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On the symmetry classes of planar self-avoiding walks

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Abstract. We present new results on the class of anisotropic, spiral walks in two dimensions. We find that these are directed problems in the sense that the usual relation, $\nu_{\|} \approx 2\nu_{\perp}$, holds between the length scale exponents. In contradistinction, however, they do not seem to fall in the usual directed universality class ($\nu_{\|}=1$). Motivated by this, the universality classes of self-avoiding walks (SAW) on the square lattice are discussed. We argue that of the 8^4 models that exist by restricting the possible two step configurations there are four major categories with a total of seven generic types. The importance of reflection symmetry in this classification is discussed.

1. *Introduction*

The problem of quantifying the properties of self-avoiding walks has received continued widespread attention, especially since their asymptotic behaviour was seen as a critical phenomenon in polymer science [1]. There has been much accomplished in the two-dimensional scene where several exact results are believed to hold [2, 3]. In the quest for a better understanding of isotropic walks (SAW), many variations on self-avoiding walks have been studied including directed (DW) [4–10], spiral (SSAW) [11, 12] and anisotropic spiral (ASSAW) walks [13–17]. While many exact results are known about the first two of these groups, the last has resisted an analytic approach and has been the least studied. Often the most interesting quantity in these problems is the mean square end-to-end distance (or radius of gyration) $\langle R_N^2\rangle$ for walks of length N. This is expected to scale with a power law; i.e.

$$\langle R_N^2\rangle \sim N^{2\nu} \tag{1}$$

possibly with a confluent logarithmic factor.

From the work of Nienhuis [2, 3] the exact value of ν is generally accepted to be $\frac{3}{4}$ for SAW and the latest series work confirms this prediction [18]. For directed walks, Cardy [7] has shown that all such problems should have two exponents: one related to the preferred direction of the walk, $\nu_{\|}$, and one perpendicular to it, $\nu_{\perp}$, and that these should be 1 and $\frac{1}{2}$ respectively. This result has been found in the exact solutions [19] of directed problems. In the isotropic spiral case Blöte and Hilhorst [12] have shown

$$\langle R_N^2\rangle \sim N \log N \tag{2}$$

and so $\nu=\frac{1}{2}$. Lastly, the numerical work on anisotropic spiral walks [13, 15] has provided estimates for ν around 0.85, which is not close to any of the other results. For one model in this class a second exponent [13] at approximately half the major value was found. This however, was not explained fully and the conclusion of [13] was that there were isotropic members of this class. In the first part of this paper we show that this is not the case. We provide convincing numerical evidence that there exists two exponents for the models of this class, and provide an argument that gives the angle of the preferred direction exactly along the lines of [16]. The relationship

$$\nu_{\|}=2\nu_{\perp} \tag{3}$$

holds for the exponents defined in the correct directions. Apparently, however, they do not have the directed values, and hence these models are not in the directed universality class.

Now, given the advanced state of knowledge about these models provided by previous work we feel that it is apposite to provide a discussion of the universality classes of these models here. Hence, in the second part of this paper an investigation of the models obtained by considering representatives of all 'two-step' rules has been undertaken. Some of these, as well as similar models have been previously considered by Manna [13, 14]. Exact enumeration coupled with the analysis technique of differential approximants has been used in this study. This has allowed us to search the 'rule' space for representatives of the universality classes. This search was fairly quick since most models display their asymptotic behaviour in short series. Here universality class refers to a differentiation simply by length scale exponents. We have chosen these rules to exemplify all possible symmetries. Of note is the fact that this search has provided another example in the ASSAW class which we show can be mapped onto one of the previously studied models. Apart from trivial cases we conclude that there are two isotropic classes (SAW and SSAW) and two anisotropic classes (DW and ASSAW). Spirality seems to be 'relevant' in both cases and we shall highlight the role of reflection symmetry in the differentiation of these classes.

