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Self-avoiding walk on a three-dimensional Manhattan lattice

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Abstract. We have extended the definition of the Manhattan lattice from two-dimensional to three-dimensional (3D) spaces. The number of self-avoiding walks on the 3D Manhattan lattice, C_n, and their mean-square end-to-end distances, $\langle R_n^2 \rangle$, were counted exactly up to 31 and 30 steps, respectively. Analysis using the method of the Dlog Padé approximant gave the exponents $\gamma = 1.1615 \pm 0.0002$ and $\nu = 0.5870 \pm 0.0025$, which are in good agreement with corresponding values for self-avoiding walks on the ordinary 3D lattice. This result suggests that self-avoiding walks on the 3D Manhattan lattice belong to the same universality class as self-avoiding walks on the ordinary 3D lattice.

The random walk on a lattice has been studied broadly and systematically since Polya [1] proposed it in 1921. In addition to its theoretical significance for mathematicians [2], the model of the lattice walk finds many applications in physics, chemistry and biology [3, 4]. Self-avoiding walks (SAWs) are a subset of random walks, where no site can be occupied more than once. This simple restriction introduces great complexity into the SAW problem. Up to now, only a few rigorous analytic solutions for the many problems of SAW have been given. Therefore, attention has turned to computer methods; especially exact enumeration and the Monte Carlo method [5–7].

Self-avoiding walks play an important role in conformational simulations, Ising models, percolation and other studies of polymer models. They have become standard tools in statistical mechanics and can be divided into two classes: SAWs on a normal (i.e. isotropic) lattice and SAWs on an oriented lattice. The latter are especially important for oriented polymers [8–10].

The Manhattan lattice is one of the simplest oriented lattices. It is a square lattice in which adjacent rows (or columns) have antiparallel orientations. It is so named for its similarity to the traffic pattern in Manhattan.

In previous studies [11–15] the investigation of SAWs on the Manhattan lattice has been confined to two-dimensional (2D) space. Here we extend the Manhattan lattice from a two-dimensional plane to three-dimensional (3D) space. First, we define a three-dimensional Cartesian coordinate system, in which the positive directions of x, y and z axes are given in a right-handed sense as shown in figure 1. The walk begins at the origin and the first step is constrained to be in one of the three positive directions of the x, y or z axes. Thus, after the first step the walker arrives at one of the three points (1, 0, 0), (0, 1, 0) or (0, 0, 1). Obviously, the walking rule here is different from that for SAWs on the simple cubic lattice. In order to determine the direction for the next step of the walker on the general point (x_i, y_i, z_i), the following rule was adopted. In the x-direction the walker goes in the positive direction when the absolute value $|y_i + z_i|$ is even and in the negative direction when $|y_i + z_i|$ is odd. Similarly,

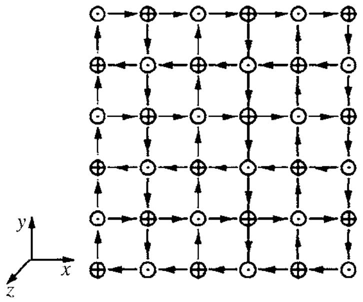

Figure 1. A plane representation of the lattice orientation for the three-dimensional Manhattan lattice (in the z-direction: $\oplus$ backward, $\odot$ forward).

Table 1. Conformational numbers C_n and the mean-square end-to-end distance $\langle R_n^2 \rangle$ obtained by the exact enumeration for SAWs with length n on the three-dimensional Manhattan lattice.

n	C_n	$\langle R_n^2 \rangle$	n	C_n	$\langle R_n^2 \rangle$
1	3	1.000 000	17	48 401 211	33.955 990
2	9	2.666 667	18	134 514 255	36.298 032
3	27	4.111 111	19	373 860 519	38.643 061
4	75	6.080 000	20	1 035 667 281	41.124 690
5	213	7.985 915	21	2 872 971 003	43.559 105
6	603	9.870 647	22	7 970 116 713	45.993 682
7	1 707	11.804 921	23	22 111 736 367	48.430 193
8	4 749	13.958 307	24	61 204 173 297	50.985 755
9	13 311	16.042 596	25	169 573 085 367	53.500 036
10	37 287	18.132 110	26	469 846 057 713	56.014 039
11	104 463	20.229 316	27	1 301 892 806 043	58.529 309
12	290 067	22.524 300	28	3 601 277 482 413	61.150 405
13	808 479	24.752 543	29	9 968 856 732 885	63.734 708
14	2 253 255	26.983 359	30	27 596 559 129 417	66.318 475
15	6 280 407	29.218 844	31	76 398 074 633 469	
16	17 416 323	31.614 959			

