\pi e^{mh}}} \right| \le \frac{N^2 + 1}{\sqrt{2\pi e^{mh}}} e^{-mh}. \tag{B.71}$$

Using this to estimate the difference of products, we obtain for $\|x\|_\infty \le 54$ the following bound on (B.70):

$$dh \sum_{m=M+1}^{\infty} e^{mh} (2\pi e^{mh})^{-d/2} 2d[(54)^2 + 1] e^{-mh} \le 2 \times 10^{-47}. \tag{B.72}$$

For $n = 2$ a similar argument gives

$$\left| S_{2,c}(x; h, M) - \frac{d^2}{(2\pi)^{d/2}} \frac{h \exp[-(M+1)(d/2 - 2)h]}{1 - \exp[-(d/2 - 2)h]} \right|$$

$$\le \frac{2[(54)^2 + 1] d^3 h}{(2\pi)^{d/2}} \frac{\exp\{-(M+1)h(d/2 - 1)\}}{1 - \exp[-(d/2 - 1)h]} \le 3 \times 10^{-26}. \tag{B.73}$$

Combining these estimates gives the bounds in the statement of the proposition for $\varepsilon = 0$.

For $\varepsilon > 0$, $F_n^{(\varepsilon)}(u) = \exp[-d\varepsilon e^u]F_n(u)$, and we can proceed in a similar fashion to what was done for the case of $\varepsilon = 0$. The only difference occurs in the treatment of $S_{n,c}^{(\varepsilon)}(x; h, M)$, and here the argument is simplified. Specifically, for $m > M = 256$, $h = 45/256$ and $\varepsilon \geq 0.001$, we have

$$S_{n,c}^{(\varepsilon)}(x; h, M) \leq S_{n,c}(x; h, M)\exp[-d(0.001)e^{45}] \leq 10^{-1000}, \tag{B.74}$$

where we have used the estimate for $S_{n,c}(x; h, M)$ provided by (B.72) and (B.73). □

B.2.3. *Numerical estimates for $I_{n,m}(x)$, $K_{n,m}(x)$, $L_n(x)$*

In the remainder of Sec. B.2, we present concrete estimates resulting from numerical integration, beginning here with $I_{n,m}(x)$, $K_{n,m}(x)$ and $L_n(x)$. A discussion of the round-off errors associated with these calculations is given in Sec. B.3.2. In presenting numerical values we use "..." to denote the result of rounding off, and write for example $x = 0.1234\ldots$ for $x \in [0.12335, 0.12345]$.

Although we do not use it in our calculations, the asymptotic behaviour of $I_{n,0}(x)$ provides a good picture of its behaviour as $|x| \to \infty$. A straightforward calculation shows that for $d > 2n$,

$$I_{n,0}(x) \sim \left(\frac{d}{2}\right)^n \frac{\Gamma(d/2 - n)}{(n-1)!\pi^{d/2}} |x|^{(2n-d)} \quad \text{as } x \to \infty\,. \tag{B.75}$$

To get some idea of the accuracy of the asymptotic formula, we checked by explicit calculation that for $d = 5$ and $\|x\|_\infty = 7$, the right side of (B.75) is within 5.6% of the left side for $n = 1$, and within 1.1% for $n = 2$.

Using Proposition B.7 to compute $I_{n,0}(x)$, and using the fact that $L_n(x)$ can be expressed in terms of $I_{n,0}(x)$ via (B.21), we obtain the values given in the following lemma. Any required values of these quantities which are not given explicitly are calculated in the same way.

Lemma B.8. *We have*

$$I_{1,0}(0) = 1.156\,308\,124\,840\,231\ldots \qquad I_{2,0}(0) = 1.934\,941\,440\,382\,351\ldots \tag{B.76}$$

with relative errors less than 10^{-16}, *as well as*

$$I_{2,2}(0) = 0.622\,325\,191\ldots \qquad I_{2,4}(0) = 0.409\,708\,941\ldots \tag{B.77}$$

$$J_{2,1} \leq 1.097\,343\,520\ldots \qquad J_{2,3} \leq 0.504\,947\,715\ldots \tag{B.78}$$

and the values for $x \in \Lambda_3$ tabulated in Table V. The values are truncated to 9 digits from calculated values with relative errors less than 2×10^{-13}.

For nonzero $x \notin \Lambda_3$, we have the bounds given in the following lemma.

Table V. Numerical values of $I_{1,0}(x)$, $I_{2,0}(x)$, $L_1(x)$, $L_2(x)$, for $x \in \Lambda_3$, truncated to 9 digits.

x	$I_{1,0}(x)$	$I_{2,0}(x)$	$L_1(x)$	$L_2(x)$
(1,0,0,0,0)	0.156 308 125	0.778 633 316	0.156 308 125	0.622 325 191
(1,1,0,0,0)	0.047 408 596 0	0.489 556 284	0.051 355 448 8	0.394 713 379
(2,0,0,0,0)	0.027 504 355 3	0.371 860 192	0.120 869 006	0.395 633 763
(1,1,1,0,0)	0.022 251 790 7	0.375 852 590	0.028 903 012 4	0.314 094 733
(2,1,0,0,0)	0.013 979 483 1	0.304 547 355	0.022 845 777 5	0.251 754 713
(3,0,0,0,0)	0.006 899 562 80	0.228 546 210	0.117 077 493	0.325 241 384
(1,1,1,1,0)	0.013 352 323 7	0.316 556 003	0.025 286 254 4	0.277 956 622
(2,1,1,0,0)	0.008 960 941 45	0.267 038 377	0.010 892 835 2	0.215 562 596
(2,2,0,0,0)	0.006 238 781 91	0.232 065 361	0.031 815 831 8	0.215 709 722
(3,1,0,0,0)	0.004 877 449 32	0.209 966 622	0.019 701 787 3	0.192 725 802
(4,0,0,0,0)	0.002 471 678 15	0.164 873 308	0.116 226 126	0.291 635 603
(1,1,1,1,1)	0.009 225 373 42	0.279 654 509	0.043 658 826 8	0.277 926 740
(2,1,1,1,0)	0.006 516 331 88	0.242 329 353	0.008 559 463 38	0.198 297 476

