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# Series Enumeration Study of the Rod-to-Coil Transition of Linear Polymer Chains

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The scaling of the number, the mean-squared end-to-end distance, and the mean displacement in the direction of the first step, for semiflexible chains on the square, triangular and simple cubic lattices are investigated by enumerating self-avoiding walks classified according to the number of turns. Simple scaling forms are found to describe adequately all the available data. Estimates of the scaling functions are obtained and compared with the Gaussian results, when available. Self-avoidance effects are suppressed but do not vanish identically in $d=3$, contrary to recent theoretical expectations.

## 1. Introduction

The rod-to-coil transition of linear polymer chains has attracted attention recently [1–5], due to unexpected scaling properties. The traditional description of chain persistency within solvable Gaussian-type models [6–8] focuses on the concept of the persistence length $\lambda$. The linear dimension, say $D$, of a chain scales with $N$, the number of monomers in the chain, as

$$D/(\mathrm{N}a) \simeq M(\mathrm{N}a/\lambda), \tag{1.1}$$

with $M(x) \to 1$ for $x \to 0$, and $M(x) \sim x^{\nu-1}$ for $x \gg 1$, and where it is assumed that all the lengths involved are much larger than a typical microscopic length scale, $a$. The chain dimensions can be measured by the even moments of the end-to-end distance vector, $\mathbf{R}$,

$$D_k \propto \langle \mathbf{R}^{2k} \rangle^{1/(2k)}, \tag{1.2}$$

where $\langle\ \rangle$ denote configurational average for fixed $N$. Recently, some surprising features of the scaling law (1.1) have been found. For Gaussian models, the scaling functions $M_k$, corresponding to $D_k$, are not universal but depend on the microscopic details of the model [9, 10] (e.g., the lattice structure). Lattice model results for $M_k$ also differ with the scaling found in the continuous "worm-like chain" theory [8, 6]. This absence of the scaling limit in the field-theoretical sense (lattice spacing going to zero) needs further investigation and understanding.

For lattice self-avoiding walk (SAW) models, a strong suppression of the self-avoidance effects as the persistence length of the chain increases was discovered both numerically and by analytic perturbative arguments [1, 3–5]. Nakanishi [4] proposed Flory-type arguments suggesting complete suppression of self-avoidance for $d>2$, i.e., the scaling functions $M_k$ should assume Gaussian values, according to his theory. It is, however, not clear if the Flory argument is valid for all $d>2$, or only in the $d \to \infty$ limit. Perturbative analyses of the type invoked in [3] suggest that the second possibility is more probable. Another interesting feature that can be easily seen by applying the techniques of [3] is that the SAW scaling functions are lattice dependent. This property is, in fact, quite common to various dimensional crossover models and suggests, as in the Gaussian case, that no all-encompassing field-theoretical continuum description exists for the rod-to-coil transition.

In this work, we consider SAW of $N$ steps on the square (SQ), triangular (TR) and simple cubic (SC) lattices. For each *turn* of a walk (90° for SQ and SC; both 60° and 120° turns for the TR), a weight $w$ is assigned. In this lattice model the elongated rod-like configurations dominate when $wN$ is small [1–3], while coiled states are dominant for $N \gg 1/w$. Thus the persistence length $\lambda$ is proportional to $1/w$.

By standard methods [11], we enumerated SAWs classified by the number of turns, $0 \leqq T \leqq N-1$, for $N \leqq 22$ on the SQ, and $N \leqq 16$ on the TR and SC lattices, and calculated $c(N, T)$, the number of walks, as well as $\langle R^2(N, T)\rangle$, the average squared end-to-end distance. In the enumeration, the *first step* of the walk is chosen along the $+X$ axis, so that the number of such walks,

$$C(N, T) \equiv c(N, T)/q, \tag{1.3}$$

and the sum of their squared end-to-end distances,

$$Q(N, T) \equiv c(N, T)\langle R^2(N, T)\rangle/q, \tag{1.4}$$

where $q$ is the lattice coordination number, are listed in Tables 1–3. For the SQ and SC lattices, we also calculated the linear moment $\langle X(N, T)\rangle$, which measures the average coordinate along the direction $(+X)$ of the first step. This quantity was studied for flexible SAWs (i.e., $w=1$) in [12]. (See also [13] for a related property of Gaussian random walks.) The data for this moment are listed as

$$S(N, T) \equiv C(N, T)\langle X(N, T)\rangle, \tag{1.5}$$

in Tables 1 and 3.

In the following sections we examine the scaling properties of the weighted averages (generating functions),

$$C_N(w) = \sum_{T=0}^{N-1} C(N, T)\, w^T, \tag{1.6}$$

$$R_N^2(w) = \left[\sum_{T=0}^{N-1} Q(N, T)\, w^T\right] \Big/ C_N(w), \tag{1.7}$$

$$X_N(w) = \left[\sum_{T=0}^{N-1} S(N, T)\, w^T\right] \Big/ C_N(w). \tag{1.8}$$

**Table 1.** Square lattice enumeration data for $N=1, \ldots, 22$. The first step is along the $+X$ axis. The quantities $C$, $Q$ and $S$ are defined in Sect. 1

| $N$ | $T$ | $C(N, T)$ | $Q(N, T)$ | $S(N, T)$ |
|---|---|---|---|---|
| 1 | 0 | 1 | 1 | 1 |
| 2 | 0 | 1 | 4 | 2 |
| 2 | 1 | 2 | 4 | 2 |
| 3 | 0 | 1 | 9 | 3 |
| 3 | 1 | 4 | 20 | 6 |
| 3 | 2 | 4 | 12 | 4 |
| 4 | 0 | 1 | 16 | 4 |
| 4 | 1 | 6 | 56 | 12 |
| 4 | 2 | 12 | 72 | 16 |
| 4 | 3 | 6 | 32 | 8 |
| 5 | 0 | 1 | 25 | 5 |
| 5 | 1 | 8 | 120 | 20 |
| 5 | 2 | 24 | 240 | 40 |
| 5 | 3 | 28 | 220 | 38 |
| 5 | 4 | 10 | 74 | 14 |
| 6 | 0 | 1 | 36 | 6 |
| 6 | 1 | 10 | 220 | 30 |
| 6 | 2 | 40 | 600 | 80 |
| 6 | 3 | 70 | 844 | 114 |
| 6 | 4 | 58 | 592 | 84 |
| 6 | 5 | 16 | 160 | 24 |
| 7 | 0 | 1 | 49 | 7 |
| 7 | 1 | 12 | 364 | 42 |
| 7 | 2 | 60 | 1260 | 140 |
| 7 | 3 | 144 | 2400 | 264 |
| 7 | 4 | 184 | 2584 | 292 |
| 7 | 5 | 116 | 1460 | 170 |
| 7 | 6 | 26 | 330 | 40 |
| 8 | 0 | 1 | 64 | 8 |
| 8 | 1 | 14 | 560 | 56 |
| 8 | 2 | 84 | 2352 | 224 |
| 8 | 3 | 252 | 5664 | 528 |
| 8 | 4 | 440 | 8264 | 780 |
| 8 | 5 | 428 | 7176 | 688 |
| 8 | 6 | 218 | 3384 | 336 |
| 8 | 7 | 42 | 656 | 68 |
| 9 | 0 | 1 | 81 | 9 |
| 9 | 1 | 16 | 816 | 72 |
| 9 | 2 | 112 | 4032 | 336 |
| 9 | 3 | 408 | 11752 | 948 |
| 9 | 4 | 900 | 21684 | 1752 |
| 9 | 5 | 1200 | 25520 | 2068 |
| 9 | 6 | 954 | 18514 | 1532 |
| 9 | 7 | 408 | 7480 | 636 |
| 9 | 8 | 68 | 1268 | 112 |
| 10 | 0 | 1 | 100 | 10 |
| 10 | 1 | 18 | 1140 | 90 |
| 10 | 2 | 144 | 6480 | 480 |
| 10 | 3 | 612 | 22184 | 1580 |
| 10 | 4 | 1636 | 49560 | 3508 |
| 10 | 5 | 2760 | 73792 | 5200 |
| 10 | 6 | 3008 | 72608 | 5176 |
| 10 | 7 | 2000 | 45136 | 3276 |
| 10 | 8 | 736 | 15928 | 1192 |
| 10 | 9 | 110 | 2396 | 186 |
| 11 | 0 | 1 | 121 | 11 |
| 11 | 1 | 20 | 1540 | 110 |
| 11 | 2 | 180 | 9900 | 660 |
| 11 | 3 | 880 | 38944 | 2480 |
| 11 | 4 | 2760 | 102216 | 6428 |
| 11 | 5 | 5656 | 184296 | 11456 |

