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# On the number of distinct sites visited in 2D lattices

Frank S. Henyey and V. Seshadri

Center for Studies of Nonlinear Dynamics, La Jolla Institute, La Jolla, California 92038  
(Received 28 January 1982; accepted 26 February 1982)

We present analytic results for the asymptotic behavior of  $S_n$ , the number of distinct sites visited in an  $n$ -step random walk on two-dimensional lattices using a combination of contour integration and saddle point techniques. We obtain results that agree very well with exact results ( $n \leq 500$ ) and numerical simulation ( $n \sim 10^3$ ).

## I. INTRODUCTION

In this paper, we analyze the asymptotic behavior of the average number of distinct sites  $S_n$  visited in an  $n$ -step random walk on two-dimensional (2D) infinite lattices.<sup>1-3</sup> The asymptotic behavior of  $S_n$  is useful, for example, in estimating the decay rate of an excitation in the presence of quenching sites or traps.<sup>4,5</sup> In one and three dimensions, the asymptotic behavior of  $S_n$  is well understood. In two dimensions, as we explain below, no satisfactory analysis of  $S_n$  exists. Such an analysis is relevant for two reasons. First, such a study should prove useful for understanding excitation transfer in quasi-one-dimensional systems with planar interchain interactions that have been proposed recently.<sup>4</sup> Second, the analysis is intrinsically interesting and, to some extent, fills a gap in our knowledge of the theory of two-dimensional random walks.

The behavior of  $S_n$  can be studied systematically using the generating function technique developed by Montroll<sup>1</sup> and Montroll and Weiss.<sup>2</sup> In this approach, the generating function

$$S(z) = \sum_{n=0}^{\infty} S_n z^n \quad |z| < 1 \quad (1.1)$$

is expressed in terms of the generating function  $P(0, z)$  for the probability of return to the origin, i. e.,

$$P(0, z) = \sum_{n=0}^{\infty} P(0, n) z^n, \quad |z| < 1, \quad (1.2)$$

and  $P(0, n)$  is the probability of return to the origin in the  $n$ th step. Montroll<sup>1</sup> has established the relation between  $S(z)$  and  $P(0, z)$  as

$$S(z) = 1/(1-z)^2 P(0, z). \quad (1.3)$$

If the analytic behavior of  $S(z)$  is known as a function of  $z$ , the asymptotic behavior of  $S_n$  for large  $n$  can be determined by the singularities of  $S(z)$  at  $z=1$ . In 1D, for a symmetric random walk,

$$P(0, z) = (1-z^2)^{-1/2}. \quad (1.4)$$

Thus, we have an expansion of  $S(z)$  in terms of half-integral powers of  $(1-z)$  as

$$S(z) = (1-z^2)^{1/2} (1-z)^{-2}. \quad (1.5)$$

Montroll<sup>1</sup> has determined the leading behavior of  $S_n$  by the somewhat complicated procedure of constructing an auxiliary sequence  $\Delta_n \equiv S_n - S_{n-1}$  and applying a Tauberian theorem to  $\Delta(z) \equiv \sum \Delta_n z^n$ . The result is

$$S_n \sim (8n/\pi)^{1/2}. \quad (1.6)$$

Correction terms in the expansion (1.6) are obtained by expanding the lower-order singularities in powers of  $z$  and using the Stirling's approximation for the coefficient of  $z^n$ . This procedure yields

$$S_n \sim \left(\frac{8n}{\pi}\right)^{1/2} \left[1 + \frac{1}{4n} + O(1/n^2)\right]. \quad (1.7)$$

In 3D, the general form of the expansion of  $P(0, z)$  is<sup>2</sup>

$$P(0, z) = u_0 - u_1(1-z)^{1/2} + u_2(1-z) - u_3(1-z)^{3/2}, \quad (1.8)$$

where the constants  $u_0, u_1, u_2, \dots$  depend on the lattice structure. The expansion of  $S(z)$  is then given by

$$S(z) = \frac{1}{u_0} (1-z)^{-2} + \frac{u_1}{u_0^2} (1-z)^{-3/2} + \frac{(u_1^2 - u_2 u_0)}{u_0^3} (1-z)^{-1} + \dots \quad (1.9)$$