Lemma B.9. *For nonzero $x \notin \Lambda_3$,*

$$\begin{aligned} I_{1,0}(x) &\leq && 0.00509\,842\,310, \\ I_{2,1}(x) &\leq I_{2,0}(x) && \leq 0.224\,302\,270, \\ K_{2,0}(x) &\leq \{I_{2,0}(0)L_2(x)\}^{1/2} && \leq 0.725\,196\,838 \\ K_{2,1}(x) &\leq \{I_{2,2}(0)L_2(x)\}^{1/2} && \leq 0.411\,273\,455. \end{aligned} \tag{B.79}$$

Proof. The first bound on $I_{2,1}(x)$ is trivial, and the first bounds on $K_{2,m}(x)$ follow from the Schwarz inequality.

To obtain the numerical bounds, we first calculate all values of $I_{n,0}(x)$ and $L_2(x)$ as in Lemma B.8, for $\|x\|_\infty \leq 5$, and find their respective maxima for $x \notin \Lambda_3$, $x \neq 0$. (By symmetry, there are fewer than the $\binom{5+d}{d} = 252$ inequivalent sites with $\|x\|_\infty \leq 5$ to be considered.) These maxima are

$$\begin{aligned} I_{1,0}(2,1,1,1,1) &= 0.00509842310\ldots, \\ I_{2,0}(2,1,1,1,1) &= 0.224302269\ldots, \\ L_2(5,0,0,0,0) &= 0.271796572\ldots. \end{aligned} \tag{B.80}$$

The desired bounds then follow, using the monotonicity obtained in Lemmas B.3 and B.4. $\square$

Bounds for larger off-axis values of x are obtained in the next lemma by a similar argument.

Lemma B.10. *For* $\|x\|_\infty \geq 7$ *with* $\operatorname{dist}(x, \text{axes}) > 0$,

$$I_{1,0}(x) \leq 0.00037697 \qquad I_{2,0}(x) \leq 0.090467 \tag{B.81}$$

$$L_1(x) \leq 0.036151 \qquad L_2(x) \leq 0.12102. \tag{B.82}$$

Proof. We first calculate $I_{n,0}(x)$ and $L_n(x)$ for the $\binom{7+d}{d} - \binom{6+d}{d} = 330$ sites with $\|x\|_\infty = 7$. The respective maxima, for off-axis x, are

$$I_{1,0}(7,1,0,0,0) = 0.0003769604506\ldots \qquad I_{2,0}(7,1,0,0,0) = 0.0904661614117\ldots \tag{B.83}$$

$$L_1(7,7,7,7,7) = 0.0361508427181\ldots \qquad L_2(7,1,0,0,0) = 0.1210137397886\ldots. \tag{B.84}$$

Then we appeal to the monotonicity shown in Lemma B.3 to obtain the desired bound on $I_{n,0}(x)$. For $L_n(x)$ we appeal to Lemma B.4. Its statement is not enough to guarantee the desired bound, but the argument of the last paragraph of its proof can easily be applied to complete the proof. □

B.2.4. *Numerical estimates for* V_4, $I_\beta^{(\varepsilon)}$ and $I_\gamma^{(\varepsilon)}$

In this section, we derive the upper bounds on V_4, $I_\beta^{(\varepsilon)}$ and $I_\gamma^{(\varepsilon)}$ which are used in Sec. 4.3.1. Definitions of these quantities can be found in (1.76) and (4.27). We recall that f_0 is defined in (4.15) by $f_0 = [(c_4/(1+c_4) - c_3/(1-c_3)]/2$.

Lemma B.11. *We have*

$$V_4^{(\varepsilon)} \leq V_4 = 0.102\,460\,190\,44\ldots, \tag{B.85}$$

and for $\varepsilon \in [0, \varepsilon_0 \equiv 0.0109388]$ *and* $f_0 \in [0, 1/3]$, *we have*

$$I_\beta^{(\varepsilon)} \leq 0.270\,561\,76, \qquad I_\gamma^{(\varepsilon)} \leq 1.653\,223\,2. \tag{B.86}$$

Proof. By (B.4) and (B.3),

$$\int \frac{d^d k}{(2\pi)^d} \frac{\sin^2 k_\mu}{\{\varepsilon + 1 - \hat{D}(k)\}^2} = d I_{1,0}^{(\varepsilon)}(e_1),$$

$$\int \frac{d^d k}{(2\pi)^d} \frac{\sin^2 k_\mu}{\{\varepsilon + 1 - \hat{D}(k)\}^3} = \frac{d}{2} I_{2,0}^{(\varepsilon)}(e_1),$$

$$\int \frac{d^d k}{(2\pi)^d} \frac{\sin^2 k_\mu \sin^2 k_\nu}{\{\varepsilon + 1 - \hat{D}(k)\}^4} = \begin{cases} (d^2/2) I_{2,0}^{(\varepsilon)}(2e_1) & (\mu = \nu) \\ (d^2/6) I_{2,0}^{(\varepsilon)}(e_1 + e_2) & (\mu \neq \nu) \end{cases}. \tag{B.87}$$

Hence by symmetry

$$V_4^{(\varepsilon)} = \frac{d-1}{6d} I_{2,0}^{(\varepsilon)}(e_1 + e_2) + \frac{1}{2d} I_{2,0}^{(\varepsilon)}(2e_1). \tag{B.88}$$

Setting $\varepsilon = 0$, this gives (B.85).

