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Critical behaviour of correlated and anisotropic self-avoiding walks

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Abstract. Here we consider self-avoiding walks (SAWS) on a square lattice for which the choice of direction at each step is not entirely random, as in the case of self-avoiding random walks. In the case of correlated SAWS, the choice of the direction (consistent with the self-avoiding restriction) for the nth step is dependent on that for the $(n-1)$th step, while for the anisotropic SAWS, the probability to choose, at any step, the particular anisotropic lattice direction is different from that for the other directions. Both the extrapolation of exact enumeration results and a small cell real space renormalisation group study indicate that finite correlation does not affect the random SAW critical behaviour, while any finite amount of lattice anisotropy induces a crossover to the 'directed' SAW critical behaviour.

1. Introduction

The long (linear) polymer molecules are quite accurately and successfully modelled by the random self-avoiding walks (random SAWS) on lattices where, at each step, a random direction for the walk on the lattice is chosen, consistent with the self-avoiding restriction which takes into account the 'excluded volume effect'. This self-avoiding restriction or the excluded volume effect leads to the well known scaling relations and exponents for the statistics of random SAWS or linear polymers (see e.g., de Gennes 1979).

Here we consider SAWS for which the choice, at each step, of the direction (consistent, of course, with the self-avoiding restriction) is not entirely random; rather they are biased in two different ways. In the first kind of walk, which we call correlated SAWS, the choice of the direction for the nth step is dependent on that for the $(n-1)$th step. For example, one might consider the case of a SAW where the nth step has got more (less) affinity to follow the same direction as that for the $(n-1)$th step, giving rise to ferro (antiferro) type correlated SAW. In the second kind of walk considered, called anisotropic SAWS, the lattice, on which the walks are performed, is assumed to be anisotropic. Consequently, the probability to choose, at any step, the particular anisotropic lattice direction is different from that for other lattice directions. In the extreme limit of the ferro type correlation for the correlated SAWS we have defined, an N stepped SAW on any dimensional lattice becomes a linear chain of length N. Consequently the critical behaviour for the SAW statistics crosses over, in this limit of correlation, to that of SAWS in one dimension. In the opposite extreme limit of

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correlation (antiferro type) the same direction is never followed for two successive steps. Enumeration results for various two-dimensional lattices suggest (Grassberger 1982) that this kind of correlated SAWs belong to the same university class as that of random SAWs. In the extreme limit of lattice anisotropy where walks are forbidden to step in directions other than the particular (anisotropic) lattice direction, the N stepped SAW again becomes a linear chain of length N. While in the opposite extreme limit of anisotropy, where the walks are forbidden to step in the particular (anisotropic) lattice direction, the SAWs reduce to 'directed' SAWs (Fisher and Sykes 1959, Chakrabarti and Manna 1983), for which the critical behaviour is anisotropic and mean-field-like (Cardy 1983, Redner and Majid 1983, Szpilka 1983). We will consider here such correlated and anisotropic SAWs on a square lattice in the entire range of correlation and anisotropy.

For exact simulation of such correlated SAWs, we simulate all the (random) SAWs of step sizes (N) upto a finite maximum, and assign a weight α^n for each walk configuration having n sites through which the walk passes straight. $\alpha > 1$ thus corresponds to ferro type correlation and $\alpha < 1$ corresponds to antiferro type correlation ($\alpha = 1$ corresponds to ordinary random SAW). In the limit $\alpha \to \infty$, the SAWs become one dimensional. In the limit $\alpha = 0$, the SAWs contributing to the total weight function will not have any two successive steps in the same direction. The total weight of the zeroth and the second moments of the distribution function are then given by

$$G_N(\alpha) = \sum_{\substack{\text{all SAWs} \\ \text{of size } N}} \alpha^n = \sum_{n=0}^{N-1} g_n(N)\alpha^n, \tag{1}$$

where $g_n(N)$ are the number of N stepped SAWs having n sites through which the SAW passes straight, without changing the direction, and

