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Universality class of trails in two dimensions

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Abstract. A trail is a walk on a lattice that may visit a site more than once but a bond at most once. We have carried out transfer-matrix studies of trails on the square lattice and of hybrid walks that interpolate between self-avoiding walks and trails. The results are in agreement with the same universal exponents as self-avoiding walks. However, the finite-size corrections are much larger than for self-avoiding walks. An explanation in terms of an irrelevant variable with scaling index $y_u = -11/12$ is given.

A trail [1–8] is defined as a walk on a lattice that may visit a site more than once but a bond at most once. Unlike a self-avoiding walk (SAW), a trail may intersect itself. Due to the restriction on the bond visits, trails are self-repelling, but not as strongly self-repelling as SAWs. It has long been suspected that trails and SAWs belong to the same universality class. The exact enumerations and Monte Carlo studies of Guttmann and others [3–7] support this interpretation. However, the convergence of the data with increasing number of steps is much slower for trails than for SAWs.

Transfer-matrix finite-size scaling methods have yielded very precise estimates of the critical exponents of SAWs in two dimensions [9–12]. For example, Derrida [9] found that phenomenological renormalization of SAWs on the square lattice from strip width 11 to 10 yields $\nu = y_t^{-1} = 0.750\,067$, compared with the exact [13, 14] value 3/4. Hoping to obtain definitive information on the question of the university class, we have carried out similar calculations for trails on the square lattice and for 'hybrid walks' that interpolate between trails and SAWs. As seen below, our data are in agreement with SAW exponents, but we also find much slower convergence with increasing system size for trails than for SAWs.

In addition to numerical evidence, a mapping onto the Coulomb gas suggests that trails and SAWs belong to the same universality class. There is a well known correspondence [15] between SAWs and the isotropic critical $O(n)$ model in the limit $n \to 0$. Nienhuis [13, 14] applied the Coulomb gas method to the $O(n)$ model in two dimensions and showed that cubic anisotropy† is an irrelevant perturbation at $n = 0$ with scaling index $y_{\mathrm{ca}} = -11/12$. In the language of SAWs or polymers this is the scaling index of a vertex where four polymers meet [14, 16]. The intersections of trails are four polymer vertices and presumably have this scaling index. Coulomb gas methods are not rigorous, but the predicted scaling index

† Shapir and Oono [8] have argued that trails on the square lattice belong to the SAW universality class on the basis of an effective $O(2n)$, $n \to 0$ field theory with an irrelevant cubic symmetry-breaking term.

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$-11/12$ for intersections is in good agreement with finite-size studies [17], so there is little reason to doubt it.

The irrelevance of intersections in the SAW model means that they do not change the universal behaviour for sufficiently low intersection fugacity. However, a higher critical point could occur at a larger fugacity, separating the trail and SAW universality classes. This gives us another reason for investigating the universal properties of models with intersections. We find no evidence for such a higher critical point in the numerical studies described later. However, the finite-size convergence is clearly slower than for the SAW model. We attribute the poorer convergence, which is observed in all finite-size studies of trails, to the irrelevant variable corresponding to the fugacity of the intersections, as discussed later.

Still another reason for our numerical studies is the controversy surrounding the correction to scaling exponent Δ for SAWs, defined by the asymptotic form $G \approx N^{\nu}(A+BN^{-\Delta})$, for large N, of the average radius of gyration G of SAWs of N steps. Here $\Delta = -y_u/y_t$, where $y_t = 4/3$ and y_u are the leading and next-to-leading thermal scaling indices of the $O(n)$, $n \to 0$ model. There are two candidates for y_u from the Coulomb gas approach, the scaling index $-11/12$ for four polymer vertices [10, 16] and a non-leading thermal scaling index -2 derived in [13]. Enumerations and Monte Carlo studies of SAWs, reviewed in [18, 19], have yielded estimates of Δ between 0.5 and 1.5, more consistent, for the most part, with $y_u = -11/12$ than -2. We know of no compelling theoretical reason why the $-11/12$ contribution should vanish for SAWs†. However, recent estimates from enumerations with larger N [20, 21] and our finite-size studies described below are more compatible with -2 than $-11/12$. Our corresponding results for trails, on the other hand, are compatible with $y_u = -11/12$.