For $I_\beta^{(\varepsilon)}$ and $I_\gamma^{(\varepsilon)}$, we first rewrite them in terms of simpler quantities. By the definitions of $\beta^{(\varepsilon)}(k)$ and $\gamma^{(\varepsilon)}(k)$ in (4.24) and (4.25),

$$I_\beta^{(\varepsilon)} = 9(1-f_0)^2 V_4^{(\varepsilon)} - 6(1-f_0) W_{3,1}^{(\varepsilon)} + I_{2,2}^{(\varepsilon)}(0),$$

$$I_\gamma^{(\varepsilon)} = 36(1-f_0)^2 V_4^{(\varepsilon)} - 12(1-f_0) W_{3,1}^{(\varepsilon)} + I_{2,2}^{(\varepsilon)}(0). \tag{B.89}$$

We rewrite $W_{3,1}^{(\varepsilon)}$ and $V_4^{(\varepsilon)}$ using (B.87), (B.88), and algebra as

$$W_{3,1}^{(\varepsilon)} = \frac{\varepsilon+1}{2} I_{2,0}^{(\varepsilon)}(e_1) - I_{1,0}^{(\varepsilon)}(e_1) = \frac{1}{2}[I_{2,2}^{(\varepsilon)}(0) - I_{1,1}^{(\varepsilon)}(0)],$$

$$V_4^{(\varepsilon)} = \frac{1}{6} I_{2,2}^{(\varepsilon)}(0) + \frac{1}{12d}[5I_{2,0}^{(\varepsilon)}(2e_1) - I_{2,0}^{(\varepsilon)}(0)]. \tag{B.90}$$

Substituting (B.90) into (B.89) gives

$$I_\beta^{(\varepsilon)} = -\frac{1-3f_0^2}{2} I_{2,2}^{(\varepsilon)}(0) + 3(1-f_0) I_{1,1}^{(\varepsilon)}(0) + \frac{3(1-f_0)^2}{4d}[5I_{2,0}^{(\varepsilon)}(2e_1) - I_{2,0}^{(\varepsilon)}(0)],$$

$$I_\gamma^{(\varepsilon)} = (1 - 6f_0 + 6f_0^2) I_{2,2}^{(\varepsilon)}(0) + 6(1-f_0) I_{1,1}^{(\varepsilon)}(0) + \frac{3(1-f_0)^2}{d}[5I_{2,0}^{(\varepsilon)}(2e_1) - I_{2,0}^{(\varepsilon)}(0)]. \tag{B.91}$$

To obtain bounds which are uniform in $\varepsilon \in [0, \varepsilon_0]$, we use the fact that $I_{2,0}^{(\varepsilon)}(x)$, $I_{2,2}^{(\varepsilon)}(0)$ and $I_{1,1}^{(\varepsilon)}(0)$ are monotone decreasing in $\varepsilon \geq 0$, by Lemma B.2. Then bounds on (B.91) which are uniform in $\varepsilon \in [0, \varepsilon_0]$ are given by

$$I_\beta^{(\varepsilon)} \leq -\frac{1-3f_0^2}{2} I_{2,2}^{(\varepsilon_0)}(0) + 3(1-f_0) I_{1,1}^{(0)}(0) + \frac{3(1-f_0)^2}{4d}[5I_{2,0}^{(0)}(2e_1) - I_{2,0}^{(\varepsilon_0)}(0)],$$

$$I_\gamma^{(\varepsilon)} \leq (1 - 6f_0 + 6f_0^2) I_{2,2}^{(0)}(0) + 6(1-f_0) I_{1,1}^{(0)}(0) + \frac{3(1-f_0)^2}{d}[5I_{2,0}^{(0)}(2e_1) - I_{2,0}^{(\varepsilon_0)}(0)]. \tag{B.92}$$

Evaluating the right sides (using $I_{2,2}^{(\varepsilon_0)} = 0.4432538877\ldots$, $I_{2,0}^{(\varepsilon_0)} = 1.704218873\ldots$), it is easily seen that the right sides are bounded by their values at $f_0 = 0$, as long as $f_0 \in [0, 1/3]$. □

B.2.5. *Numerical estimates for* $|x|^2 I_{1,0}(x)$

This section contains a proof of the following lemma.

Lemma B.12. *For* $\|x\|_\infty \geq 7$,

$$|x|^2 I_{1,0}(x) \leq 0.0191625. \tag{B.93}$$

For $x = ne_1$, *with* $n \geq 9$,

$$|x|^2 I_{1,0}(x) \leq 0.0145427. \tag{B.94}$$

We have not succeeded in exploiting any simple monotonicity in the following proof, but instead combine several different arguments.