$$R_N^2(\alpha) = \sum_{\substack{\text{all SAWs} \\ \text{of size } N}} R^2_{\text{end-to-end}}\alpha^n = \sum_{n=0}^{N-1} r_n^2(N)\alpha^n, \tag{2}$$

where $r_n^2(N)$ is the sum of the squares of end-to-end distances of the SAWs having the same n, the number of sites through which the SAW passes straight. In the limit $\alpha = 1$, $G_N(\alpha)$ and $R_N^2(\alpha)/G_N(\alpha)$ reduces respectively to the total number of SAWs of N steps and the average end-to-end distance. Extrapolating the results for finite step sizes N (the maximum value of $N = 17$ here), we tried to fit these two moments with the asymptotic scaling forms

$$G_N(\alpha) \sim [\mu(\alpha)]^N N^{\gamma-1} \tag{3}$$

$$R_N^2(\alpha) \sim C(\alpha) N^{2\nu} \tag{4}$$

and found that the exponents γ and ν do not change with the correlation weight factor α for $0 \leqslant \alpha \ll \infty$, showing that finite correlation does not affect the SAW critical behaviour. This has also been shown using a small cell real space renormlisation group (RSRG) technique. A similar situation also occurs for the random percolation problem, where such (quenched) correlation does not affect the critical behaviour (Chakrabarti *et al* 1981, Zhang 1982, Tuthill and Klein 1983 and references therein). The phase diagram ($\mu(\alpha)$ against α) for the correlated SAW, obtained here from extrapolation of the exact enumeration results have been compared with that obtained employing the RSRG technique.

To study the critical behaviour of SAWs on anisotropic lattices, we enumerate again all the (random) SAWs of a finite number of steps (N) on a square lattice and assign an anisotropy weight factor α for each step in the particular anisotropic lattice direction (e.g., the vertical upward direction). In the limit $\alpha = 1$, the problem reduces to that of ordinary SAWs, while for $\alpha = 0$ no step in the vertical upward direction is permitted and the remaining SAWs, contributing to the total weight function, will be 'directed' SAWs. Here also we define $G_N(\alpha)$ and $R_N^2(\alpha)$ as the total weights for the zeroth and the second moment of the distribution function respectively, in an exactly similar way as in equations (1) and (2). Here n corresponds to the number of steps in the specified (anisotropic) lattice direction (vertical up direction in our example), $g_n(N)$ corresponds to the number of N stepped SAWs having n steps in that specified direction and $r_n^2(N)$ corresponds to the sum of the squares of their end-to-end distances. We then tried to fit our extrapolated simulation results to the asymptotic scaling forms like (3) and (4) and the results indicate that the crossover to 'directed' SAW critical behaviours occurs for any finite amount of lattice anisotropy ($\alpha \neq 1$). The same has been confirmed, using a small cell RSRG technique. The phase diagram ($\mu(\alpha)$ against α) for the anisotropic SAW, obtained by extrapolating the exact enumeration results has been compared with that obtained by employing the RSRG technique.

2. Simulation results for correlated and anisotropic SAWS

In order to obtain $g_n(N)$ and $r_n^2(N)$, as defined in equations (1) and (2), for correlated and anisotropic SAWs, we first enumerate all the (random) SAW configurations, for a finite step size N, following Martin (1974). For each of these configurations, we count the number (n) of sites through which the SAW passes straight (without changing direction). Collecting the number of such SAW configurations having the same value of n, and summing up the squares of their end-to-end distances, we get $g_n(N)$ and $r_n^2(N)$ respectively for the correlated SAW. To determine the same quantities $g_n(N)$ and $r_n^2(N)$ for anisotropic SAWs, we count, for each (random) SAW configuration, the number n of bonds traced in the (specified) anisotropic lattice direction. For step size up to 17, the results for $g_n(N)$ and $r_n^2(N)$ for both correlated and anisotropic SAWs are given in tables 1(a), 1(b) and 2(a), 2(b) respectively. It may be noted that for correlated SAWs $g_0(N)$ and $r_0^2(N)$ correspond respectively to the number and sum of the squares of the end-to-end distances of N stepped 'two choice' SAWs on square lattice (Grassberger 1982) and for anisotropic SAWs, $g_0(N)$ and $r_0^2(N)$ correspond respectively to the number and sum of the squares of the end-to-end distances of N stepped 'directed' SAWs on a square lattice (Chakrabarti and Manna 1983, Blöte and Hilhorst 1983).