**Table 1** (continued)

| $N$ | $T$ | $C(N,T)$ | $Q(N,T)$ | $S(N,T)$ |
|---|---|---|---|---|
| 11 | 6 | 7834 | 229554 | 14336 |
| 11 | 7 | 7136 | 193632 | 12188 |
| 11 | 8 | 4100 | 105156 | 6760 |
| 11 | 9 | 1328 | 32912 | 2168 |
| 11 | 10 | 178 | 4450 | 304 |
| 12 | 0 | 1 | 144 | 12 |
| 12 | 1 | 22 | 2024 | 132 |
| 12 | 2 | 220 | 14520 | 880 |
| 12 | 3 | 1210 | 64544 | 3720 |
| 12 | 4 | 4360 | 194712 | 11028 |
| 12 | 5 | 10492 | 412544 | 22988 |
| 12 | 6 | 17656 | 622608 | 34660 |
| 12 | 7 | 20448 | 665136 | 37116 |
| 12 | 8 | 16094 | 490296 | 27708 |
| 12 | 9 | 8106 | 236096 | 13596 |
| 12 | 10 | 2342 | 66344 | 3928 |
| 12 | 11 | 282 | 8144 | 500 |
| 13 | 0 | 1 | 169 | 13 |
| 13 | 1 | 24 | 2600 | 156 |
| 13 | 2 | 264 | 20592 | 1144 |
| 13 | 3 | 1620 | 102084 | 5370 |
| 13 | 4 | 6590 | 348078 | 17918 |
| 13 | 5 | 18252 | 847772 | 42742 |
| 13 | 6 | 36164 | 1504196 | 75432 |
| 13 | 7 | 50904 | 1947704 | 97332 |
| 13 | 8 | 51026 | 1819042 | 91590 |
| 13 | 9 | 35156 | 1189268 | 60502 |
| 13 | 10 | 15806 | 514086 | 26712 |
| 13 | 11 | 4116 | 131012 | 6966 |
| 13 | 12 | 452 | 14716 | 808 |
| 14 | 0 | 1 | 196 | 14 |
| 14 | 1 | 26 | 3276 | 182 |
| 14 | 2 | 312 | 28392 | 1456 |
| 14 | 3 | 2106 | 155316 | 7518 |
| 14 | 4 | 9550 | 590744 | 27888 |
| 14 | 5 | 29876 | 1626496 | 74960 |
| 14 | 6 | 68132 | 3318832 | 151588 |
| 14 | 7 | 112972 | 5054104 | 229200 |
| 14 | 8 | 137698 | 5723712 | 260204 |
| 14 | 9 | 120790 | 4742588 | 216914 |
| 14 | 10 | 74266 | 2783536 | 129056 |
| 14 | 11 | 30034 | 1090812 | 51566 |
| 14 | 12 | 7124 | 254184 | 12316 |
| 14 | 13 | 724 | 26312 | 1312 |
| 15 | 0 | 1 | 225 | 15 |
| 15 | 1 | 28 | 4060 | 210 |
| 15 | 2 | 364 | 38220 | 1820 |
| 15 | 3 | 2688 | 228704 | 10248 |
| 15 | 4 | 13440 | 960064 | 41832 |
| 15 | 5 | 46932 | 2949012 | 125050 |
| 15 | 6 | 121106 | 6804810 | 285104 |
| 15 | 7 | 231268 | 11920884 | 494026 |
| 15 | 8 | 332472 | 15883336 | 657580 |
| 15 | 9 | 354584 | 15963064 | 661480 |
| 15 | 10 | 277706 | 11876394 | 496840 |
| 15 | 11 | 153528 | 6319304 | 267544 |
| 15 | 12 | 56568 | 2263816 | 97840 |
| 15 | 13 | 12304 | 485776 | 21444 |
| 15 | 14 | 1160 | 46632 | 2120 |
| 16 | 0 | 1 | 256 | 16 |
| 16 | 1 | 30 | 4960 | 240 |
| 16 | 2 | 420 | 50400 | 2240 |
| 16 | 3 | 3360 | 327488 | 13664 |