We first check by direct computer calculation that:

1. (B.93) is satisfied for $\|x\|_\infty \leq 13$.
2. For $\|x\|_\infty = 14, 20$,

$$I_{1,0}(x) \leq \frac{0.13}{|x|^3}. \tag{B.95}$$

3. (B.94) and (B.95) hold for $x = ne_1$, with $9 \leq n \leq 54$. Also

$$I_{2,0}(54e_1) \leq \frac{0.66}{54}. \tag{B.96}$$

To handle large x, we use the following lemma.

Lemma B.13. *The identity*

$$(|x|^2 + 1) I_{1,0}(x) = \left(1 - \frac{4}{d}\right) I_{2,0}(x) + R_1(x) \tag{B.97}$$

holds, where

$$R_1(x) \equiv \frac{2}{d^2} \int \frac{d^d k}{(2\pi)^d} \frac{e^{ik\cdot x}}{\{1 - \hat{D}(k)\}^3} \sum_{\mu=1}^{d} (1 - \cos k_\mu)^2. \tag{B.98}$$

Also, $R_1(x)$ *obeys the bound*

$$R_1(x) \leq \frac{34}{|x|^2}. \tag{B.99}$$

Proof of Lemma B.12, given Lemma B.13. We begin with (B.94), which is the easier of the two bounds. The third item above takes care of $9 \leq n \leq 54$. For $n \geq 54$, we use

(B.96) and the monotonicity given in Lemma B.3 to conclude that $I_{2,0}(x) \le 0.66/54$ for all $\|x\|_\infty \ge 54$. This, combined with Lemma B.13, implies that for all $\|x\|_\infty \ge 54$,

$$|x|^2 I_{1,0}(x) \le \frac{0.66}{(54)(5)} + \frac{34}{54^2} \le 0.01411. \tag{B.100}$$

We turn now to (B.93). The first and second items above take care of $\|x\|_\infty \le 14$. In particular, for $\|x\|_\infty = 14$,

$$|x|^2 I_{1,0}(x) \le \frac{0.13}{14}. \tag{B.101}$$

We next consider a site y with $\|y\|_\infty \in [15, 19]$, and without loss of generality assume $y_1 \ge y_2 \ge \cdots \ge y_d \ge 0$. We define $z \in \mathbf{Z}^d$ by setting $z_\mu = \max\{y_\mu - 14, 0\}$, and let $x = y - z$. Then z_μ is nonzero only when $y_\mu \ge 14$ (in which case $x_\mu = 14$), and because $\|y\|_\infty \le 19$ we have $y_\mu/x_\mu \le 19/14$ (taking $0/0 = 1$). By construction, $\|x\|_\infty = 14$, and so (B.101) holds. On the other hand, each component of z is nonnegative, so by the monotonicity given in Lemma B.3, $I_{1,0}(y) \le I_{1,0}(x)$. Therefore

$$|y|^2 I_{1,0}(y) \le |y|^2 I_{1,0}(x) \le \frac{|y|^2}{|x|^2} \cdot \frac{0.13}{14} \le \frac{19^2}{14^2} \cdot \frac{0.13}{14} \le 0.01711. \tag{B.102}$$

Similarly, using the bounds for $\|x\|_\infty = 20$ given in the second item above, for $\|y\|_\infty \le 33$ we have

$$|y|^2 I_{1,0}(y) \le |y|^2 I_{1,0}(x) \le \frac{33^2}{20^2} \cdot \frac{0.13}{20} \le 0.01770, \tag{B.103}$$

which gives (B.93) for $\|x\|_\infty \le 33$.

For $\|x\|_\infty \in [34, 54]$, it follows from monotonicity and the third item above that

$$|x|^2 I_{1,0}(x) \le |x|^2 I_{1,0}(\|x\|_\infty e_1) \le \frac{|x|^2}{\|x\|_\infty^2} \frac{0.13}{\|x\|_\infty} \le d \frac{0.13}{34} \le 0.019118. \tag{B.104}$$

Finally, $\|x\|_\infty \ge 55$ has already been taken care of by (B.100). □

It remains only to prove Lemma B.13.

Proof of Lemma B.13. It is a straightforward calculation to derive (B.97) from the integral representation

$$(1 + |x|^2) I_{1,0}(x) = \int \frac{d^d k}{(2\pi)^d} \frac{e^{ik\cdot x}}{\{1 - \hat{D}(k)\}^2} \left\{1 - \frac{2}{1 - \hat{D}(k)} \sum_{\mu=1}^{d} \left(\frac{\sin k_\mu}{d}\right)^2\right\}. \tag{B.105}$$

To bound $R_1(x)$, we use the fact that

$$|x|^2 R_1(x) = -\frac{2}{d^2}\int \frac{d^d k}{(2\pi)^d} e^{ik\cdot x} \sum_{\mu=1}^{d} \partial_\mu^2 \left(\frac{1}{\{1-\hat{D}(k)\}^3} \sum_{\nu=1}^{d} (1-\cos k_\nu)^2 \right)$$

$$= -\frac{4}{d} I_{2,0}(x) + \frac{2}{d}\int \frac{d^d k}{(2\pi)^d} \frac{e^{ik\cdot x}}{\{1-\hat{D}(k)\}^3} \left\{ -\frac{12\cdot ST}{d\{1-\hat{D}(k)\}^2} + \frac{3T}{1-\hat{D}(k)} + \frac{12}{d^2}\sum_{\mu=1}^{d} \frac{\sin^2 k_\mu}{1-\hat{D}(k)}(1-\cos k_\mu) - T - 2S \right\}, \tag{B.106}$$

where

$$S \equiv \frac{1}{d}\sum_{\mu=1}^{d} \sin^2 k_\mu, \qquad T \equiv \frac{1}{d}\sum_{\mu=1}^{d} (1-\cos k_\mu)^2. \tag{B.107}$$