2.1. *Analysis of the simulation data*

The values of the scaling exponent γ and the connectivity constant $\mu(\alpha)$ (equation (3)) are determined, from these simulation results for finite steps N, following the extrapolation method of Martin (1974). To find the value of the average end-to-end distance

Table 1. (*a*) $g_n(N)$, as defined in equation (1), for correlated SAWS on a square lattice. (*b*) $r_n^2(N)$, as defined in equation (2), for correlated SAWS on a square lattice.

(*a*)

n \ N	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0	—	8	16	24	40	64	104	168	272	440	712	1128	1808	2896	4640	7368	11 744
1		4	16	48	112	232	464	872	1632	2944	5312	9368	16 464	28 496	49 216	84 144	143 504
2			4	24	96	280	736	1712	3816	8000	16 400	32 424	63 224	120 136	226 272	418 344	768 544
3				4	32	160	576	1760	4800	12 032	28 544	64 376	140 624	297 064	614 112	1239 496	2463 648
4					4	40	240	1008	3600	11 040	31 336	81 792	204 104	483 160	1110 824	2461 528	5344 744
5						4	48	336	1632	6544	22 624	70 624	203 616	550 792	1418 336	3496 632	8333 872
6							4	56	448	2448	11 040	41 968	144 656	451 888	1329 888	3671 040	9734 328
7								4	64	576	3520	17 440	73 008	272 528	925 072	2917 984	8659 104
8									4	72	720	4840	26 360	119 504	484 424	1761 952	5973 528
9										4	80	880	6480	38 200	187 728	815 136	3183 504
10											4	88	1056	8424	53 760	282 992	1318 664
11												4	96	1248	10 752	73 472	414 528
12													4	104	1456	13 440	98 336
13														4	112	1680	16 576
14															4	120	1920
15																4	128
16																	4

(*b*)

n \ N	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0	—	16	48	128	296	640	1320	2624	5072	9584	17 800	32 576	58 864	105 248	186 528	327 936	572 448
1		16	80	288	880	2368	5840	13 356	29 920	63 712	131 648	265 376	524 048	1016 736	1943 104	3665 184	6834 576
2			36	224	960	3376	10 336	28 704	74 056	180 544	420 624	944 384	2056 344	4363 248	9055 264	18 436 832	36 916 160
3				64	480	2400	9600	33 056	102 080	290 432	774 528	1961 184	4757 072	11 134 144	25 277 216	55 907 424	120 870 624
4					100	880	5040	22 656	86 736	295 168	918 216	2660 544	7276 168	18 970 352	47 505 576	114 945 664	269 979 496
5						144	1456	9408	47 008	198 240	737 184	2490 432	7790 816	22 894 848	63 852 256	170 398 496	437 802 096
6							196	2240	16 128	88 736	408 864	1650 176	6016 784	20 216 416	63 533 344	188 775 040	534 839 224
7								256	3264	25 920	155 776	778 848	3391 088	13 275 328	47 683 536	159 602 112	503 338 528
8									324	4560	39 600	258 176	1392 312	6505 984	27 219 240	104 092 640	369 704 920
9										400	6160	58 080	408 336	2362 976	11 796 048	52 529 408	213 096 208
10											484	8096	82 368	621 264	3840 256	20 398 592	96 337 032
11												576	10 400	113 568	914 816	6016 192	33 881 920
12													676	13 104	152 880	1309 952	9132 704
13														784	16 240	201 600	1830 976
14															900	19 840	261 120
15																1024	23 936
16																	1156

Table 2. (*a*) $g_n(N)$, as defined in equation (1), for anisotropic SAWs on a square lattice. (*b*) $r_n^2(N)$, as defined in equation (2), for anisotropic SAWs on a square lattice.