**Table 1** (continued)

| $N$ | $T$ | $C(N,T)$ | $Q(N,T)$ | $S(N,T)$ |
|---|---|---|---|---|
| 16 | 4 | 18368 | 1504048 | 60872 |
| 16 | 5 | 70748 | 5099648 | 200388 |
| 16 | 6 | 203784 | 13132352 | 508568 |
| 16 | 7 | 440488 | 26023160 | 994216 |
| 16 | 8 | 729496 | 39900528 | 1517920 |
| 16 | 9 | 917760 | 47193760 | 1791604 |
| 16 | 10 | 874158 | 42599624 | 1625056 |
| 16 | 11 | 615382 | 28736416 | 1105604 |
| 16 | 12 | 309874 | 13976856 | 545356 |
| 16 | 13 | 104586 | 4609208 | 183296 |
| 16 | 14 | 21036 | 916296 | 37264 |
| 16 | 15 | 1842 | 81984 | 3432 |
| 17 | 0 | 1 | 289 | 17 |
| 17 | 1 | 32 | 5984 | 272 |
| 17 | 2 | 480 | 65280 | 2720 |
| 17 | 3 | 4144 | 457744 | 17864 |
| 17 | 4 | 24584 | 2283176 | 86240 |
| 17 | 5 | 103632 | 8470480 | 309924 |
| 17 | 6 | 329666 | 24084258 | 866544 |
| 17 | 7 | 795876 | 53274052 | 1886010 |
| 17 | 8 | 1493382 | 92426230 | 3250082 |
| 17 | 9 | 2164776 | 125834632 | 4400668 |
| 17 | 10 | 2433582 | 133709806 | 4685292 |
| 17 | 11 | 2083468 | 109450524 | 3849982 |
| 17 | 12 | 1336186 | 67494874 | 2399986 |
| 17 | 13 | 615912 | 30217656 | 1088244 |
| 17 | 14 | 192136 | 9229040 | 339044 |
| 17 | 15 | 35876 | 1708644 | 64030 |
| 17 | 16 | 2936 | 143112 | 5512 |
| 18 | 0 | 1 | 324 | 18 |
| 18 | 1 | 34 | 7140 | 306 |
| 18 | 2 | 544 | 83232 | 3264 |
| 18 | 3 | 5032 | 626448 | 22968 |
| 18 | 4 | 32200 | 3372432 | 119448 |
| 18 | 5 | 147340 | 13589752 | 465420 |
| 18 | 6 | 512974 | 42290016 | 1421544 |
| 18 | 7 | 1368070 | 103308836 | 3410206 |
| 18 | 8 | 2867640 | 200126536 | 6546824 |
| 18 | 9 | 4710626 | 308375172 | 10010594 |
| 18 | 10 | 6103342 | 377271120 | 12233772 |
| 18 | 11 | 6167174 | 363612964 | 11806054 |
| 18 | 12 | 4810672 | 272135272 | 8893908 |
| 18 | 13 | 2823332 | 154477240 | 5099468 |
| 18 | 14 | 1202452 | 64043944 | 2144380 |
| 18 | 15 | 347864 | 18209664 | 621184 |
| 18 | 16 | 60698 | 3153944 | 109800 |
| 18 | 17 | 4688 | 248288 | 8864 |
| 19 | 0 | 1 | 361 | 19 |
| 19 | 1 | 36 | 8436 | 342 |
| 19 | 2 | 612 | 104652 | 3876 |
| 19 | 3 | 6048 | 841536 | 29088 |
| 19 | 4 | 41520 | 4863408 | 162120 |
| 19 | 5 | 205092 | 21154100 | 680654 |
| 19 | 6 | 775808 | 71518440 | 2254776 |
| 19 | 7 | 2265524 | 191249636 | 5909630 |
| 19 | 8 | 5249822 | 409255470 | 12509202 |
| 19 | 9 | 9636192 | 704293344 | 21311400 |
| 19 | 10 | 14155602 | 975442730 | 29421464 |
| 19 | 11 | 16487416 | 1082638040 | 32594284 |
| 19 | 12 | 15183378 | 954184306 | 28845550 |
| 19 | 13 | 10837688 | 657423400 | 19989628 |
| 19 | 14 | 5876904 | 345579696 | 10630576 |
| 19 | 15 | 2320512 | 133362752 | 4156412 |

**Table 1** (continued)

| $N$ | $T$ | $C(N, T)$ | $Q(N, T)$ | $S(N, T)$ |
|---|---|---|---|---|
| 19 | 16 | 626972 | 35462756 | 1126480 |
| 19 | 17 | 102548 | 5769364 | 186702 |
| 19 | 18 | 7480 | 428432 | 14228 |
| 20 | 0 | 1 | 400 | 20 |
| 20 | 1 | 38 | 9880 | 380 |
| 20 | 2 | 684 | 129960 | 4560 |
| 20 | 3 | 7182 | 1111968 | 36360 |
| 20 | 4 | 52656 | 6866640 | 216216 |
| 20 | 5 | 279096 | 32066360 | 973228 |
| 20 | 6 | 1139686 | 117043592 | 3475620 |
| 20 | 7 | 3616786 | 340097800 | 9883356 |
| 20 | 8 | 9178452 | 796859664 | 22867936 |
| 20 | 9 | 18627866 | 1515157720 | 42972340 |
| 20 | 10 | 30583370 | 2344164944 | 66129060 |
| 20 | 11 | 40391102 | 2945976728 | 82791820 |
| 20 | 12 | 42883506 | 2990562344 | 84148308 |
| 20 | 13 | 36135764 | 2426753288 | 68531488 |
| 20 | 14 | 23832792 | 1548434440 | 44066956 |
| 20 | 15 | 11977978 | 757628928 | 21798876 |
| 20 | 16 | 4415902 | 273396672 | 7977556 |
| 20 | 17 | 1117420 | 68262960 | 2028028 |
| 20 | 18 | 172166 | 10468664 | 316972 |
| 20 | 19 | 11844 | 735632 | 22852 |
| 21 | 0 | 1 | 441 | 21 |
| 21 | 1 | 40 | 11480 | 420 |
| 21 | 2 | 760 | 159600 | 5320 |
| 21 | 3 | 8460 | 1447788 | 44910 |
| 21 | 4 | 65970 | 9514002 | 283806 |
| 21 | 5 | 373668 | 47477812 | 1363230 |
| 21 | 6 | 1638510 | 186088838 | 5220828 |
| 21 | 7 | 5615504 | 583873680 | 16006712 |
| 21 | 8 | 15495528 | 1486827352 | 40194176 |
| 21 | 9 | 34449452 | 3096001260 | 82570418 |
| 21 | 10 | 62564324 | 5293443980 | 140193996 |
| 21 | 11 | 92362700 | 7432590604 | 195667754 |
| 21 | 12 | 111225932 | 8544765668 | 224806708 |
| 21 | 13 | 108061712 | 7987431984 | 210290464 |
| 21 | 14 | 84148106 | 6003133602 | 158947440 |
| 21 | 15 | 51435656 | 3565513608 | 95078148 |
| 21 | 16 | 24134822 | 1631236798 | 44026566 |
| 21 | 17 | 8328628 | 552640068 | 15112454 |
| 21 | 18 | 1984284 | 130030524 | 3621432 |
| 21 | 19 | 288624 | 18857632 | 534512 |
| 21 | 20 | 18826 | 1257362 | 36518 |
| 22 | 0 | 1 | 484 | 22 |
| 22 | 1 | 42 | 13244 | 462 |
| 22 | 2 | 840 | 194040 | 6160 |
| 22 | 3 | 9870 | 1860188 | 54890 |
| 22 | 4 | 81570 | 12961344 | 367356 |
| 22 | 5 | 491484 | 68836672 | 1875776 |
| 22 | 6 | 2303060 | 288366656 | 7669060 |
| 22 | 7 | 8477132 | 971713144 | 25221712 |
| 22 | 8 | 25265132 | 2672423576 | 68312032 |
| 22 | 9 | 61084844 | 6049014552 | 152341408 |
| 22 | 10 | 121544920 | 11328446376 | 282867444 |
| 22 | 11 | 198508008 | 17581450512 | 435711532 |
| 22 | 12 | 267259406 | 22586589608 | 558257520 |
| 22 | 13 | 294527078 | 23914296468 | 590479014 |
| 22 | 14 | 264465928 | 20706942968 | 512798860 |
| 22 | 15 | 190850728 | 14487600280 | 360672992 |
| 22 | 16 | 108912908 | 8046030680 | 202019896 |
| 22 | 17 | 47822468 | 3455724056 | 87767868 |
| 22 | 18 | 15532710 | 1103071008 | 28405024 |
| 22 | 19 | 3490738 | 245357772 | 6429458 |
| 22 | 20 | 481298 | 33745592 | 900020 |
| 22 | 21 | 29956 | 2140520 | 58408 |