for the y coordinate the walker moves in the positive direction for even $|x_i + z_i|$ and in the negative direction for odd $|x_i + z_i|$ and in the z-direction the walker moves in the positive direction for even $|x_i + y_i|$ and in the negative direction for odd $|x_i + y_i|$. With this convention the 3D Manhattan lattice is a natural extension of the familiar 2D Manhattan lattice and if $z_i \equiv 0$, the 3D Manhattan lattice reduces to the 2D one.

Exact enumeration [16] is a computer method in which one fully enumerates all the possible conformations for self-avoiding walks from a given origin and is then able to evaluate the properties of each conformation. The number of conformations, C_n, and the mean-square end-to-end distances, $\langle R_n^2 \rangle$, obtained by the exact enumeration for SAWs on the 3D Manhattan lattice are listed in table 1.

The generating function for a SAW can be written as [16]

$$f(x) = 1 + \sum_{n\geqslant 1} C_n x^n \sim A(1 - \mu x)^{-\gamma} \tag{1}$$

where n is the step number (the chain length). The number of conformations is given by $C_n \sim \mu^n n^{\gamma-1}$, where μ is the connective constant and γ is a universal critical exponent. Defining a parameter

$$\mu_n \equiv C_n / C_{n-1} \sim [1 + (\gamma - 1)/n]\mu \tag{2}$$

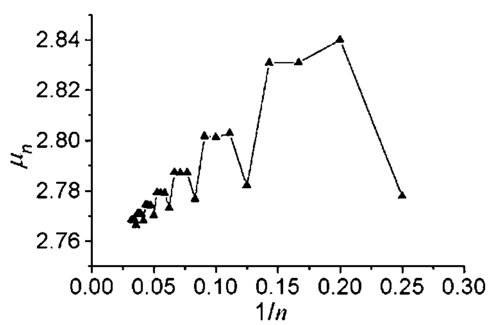

Figure 2. A plot of μ_n as a function of $1/n$ for self-avoiding walks with length n on the three-dimensional Manhattan lattice.

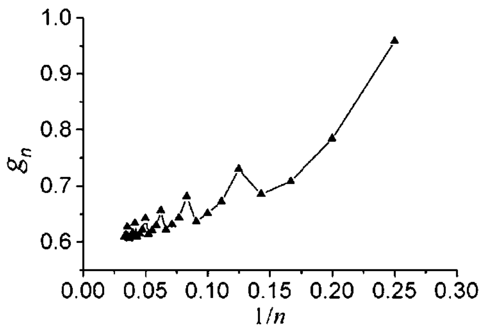

Figure 3. A plot of g_n as a function of $1/n$ for self-avoiding walks with length n on the three-dimensional Manhattan lattice.

and plotting μ_n against $1/n$, we extract μ and γ by extrapolating to $1/n = 0$.

Similarly, the generating function for the mean-square end-to-end distance can be written as

$$g(x) = 1 + \sum_{n\geqslant 1} \langle R_n^2 \rangle x^n \sim B(1-x)^{-\gamma} \tag{3}$$

where $\langle R_n^2 \rangle \sim n^{2\nu}$ is the mean-square end-to-end distance of n-step SAWs and ν is a universal critical exponent. Through the parameter

$$g_n = \tfrac{1}{2} n (\langle R_{n+1}^2 \rangle / \langle R_n^2 \rangle - 1) \tag{4}$$

the extrapolation to $1/n = 0$ gives an estimate for ν.