The models we have studied can be understood from the following ruminations. Consider the construction of a configuration of a self-avoiding walk on a square lattice. At each step we have three possible directions in which to proceed so long as the self-avoiding condition is satisfied. Now consider restricting the possible choices for continuation. The present step can be in one of the four lattice directions and for each of these directions there are 2^3 choices of constraint (reflecting the three possible ways of proceeding for the SAW). Hence there are $(2^3)^4=4096$ possible constraints we can consider. Many produce trivial models and most give essentially one-dimensional results. In fact, we have found that there are only 11 rules in classes other than the directed or trivial ones. Figure 1 catalogues 12 representative cases which include most of these 11 rules and some of the directed and trivial classes so as to cover all universality classes. These were chosen from the much smaller number of 'balanced' rules that have the same number of north as south and west as east steps in their rules. All but one have the 180°, rotation symmetry necessary to give a non-directed rule and this condition reduces the rule space from 4096 to 64. Note that the self-avoiding constraint always takes precedence over the rule. Rule (a) is simply the unconstrained SAW while rule (d) gives pure spiral walks. Rules (g) and (i) are Manna's three-choice anisotropic spiral and two-choice anisotropic spiral cases respectively. Rule (h) is also in the anisotropic spiral class. Rules (b) and (c) behave as the unconstrained SAW and (e), (f), (j), (k) and (l) are either directed or trivial in some fashion. We shall discuss these in more detail after giving the new results for the ASSAW class.

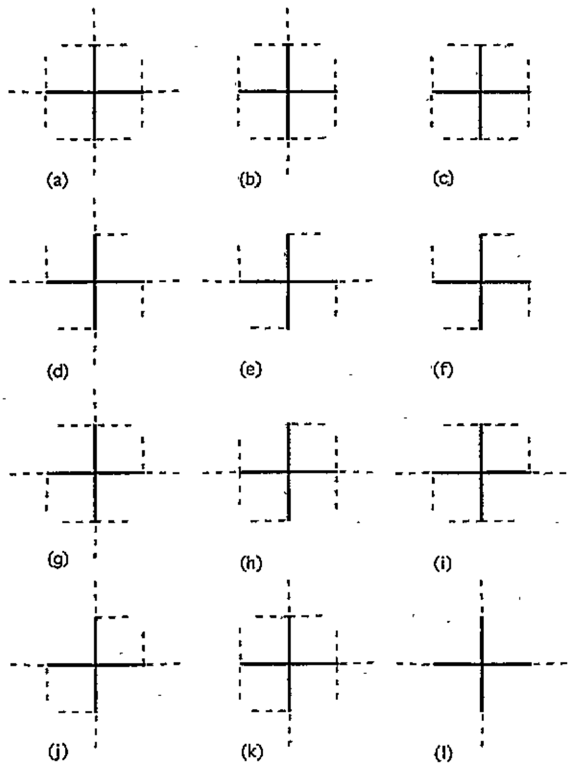

Figure 1. Each of the above diagrams illustrates a two-step rule for self-avoiding walks. In each case the bold line signifies the present state of the walk while the dashed lines the allowed continuations from that given step.

2. Anisotropic, spiral walks

Whittington [16] has provided an argument for the value of the connective constants of the two-choice and three-choice models of Manna (rules (g) and (i)). This was accomplished in part by considering a subset of configurations in which south or west steps are excluded. This is equivalent to considering the total rule space without self-avoidance. In both models one is left with a concatenation of staircase walks which are of differing types for the two models. For the three-choice model the walks are normal staircase walks that can move in the vertical or horizontal direction at each step while the two-choice case gives rise to staircase walks that are free to move vertically only if the previous step has been a horizontal one. It is simple to see that in the three-choice case a random walk version will have a major axis along the 45 degree line to the horizontal. Denoting this angle for the two-choice as θ_{2c}, its value can be derived from the two variable generating function for this type of staircase walk. The generating function for these horizontal-preferring staircase walks can be found from the recurrence relation

$$G_x = x(1 + G_x + y + yG_x) \tag{4}$$

where G_x is the generating function for walks starting with a horizontal step and $x(y)$ is the fugacity attached to horizontal (vertical) steps. This can be solved immediately to give

$$G_x = \frac{x(1+y)}{1-x(1+y)}. \tag{5}$$

Hence the full generating function is

$$G(x,y) = 1 + G_x + y(1+G_x) = \frac{1+y}{1-x(1+y)}. \tag{6}$$

We can evaluate the average slope via the generating function as

$$\tan(\theta_{2c}) = x\frac{\partial G}{\partial y} \bigg/ y\frac{\partial G}{\partial x} = \frac{x}{y(1+y)^2}. \tag{7}$$