We also use the crude estimates

$$T \le \frac{1}{d}\sum_{\mu,\nu} (1-\cos k_\mu)(1-\cos k_\nu) = d\{1-\hat{D}(k)\}^2,$$

$$T \le 2\{1-\hat{D}(k)\}, \tag{B.108}$$

and

$$\sum_{\mu=1}^{d} \sin^2 k_\mu \{1-\cos k_\mu\} \le \sum_{\mu,\nu=1}^{d} \sin^2 k_\mu (1-\cos k_\nu) = d^2 S\{1-\hat{D}(k)\}. \tag{B.109}$$

Combining this with the fact that $\int \frac{d^d k}{(2\pi)^d}\frac{S}{(1-\hat{D})^3} = dW_{3,0}$ gives

$$|x|^2 R_1(x) \le \frac{2}{d}\int \frac{d^d k}{(2\pi)^d}\left\{ \frac{26S}{\{1-\hat{D}(k)\}^3} + \frac{3d+2}{\{1-\hat{D}(k)\}^2} \right\} = (52)(W_{3,0}) + \frac{2(3d+2)}{d} I_{2,0}(0). \tag{B.110}$$

Substituting numerical values into the right side gives the bound on $R_1(x)$ of the lemma. □

B.3. *Control of round-off errors*

In this section, we briefly discuss rigorous bounds on the round-off errors involved in the numerical calculation of the integrals $I_{n,0}(x)$, and in the numerical calculations in the remainder of the paper. We omit any detailed description of the analysis we used, and merely give an overview. One approach to the rigorous control of round-off errors is to use interval arithmetic, but in view of the fact that our computer program was not originally written using interval arithmetic, we found it easier to perform the analysis of round-off errors after the fact. We begin with a brief background on round-off errors in numerical computations.

B.3.1. *Background on round-off errors*

Final numerical calculations were performed using VAX FORTRAN on VAX6440 at the Meson Science Laboratory, Faculty of Science, University of Tokyo, running the VAX/VMS operating system. On the computer, real numbers are approximated by floating point binary numbers consisting of mantissa and exponent. Using a mantissa of length L, the relative error incurred in converting a real number to binary is at most 2^{-L}. In addition to this truncation error, there is round-off error involved in each operation of addition, subtraction, multiplication and division. Given two floating point binary numbers X and Y, let $a(X \cdot Y)$ denote the floating point binary product produced by the computer, and similarly for the other three arithmetic operations. Then the relative error generated in one of these operations is at most 2^{-L+1} (see e.g. [6]). More precisely,

$$\left| \frac{a(X+Y)}{X+Y} - 1 \right| \le 2^{-L+1} \tag{B.111}$$

and similarly for the other three operations. To simplify the notation, we will write $\varepsilon \equiv 2^{-L+1}$ to denote this basic unit of error.

We next consider the propagation of errors in calculations involving several steps. To be specific, we consider two nonnegative real numbers x and y, and denote their representations on the computer as binary floating point numbers by X and Y. These can be results of preceding algebraic operations on the computer. We now estimate the relative errors involved in approximating $x + y$ by $X + Y$, and similarly for subtraction, multiplication and division. To distinguish between round-off and truncation errors, we will denote the relative error in representing x by X as

$$\delta(x) \equiv \left| \frac{X}{x} - 1 \right| . \tag{B.112}$$

To simplify the estimates, we assume that

$$\varepsilon,\ \delta(x),\ \delta(y) \le 10^{-6}, \tag{B.113}$$

which will be the case for our applications.

For addition, we have

$$\left|\frac{a(X+Y)}{x+y}-1\right| \le \left|\frac{a(X+Y)}{X+Y}-1\right| \cdot \left|\frac{X+Y}{x+y}\right| + \left|\frac{X+Y}{x+y}-1\right|$$

$$\le (1.00001)\varepsilon + \max\{\delta(x), \delta(y)\}. \tag{B.114}$$

Here we used (for a, b, A, $B > 0$)

$$\frac{A+B}{a+b} = \frac{\frac{A}{a} + \frac{B}{b}\frac{b}{a}}{1+\frac{b}{a}} \le \max\left\{\frac{A}{a}, \frac{B}{b}\right\}. \tag{B.115}$$

For multiplication and division, we have

$$\left|\frac{a(X\cdot Y)}{x\cdot y}-1\right| \le \left|\frac{a(X\cdot Y)}{X\cdot Y}-1\right| \cdot \left|\frac{X\cdot Y}{x\cdot y}\right| + \left|\frac{X\cdot Y}{x\cdot y}-1\right|$$

$$\le (1.00001)\{\varepsilon + \delta(x) + \delta(y)\} \tag{B.116}$$

and

$$\left|\frac{a(X/Y)}{x/y}-1\right| \le (1.00001)\{\varepsilon + \delta(x) + \delta(y)\}. \tag{B.117}$$

Subtraction is most conveniently treated in terms of *absolute* errors:

$$|a(X-Y)-(x-y)| \le |a(X-Y)-(X-Y)| + |X-Y-(x-y)|$$

$$\le \varepsilon|X-Y| + \delta(x)x + \delta(y)y$$

$$\le (1.00001)\{\varepsilon|x-y| + \delta(x)x + \delta(y)y\}. \tag{B.118}$$

The terms $\delta(x)x$ and $\delta(y)y$ can be interpreted as absolute errors of x and y.