Our numerical calculations consider hybrid walks on the square lattice, where at most two visits per site are allowed. We work in the grand canonical ensemble, assigning a bond fugacity K to each step of the walk and a fugacity α to each site visited more than once. Both intersections and 'collisions', where a walk returns to a site without crossing itself, have Boltzmann weight α. The values $\alpha = 0$ and $\alpha = 1$ correspond to SAWs and trails, respectively, and by varying α, one may interpolate between these two special cases. If there is a higher critical point separating the trail and SAW universality classes, it thus becomes accessible.

We have obtained the exact transfer matrix for one hybrid walk on a strip of width L with periodic (cylindrical) boundary conditions by extending Derrida's procedure [9] for SAWs to include non-nested as well as nested configurations, using methods described for example by Blöte and Nienhuis [11]. The largest eigenvalue $\lambda_L^{(1)}$ of the one-walk transfer matrix determines a correlation length $\xi_L^{(1)}$ according to [9]

$$\xi_L^{(1)}(K,\alpha) = -[\ln \lambda_L^{(1)}(K,\alpha)]^{-1}. \tag{1}$$

For fixed intersection fugacity α we generate sequences of estimates $K_{\mathrm{c}}(\alpha, L)$, $y_t(\alpha, L)$ for the critical bond fugacity (inverse connectivity) and the thermal scaling index that approach exact bulk values $K_{\mathrm{c}}(\alpha)$ and $y_t = 2 - x_{\mathrm{eng}} = \nu^{-1}$, respectively, in the limit $L \to \infty$ from the phenomenological renormalization equations [22]

$$L^{-1}\xi_L^{(1)}(K_{\mathrm{c}}(\alpha, L), \alpha) = (L-1)^{-1}\xi_{L-1}^{(1)}(K_{\mathrm{c}}(\alpha, L), \alpha) \tag{2}$$

† The close encounters or near collisions of a SAW with itself correspond to four polymer vertices with scaling index $-11/12$. In the $O(n)$ model the index $y_{\mathrm{ca}} = -11/12$ is not only associated with cubic anisotropic interactions but also with isotropic interactions such as $(s_1 \cdot s_2)^2$ and $s_1 \cdot s_3 s_2 \cdot s_4$, where $s_1, \ldots, s_4$ are spins at the corners of an elementary square of the lattice [13, 14]. If absent in the starting Hamiltonian, such interactions are presumably generated by the renormalization group.

$$1 + y_t(\alpha, L) = \frac{\ln[(\partial\xi_L^{(1)}/\partial K)(\partial\xi_{L-1}^{(1)}/\partial K)^{-1}]}{\ln[L(L-1)^{-1}]}. \tag{3}$$

The partial derivatives in equation (3) are evaluated at $K = K_c(\alpha, L)$.

To estimate the magnetic scaling dimension $x_{mag} = 2 - y_h = 1 - \gamma/2\nu$, we make use of the relation $\lim_{L\to\infty} L^{-1}\xi_L^{(1)}(K_c(\alpha), \alpha) = (2\pi x_{mag})^{-1}$, implied by conformal invariance [23], and calculate the sequence

$$x_{mag}(L) = L[2\pi\xi_L^{(1)}(K_c(\alpha, L), \alpha)]^{-1} \tag{4}$$

which approaches x_{mag} in the limit $L \to \infty$. Another sequence of estimates of the scaling dimension of the energy density $x_{eng} = 2 - y_t$, in addition to the sequence based on equation (3), follows from the relation

$$x_{eng}(L) = L[2\pi\xi_L^{(2)}(K_c(\alpha, L), \alpha)]^{-1} \tag{5}$$

analogous to (4). Here $\xi_l^{(2)}$ is the correlation length associated with two walks on the strip [10, 12].

In table 1 estimates of K_c, y_t, x_{mag}, and x_{eng} for SAWs ($\alpha = 0$), calculated from equations (2)–(5), respectively, are given for strip widths $L \leqslant 13$. (Strips with $L \leqslant 11$ are analysed in [9].) Extrapolation of K_c on the basis of iterated fits [24] with a finite-size correction exponent $y_u - y_t = -10/3$ (see below) yields $K_c = 0.379\,052 \pm 0.000\,001$, in excellent agreement with the [20] estimate $K_c = 0.379\,05228 \pm 0.000\,00014$ of the critical fugacity or inverse connectivity of SAWs on the square lattice. The data in table 1 are also in good agreement with the accepted exact values [13, 14]

$$y_t = 2 - x_{eng} = 4/3 \qquad x_{mag} = 5/48 = 0.104\,166\,666\ldots \tag{6}$$

of the SAW exponents. Note that the sequence for y_t is not monotonic but must pass through a minimum for $L > 12$ in order to extrapolate to 4/3.