The asymptotic behavior of  $S_n$  is then given by

$$S_n \sim \frac{n}{u_0} + \frac{2u_1}{u_0^2} \left(\frac{n}{\pi}\right)^{1/2} + (u_1^2 - u_2 u_0 + u_0^3)/u_0^3 \dots \quad (1.10)$$

The most important feature to note in results (1.7) and (1.10) for  $S_n$  is that the successive terms in the expansion decrease by factors  $\text{const}/n$  in Eq. (1.6) and  $\text{const}/\sqrt{n}$  in Eq. (1.10), respectively, leading to a sharply convergent series. Thus, the corrections to the leading-order terms are quite small for large  $n$ .

The situation in 2D is more complicated. Let us consider the well-known case of a 2D square lattice. In this case,  $P(0, z)$  is known in a closed form (see Ref. 5),

$$P^{sq}(0, z) = F\left(\frac{1}{2}, \frac{1}{2}, 1, z^2\right) = (2/\pi) K(z^2), \quad (1.11)$$

where  $F$  is the hypergeometric function and  $K$  is the elliptic integral of the first kind. An expansion of  $P^{sq}(0, z)$  in powers of  $(1-z)$  yields

$$P^{sq}(0, z) = \frac{2}{\pi} \left[ -\frac{1}{2} \ln(1-z^2) + \psi(1) - \psi\left(\frac{1}{2}\right) \right] + \frac{1}{2\pi} \left[ -\frac{1}{2} \ln(1-z^2) + \psi(2) - \psi\left(\frac{3}{2}\right) \right] (1-z)^2 + \dots, \quad (1.12)$$

where  $\psi$ 's are the digamma functions. Substitution of Eq. (1.12) in Eq. (1.3) leads to the expansion

$$S^{sq}(0, z) = \frac{-\pi}{(1-z)^2 \ln(1-z^2)} \times \left[ \sum_{n=0}^{\infty} \left\{ \frac{2[\psi(1) - \psi(\frac{1}{2})]}{\ln(1-z)} \right\}^n + O(1-z)^2 + \dots \right]. \quad (1.13)$$

The leading term in the asymptotic behavior is

$$S_n \sim \pi n / \log n, \quad (1.14)$$

a result obtained by Montroll by using the Tauberian theorem.<sup>1</sup> The problem is, however, that the correction terms from the infinite sum in Eq. (1.13) die down only logarithmically with  $n$  and are quite important. This correction is important for *all* two-dimensional lattices. Zumofen and Blumen<sup>5</sup> recognize this problem and have replaced Eq. (1.14) by the formula

$$S_n \sim \pi n / \ln c_2 n, \quad (1.15)$$

and obtained  $c_2$  by Monte Carlo techniques for square, triangular, and hexagonal lattices. So far, their numerical estimate of  $c_2$  is the only correction available for the asymptotic behavior of  $S_n$ . Zumofen and Blumen have, however, computed  $S_n$  exactly for up to 500 steps using a recursion relation.

In this paper, we give an exact expansion of  $S_n$  for square, triangular, and hexagonal lattices, taking all logarithmic corrections into account. Since it does not appear in the random-walk literature that the generating function  $P(0, z)$  is known analytically for the triangular and hexagonal lattices, we first determine these results in Sec. II. Once  $S(z)$  is known, we analyze the asymptotic behavior of  $S_n$  using a contour integration and the saddle-point technique. The saddle-point method was introduced by Debye<sup>6</sup> for the purpose of evaluating integrals which are closely related to the contour integral of the Bessel function generating function. It has recently been used by Lipatov<sup>7</sup> and others<sup>8</sup> in a quantum theory context involving generating functions. It appears to be a very useful tool to problems in random-walk theory, also. Since in the random-walk literature there has been no mention of this technique, a somewhat pedagogical exposition is presented in Sec. III. In Sec. IV, an analysis of the results is presented.