(*a*)

n \ N	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0	3	7	17	41	99	239	577	1393	3363	8119	19 601	47 321	114 243	275 807	665 857	1607 521	3880 899
1	1	4	12	28	74	184	478	1216	3122	7956	20 272	51 468	130 426	329 720	831 938	2095 136	5267 426
2		1	6	22	64	166	442	1100	2882	7310	19 052	49 010	127 174	328 134	847 672	2183 072	5616 248
3			1	8	36	124	368	1016	2724	7000	18 310	46 488	121 262	310 900	811 398	2099 036	5471 732
4				1	10	54	216	724	2190	6220	16 978	44 952	118 178	304 066	792 194	2030 110	5294 198
5					1	12	76	348	1308	4336	13 250	38 272	106 412	287 664	765 084	2000 532	5228 266
6						1	14	102	528	2208	8010	26 370	81 050	237 044	668 802	1836 470	4948 518
7							1	16	132	764	3528	13 956	49 482	162 020	500 046	1476 236	4213 312
8								1	18	166	1064	5388	23 142	88 210	307 662	1003 150	3105 618
9									1	20	204	1436	7924	36 792	150 386	558 144	1922 766
10										1	22	246	1888	11 288	56 418	246 594	972 322
11											1	24	292	2428	15 648	83 852	390 778
12												1	26	342	3064	21 188	121 278
13													1	28	396	3804	28 108
14														1	30	454	4656
15															1	32	516
16																1	34
17																	1

(*b*)

n \ N	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0	3	20	89	336	1155	3740	11 617	34 992	102 931	297 108	844 441	2369 312	6575 411	18 077 436	49 294 209	133 454 240	359 006 819
1	1	8	36	144	530	1856	6222	20 184	63 754	197 024	597 792	1785 464	5260 474	15 314 216	44 111 722	125 862 416	356 071 666
2		4	30	128	448	1472	4730	15 008	46 970	145 304	444 188	1343 544	4023 086	11 935 704	35 105 800	102 426 864	296 607 200
3			9	80	388	1432	4648	14 296	43 020	128 392	381 398	1130 008	3335 750	9813 680	28 751 958	83 889 960	243 693 660
4				16	170	960	3968	13 776	43 470	130 352	380 914	1100 040	3161 250	9073 808	26 029 794	74 669 944	214 046 486
5					25	312	2036	9504	36 260	122 056	380 162	1128 840	3258 988	9262 416	26 122 380	73 451 240	206 393 962
6						36	518	3856	20 224	85 184	310 362	1025 776	3173 794	9394 808	27 015 226	76 279 144	213 103 590
7							49	800	6708	39 208	181 792	719 160	2543 954	8307 632	25 616 286	75 815 360	218 008 192
8								64	1170	10 928	70 592	358 448	1537 334	5833 120	20 215 246	65 468 384	201 516 554
9									81	1640	16 900	119 728	662 076	3068 552	12 478 962	45 966 552	156 931 294
10										100	2222	25 056	193 344	1158 080	5778 306	25 133 376	98 359 562
11											121	2928	35 876	299 704	1934 744	10 352 664	48 036 322
12												144	3770	49 888	448 768	3108 112	17 770 078
13													169	4760	67 668	652 352	4827 348
14														196	5910	89 840	924 288
15															225	7232	117 076
16																256	8738
17																	289

exponent ν (equation (4)), we calculate

$$\rho_N(\alpha) = R_N^2(\alpha)/G_N(\alpha) \tag{5}$$

and

$$\nu_N(\alpha) = \tfrac{1}{2}N(\rho_{N+1}(\alpha)/\rho_N(\alpha) - 1). \tag{6}$$

Plotting these $\nu_N(\alpha)$ values against $1/N$, we find the average ν (for $1/N \to 0$) from separate extrapolations for even and odd N values. These average ν values are then found for different values of α. These results for exponents γ and ν, for both correlated and anisotropic SAWs, for various values of α are shown in figures 1 and 2 respectively.