B.3.2. *Round-off errors in the numerical calculation of $I_{n,0}(x)$*

Here we concentrate on the evaluation of $I_{n,0}^{(\varepsilon)}(x)(n = 1, 2)$ with $\varepsilon = 0$. The case of $\varepsilon > 0$ can be treated similarly. Values of $I_{n,0}(x)$ are computed using Proposition B.7, in which $I_{n,0}(x)$ is approximated by the finite sum $A_n(x; h = 45/256, M = 256)$ defined in (B.51). For $x = 0$, which is the most fundamental value in our applications, all computations are done using quad precision (real $*$ 16), which involves a 112 digit binary mantissa, and hence $\varepsilon = 2^{-111}$. For $x \neq 0$ we compute the values of $f_N(e^{mh})$ via Proposition B.5, using quad precision, but to save time we compute $A_n(x; h = 45/256, M = 256)$ using double precision (real $*$ 8) (with 52 digit binary mantissa, so $\varepsilon = 2^{-51}$). The round-off errors in these calculations are such that the overall round-off error in the evaluation of $I_{n,0}(x)$ ($n = 1, 2$) is less than 3×10^{-13}.

To see this, we first bound the errors involved in generating the integration points e^{mh}. Then we consider the round-off errors involved in the computation of $f_N(t)$, where $t \equiv e^{mh}$. For $t \leq 2000$, by Proposition B.5 $f_N(t)$ can be approximated by $T(t; N, M)$ of (B.33) with $M \leq 4001$. The resulting round-off error can be estimated using the bounds given in the previous subsection, with the result that for $N \leq 100$ and $M \leq 4001$ the relative error in the evaluation of $T(t; N, M)$ is less than 10^{-24}. Similarly, for $t \geq 2000$, $f_N(t)$ is approximated by $A(t; N, M)$ of (B.34). It can be shown that the relative error due to round-off in the computation of $A(t; N, M)$ is at most 5×10^{-24}.

Finally, the round-off errors in the numerical computation of $A_n(x; h, m)$ of (B.51) are treated similarly. The result is that the relative error due to round-off is at most 3×10^{-13}.

In conclusion, the values of $I_{1,0}(x)$ and $I_{2,0}(x)(0 < \|x\|_\infty \leq 54)$ used in Sec. B.2 are accurate up to the sum of absolute error 2×10^{-19} (see Proposition B.7) and relative (round-off) error 3×10^{-13}. For $I_{1,0}(0)$ and $I_{2,0}(0)$ quad precision was used throughout, reducing the relative (round-off) error to 10^{-20}. All these errors in Gaussian quantities are taken into account in the remaining numerical calculations explained in the next subsection.

B.3.3. *Round-off errors in other numerical calculations*

All remaining numerical calculations presented in Secs. 2 through 5 were performed using double precision. These calculations can all be written as inequalities, in which either an upper bound or a lower bound (but not both) is required. This makes it relatively easy to write a computer program which always gives a rigorous upper or lower bound in each operation, taking round-off errors into account "by hand". We used such a program, thereby reducing round-off errors to zero.

To illustrate this approach we consider as a specific example the inequality (2.10), which reads

$$R'_p(x) \leq [1 - 2dp^2 + 2pG_p(e_1)\{1 + 2dpG_p(e_1)\}]B'_p(x). \tag{B.119}$$

In our numerical upper bound we compute a bound on the right side and then multiply by a factor slightly greater than one, to restore any possible diminution due to round-off error. To be specific, for this inequality we use the values in $P_p(1)$ for $G_p(e_1)$ and $B'_p(x)$. This entails conversion errors from decimal to binary of ε in each case. The relative error in the calculation of $2dp$ is about 3ε (being two multiplications, plus a conversion error for d). Although there is one subtraction, the result of the subtraction is more than 0.8 so there is little difference between absolute and relative errors. Proceeding this way for the other operations, we can conclude that the overall relative error involved in the calculation of the right side of (B.119) is less than 20ε. Therefore a rigorous upper bound on $R'_p(x)$ can be obtained by multiplying the computer generated bound by $(1 + 20\varepsilon)$.

Our computer program has been written to modify each calculation in a similar fashion to remove any possible underestimate in an upper bound (or overestimate in the case of a lower bound) due to round-off error.

A word on the use of (3.23) and (3.24) is in order. Although these inequalities each involve subtractions, the values of $\bar{f}$ on the machine are true upper bounds on f (being generated according to the above procedure of obtaining rigorous bounds), and hence their relative errors can be considered to be zero. Therefore we have only to account for a relative error of ε in each of these subtractions.

C. Analysis for Six or More Dimensions

The numerical estimates given throughout the paper are for $d = 5$. In this appendix, we discuss the modifications used for the treatment of higher dimensions. As explained in Sec. 1.5, the method of proof relies on the fact that various Gaussian quantities are small. Because these Gaussian quantities become smaller as the dimension increases, the proof becomes relatively easier. In fact, if the $d = 5$ Gaussian values had been a little smaller, the arguments in this paper could have been made less elaborate. To give an indication of the effect of increasing the dimension, we note that the $d = 5$ value $I_{2,2}(0) = 0.6223\ldots$ is reduced to $I_{2,2}(0) = 0.2802\ldots$ in $d = 6$, and asymptotically $I_{2,2}(0) \sim 1/(2d)$ as $d \to \infty$.