It is interesting that there are period-four oscillations in figures 2 and 3. This is significantly different from the well known odd–even oscillation of SAWs on the simple cubic lattice. Similar period-four oscillations which correspond to singularities of $f(x)$ and $g(x)$ at poles $x = -x_c$ are also observed for SAWs on the 2D Manhattan lattice [11, 12]. These oscillations complicate the estimation of γ or ν by simple extrapolation, so we have applied the Padé approximant method [17] to analyse the critical exponents.

The Padé approximant is a series analysis method widely used in statistical mechanics. The $[N/D]$ Padé approximant for $f(x)$ is the quotient of two polynomials of degrees N and D, the coefficients of which are chosen in such a way that the expansion of the $P_N(x)/Q_D(x)$ agrees with the exact expansions of $f(x)$ up to the x^{N+D} term. Ordinarily one sets

$$f(x) = \frac{P_N(x)}{Q_D(x)} = \frac{p_0 + p_1 x + \cdots + p_N x^N}{1 + q_1 x + \cdots + q_D x^D} \tag{5}$$

and requires $P_N(x)$ and $Q_D(x)$ to satisfy

$$Q_D(x) f(x) - P_N(x) = \mathrm{O}\big(x^{N+D+1}\big). \tag{6}$$

However, this method is effective only if $f(x)$ has at most one singularity. For a chain-generating function of SAWs on the 3D Manhattan lattice with their multiple singularities one should use the Dlog Padé approximant [17], where the generating function $f(x)$ is replaced by its logarithmic derivative

$$F(x) = \frac{\mathrm{d}}{\mathrm{d}x} \ln f(x) = \frac{f'(x)}{f(x)} = \frac{P(x)}{Q(x)}. \tag{7}$$

Table 2. Unbiased estimated values of μ, γ and ν for the three-dimensional Manhattan lattice using the method of the $[N/D]$ Dlog Padé approximant.

$[N/D]$	μ	γ	ν	$[N/D]$	μ	γ	ν
[13/12]	2.752 819	1.161 433	0.588 393	[14/14]	2.752 804	1.161 576	0.588 248
[13/13]	2.752 629	1.164 339	0.582 343	[14/15]	2.752 804	1.161 624	0.588 827
[13/14]	2.752 789	1.161 746	0.588 964	[15/14]	2.752 804	1.161 566	0.593 153
[14/13]	2.752 804	1.161 567	0.581 177	[15/15]	2.752 834	1.161 338	

The pole of the $[N/D]$ approximants closest to the origin on the positive real axis and the residue at this pole provide estimated values for x_c and $-\gamma$, respectively.

Similarly, we have

$$G(x) = \frac{\mathrm{d}}{\mathrm{d}x} \ln g(x) = \frac{g'(x)}{g(x)} = \frac{P(x)}{Q(x)}. \tag{8}$$

The residue at the pole $x_c = 1$ is equal to $-1 - 2\nu$.

The connective constant μ and the critical exponents γ and ν obtained by using the Dlog Padé approximant are listed in table 2.

Summarizing the calculated results for self-avoiding walks on the 3D Manhattan lattice, we obtain

$$\begin{aligned} \mu &= 2.7528 \pm 0.0001 \\ \gamma &= 1.1615 \pm 0.0002 \\ \nu &= 0.5870 \pm 0.0025. \end{aligned} \tag{9}$$

In comparison with the existing theoretical predictions for the exponents γ and ν obtained using the renormalization group (RG), Monte Carlo (MC) and exact enumeration (EE),

$$\gamma = \begin{cases} 1.1613 \pm 0.0021 & \text{EE [18]} \\ 1.1619 \pm 0.0001 & \text{EE [19]} \\ 1.1608 \pm 0.0003 & \text{MC [20]} \end{cases} \tag{10}$$

$$\nu = \begin{cases} 0.5880 \pm 0.0010 & \text{RG [21]} \\ 0.5877 \pm 0.0013 & \text{MC [22]} \\ 0.5880 \pm 0.0018 & \text{MC [23]} \end{cases} \tag{11}$$

it was found that our results of SAWs on the 3D Manhattan lattice are consistent with the above values. This conclusion indicates that SAWs on the 3D Manhattan lattice belong to the same universality class as that of the ordinary SAWs, which provides substantial support to the recently proposed view of Caracciolo *et al* [11].

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