## II. GENERATING FUNCTIONS

The general behavior of 2D generating function  $P(0, z)$  for square, triangular, and hexagonal lattices near  $z=1$  can be expressed as

$$P(0, z) = c_1 \ln(1-z) + c_2 + c_3 \ln(1-z)(1-z)^2 \dots \quad (2.1)$$

In earlier analyses of  $P(0, z)$  for triangular and hexagonal lattices, only  $c_1$  has been computed. For calculating the logarithmic corrections, it is necessary to calculate  $c_2$  also. Hence, we proceed as follows. The expression for  $P(0, z)$ , in terms of the structure factor  $\lambda(\theta)$ , is given by<sup>5</sup>

$$P(0, z) = \frac{1}{V_{Bz}} \int \frac{d\theta}{1 - z\lambda(\theta)} \quad z < 1 \quad (2.1a)$$

for a triangular lattice and by

$$P(0, z) = \frac{1}{V_{Bz}} \int \frac{d\theta}{1 - z^2 |\lambda(\theta)|^2} \quad z < 1 \quad (2.1b)$$

for a hexagonal lattice. In order to obtain both a simple form for  $\lambda(\theta)$  as well as a convenient Brillouin zone, the shape of the unit cell is transformed so that all lattice sites lie on a square lattice of length 1. For this lattice,

$$V_{Bz} = (2\pi)^2, \quad (2.2a)$$

$$\lambda^{\text{tr}}(\theta) = \frac{1}{3} [\cos \theta_x + \cos \theta_y + \cos(\theta_x + \theta_y)] \quad (2.2b)$$

and

$$\lambda^{\text{hex}}(\theta) = \frac{1}{3} [e^{i\theta_x} + 2 \cos \theta_y]. \quad (2.2c)$$

The generating function  $P(0, z)$  for the triangular lattice can be evaluated by substituting Eqs. (2.2a) and (2.2b) in Eq. (2.1a) to obtain

$$P^{\text{tr}}(0, z) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} d\theta_x d\theta_y \times \frac{1}{1 - \frac{1}{3} z [\cos \theta_x + \cos \theta_y + \cos(\theta_x + \theta_y)]} \quad (2.3)$$

Using the identity

$$\frac{1}{x} = \int_0^{\infty} e^{-tx} dt \quad (2.4)$$

in Eq. (2.3) and performing the integration over  $\theta_x$ , we obtain

$$P^{\text{tr}}(0, z) = \frac{1}{2\pi} \int_0^{\infty} dx \int_{-\pi}^{\pi} d\theta_y \exp[-x[1 - (z/3) \cos \theta_y]] \times I_0\left(\frac{xz}{3} \sqrt{(1 + \cos \theta_y)^2 + \sin^2 \theta_y}\right) \quad (2.5)$$

where  $I_0$  is the Bessel function. The  $x$  integration in Eq. (2.5) can now be performed yielding

$$P^{\text{tr}}(0, z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta_y \frac{1}{\sqrt{[1 - (z/3) \cos \theta_y]^2 - (2z^2/9)(1 + \cos \theta_y)}} \quad (2.6)$$

The expression on the right-hand side of Eq. (2.6) can be cast as an elliptic function by the transformation  $y = \cos \theta_y$ . The result is

$$P^{\text{tr}}(0, z) = \frac{3}{z\pi} \int_a^c \frac{dy}{\sqrt{(a-y)(b-y)(c-y)(y-d)}} \quad (2.7)$$

where

$$\begin{aligned} \frac{a}{b} &= \frac{3}{z} + 1 \pm \sqrt{\frac{6}{z} + 3} \\ c &= 1, \quad d = -1 \\ a > b > c > y > d, \quad \text{for } z < 1. \end{aligned} \quad (2.8)$$