We first consider $6 \le d \le 9$, and then discuss $d \ge 10$. For $6 \le d \le 9$ we perform calculations similar to (but considerably simpler than) those for $d = 5$, while for $d \ge 10$ we work with bounds which are uniform in d.

C.1. *Dimensions 6, 7, 8, 9*

For $6 \le d \le 9$, we proceed essentially as for $d = 5$, but with many simplifications. For the inequalities $P_p(\alpha)$ we now take just the three inequalities

$$B_p(0) \le (0.26)\cdot\alpha, \qquad \sup_{x\neq 0} B_p'(x) \le (0.26)\cdot\alpha, \qquad \sup_{x\neq 0} |x|^2 G_p(x) \le (0.11)\cdot\alpha. \quad \text{(C.1)}$$

We use $p_0 \equiv 1/(2d - 1)$, and $z_c(d) \le (1.01185)/(2d - 1)$. The latter follows from Corollary A.2, using explicit numerical values of Gaussian quantities calculated via Proposition B.7.

We then perform the calculations of Secs. 2–3, with many simplifications. For example, we simply use $R(0) \le B(0)$ and $R_p'(x) \le B_p'(x)$, and thus do not require most of Sec. 2.1. Also most of Sec. 3.3 can be omitted, because we just employ

$$\sum_x \Pi_p^{(n)}(x) \le \left[\sup_{x\neq 0} G_p(x)\right] R_p(0) \left[\sup_{y\neq 0} R_p'(y)\right]^{n-2} \qquad \text{(C.2)}$$

and (3.69) and (3.70) to bound $\sum_x \Pi_p^{(n)}(x)$ and $\sum_x |x|^2 \Pi_p^{(n)}(x)$. Then we proceed to bound $B_p(0)$, $B_p'(x)$, and $|x|^2 G_p(x)$ as was done in Sec. 4 for $d = 5$. Because the Gaussian quantities are so small, the values of $I_{n,0}(x)$ and $L_n(x)$ $(n = 1, 2)$ turn out to be needed only for $\|x\|_\infty \le 2$.

We omit any detailed account of the calculation, but only give the resulting bounds on $B_p(0)$ and $c_1' - c_4'$ (defined in Lemma 3.1):

$$c_1' \le 0.13, \quad c_2' \le 0.031, \quad c_3' \le 0.010, \quad c_4' \le 0.038, \quad B_p(0) \le 0.26. \quad \text{(C.3)}$$

C.2. *Dimensions 10 and higher*

For dimensions 10 and higher, we use estimates which are uniform in d. For this we use the following lemma, whose proof is deferred to the end of the section.

Lemma C.1. *The integrals $I_{n,m}(0)$ ($n \ge 1$, $m = 0, 1$) are monotone decreasing in d. Moreover for $d \ge 10$,*

$$I_{1,0}(0) \le 1.06, \qquad I_{2,0}(0) \le 1.21, \qquad I_{2,2}(0) \le 0.09 \qquad \text{(C.4)}$$

and

$$\sup_x |x|^2 I_{1,0}(x) \le 0.085, \qquad \sup_{x \ne 0} L_2(x) \le 0.20. \qquad \text{(C.5)}$$

For $d \ge 10$, we take for $P_p(\alpha)$ simply

$$B_p(0) \le 0.10, \qquad \sup_x |x|^2 G_p(x) \le 0.10. \qquad \text{(C.6)}$$

We do not explicitly extract the 2-loop or 3-loop contributions from Π, so that in Sec. 3.1 we now take $\pi_0 = \pi_1 = 0$. It then follows that N_p, X_p, $Y_p \le 1$. We use

$$B_p'(x) = B_p(x) + G_p(x) \le B_p(0) + \left(\frac{B_p(0)}{2d}\right)^{1/2} \le 0.17072 \qquad \text{(C.7)}$$

to bound $B_p'(x)$, and then proceed as for $d < 10$. Using $d \ge 10$, we obtain the inequalities

$$c_1 = 0.00176, \qquad c_2 = 0.01031, \qquad c_3 = 0.00113, \qquad c_4 = 0.01099 \qquad \text{(C.8)}$$

for the constants c_i of Lemma 3.1.

Then we proceed as in Sec. 4, using Lemma C.1, to estimate $B_p(0)$ and $|x|^2 G_p(x)$. The bound (4.7) on $B(0)$ is straightforward [using $J_{2,1} \le (I_{2,0} I_{2,2})^{1/2}$]. The bound (4.26) on $|x|^2 G(x)$ requires bounds on V_4, I_β, I_γ and $I_{2,1}(x)$, in addition to the bounds of Lemma C.1. To bound the first three of these, we use the fact that for $x \ne 0$ we have by monotonicity in x and d $I_{2,0}(x) \le I_{2,0}(e_1) = I_{2,1}(0) \le 0.15$, together with the formulas in the proof of Lemma B.11. For example,

$$V_4 \le \frac{d+2}{6d} I_{2,0}(e_1) \le \frac{1}{5}(0.15). \qquad \text{(C.9)}$$

In bounding $|x|^2 G_p(x)$, we use $I_{2,1}(x) \le I_{2,1}(x) + I_{1,0}(x) = I_{2,0}(x) \le 0.15$. Using the fact that $z_c \le (1.08)/(2d-1)$, which follows from Corollary A.2 and Lemma C.1 (using

$C_{p,2}(x) \le I_{1,0}(x) \le I_{1,0}(0) - 1$), we obtain

$$c_1' \le 0.1155, \quad c_2' \le 0.0104, \quad c_3' \le 0.00113, \quad c_4' \le 0.01099, \quad B(0) \le 0.1 \quad \text{(C.10)}$$

and can complete the proof that $P_p(0.999)$ is satisfied.