Setting $x=y$ and noting that the generating function diverges at the golden mean

$$y = \frac{1}{1+y} = (\sqrt{5}-1)/2 \tag{8}$$

we have

$$\theta_{2c} = \tan^{-1}((3-\sqrt{5})/2) \approx 0.364\,86. \tag{9}$$

Returning to the full models, one can evaluate for walks of any (given sufficient computer time) length an average angle of the line of maximum square end-to-end distance. One immediately can see that these values converge to $\theta_{3c} = \pi/4$ and $\theta_{2c} = 0.364\,86\ldots$ fairly quickly and hence we are confident that these values are exact when self-avoidance is included.

We have enumerated two-choice and three-choice walks with end-to-end distances along the major and minor (perpendicular to those angles) axes up to lengths (n) 44 and 32, respectively. The results are given in tables 1 and 2, respectively. These enumerations add new information to the old series and also increase the lengths considered slightly. For comparison, enumerations up to lengths 42 and 30 for the two-choice and three-choice models, respectively, both took approximately 9 cpu hours on an IBM RISC 6000/560.

The first result from this data is contained in figure 2 where $\sqrt{\langle R_{\parallel}^2\rangle_n}$ is plotted against $\langle R_{\perp}^2\rangle_n$. The near-perfect straight line fit for this relationship clearly indicates that

$$\nu_{\parallel} = 2\nu_{\perp} \tag{10}$$

holds. This immediately enables us to discount the possibility that ASSAW is in either the spiral or SAW universality classes. We note here that because the angle is 45 degrees for the three choice model Manna fortuitously extracted two exponents for that model and not for the other.

Using the new enumerations we have extracted the best estimates for $\nu_{\parallel}$ for each model. The best results using differential approximates is

$$\nu_{\parallel} = 0.845(5) \tag{11}$$

which differs little from earlier estimates [17]. The exponent estimates for the two models are in good correspondence. We offer no 'rational fraction' conjecture for this exponent although the existence of such a fraction is likely given the values of exponents in the other two-dimensional models. The differential approximants used were inhomogeneous second, third, and fourth order approximants with biasing.

Table 1. 2-choice model: enumerations.