**Table 2.** Tringular lattice enumeration data for $N$ upto 16. The first step is along the $+X$ axis. The quantities $C$ and $Q$ are defined in Sect. 1

| $N$ | $T$ | $C(N, T)$ | $Q(N, T)$ |
|---|---|---|---|
| 1 | 0 | 1 | 1 |
| 2 | 0 | 1 | 4 |
| 2 | 1 | 4 | 8 |
| 3 | 0 | 1 | 9 |
| 3 | 1 | 8 | 40 |
| 3 | 2 | 14 | 48 |
| 4 | 0 | 1 | 16 |
| 4 | 1 | 12 | 112 |
| 4 | 2 | 44 | 284 |
| 4 | 3 | 46 | 242 |
| 5 | 0 | 1 | 25 |
| 5 | 1 | 16 | 240 |
| 5 | 2 | 90 | 942 |
| 5 | 3 | 196 | 1672 |
| 5 | 4 | 152 | 1098 |
| 6 | 0 | 1 | 36 |
| 6 | 1 | 20 | 440 |
| 6 | 2 | 150 | 2352 |
| 6 | 3 | 512 | 6414 |
| 6 | 4 | 818 | 8710 |
| 6 | 5 | 490 | 4672 |
| 7 | 0 | 1 | 49 |
| 7 | 1 | 24 | 728 |
| 7 | 2 | 226 | 4936 |
| 7 | 3 | 1048 | 18256 |
| 7 | 4 | 2568 | 38034 |
| 7 | 5 | 3208 | 41880 |
| 7 | 6 | 1572 | 18938 |
| 8 | 0 | 1 | 64 |
| 8 | 1 | 28 | 1120 |
| 8 | 2 | 318 | 9210 |
| 8 | 3 | 1852 | 43122 |
| 8 | 4 | 6204 | 121746 |
| 8 | 5 | 11822 | 205012 |
| 8 | 6 | 12086 | 189700 |
| 8 | 7 | 5044 | 74108 |
| 9 | 0 | 1 | 81 |
| 9 | 1 | 32 | 1632 |
| 9 | 2 | 424 | 15786 |
| 9 | 3 | 2996 | 89540 |
| 9 | 4 | 12644 | 319866 |
| 9 | 5 | 32860 | 729084 |
| 9 | 6 | 51312 | 1029546 |
| 9 | 7 | 44300 | 820976 |
| 9 | 8 | 16120 | 282228 |
| 10 | 0 | 1 | 100 |
| 10 | 1 | 36 | 2280 |
| 10 | 2 | 546 | 25368 |
| 10 | 3 | 4522 | 169132 |
| 10 | 4 | 23142 | 731900 |
| 10 | 5 | 76000 | 2109760 |
| 10 | 6 | 161154 | 4027990 |
| 10 | 7 | 212832 | 4894472 |
| 10 | 8 | 159252 | 3427744 |
| 10 | 9 | 51376 | 1051902 |
| 11 | 0 | 1 | 121 |
| 11 | 1 | 40 | 3080 |
| 11 | 2 | 684 | 38754 |
| 11 | 3 | 6496 | 297080 |
| 11 | 4 | 39012 | 1511156 |
| 11 | 5 | 155296 | 5275688 |
| 11 | 6 | 416958 | 12732026 |
| 11 | 7 | 746080 | 20896820 |
| 11 | 8 | 853202 | 22273844 |
| 11 | 9 | 563796 | 13902800 |

**Table 2** (continued)

| $N$ | $T$ | $C(N, T)$ | $Q(N, T)$ |
|---|---|---|---|
| 11 | 10 | 163258 | 3852488 |
| 12 | 0 | 1 | 144 |
| 12 | 1 | 44 | 4048 |
| 12 | 2 | 836 | 56838 |
| 12 | 3 | 8964 | 492604 |
| 12 | 4 | 61896 | 2881288 |
| 12 | 5 | 289538 | 11823650 |
| 12 | 6 | 941954 | 34552680 |
| 12 | 7 | 2134130 | 71649192 |
| 12 | 8 | 3303244 | 103070166 |
| 12 | 9 | 3330248 | 97815462 |
| 12 | 10 | 1970536 | 55057782 |
| 12 | 11 | 517810 | 13906386 |
| 13 | 0 | 1 | 169 |
| 13 | 1 | 48 | 5200 |
| 13 | 2 | 1004 | 80606 |
| 13 | 3 | 12000 | 779440 |
| 13 | 4 | 93518 | 5154996 |
| 13 | 5 | 503112 | 24326372 |
| 13 | 6 | 1924718 | 83558692 |
| 13 | 7 | 5284624 | 209764712 |
| 13 | 8 | 10349588 | 381054600 |
| 13 | 9 | 14110336 | 487711640 |
| 13 | 10 | 12721712 | 417022380 |
| 13 | 11 | 6816104 | 213715532 |
| 13 | 12 | 1639016 | 49589048 |
| 14 | 0 | 1 | 196 |
| 14 | 1 | 52 | 6552 |
| 14 | 2 | 1188 | 111138 |
| 14 | 3 | 15636 | 1186316 |
| 14 | 4 | 135954 | 8755178 |
| 14 | 5 | 826602 | 46721926 |
| 14 | 6 | 3637446 | 184560186 |
| 14 | 7 | 11745974 | 544540872 |
| 14 | 8 | 27878746 | 1197265506 |
| 14 | 9 | 48061714 | 1934185646 |
| 14 | 10 | 58542252 | 2229060042 |
| 14 | 11 | 47737532 | 1734009442 |
| 14 | 12 | 23368942 | 815563862 |
| 14 | 13 | 5179836 | 174996560 |
| 15 | 0 | 1 | 225 |
| 15 | 1 | 56 | 8120 |
| 15 | 2 | 1386 | 149610 |
| 15 | 3 | 19952 | 1747424 |
| 15 | 4 | 191302 | 14237932 |
| 15 | 5 | 1297752 | 84796124 |
| 15 | 6 | 6458860 | 378832102 |
| 15 | 7 | 23996104 | 1285421496 |
| 15 | 8 | 66983216 | 3321317840 |
| 15 | 9 | 139912028 | 6492431668 |
| 15 | 10 | 215378466 | 9440100104 |
| 15 | 11 | 237067876 | 9892087284 |
| 15 | 12 | 176455672 | 7057537302 |
| 15 | 13 | 79514824 | 3066998128 |
| 15 | 14 | 16350102 | 612021142 |
| 16 | 0 | 1 | 256 |
| 16 | 1 | 60 | 9920 |
| 16 | 2 | 1600 | 197290 |
| 16 | 3 | 24986 | 2502902 |
| 16 | 4 | 262038 | 22318006 |
| 16 | 5 | 1962078 | 146767128 |
| 16 | 6 | 10897650 | 731859970 |
| 16 | 7 | 45803820 | 2808705528 |
| 16 | 8 | 147120662 | 8345793114 |
| 16 | 9 | 361397702 | 19169457220 |
| 16 | 10 | 673819246 | 33717096634 |
| 16 | 11 | 936817752 | 44558843562 |