For the correlated SAW, γ remains practically unchanged (from $\gamma = 1.324$ for $\alpha = 1$, compared with the exact value $\frac{43}{32}$ (Nienhuis 1982)) with the variation of the correlation weight factor $\alpha (0 \leq \alpha \leq 2)$. The systematic decrease in the γ value for the correlated SAWs for $\alpha \to 0$ is due to the finite size effect. This was confirmed when, using the enumeration results of Grassberger (1982) for his 'two choice' SAWs on a square lattice (which are the only contributing terms for $\alpha = 0$ in our case) for step sizes N up to 44, we found the same value of γ (see figure 1). It was seen that for $\alpha \geq 40$, the exponent γ becomes equal to 1 (linear chain value), as expected for these large correlations. The average end-to-end distance exponent ν for the correlated SAW also remains unchanged (remaining very nearly equal to 0.739 for $\alpha = 1$, compared with the exact value $\nu = 0.75$ (Nienhuis 1982)) for $0 \leq \alpha \leq 2$, as shown in figure 2. It was seen that the crossover to linear chain behaviour in ν occurs for $\alpha \geq 100$. This shows that for finite amount of correlation, the SAW critical behaviour remains unchanged. This has been further confirmed in the next section, using small cell RSRG results.

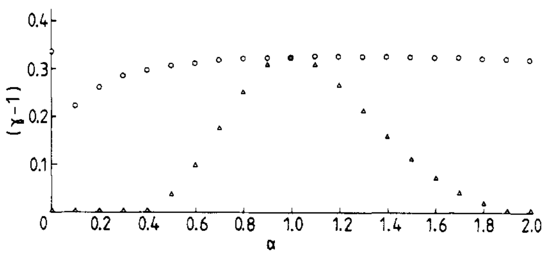

Figure 1. Plot of the values of the exponent γ against the weight factor α for correlated (○) and anisotropic (△) SAWs.

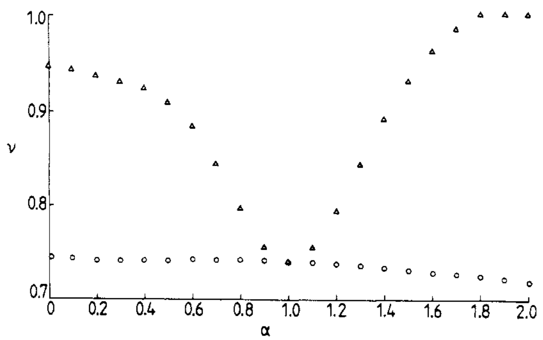

Figure 2. Plot of the values of the exponent ν against the weight factor α for correlated (○) and anisotropic (△) SAWs.

For anisotropic SAWs, both γ and ν immediately change as the isotropy of the lattice is disturbed (α is different from unity). Although γ and ν are found respectively to decrease and increase gradually and assume the 'directed' SAW exponent values ($\gamma = \nu = 1$, see e.g., Cardy 1983) for $0 \leq \alpha < 0.4$ and $\alpha > 1.9$ (see figures 1 and 2), we believe, this gradual crossover is a manifestation of the finite size effect. In fact, the crossover was observed to become sharper as the step size N was increased (see figure 3). It may be noted that even for completely 'directed' SAWs ($\alpha = 0$), the extrapolated γ value did not reach the 'directed' SAW exponent value ($\gamma = 1$). This is also due to the finite size (up to $N = 17$) of the walks we have simulated, as indicated by figure 3. Thus, these enumeration results for anisotropic SAWs indicate that the crossover to directed SAW critical behaviour occurs for any finite amount of lattice anisotropy ($\alpha \neq 1$). This is also in agreement with the small cell RSRG results, obtained in the next section.