n	c_n	$\langle R_x^2\rangle_n$	$\langle R_xR_y\rangle_n$	$\langle R_y^2\rangle_n$	$\langle R^2\rangle_n$	$\langle R_\parallel^2\rangle_n$	$\langle R_\perp^2\rangle_n$
1	4	0.500 00	0.000 00	0.500 00	1.000 00	0.500 00	0.500 00
2	8	1.750 00	-0.250 00	0.750 00	2.500 00	1.789 34	0.710 66
3	16	3.375 00	0.750 00	1.125 00	4.500 00	3.588 53	0.911 47
4	28	5.928 57	1.500 00	1.642 86	7.571 43	6.382 91	1.188 52
5	52	8.576 92	2.384 62	2.115 38	10.692 31	9.343 97	1.348 34
6	90	12.200 00	3.577 78	2.777 78	14.977 78	13.385 53	1.592 25
7	160	15.900 00	4.850 00	3.400 00	19.300 00	17.541 81	1.758 19
8	276	20.413 04	6.398 55	4.181 16	24.594 20	22.612 07	1.982 13
9	484	24.900 83	7.975 21	4.909 09	29.809 92	27.672 24	2.137 67
10	826	30.368 04	9.888 62	5.825 67	36.193 70	33.835 67	2.358 04
11	1 434	35.601 12	11.754 53	6.659 69	42.260 81	39.752 59	2.508 22
12	2 438	41.842 49	13.970 47	7.680 07	49.522 56	46.806 51	2.716 05
13	4 194	47.845 49	16.130 66	8.626 13	56.471 63	53.605 78	2.865 84
14	7 104	54.832 21	18.636 82	9.748 87	64.581 08	61.516 66	3.064 42
15	12 150	61.518 19	21.059 42	10.793 09	72.311 28	69.099 38	3.211 89
16	20 506	69.243 05	23.850 48	12.018 82	81.261 87	77.857 47	3.404 41
17	34 898	76.605 54	26.532 64	13.161 04	89.766 58	86.216 08	3.550 50
18	58 740	85.018 35	29.589 27	14.482 84	99.501 19	95.763 81	3.737 38
19	99 568	93.031 17	32.520 73	15.719 11	108.750 28	104.868 13	3.882 15
20	167 186	102.115 92	35.836 49	17.135 69	119.251 61	115.187 06	4.064 55
21	282 468	110.753 57	39.007 42	18.462 21	129.215 78	125.007 80	4.207 99
22	473 318	120.485 33	42.572 41	19.970 36	140.455 69	136.069 16	4.386 52
23	797 462	129.732 52	45.977 00	21.385 08	151.117 60	146.588 84	4.528 76
24	1 333 866	140.091 39	49.783 36	22.982 26	163.073 66	158.369 73	4.703 93
25	2 241 980	149.930 85	53.414 87	24.482 65	174.413 51	169.568 45	4.845 05
26	3 744 048	160.900 06	57.456 07	26.166 79	187.066 85	182.049 60	5.017 25
27	6 279 996	171.317 01	61.308 84	27.750 75	199.067 76	193.910 42	5.157 33
28	10 472 560	182.880 80	65.578 67	29.519 78	212.400 58	207.073 68	5.326 90
29	17 533 852	193.862 32	69.647 74	31.185 50	225.047 82	219.581 81	5.466 01
30	29 202 420	206.006 26	74.140 59	33.037 53	239.043 79	233.410 59	5.633 19
31	48 813 440	217.540 41	78.421 36	34.783 30	252.323 71	246.552 31	5.771 40
32	81 204 864	230.251 69	83.132 24	36.716 65	266.968 33	261.031 91	5.936 42
33	135 541 920	242.327 35	87.620 45	39.540 90	280.868 25	274.794 48	6.073 77
34	225 249 074	255.594 16	92.544 77	40.553 99	296.148 15	289.911 33	6.236 82
35	375 481 028	268.201 39	97.236 60	42.455 32	310.656 71	304.283 35	6.373 36
36	623 395 676	282.012 70	102.370 07	44.546 66	326.559 36	320.024 76	6.534 60
37	1 037 947 386	295.142 29	107.262 00	46.523 77	341.666 06	334.995 68	6.670 38
38	1 721 755 690	309.488 05	112.600 73	48.692 01	358.180 06	351.350 13	6.829 93
39	2 863 621 286	323.131 33	117.689 42	50.743 67	373.875 00	366.910 00	6.964 99
40	4 746 373 644	338.002 23	123.229 81	52.987 55	390.989 78	383.866 79	7.122 98
41	7 886 384 910	352.151 25	128.512 22	55.112 63	407.263 88	400.006 51	7.257 36
42	13 061 734 390	367.538 48	134.250 85	57.430 94	424.969 43	417.555 54	7.413 89
43	21 683 197 766	382.185 85	139.724 15	59.628 39	441.814 24	434.266 62	7.547 62
44	35 887 723 320	398.081 29	145.657 87	62.020 04	460.101 33	452.398 55	7.702 78

Assuming confluent exponents tended to stablize the leading exponent, although there was no indication of a simple confluent correction term. This can be seen as an indication that the precise asymptotic form cannot be approximated by differential approximants, and that therefore the extrapolated exponent values have to be interpreted carefully. We also considered the possibility of logarithmic corrections to the power law as in the spiral case [12]. We found that there is no consistent way of assigning a value to the power of such a confluent logarithmic factor if, with the