**Table 2** (continued)

| $N$ | $T$ | $C(N, T)$ | $Q(N, T)$ |
|---|---|---|---|
| 16 | 12 | 940523714 | 42801542806 |
| 16 | 13 | 643899436 | 28197869358 |
| 16 | 14 | 268812158 | 11387593994 |
| 16 | 15 | 51545484 | 2123713276 |

**Table 3.** Simple Cubic lattice enumeration data for $N$ upto 16. The first step is along the $+X$ axis. The quantities $C$, $Q$ and $S$ are defined in Sect. 1

| $N$ | $T$ | $C(N, T)$ | $Q(N, T)$ | $S(N, T)$ |
|---|---|---|---|---|
| 1 | 0 | 1 | 1 | 1 |
| 2 | 0 | 1 | 4 | 2 |
| 2 | 1 | 4 | 4 | 4 |
| 3 | 0 | 1 | 9 | 3 |
| 3 | 1 | 8 | 20 | 12 |
| 3 | 2 | 16 | 24 | 16 |
| 4 | 0 | 1 | 16 | 4 |
| 4 | 1 | 12 | 56 | 24 |
| 4 | 2 | 48 | 144 | 64 |
| 4 | 3 | 60 | 112 | 64 |
| 5 | 0 | 1 | 25 | 5 |
| 5 | 1 | 16 | 120 | 40 |
| 5 | 2 | 96 | 480 | 160 |
| 5 | 3 | 248 | 780 | 316 |
| 5 | 4 | 228 | 524 | 244 |
| 6 | 0 | 1 | 36 | 6 |
| 6 | 1 | 20 | 220 | 60 |
| 6 | 2 | 160 | 1200 | 320 |
| 6 | 3 | 620 | 3004 | 948 |
| 6 | 4 | 1188 | 4216 | 1472 |
| 6 | 5 | 832 | 2336 | 928 |
| 7 | 0 | 1 | 49 | 7 |
| 7 | 1 | 24 | 364 | 84 |
| 7 | 2 | 240 | 2520 | 560 |
| 7 | 3 | 1248 | 8560 | 2208 |
| 7 | 4 | 3600 | 18480 | 5160 |
| 7 | 5 | 5384 | 21172 | 6564 |
| 7 | 6 | 3068 | 10088 | 3432 |
| 8 | 0 | 1 | 64 | 8 |
| 8 | 1 | 28 | 560 | 112 |
| 8 | 2 | 336 | 4704 | 896 |
| 8 | 3 | 2184 | 20224 | 4416 |
| 8 | 4 | 8464 | 59216 | 13784 |
| 8 | 5 | 19192 | 103976 | 26480 |
| 8 | 6 | 23236 | 102824 | 28384 |
| 8 | 7 | 11220 | 42888 | 12720 |
| 9 | 0 | 1 | 81 | 9 |
| 9 | 1 | 32 | 816 | 144 |
| 9 | 2 | 448 | 8064 | 1344 |
| 9 | 3 | 3504 | 41992 | 7944 |
| 9 | 4 | 17000 | 155576 | 31040 |
| 9 | 5 | 51968 | 369776 | 79800 |
| 9 | 6 | 96548 | 560624 | 129448 |
| 9 | 7 | 98288 | 482384 | 119088 |
| 9 | 8 | 41192 | 178568 | 46768 |
| 10 | 0 | 1 | 100 | 10 |
| 10 | 1 | 36 | 1140 | 180 |
| 10 | 2 | 576 | 12960 | 1920 |
| 10 | 3 | 5256 | 79304 | 13240 |
| 10 | 4 | 30696 | 355840 | 62136 |
| 10 | 5 | 117808 | 1069088 | 200272 |
| 10 | 6 | 295440 | 2194960 | 436208 |
| 10 | 7 | 462480 | 2892808 | 610400 |
| 10 | 8 | 405928 | 2207688 | 492112 |
| 10 | 9 | 150092 | 735276 | 172180 |