Table 1. Estimates of K_c, y_t, x_{mag} and x_{eng} for SAWs ($\alpha = 0$) from equations (2)–(5).

L	K_c	y_t	x_{mag}	x_{eng}
3	0.365 304 779	1.380 306 95	0.145 960 861	0.699 759 482
4	0.373 399 472	1.352 952 14	0.128 532 404	0.692 670 246
5	0.376 632 894	1.342 272 25	0.118 351 629	0.684 192 681
6	0.377 909 540	1.337 471 12	0.112 940 779	0.678 737 907
7	0.378 447 688	1.335 241 59	0.110 031 096	0.675 502 494
8	0.378 698 393	1.334 174 75	0.108 365 532	0.673 508 762
9	0.378 827 984	1.333 641 92	0.107 336 457	0.672 191 684
10	0.378 901 312	1.333 363 70	0.106 655 017	0.671 262 850
11	0.378 945 913	1.333 213 53	0.106 177 949	0.670 573 556
12	0.378 974 611	1.333 131 46	0.105 829 338	0.670 042 355
13	0.378 993 914	1.333 087 45	0.105 566 001	0.669 621 276

In table 2 estimates of K_c, y_t, x_{mag} and x_{eng} for trails ($\alpha = 1$) from equations (2)–(5), respectively, are given for $L \leqslant 11$. Extrapolation of the K_c data, using an iterated fit with a finite-size correction exponent $y_u - y_t = -9/4$ (see below), yields $K_c = 0.367\,57 \pm 0.000\,01$, in excellent agreement with the estimate $K_c = 0.367\,563 \pm 0.000\,001$ of Conway and Guttmann [6]. The finite-size extrapolation reproduces the minimum that the finite-size data must pass through for $L > 10$ in order to be consistent with Conway and Guttmann's result.

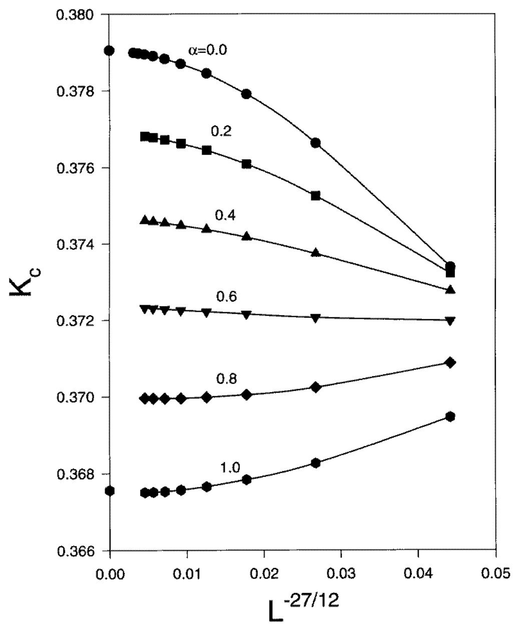

Figure 1. Data for the critical bond fugacity $K_c(\alpha)$ of type 1 walks from equation (2) with $\alpha = 0, 0.2, \ldots, 1$ and $L \leqslant 13$ for $\alpha = 0$, $L \leqslant 11$ for $\alpha > 0$. The best estimates of [20] for SAWs ($\alpha = 0$) and of [6] for trails ($\alpha = 1$) are indicated on the vertical $L = \infty$ axis.

Table 2. Estimates of K_c, y_t, x_{mag} and x_{eng} for trails ($\alpha = 1$) from equations (2)–(5).