Table 2. 3-choice model: enumerations.

n	c_n	$\langle R_x^2\rangle_n$	$\langle R_xR_y\rangle_n$	$\langle R_y^2\rangle_n$	$\langle R^2\rangle_n$	$\langle R_\parallel^2\rangle_n$	$\langle R^2{}_\perp\rangle_n$
1	4	0.500 00	0.000 00	0.500 00	1.000 00	0.500 00	0.500 00
2	10	1.400 00	0.200 00	1.400 00	2.800 00	1.600 00	1.200 00
3	24	2.500 00	0.666 66	2.500 00	5.000 00	3.166 66	1.833 33
4	54	3.925 92	1.407 40	3.925 92	7.851 85	5.333 33	2.518 51
5	124	5.403 22	2.322 58	5.403 22	10.806 45	7.725 80	3.080 64
6	272	7.250 00	3.514 70	7.250 00	14.500 00	10.764 70	3.735 29
7	608	9.065 78	4.802 63	9.065 78	18.131 57	13.868 42	4.263 15
8	1 314	11.287 67	6.392 69	11.287 67	22.575 34	17.680 36	4.894 97
9	2 884	13.426 49	8.022 19	13.426 49	26.852 98	21.448 68	5.404 29
10	6 178	15.978 31	9.966 65	15.978 31	31.956 62	25.944 96	6.011 65
11	13 388	18.424 11	11.915 14	18.424 11	36.848 22	30.339 25	6.508 96
12	28 486	21.284 42	14.187 88	21.284 42	42.568 84	35.472 30	7.096 53
13	611 68	24.019 35	16.435 65	24.019 35	48.038 71	40.455 00	7.583 70
14	129 446	27.173 13	19.017 73	27.173 13	54.346 27	46.190 87	8.155 40
15	276 020	30.184 02	21.549 94	30.184 02	60.368 04	51.733 96	8.634 07
16	581 572	33.617 69	24.425 46	33.617 69	67.235 39	58.043 16	9.192 23
17	1 233 204	36.894 14	27.230 38	36.894 14	73.788 29	64.124 53	9.663 75
18	2 588 906	40.596 82	30.386 54	40.596 82	81.193 64	70.983 37	10.210 27
19	5 464 816	44.129 53	33.454 03	44.129 53	88.259 06	77.583 56	10.675 49
20	11 437 088	48.092 10	36.880 19	48.092 10	96.184 20	84.972 29	11.211 90
21	24 050 760	51.873 34	40.201 77	51.873 34	103.746 68	92.075 12	11.671 56
22	50 201 640	56.087 56	43.888 58	56.087 56	112.175 13	99.976 14	12.198 98
23	105 228 216	60.110 75	47.457 04	60.110 75	120.221 51	107.567 80	12.653 70
24	219 139 194	64.569 51	51.396 43	64.569 51	129.139 02	115.965 94	13.173 07
25	458 067 944	68.828 64	55.205 30	68.828 64	137.657 28	124.033 94	13.623 33
26	951 999 224	73.525 69	59.390 25	73.525 69	147.051 39	132.915 95	14.135 44
27	1 985 163 932	78.015 48	63.433 81	78.015 48	156.030 96	141.449 30	14.581 66
28	4 118 332 532	82.945 13	67.857 98	82.945 13	165.890 26	150.803 11	15.087 14
29	8 569 510 852	87.660 86	72.131 19	87.660 86	175.321 72	159.792 05	15.529 68
30	17 749 322 414	92.818 00	76.788 92	92.818 00	185.636 00	169.606 92	16.029 09
31	36 863 339 520	97.755 32	81.287 10	97.755 32	195.510 64	179.042 43	16.468 22
32	76 241 288 094	103.135 35	186.173 32	103.135 35	206.270 70	189.308 67	16.962 04

present data, one fits using each model, and to each of the major and minor end-to-end distance enumerations. The only other possibility left is that the series are so short compared to where the true asymptotic behaviour sets in that there exist turning points and other exotic changes in the exponent estimates. We do caution that this does happen in the case of spiral walks when considering series of length 40 or so! We note that the addition of the logarithmic confluency in the fitting form *decreases* the exponent estimates and so move them away from the directed values. Assuming that the ASSAW are in a separate universality class (the possibility, though remote, remains that they are in the directed class with added logarithmic corrections) this demonstrates that there is competition between the spirality and the anisotropy, and indicates a particular fixed point structure in a renormalisation group study.