**Table 3** (continued)

| $N$ | $T$ | $C(N,T)$ | $Q(N,T)$ | $S(N,T)$ |
|---|---|---|---|---|
| 11 | 0 | 1 | 121 | 11 |
| 11 | 1 | 40 | 1 540 | 220 |
| 11 | 2 | 720 | 19 800 | 2 640 |
| 11 | 3 | 7 520 | 139 264 | 20 800 |
| 11 | 4 | 51 280 | 734 288 | 113 976 |
| 11 | 5 | 237 200 | 2 670 184 | 441 712 |
| 11 | 6 | 749 852 | 6 931 608 | 1 207 760 |
| 11 | 7 | 1 589 568 | 12 363 760 | 2 272 648 |
| 11 | 8 | 2 147 464 | 14 443 536 | 2 789 416 |
| 11 | 9 | 1 656 992 | 9 884 584 | 1 999 784 |
| 11 | 10 | 548 388 | 2 985 968 | 629 728 |
| 12 | 0 | 1 | 144 | 12 |
| 12 | 1 | 44 | 2 024 | 264 |
| 12 | 2 | 880 | 29 040 | 3 520 |
| 12 | 3 | 10 340 | 230 864 | 31 200 |
| 12 | 4 | 80 720 | 1 399 216 | 195 496 |
| 12 | 5 | 436 632 | 5 976 800 | 885 384 |
| 12 | 6 | 1 665 256 | 18 784 528 | 2 915 248 |
| 12 | 7 | 4 455 808 | 42 359 344 | 6 900 936 |
| 12 | 8 | 8 158 532 | 66 979 848 | 11 412 400 |
| 12 | 9 | 9 680 372 | 70 112 424 | 12 468 656 |
| 12 | 10 | 6 657 580 | 43 479 928 | 8 046 936 |
| 12 | 11 | 1 994 292 | 12 024 824 | 2 305 504 |
| 13 | 0 | 1 | 169 | 13 |
| 13 | 1 | 48 | 2 600 | 312 |
| 13 | 2 | 1 056 | 41 184 | 4 576 |
| 13 | 3 | 13 800 | 365 204 | 45 060 |
| 13 | 4 | 121 260 | 2 501 924 | 317 796 |
| 13 | 5 | 751 352 | 12 281 692 | 1 646 940 |
| 13 | 6 | 3 357 504 | 45 352 848 | 6 342 504 |
| 13 | 7 | 10 859 984 | 123 816 200 | 18 097 784 |
| 13 | 8 | 25 143 524 | 247 547 924 | 37 686 364 |
| 13 | 9 | 40 471 112 | 350 596 196 | 55 505 708 |
| 13 | 10 | 42 793 156 | 332 309 384 | 54 581 608 |
| 13 | 11 | 26 551 480 | 188 274 228 | 32 000 044 |
| 13 | 12 | 7 264 808 | 47 964 296 | 8 405 872 |
| 14 | 0 | 1 | 196 | 14 |
| 14 | 1 | 52 | 3 276 | 364 |
| 14 | 2 | 1 248 | 56 784 | 5 824 |
| 14 | 3 | 17 940 | 555 716 | 63 084 |
| 14 | 4 | 175 340 | 4 246 872 | 494 536 |
| 14 | 5 | 1 224 040 | 23 561 376 | 2 886 304 |
| 14 | 6 | 6 269 928 | 100 010 808 | 12 730 344 |
| 14 | 7 | 23 782 680 | 320 822 992 | 42 535 064 |
| 14 | 8 | 66 616 268 | 776 738 056 | 106 900 816 |
| 14 | 9 | 135 660 836 | 1 390 934 628 | 198 473 212 |
| 14 | 10 | 194 557 140 | 1 783 500 048 | 263 309 896 |
| 14 | 11 | 185 383 188 | 1 543 474 124 | 235 322 892 |
| 14 | 12 | 104 752 528 | 804 719 096 | 126 408 496 |
| 14 | 13 | 26 377 424 | 190 068 688 | 30 666 536 |
| 15 | 0 | 1 | 225 | 15 |
| 15 | 1 | 56 | 4 060 | 420 |
| 15 | 2 | 1 456 | 76 440 | 7 280 |
| 15 | 3 | 22 848 | 818 384 | 86 016 |
| 15 | 4 | 245 728 | 6 902 784 | 742 000 |
| 15 | 5 | 1 908 712 | 42 716 308 | 4 815 892 |
| 15 | 6 | 11 027 436 | 204 963 592 | 23 935 704 |
| 15 | 7 | 48 006 920 | 755 844 404 | 91 656 948 |
| 15 | 8 | 157 891 240 | 2 150 709 816 | 269 928 928 |
| 15 | 9 | 389 425 904 | 4 664 081 504 | 605 215 784 |
| 15 | 10 | 707 139 188 | 7 561 391 008 | 1 012 548 920 |
| 15 | 11 | 914 022 384 | 8 849 181 992 | 1 220 950 688 |
| 15 | 12 | 792 478 184 | 7 042 302 328 | 999 368 384 |
| 15 | 13 | 411 128 432 | 3 399 129 488 | 495 148 920 |
| 15 | 14 | 95 892 520 | 747 961 688 | 111 564 104 |
| 16 | 0 | 1 | 256 | 16 |
| 16 | 1 | 60 | 4 960 | 480 |
| 16 | 2 | 1 680 | 100 800 | 8 960 |
| 16 | 3 | 28 560 | 1 171 968 | 114 688 |
| 16 | 4 | 335 328 | 10 814 944 | 1 079 568 |
| 16 | 5 | 2 868 024 | 73 861 952 | 7 713 256 |
| 16 | 6 | 18 446 224 | 395 388 288 | 42 656 592 |
| 16 | 7 | 90 629 056 | 1 648 405 336 | 184 202 848 |
| 16 | 8 | 342 311 880 | 5 393 257 584 | 622 230 240 |
| 16 | 9 | 991 906 320 | 13 747 970 776 | 1 636 114 976 |
| 16 | 10 | 2 182 299 212 | 26 994 678 456 | 3 308 107 088 |
| 16 | 11 | 3 571 702 332 | 39 941 612 344 | 5 033 348 448 |
| 16 | 12 | 4 199 050 708 | 42 974 149 944 | 5 560 551 376 |
| 16 | 13 | 3 338 798 836 | 31 643 370 160 | 4 197 695 704 |
| 16 | 14 | 1 600 887 728 | 14 215 872 264 | 1 930 121 152 |
| 16 | 15 | 347 713 380 | 2 928 164 872 | 406 045 096 |

## 2. Scaling of the Number of Walks

In this section we consider the scaling properties of the generating function $C_N(w)$ defined by (1.6) with (1.3). For large $N$ and $w^{-1}$, such that the product $wN$ is finite, we expect [1–4]

$$C_N(w) \cong F(x), \tag{2.1}$$

where

$$x \equiv (q-2)\, wN. \tag{2.2}$$

The scaling function $F(x)$ is lattice and model dependent. The factor $(q-2)$ is introduced to facilitate presentation of the results for a Gaussian model of non-self-avoiding walks with no immediate returns [1, 2]. Then [3]

$$C_N(w) \equiv [1+(q-2)\, w]^{N-1} \cong F^G(x) \equiv \mathrm{e}^x, \tag{2.3}$$

for any regular lattice. The scaling combination used in [1] is identical to $x$ in terms of the leading behavior. Differences are of higher order and manifest themselves only in corrections to scaling.

For SAW models, we have

$$F(x) = 1 + x + f_2 x^2 + f_3 x^3 + \dots \quad (x \ll 1), \tag{2.4}$$

$$F(x) \simeq A x^{\gamma-1} \mathrm{e}^{\sigma x} \quad (x \gg 1). \tag{2.5}$$

The constants $A$, $\sigma$, $f_2$, $f_3$, ... are lattice dependent; $\gamma$ is an isotropic SAW critical exponent. Corrections to scaling for $C_N(w)$ take the forms [1–4]

$$C_N(w) - F(x) \cong \sum_{k>0} \frac{1}{N^k} F^{(k)}(x). \tag{2.6}$$

For the SQ and SC lattices, even-odd oscillations are anticipated [3],

$$C_N(w) - F(x) \cong \sum_{k>0} \frac{1}{N^k} [F^{(k)}(x) + (-1)^k \tilde{F}^{(k)}(x)]. \quad (2.7)$$

Since we are working with $N \lesssim O(20)$, cancellation of at least the $O(N^{-1})$ correction term is needed to obtain accurate estimates of the leading scaling behavior. Thus, we form approximants

$$F_N(x) \equiv [N C_N(w) - (N-k)\, C_{N-k}(w)]/k, \quad (2.8)$$

where we set $k=1$, except for the SQ lattice for which $k=2$ was used. Indeed, the choice $k=2$ cancels the oscillatory $O(N^{-1})$ correction which is apparently appreciable in the SQ data. The SC lattice results also show some fluctuations but to order $N \leqq 16$ they are not very regular, and the use of $k=2$ does not improve the consistency of the results. We tried two more elaborations: shifting $N \to N-1$, $N-2, \ldots$ in the RHS of (2.8), and use of more complicated linear combinations of $C_N(w)$ to attempt cancellation of $O(1/N^2)$ contribution in (2.6). However, the results did not seem to improve compared with a simpler form (2.8). Figures 1, 2 and 3 show the range of the approximants $F_N(x)$ for $0 \leqq x \leqq 10$, for the SQ, TR and SC lattices, respectively ($k=2$, 1 and 1). We plotted $L_N(x) \equiv \ln F_N(x)$ for the four largest $N$ values available ($N = 22$, 21, 20, 19 and $N=16$, 15, 14, 13, for the SQ and the TR or SC, respectively). The Gaussian answer $L^G \equiv \ln F^G(x) \equiv x$ is also shown. Note that the four largest-$N$ curves are very close, and we reproduce only the range covered by these four sets of data. The available data provide rather stable estimates of the scaling functions $F(x)$, for at least $x \lesssim 6$.