From the tables of elliptic function,<sup>9(a),(b)</sup> we have the formulas

$$\int_u^c \frac{dx}{\sqrt{(a-x)(b-x)(c-x)(x-d)}} = \frac{2}{\sqrt{(a-c)(b-d)}} F(\gamma, r), \quad (2.9a)$$

$$\gamma = \arcsin \sqrt{\frac{(b-d)(c-u)}{(c-d)(b-u)}}, \quad (2.9b)$$

$$r = \sqrt{\frac{(a-b)(c-d)}{(a-c)(b-d)}}. \quad (2.9c)$$

When the lower limit  $u=d$ ,  $\gamma = \arcsin(1) = \pi/2$ . Using the identity  $F(\pi/2, r) = K(r)$ , where  $K(r)$  is a complete elliptic integral and  $r$  is the modulus, we obtain

$$P^{\text{tr}}(0, z) = \frac{6}{\pi z \sqrt{(a-c)(b-d)}} K \left( \sqrt{\frac{(a-b)(c-d)}{(a-c)(b-d)}} \right)^{1/2}. \quad (2.10)$$

As  $z \rightarrow 1$ , using the values [Eq. (2.8)] in Eq. (2.9c), it can be seen that the complementary modulus

$$r' \equiv \sqrt{1 - r^2} \quad (2.11a)$$

approaches zero as

$$r' = \sqrt{\frac{4}{3}(1-z)} \left[ 1 - \frac{1}{12}(1-z) + O(1-z)^2 \right]. \quad (2.11b)$$

Thus, as  $z \rightarrow 1$ , the following expansion of  $K(r)^{3(b)}$  can be made:

$$K(r) = \ln\left(\frac{4}{r'}\right) + \left(\frac{1}{2}\right)^2 \left( \ln \frac{4}{r'} - \frac{2}{1.2} \right) r'^2 + O(r')^4 + \dots \quad (2.12)$$

Thus, we can write

$$P^{\text{tr}}(0, z) = \frac{-\sqrt{3}}{2\pi z} \ln\left(\frac{1-z}{12}\right) [1 + O(1-z)]. \quad (2.13)$$

The generating function for the hexagonal lattice can be computed in a similar fashion. Substituting Eq. (2.2c) in Eq. (2.1b) and carrying out the algebra parallel to that from Eqs. (2.3)–(2.5), we arrive at

$$P^{\text{hex}}(0, z) = \frac{1}{\pi} \int_0^\pi \frac{d\theta_y}{\left\{ \left[ 1 - \frac{z^2}{9} (1 + 4 \cos^2 \theta_y) \right]^2 - \left( \frac{4z^2}{9} \cos \theta_y \right)^2 \right\}^{1/2}}. \quad (2.14)$$

The transformation  $\cos^2 \theta = y$  leads to the result

$$P^{\text{hex}}(0, z) = \frac{9}{4\pi z^2} \int_0^1 \frac{dy}{\sqrt{(a-y)(b-y)(c-y)(y-d)}}, \quad (2.15)$$

where

$$\left. \begin{matrix} a \\ b \end{matrix} \right\} = \frac{1}{4} \left[ 1 \pm \frac{3}{z} \right]^2, \quad c = 1, \quad d = 0. \quad (2.16)$$

Once again, paralleling the development from Eqs. (2.9)–(2.12), we arrive at the result

$$P^{\text{hex}}(0, z) = -\frac{3\sqrt{3}}{4\pi} \ln\left(\frac{1-z}{4}\right) [1 + O(1-z)]. \quad (2.17)$$

### III. EXPANSION IN INVERSE POWERS OF $\ln n$

For each 2D lattice, the generating function  $S(z)$  for the average number of distinct sites visited is of the form

$$S(z) = \frac{-A}{(1-z)^2 \ln(1-z/B)} [1 + O(1-z)], \quad (3.1)$$

and no other singularity is closer to the origin than that at  $z=1$ , and the singularity at  $z=-1$  has only the logarithmic singularity without the double pole multiplying it. The values of  $A$ ,  $B$  are  $\pi$ , 8 for the square lattice,  $2\pi/\sqrt{3}$ , 12 for the triangular lattice, and  $4\pi/3\sqrt{3}$ , 4 for the hexagonal lattice. In the technique to be presented it is important that  $S(z) \rightarrow \infty$  as  $z \rightarrow 1$  from the left.