3. Discussion

In the previous section we have given several results on the class of ASSAW which indicate that it is a separate universality class. Naturally two questions arise. Given the

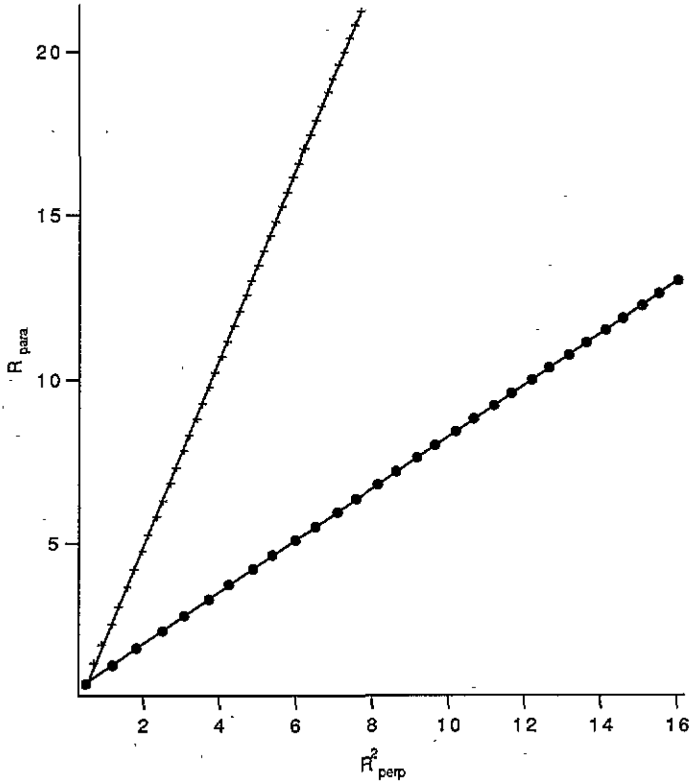

Figure 2. This figure plots the parallel end-to-end distance against the square of the perpendicular end-to-end distance for both the two choice and three choice models of Manna. The straight line is the least squares fit for each set of points. The fit is remarkably good even for short walks.

rule space of two step restrictions on the square lattice how many universality classes are there? Secondly, what factors determine the universality class of a particular rule? We shall attempt to answer these two questions here.

Table 3 catalogues the length scale exponents for the 12 models of figure 1. They fall into seven classes of which three have $\nu_\parallel = 1$ while one (rule (f)) is completely trivial. The important classes are those previously mentioned: SAW ($\nu_\parallel = \nu_\perp = 3/4$); SSAW ($\nu_\parallel = \nu_\perp = 1/2$); DW ($\nu_\parallel = 1, \nu_\perp = 1/2$); ASSAW ($\nu_\parallel = 0.845$, $\nu_\perp = 0.4225$). There is only one member of the SSAW class and four members of SAW (the fourth being a 90 degree rotation of rule (b)). Rule (h) is a new member of the ASSAW class although we have subsequently found that it can be mapped exactly onto the two-choice model (appendix A). This gives six members of the ASSAW while the rest of the 4096 rules are either in the directed classes or one of the trivial classes (where either one exponent is 0 or both are 1). The small number of non-trivial rules has clearly facilitated our work. Given that these are indeed the only classes (we have not done an exhaustive study); we proceed to the second question.

One condition for producing a non-trivial rule is that there must be sufficient options in each direction. For example, any rule with one direction blocked altogether will be directed. Balance is also a criterion: rules that do not have equal numbers of

Table 3. Length scale exponents and symmetries for 12 representative rules.