L	K_c	y_t	x_{mag}	x_{eng}
3	0.373 913 736	1.377 402 30	0.088 156 273	0.479 376 773
4	0.369 462 256	1.379 958 49	0.099 072 006	0.524 999 724
5	0.368 264 648	1.375 897 06	0.103 448 333	0.553 038 507
6	0.367 836 824	1.371 450 09	0.105 573 002	0.572 883 716
7	0.367 655 441	1.367 482 36	0.106 729 231	0.587 836 947
8	0.367 571 856	1.364 052 81	0.107 386 876	0.599 478 530
9	0.367 532 339	1.361 107 89	0.107 759 842	0.608 741 185
10	0.367 514 159	1.358 578 68	0.107 961 227	0.616 237 060
11	0.367 506 746	1.356 399 60	0.108 055 983	0.622 389 784

In Figure 1 data for the critical bond fugacity $K_c(\alpha)$, calculated according to equation (2) for $\alpha = 0, 0.2, \ldots, 1$, are plotted against $L^{-9/4}$. The reason for this particular power of L is given below. The best estimates $K_c(0) = 0.379\,05228 \pm 0.000\,00014$ for SAWs [20] and $K_c(1) = 0.367\,563 \pm 0.000\,001$ for trails [6] are indicated on the vertical $L = \infty$ axis. As mentioned in the previous paragraph, the data for trails must pass through a minimum for $L > 10$ for consistency with the best estimate. There are minima at $L = 4$ and 9 in the K_c data for $\alpha = 0.6$ and 0.8, respectively, and the minimum presumably moves out to $L > 10$ for $\alpha = 1$.

In figures 2–4 estimates of the exponents y_t, x_{mag} and x_{eng}, calculated according to equations (3)–(5) for $\alpha = 0, 0.2, \ldots, 1$, are plotted against $L^{-11/12}$. The reason for this particular power of L is given below. The point on the vertical axis corresponding to

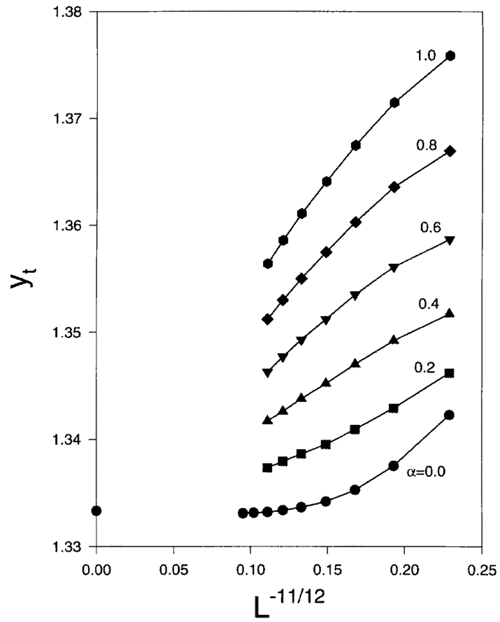

Figure 2. Data for the scaling index y_t of type 1 walks from equation (3) with $\alpha = 0, 0.2, \ldots, 1$ and $L \leqslant 13$ for $\alpha = 0$, $L \leqslant 11$ for $\alpha > 0$. The exact result 4/3 for the SAW ($\alpha = 0$) is indicated on the vertical $L = \infty$ axis.

$L = \infty$ in each of the figures indicates the exact result (6) for SAWs. The data the for y_t in figure 2 support the interpretation that SAWs and trails belong to the same universality class convincingly.

The estimates of x_{mag} for hybrid walks with $\alpha = 0.6$ and 0.8 in figure 3 are non-monotonic, with maxima at $L = 4$ and 9, respectively. Presumably the maximum moves out to $L > 10$ for $\alpha = 1$. For this reason it is difficult to extrapolate the x_{mag} sequence for trails, given in table 2, reliably. Guttman [3, 4] also found better behaved data, based on exact enumerations, for $\nu = y_t^{-1}$ than for $\gamma = 2y_t^{-1}(1 - x_{\mathrm{mag}})$.

The data x_{eng} data for $\alpha > 0$ in figure 4, which are based on equation (5), are not as clearly consistent with the SAW prediction 2/3 as the data for $y_t = 2 - x_{\mathrm{eng}}$ in figure 2, based on (3). Linear extrapolation through the points for $L = 10,\ 11$ in figure 4 leads to values slightly larger than 2/3 that increase with increasing α, for example 0.690 for $\alpha = 1$. The slight downward curvature of the data with increasing L must increase for $L > 11$ for consistency with the SAW prediction. Fitting procedures with the predicted finite-size exponent $y_u = -11/12$ and an additional finite-size correction with exponent -2 yield results that are consistent with $x_{\mathrm{eng}} = 2/3$, but with a relatively poor accuracy of a few times 10^{-2}.