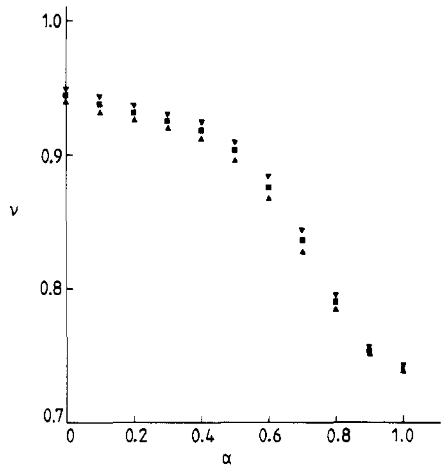

Figure 3. Plot of the values of the exponent ν, obtained by extrapolating the results for various step sizes, (▼, 7–16; ■, 7–14; ▲, 7–12) against the anisotropy weight factor α (shows the finite size effect).

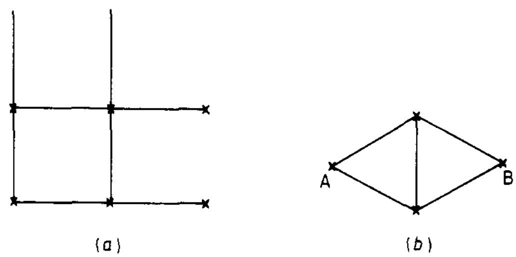

Figure 4. (a) Basic cell, of the square lattice, which scales to a single bond in each direction under renormalisation. (b) 'Wheatstone Bridge' construction; a single bond AB is left after rescaling.

3. RSRG treatment for correlated and anisotropic SAWS

The scaling transformations (see e.g., Stanley *et al* 1982) for the fugacity (f) of the monomers and their correlation or anisotropy parameter (α) are derived here using first a reconstruction (following Bernasconi 1978 and Yeomans and Stinchcombe 1979) of the square lattice cell, shown in figure 4(a), to a 'Wheatstone bridge' type cell as shown in figure 4(b), and then rescaling this cell to a single horizontal bond AB (scale factor $b = 2$). The renormalised bond AB is assigned a renormalised fugacity f' if SAWs starting from A reach B.

Using the cell shown in figure 4(b), the recursion relation for f in the case of the correlated SAW may be written as

$$f' = 2f^2\alpha + 2f^3, \tag{7}$$

where α is the correlation weight factor contributing at each site through which the SAW passes straight (strictly speaking, passing straight through a site is only possible in the original cell; figure 4(a)). Considering an adjacent similar cell, renormalisable to another horizontal bond BC, we get the recursion relation for α

$$\alpha' f'^2 = (2f^{2\alpha} + 2f^3)[(\alpha^2 + \alpha)f^2 + (1+\alpha)f^3]. \tag{8}$$

Similarly, considering the lattice anisotropy in the vertical up direction, the recursion relation for f, in the case of anisotropic SAW, can be written, using the cell shown in figure 4(b), as

$$f' = 2f^2 + f^3(1+\alpha), \tag{9}$$

where α is here the anisotropy weight factor for each step in the vertical up direction. Considering a similar cell (as in figure 4(b)) in the vertical direction, the recursion relation for α may be written as

$$\alpha' f' = \alpha^2(2f^2 + 2f^3). \tag{10}$$

It may be noted that all these recursion relations (7)–(8) and (9)–(10) become degenerate, in the random SAW limit ($\alpha = 1$), which, especially in the case of the correlated SAW, is the reason for our choice of the 'Wheatstone bridge' type reconstructed cell.