The coefficient  $S_n$  is given by the Cauchy–Taylor formula

$$S_n = \frac{1}{2\pi i} \oint \frac{dz S(z)}{z^{n+1}}, \quad (3.2)$$

where the integration contour is a circle centered on the origin with a radius less than 1. The integrand is infinite at both  $z=0$  and  $z=1$ , and therefore has a saddle in between. As  $n$  is increased, the saddle gets sharper (i. e., the second derivative of the integrand approaches infinity). Therefore, saddle-point integration<sup>10</sup> provides an asymptotic expansion of  $S_n$ .

We write the integrand as

$$S(z)/z^{n+1} = f(z)g(z), \quad (3.3)$$

where the first factor

$$f(z) = 1/z^n (1-z)^2 \quad (3.4)$$

contains the most rapid variation of the integrand near the saddle. The second factor in the right-hand side of Eq. (3.2):

$$g(z) = \frac{S(z)(1-z)^2}{z} = \frac{-A}{\ln(1-z/B)} [1 + O(1-z)] \quad (3.5)$$

varies much more slowly. One factor of  $z^{-1}$  has been included in  $g$  so that the expansion will involve  $n$  rather than  $n+1$ .

It is not essential, and it only causes complications, to find the exact saddle of the integrand. It suffices to find the saddle of the rapidly varying part  $f$ . This saddle is at  $f'(z_s) = 0$ , which gives

$$n/z_s = 2/1 - z_s. \quad (3.6)$$

The solution for  $z_s$  is nearly  $z_s = 1$ , so the  $z_s$  on the left-hand side of Eq. (3.6) can be dropped. Moreover, dropping it makes the expansion variable more simple. Thus, we determine

$$z_s = 1 - (2/n). \quad (3.7)$$

The saddle-point integration is carried out by distorting the contour to lie on the line  $z = z_s + iy$ . Any singularities of  $S(z)$  that have been crossed in this distortion will provide corrections which fall exponentially in  $n$ , except for that at  $z = -1$ . The singularity at  $z = -1$  could be handled exactly as the one at  $z = 1$ , with the result that its contribution is down by a factor proportional to  $(-)^n/n^2$  from the  $z = 1$  contribution. It is also convenient to scale  $y$  in such a way that the shape of the saddle is independent of  $n$  for large  $n$ . This is accomplished by setting  $y = (2/n)\tau$ . The expansion can then be carried out under the assumption that  $\tau = O(1)$ .

In terms of the new contour parameterized by the variable  $\tau$ , the expression for  $S_n$  is

$$S_n = -\frac{1}{\pi n} \int_{-\infty}^{\infty} d\tau \frac{A[1 + O(1/n)]}{[(2/n)(1-i\tau)]^2 \ln[(2/Bn)(1-i\tau)] [1 - (2/n)(1-i\tau)]^n}. \quad (3.8)$$

In the denominator of the integrand, the factor

$$\left[1 - \frac{2}{n}(1-i\tau)\right]^n = \exp[-2(1-i\tau)] \left[1 + O\left(\frac{1}{n}\right)\right] \quad (3.9)$$

is nearly independent of  $n$ . Thus,

$$S_n = \frac{An}{4\pi} \int_{-\infty}^{\infty} d\tau \frac{\exp[-2(1-i\tau)] [1 + O(1/n)]}{(1-i\tau)^2 [\ln(Bn/2) - \ln(1-i\tau)]} \\ \sim \frac{An}{4\pi \ln(Bn/2)} \sum_{j=0}^{\infty} \int_{-\infty}^{\infty} d\tau \left(\frac{\ln(1-i\tau)}{\ln(Bn/2)}\right)^j \\ \times \frac{\exp[-2(1-i\tau)]}{(1-i\tau)^2} \left[1 + O\left(\frac{1}{n}\right)\right], \quad (3.10)$$

which already exhibits the expansion in inverse powers of  $\ln(Bn/2)$ . The interchange of the summation and integration leads to a divergent asymptotic series.<sup>11</sup>