Rule	$\nu_\parallel$	$\nu_\perp$	Rotation by 90°	Rotation by 180°	Reflection
(a)	3/4	3/4	y	y	y
(b)	3/4	3/4	n	y	y
(c)	3/4	3/4	y	y	y
(d)	1/2 (log)	1/2 (log)	y	y	n
(e)	1	0	n	y	n
(f)	0	0	y	y	n
(g)	0.845 (5)	0.423 (3)	n	y	n
(h)	0.845 (5)	0.423 (3)	n	y	n
(i)	0.845 (5)	0.423 (3)	n	y	n
(j)	1	1/2	n	y	y
(k)	1	1/2	n	n	n
(l)	1	1	y	y	y

possible steps in opposite directions of the two axes will also be directed. These conditions significantly reduce the number of possible rules.

The symmetries of the non-trivial rules provide a sign of their universality class. Table 3 catalogues the symmetries possessed by the 12 rules of figure 1. All the non-trivial rules possess the symmetry of 180°-rotation and so the absence of this symmetry can be used to exclude the unbalanced rules mentioned before and rules similar to rule (k) which are balanced but possess no symmetries (that is all rules where $\langle R_{x,y}\rangle_n \neq 0$). Then the rules in the SSAW and ASSAW classes can be distinguished from the SAW class rules by the lack of a reflection symmetry. (Note that in two dimensions any spirality breaks all reflection symmetries. This is not the case in three dimensions and it seems that there is a three-dimensional two-step rule with reflection symmetry but also spirality that falls into the three-dimensional SAW class [15].) However, there are rules that fall in the directed or trivial classes that possess the same symmetries as those in the non-trivial classes. If one could exclude all members of the DW then one could decide on the universality class simply by symmetry arguments. That is, it would leave only those rules in the SAW, SSAW and ASSAW classes and the occurrence of reflection symmetry then uniquely determines the SAW class and the possession of 90° rotation symmetry distinguishes the SSAW class rule from the ASSAW rules. Let us discuss briefly those rules in the directed/trivial classes that possess the same symmetries as the non trivial rules. If they do not have a reflection symmetry such as rules (e) and (f) then they seem to always be trivial (one exponent is zero and the number of configurations is bounded for any length). If, on the other hand they do possess reflection symmetry like rules (j) and (l) they can be distinguished from the SAW class because there are clearly no configurations that have steps in all four directions and this indicates directedness. Hence, we have given a recipe so that any rule can be classified using quickly obtainable information (directed models are easily identified by inspection) and the symmetries possessed by the rules.

To summarize: In the present article we have explained that anisotropic walks are truly *anisotropic* with respect to length scale exponents essentially because they are concatenations of types of self-avoiding staircase walks. Also, that spirality, which is linked to the absence of reflection symmetry, is a relevant constraint in self-avoiding walk models when coupled with anisotropy: it would seem that the ASSAW universality class is different to the DW class. The presence or absence of reflection and rotation symmetries delineates the non-trivial self-avoiding restricted-rule walks in two dimensions.

Acknowledgments

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Appendix. Proof of mapping rule (h) onto rule (i)

Here we prove that the configurations produced by rule (h) can be mapped bijectively onto the configurations of rule (i) (Manna's two-choice rule). Each rule-(i) configuration can be produced from rule (h) by traversing the configuration backwards.

Proof. Consider a configuration of rule (h). After a step
east (E) the walk can continue N, S, or E;
west (W) the walk can continue N, S, or W;
north (N) the walk can continue E;
south (S) the walk can continue W.
Hence a step from the
east (E) can come from the N, or the E;
west (W) can come from the S, or the W;
north (N) can come from the E, or the W;
south (S) can come from the E, or the W.
Now consider making the step in reverse: this is done precisely according to rule (i). The argument is clearly symmetric and therefore, each configuration produced by rule (h) is produced by rule (i) in reverse and visa versa. Hence, the configurations are identical, ignoring the rooting, which is irrelevant for physical properties.

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