The non-trivial fixed points and exponents for these recursion relations are given in table 3. The corresponding flow diagrams for correlated and anisotropic SAWs are shown in figures 5 and 6 respectively. Both the table (positive crossover exponent

Table 3. Non-trivial fixed points and exponents for correlated and anisotropic SAWs.

Type of walk	Correlated SAW	Anisotropic SAW	
Fixed points (FP)	$\alpha^* = 1, f^* = 0.366$ ($\mu \equiv 1/f^* = 2.732$) (random SAW FP)	$\alpha^* = 1, f^* = 0.366$ ($\mu = 2.732$) (random SAW FP)	$\alpha^* = 0, f^* = 0.414$ ($\mu = 2.414$) ('directed' SAW FP)
End-to-end distance exponent (ν)	0.846	0.846	0.894
Crossover exponent (φ_α/ν)	-1.182	1.628	$-\infty$

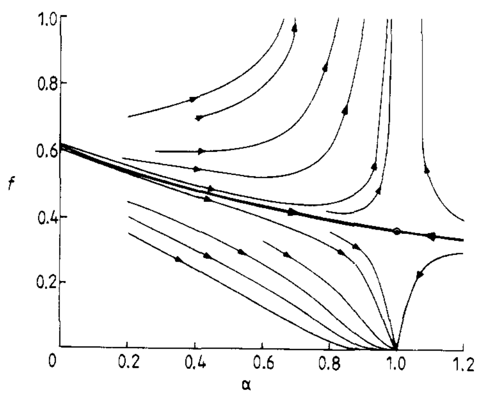

Figure 5. Flow diagram for correlated SAWs (RSRG equations (7) and (8)).

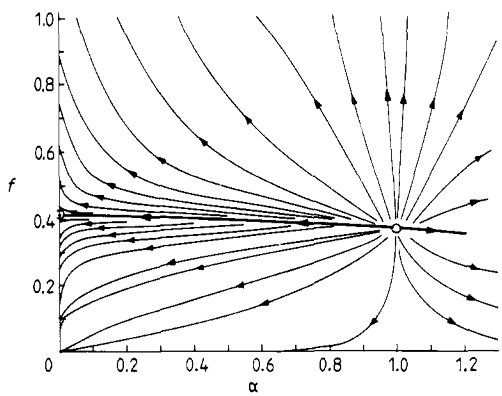

Figure 6. Flow diagram for anisotropic SAWs (RSRG equations (9) and (10)).

indicating instability) as well as the flow diagrams support our conclusions in the previous section: finite correlation does not affect the SAW critical behaviour, while any finite amount of lattice anisotropy induces a cross over to 'directed' SAW critical behaviour.

The phase diagrams (plot of $\mu(\alpha)$ against α), for both correlated and anisotropic SAWs, obtained from the above flow diagrams (figures 5 and 6) are compared in figure 7 with those obtained from the extrapolation of exact enumeration results of the previous section.

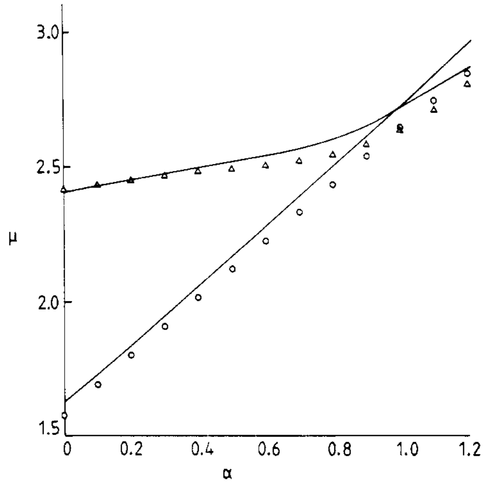

Figure 7. Comparison of the phase diagram ($\mu(\alpha)$ against α) for both correlated (○) and anisotropic (△) SAWs, obtained using RSRG (full curves) and extrapolating the exact enumeration results.

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