The quadratures involved in Eq. (3.10) can be simplified by the observation that  $\ln(1-i\tau)$  is the derivative of a power  $(1-i\tau)$  with respect to the power:

$$\ln(1-i\tau)(1-i\tau)^{-\beta} = -\partial_{\beta}(1-i\tau)^{-\beta}. \quad (3.11)$$

So,

$$S_n = \frac{An}{4\pi} \frac{1}{[\ln(Bn/2) + \partial_{\beta}]} \int_{-\infty}^{\infty} d\tau \frac{\exp[-2(1-i\tau)]}{(1-i\tau)^{\beta}} \Big|_{\beta=2} \\ \times \left[1 + O\left(\frac{1}{n}\right)\right]. \quad (3.12)$$

The remaining integral can be analytically evaluated:

$$S_n = \frac{An}{4} \frac{1}{[\ln(Bn/2) + \partial_{\beta}]} \frac{2^{\beta}}{\Gamma(\beta)} \Big|_{\beta=2} \left[1 + O\left(\frac{1}{n}\right)\right] \\ = An \frac{1}{(\ln Bn + \partial_{\beta})} \frac{1}{\Gamma(\beta)} \Big|_{\beta=2} \left[1 + O\left(\frac{1}{n}\right)\right], \quad (3.13)$$

where  $2^{\beta}$  has been commuted through the operator,

$$\partial_{\beta}[2^{\beta}F(\beta)] = 2^{\beta}(\ln 2 + \partial_{\beta})F(\beta).$$

TABLE I. The expansion coefficients for the leading series in  $S_n$  [Eq. (3.13)].

$j$	$(-\partial_{\beta})^j \frac{1}{\Gamma(\beta)} \Big _{\beta=2}$
0	1.000 000
1	0.422 784
2	-0.466 187
3	-1.146 547
4	-0.589 260
5	2.117 429
6	5.776 76
7	4.053 82
8	-14.549 0
9	-52.833 9
10	-63.670 4
11	103.344
12	641.144
13	1279.49
14	-13.91
15	-8206.5
16	-26 647.0
17	-32 844.0
18	76 848.0
19	513 400.0
20	1 275 000.0

TABLE II.  $S_n$ , the series of inverse logs, and the fit to  $S_n$ , including the next leading terms.

Hexagonal	Exact	$[nc_j/(\ln n)^j]$	Fit
2	2.6667	(2, 37)	2.69
5	4.5185	(4, 2527)	4.5161
10	7.1733	6, 9450	7.1757
20	11.8944	11, 6895	11.8947
50	24.2683	24, 0889	24.2680
100	42.6343	42, 4706	42.6339
200	76.0461	76, 8958	76.0459
500	166.3616	166, 2262	166.3618
Square			
2	2.7500	(2, 3774)	2.7822
5	4.8437	4, 5109	4.8421
10	7.8814	7, 5925	7.8837
20	13.3396	13, 0797	13.3395
50	27.8136	27, 5855	27.8129
100	49.5041	49, 2958	49.5036
200	89.2576	89, 0661	89.2574
500	197.5412	197, 3684	197.5415
Triangular			
2	2.8333	2, 4109	2.8514
5	5.0555	4, 6940	5.0585
10	8.3371	8, 0144	8.3368
20	14.2514	13, 9612	14.2502
50	30.0342	29, 7790	30.0332
100	53.8063	53, 5728	53.8058
200	97.5448	97, 3297	97.5448
500	217.1643	216, 9698	217.1650

The expansion is

$$S_n \sim \frac{An}{\ln Bn} \sum_{j=0}^{\infty} \left(-\frac{\partial_{\beta}}{\ln Bn}\right)^j \frac{1}{\Gamma(\beta)} \Big|_{\beta=2} \left[1 + O\left(\frac{1}{n}\right)\right]. \quad (3.14)$$