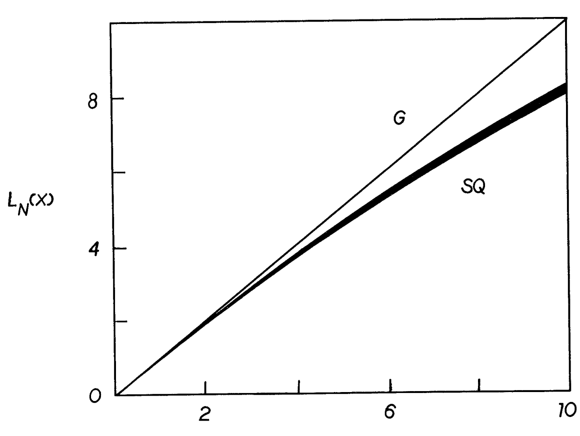


**Fig. 1.** Estimation of the scaling function for the number of walks, on the SQ lattice. The Gaussian result is also shown. (See Sect. 2 for details)

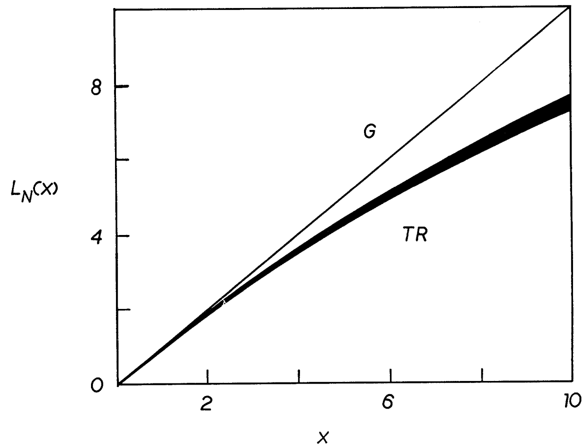


**Fig. 2.** TR-lattice scaling function for the number of walks. (See Sect. 2 for details)

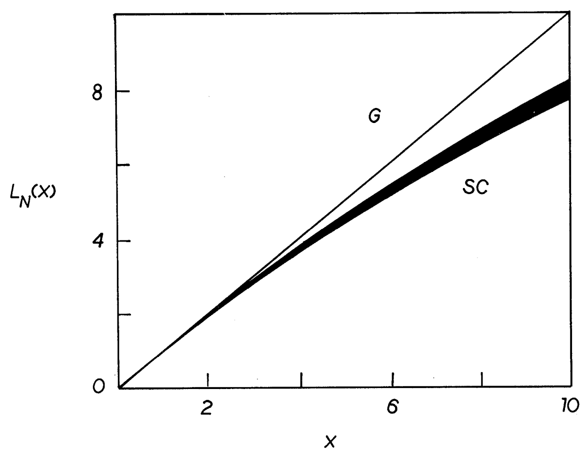


**Fig. 3.** SC-lattice scaling function for the number of walks. (See Sect. 2 for details)

In Fig. 4 we plot the difference

$$L(x) - x = \ln [F(x)/F^G(x)], \quad (2.9)$$

where for $F(x)$ we use $F_{22}^{SQ}$, $F_{16}^{TR}$ and $F_{16}^{SC}$. All three SAW scaling functions are close to the Gaussian one, even for $x \sim 2$. Note, however, that the SC deviation is comparable with the $d=2$ lattice deviations, contrary to the prediction of [4]. Another interesting feature of Figs. 1–4 is a difference between $F^{SQ}$ and $F^{TR}$: evidently there is no universality in the normal critical phenomena sense. (The difference cannot be repaired by rescaling $x \to \text{const} \cdot x$.)

For small $x$, the scaling functions, Figs. 1–3, were obtained with high accuracy. The reason for this is very simple: one can easily verify that all the corrections to scaling in this problem, i.e., $F^{(j)}$ in (2.6), etc. actually *vanish* as $x \to 0$; indeed, for the fully extended "rods" the scaling expressions coincide with the full

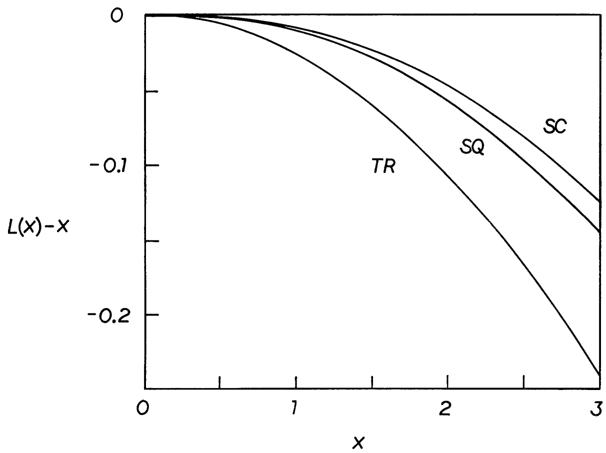


**Fig. 4.** Deviation of the SAW scaling functions for the number of walks from their Gaussian values

answers. In the opposite limit of large $x$, the form (2.5) does not adequately fit the ranges of Figs. 1–3. (We tried the fit for $6 \lesssim x \lesssim 10$. Accurate data for larger $x$ values are needed to see the asymptotic behavior.)

## 3. Scaling of the End-to-End Distance Moments

Let us first consider the scaling of the quantity $R_N^2(w)$ defined via (1.7). It was studied in [1, 2] by Monte Carlo (MC) techniques. The appropriate scaling relation takes the form

$$R_N^2(w)/N^2 \cong G(x), \tag{3.1}$$

where

$$G(x \to 0) = 1, \tag{3.2}$$

$$G(x \to \infty) \simeq B x^{2(\nu-1)}. \tag{3.3}$$

Here $\nu$ is the universal correlation length exponent of isotropic SAWs, while $G(x)$ and the constant $B$ are lattice (model) dependent. Following [1, 2], we study the function

$$H(x) = x^{2(1-\nu)} G(x) \tag{3.4}$$

which approaches a constant ($B$) as $x \to \infty$. We form the approximants

$$H_N(x) \equiv x^{2(1-\nu)} [R_N^2(w)/N - R_{N-k}^2(w)/(N-k)]/k, \tag{3.5}$$

similar to (2.8). The values of $\nu$ are required as an input. We used the exact value [14] for $d=2$, and the central numerical estimate [15] for $d=3$,

$$\nu(d=2) = 3/4, \tag{3.6}$$

$$\nu(d=3) \cong 0.5875. \tag{3.7}$$

The Gaussian scaling function [1, 6], for the squared end-to-end distance generating function of lattice random walks with no *immediate* returns,

$$G^G(x) = 2(e^{-x} + x - 1)/x^2, \tag{3.8}$$

is to be compared with $G(x)$ of (3.1). Since we use $H(x)$ instead, we define

$$\tilde{H}^G(x) \equiv x^{2(1-\nu)} G^G(x), \tag{3.9}$$

with the SAW exponent $\nu$. Thus $\tilde{H}^G$ is *not* the appropriate scaling function $H$ for the Gaussian case. (Note $\nu^G = 1/2$.)