Proof of Lemma C.1. We follow the argument of [13, Appendix A] to prove monotonicity of $I_{n,m}(0)$, using the integral representation (B.3) to write, for $m = 0, 1$,

$$I_{n,m}(0) = \frac{1}{(n-1)!} \int_0^\infty ds\, s^{n-1} f_0(s/d)^d \frac{f_m(s/d)}{f_0(s/d)}. \tag{C.11}$$

Denoting the $L_p(-\pi, \pi)$ norm of $g_s(\theta) \equiv \exp(-s(1 - \cos\theta))$ by $\|g_s(\theta)\|_p$, the middle factor of the integrand can be expressed as $f_0(s/d)^d = \|g_s(\theta)\|_{1/d}$, which is monotone decreasing in d for fixed s. This proves the monotonicity of $I_{n,0}(0)$.

For $m = 1$, the last factor of the integrand is also monotone decreasing in d for fixed s, because $f_1(x)/f_0(x)$ is monotone increasing in $x > 0$. This can be seen from direct calculation of its derivative, which gives

$$\frac{d}{dx}\left(\frac{f_1(x)}{f_0(x)}\right) = \langle \cos^2\theta \rangle - \langle \cos\theta \rangle^2 \ge 0 \tag{C.12}$$

where $\langle f(\theta) \rangle \equiv \int_0^{2\pi} d\theta\, f(\theta) e^{x\cos\theta} / \int_0^{2\pi} d\theta\, e^{x\cos\theta}$. This completes the proof of monotonicity.

The first two inequalities of (C.4) then follow from monotonicity and the fact that $I_{1,0}(0) \le 1.06$ and $I_{2,0}(0) \le 1.21$ for $d = 10$, by direct computation. For the third inequality of (C.4), we check by direct calculation that $I_{2,2}(0) \le 0.09$ for $10 \le d \le 14$, while for $d \ge 15$ we note that by monotonicity in d and direct computation $I_{2,1}(0) \le 0.09$, and hence $I_{2,2}(0) = I_{2,1}(0) - I_{1,1}(0) \le 0.09$ for $d \ge 15$.

To prove the inequality for $L_2(x)$ we first recall (B.21), which expresses $L_2(x)$ as an average over $I_{2,0}(y)$. By monotonicity in $|y_\mu|$, $I_{2,0}(y) \le I_{2,0}(e_1) = I_{2,1}(0) \le 0.21$, for $y \ne 0$. Since on the right side of (B.21) at most a fraction $1/(2d)$ of the terms has $x + p(x; v, \delta) = 0$ for $x \ne 0$, we have

$$L_2(x) \le \frac{1}{2d} I_{2,0}(0) + \frac{2d-1}{2d} I_{2,0}(e_1) \le 0.20. \tag{C.13}$$

Finally, we turn to the bound on $|x|^2 I_{1,0}(x)$. Since $|\omega| \ge |x|$ when ω is a walk from 0 to x, we have (the following sums are over simple random walks)

$$\begin{aligned} |x|^2 I_{1,0}(x) &= |x|^2 \sum_{\omega: 0 \to x} \left(\frac{1}{2d}\right)^{|\omega|} \\ &\le \sum_{\omega: 0 \to x} |\omega|^2 \left(\frac{1}{2d}\right)^{|\omega|} = \left(p^2 \frac{\partial^2}{\partial p^2} + p \frac{\partial}{\partial p}\right) \sum_{\omega: 0 \to x} p^{|\omega|} \Bigg|_{p = 1/(2d)}. \end{aligned} \tag{C.14}$$

After a little algebra, for $x \neq 0$ this gives

$$|x|^2 I_{1,0}(x) \leq I_{3,2}(x) + I_{2,1}(x) = I_{3,1}(x) \leq I_{3,1}(0). \tag{C.15}$$

For $10 \leq d \leq 22$, we proceed essentially as for $d = 5$ in the proof of Lemma B.12, also making use of (C.15). For $d \geq 23$, by monotonicity in d and direct calculation for $d = 23$ we have $I_{3,1}(0) \leq 0.0832$, and thus $|x|^2 I_{1,0}(x) \leq 0.084$. □

Acknowledgements

We thank David Brydges, Alan Sokal, and Michael Aizenman for stimulating discussions and encouragement. In particular, the methods of Appendix A arose out of discussions with Alan Sokal. T.H. would also like to thank Hal Tasaki for continual encouragement, and Tsuneyoshi Kamae, Ryugo S. Hayano and Tadayuki Takahashi for their assistance in programming in FORTRAN and in using INTERNET, which proved to be a vital tool for our collaboration. T.H. also thanks Tetsuya Hattori, who first taught him how to evaluate Gaussian integrals about a decade ago.

Part of this work was done while T.H. was at the Department of Mathematics of the University of Texas at Austin, and while visiting the Courant Institute of Mathematical Sciences, N.Y.U. and the Department of Mathematics and Statistics, McMaster University.

Numerical computations were carried out at the Academic Computing Facility of the Courant Institute, the Computer Center of the University of Texas at Austin, the Department of Mathematics and Statistics, McMaster University, and at the Meson Science Laboratory, University of Tokyo. We are particularly grateful to the Meson Science Laboratory, University of Tokyo, for having generously provided computer time.

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