If more care had been taken in the various expansions, the  $1/n$  terms could have been retained. The only fact we note here is that the correction terms are

$$\frac{n}{\ln n} O(1/n) = O(1/\ln n).$$

#### IV. NUMERICAL EXPRESSIONS

From the solution (3.14) for  $S_n$ , it is clear that two improvements can be made on the existing fit of Zumofen and Blumen. They assumed the form

$$S_n \approx \frac{An}{\ln c_2 n} + c_3.$$

We now know that the first term can be replaced by the entire series in Eq. (3.14), and that the second term actually should be  $O(1/\ln n)$  rather than constant. As a result of these improvements, the details of their fit, such as the values of  $c_2$  and the amount of correction ( $c_3$  in the above expression), differ slightly.

The coefficients of  $(-1/\ln Bn)^j$  in Eq. (3.14) differ by a factor of  $j!$  from the Taylor coefficients of  $1/\Gamma(2+z)$ . The Taylor coefficients of  $1/\Gamma(z)$  are tabulated in Ref. 12 and, by use of the recursion formula for the gamma function, the coefficients in Eq. (3.14) can easily be constructed. They are tabulated in Table I.

TABLE III. The determined values  $A$  and  $B$ , and the fit parameters  $C$  and  $D$ .  $A^{-1}$ ,  $B^{-1}$ ,  $C$ , and  $D$  all decrease as the number of nearest lattice neighbors increases.

Lattice	$A$	$B$	$C$	$D$
Hexagonal	2.4184	4	2.5465	0.7767
Square	3.1416	8	2.0556	0.5987
Triangular	3.6276	12	1.9119	0.5167

For large values of  $n$ , the sum in Eq. (3.14) can then be evaluated. For the very smallest values of  $n$ , a re-summation of this asymptotic series is necessary, since the terms increase from the beginning. In Table II, this sum is compared to the exact  $S_n$  as evaluated by Zumofen and Blumen, for the three lattices. Their proposed form,  $An/\ln c_2 n$ , for the part of  $S_n$  given by this sum, can incorporate the second term in the series, but does not do well with the remainder. The third coefficient, in an expansion of this form in powers of  $1/\ln Bn$  is 0.17875 if the second term is 0.42278, while the actual coefficient -0.46619 has the opposite sign. If the second term is made to be exactly correct,

$$c_2 = Be^\gamma/e = 5.24176, \quad (4.1)$$

where  $\gamma$  is Euler's constant 0.57722, rather than

$$c_2 = 2B/e = 5.88607, \quad (4.2)$$

as suggested by their fit. ( $B=8$  for the numerical values.)

If the sum is equated to

$$An/\ln[c_2(n)n], \quad (4.3)$$

where  $c_2$  is allowed to be a function of  $n$ ,  $c_2(n)$  varies from 6.51 at  $n=5$  to 5.29 at  $n=10^{32}$  to 5.24 at  $n=\infty$  for the square lattice, and is approximately, but not very accurately, a constant. Its value at  $\infty$  is approached rather slowly.

An important consequence of Eq. (3.13) is that the corrections to the  $n/(\ln n)^j$  series is  $O(1/\ln n)$  rather than  $O(1)$ . We have not evaluated these terms explicit-

ly, but rather we have fit

$$S_n - \text{series in } \frac{n}{(\ln n)^j} = \frac{1}{C + D \ln n}.$$

The fit values of  $C$  and  $D$  are listed in Table III, along with the determined constants  $A$  and  $B$  of Eq. (3.13). The precise values of  $C$  and  $D$  are of no particular significance, since they result from a fit, but their trend is clear. The fit values of  $S_n$  are listed in Table II and are seen to fit extremely well except at  $n=2$ .

In conclusion, the contour integration combined with the saddle point technique yields very accurate results for  $S_n$  for 2D lattices.

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