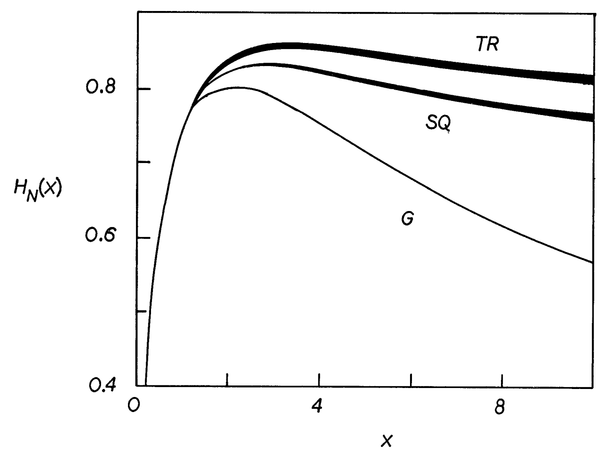


**Fig. 5.** Mean-squared end-to-end distance scaling functions for the SQ and TR lattices, as well as the Gaussian answer. (See Sect. 3)

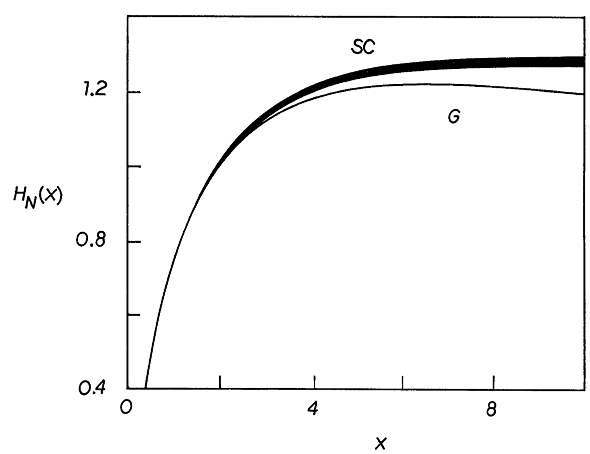


**Fig. 6.** SC-lattice scaling, for the mean-squared end-to-end distance

Figure 5 shows approximants $H_N(x)$ for the SQ ($N=22$, 21, 20, 19; $k=2$) and the TR ($N=16$, 15, 14, 13; $k=1$) lattices, as well as $\tilde{H}^G(x)$. Figure 6 displays the SC lattice results ($N=16$, 15, 14, 13; $k=1$) and $\tilde{H}^G(x)$. Only the spreads of the curves for different $N$ for $H_N(x)$ are indicated. The data for $H(x)$ are well-converged and represent $H^{SQ}$ and $H^{TR}$ accurately up to at least $x \sim 8$. The SC data are more disperse and seem convergent up to about $x \sim 5$. The SC scaling function is indeed very close to the Gaussian one as observed in MC studies (1). Our results are consistent with the MC values to the extent that comparison is possible. The $x \leqq 10$ data have not yet reached the asymptotically constant behavior.

We turn now to the linear moment $X_N(w)$ defined by (1.8). If this quantity scales, then

$$X_N(w) \cong N\,Y(x), \tag{3.10}$$

with

$$Y(0)=1. \tag{3.11}$$

The large-$x$ behavior is more interesting since for the appropriate unbiased SAW moment, $X_N(1)$, the asymptotic $N$ dependence is not fully understood. According to [12],

$$X_N(1) \sim N^{\omega} \quad (d=2), \tag{3.12}$$

with a very small $\omega$ ($\sim 0.06$). Preliminary evidence indicates also [12] that

$$X_N(1) \sim \text{const} \ \text{as}\ N \to \infty \quad (d=3). \tag{3.13}$$

Due to small value of the exponent $\omega$ estimate, logarithmic behavior of $X_N^{(d=2)}(1)$ has not been excluded. In fact, the behavior of $X_N(1)$ for Gaussian walks [13] are $\ln N$ and *const*, for $d=2$ and 3, respectively. (The appropriate model in that case must exclude revisits of the origin, in addition to having the first step fixed along the $+X$ axis.) Thus, a good guess for $Y(x \to \infty)$, at the present time is

$$Y(x) \sim x^{-1} \quad (d=3), \tag{3.14}$$

$$Y(x) \sim x^{\omega-1} \ \text{or}\ x^{-1}\ln x \quad (d=2). \tag{3.15}$$

According to these relations, the product $x\,Y(x)$ is an interesting quantity to be considered.

We use the approximants

$$x\,Y_N(x) \equiv [X_N(w) - X_{N-k}(w)]/k. \tag{3.16}$$

The spread of the four, having largest-$N$, is indicated in Fig. 7, for the SQ and the SC lattices. The linear moments indeed scale as conjectured in (3.10). The trend in Fig. 7 is consistent with $x\,Y^{SC} \to$ const for large $x$. The SQ data show an upward trend but consistency with (3.15) cannot be claimed since several decades in $x$ would be needed for a quality fit.

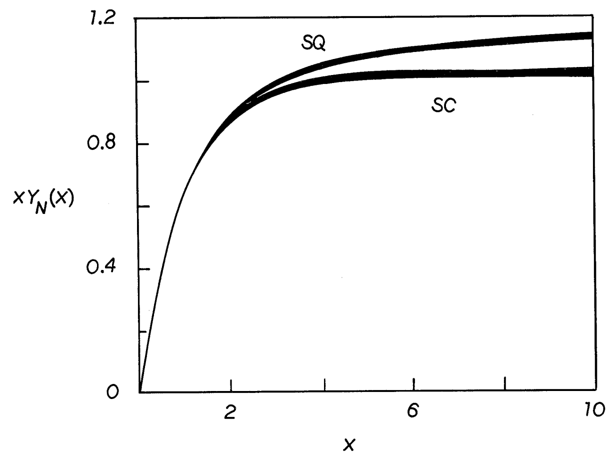


**Fig. 7.** Scaling function estimates for the first moment of the end displacement for the SQ and SC lattices

## 4. Summary

Our results indicate that the rod-to-coil transition can be described by scaling laws and is governed by the combination $wN$. The prediction of [4] that the $d=3$ scaling functions take on Gaussian values was not confirmed with the available data, i.e., for $N < O(20)$. All the scaling functions calculated are, however, rather close to the Gaussian results (when available) for $x \equiv (q-2)\,wN \lesssim 3$, at least. This suppression of self-avoidance effects was found in other studies [1–4] as well.

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