In figures 2–4 one sees that the finite-size corrections generally increase as α increases. The sequences for $\alpha = 0$ and $\alpha \neq 0$ seem to vary, for large L, according to different power laws. The leading power-law correction follows from the standard finite-size scaling ansatz [25]

$$L^{-1}\xi_L^{(i)}(K, \alpha) = f^{(i)}(L^{y_t}t, L^{y_u}u) \tag{7}$$

for the correlation lengths $\xi_L^{(i)}$, $i = 1, 2$. Here $t(K, \alpha)$ is the relevant thermal variable,

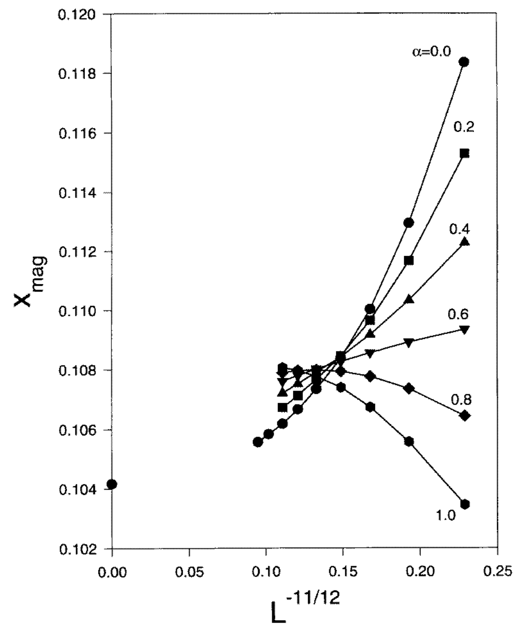

Figure 3. Data for the scaling dimension x_{mag} of type 1 walks from equation (4) with $\alpha = 0, 0.2, \dots, 1$ and $L \leqslant 13$ for $\alpha = 0$, $L \leqslant 11$ for $\alpha > 0$. The exact result $5/48$ for the SAW ($\alpha = 0$) is indicated on the vertical $L = \infty$ axis.

which vanishes on the critical line $K = K_{\mathrm{c}}(\alpha)$, and $u(K, \alpha)$ is the leading irrelevant variable. The ansatz (7) is valid in the critical region $|t| << 1$, $L >> 1$. Since there are no thermodynamic singularities for finite L, the right-hand side of equation (7) may be expanded in a double Taylor series in t and u. Equations (2)–(5) and (7) imply leading finite-size corrections of order $L^{-y_t+y_u}$ to the estimates of K_{c} and of order L^{y_u} to the exponents y_t, x_{mag} and x_{eng} for large L.

Substituting the scaling index $y_u = -11/12$ for four polymer vertices in these results, we obtain corrections to the critical bond fugacity and exponents that fall off as $L^{-9/4}$ and $L^{-11/12}$, respectively. The data for $0 < \alpha \leqslant 1$, i.e. walks with intersections, in figures 1 and 2 seem compatible with these power laws. Presumably the $L^{-11/12}$ behaviour of the data for larger α in figures 3 and 4 becomes apparent for greater values of L than we have considered.

For $\alpha = 0$ or SAWs our numerical data are more compatible with $y_u = -2$, i.e. with leading corrections to the critical bond fugacity and exponents that fall off as $L^{-10/3}$ and L^{-2}, respectively, than with $y_u = -11/12$. As mentioned above, we have no theoretical proof why the $y_u = -11/12$ corrections should vanish identically for SAWs. However, our numerical data show that if the $-11/12$ corrections exist at all, they have a small amplitude. One can estimate the leading irrelevant scaling index y_u for SAWs by fitting the SAW data for x_{mag} and x_{eng} in table 1 to power laws of the from $A + BL^{-y_u}$, using the exact values (6) for A. For $L = 10$–11, 11–12 and 12–13 the estimates of y_u are -2.233, -2.188 and -2.154, respectively, from the x_{mag} data and -1.705, -1.680 and -1.665 from the x_{eng} data. These numbers are closer to -2 than to $-11/12$, but for $L = 10$–13 the finite-size corrections are not well fit by a single power law.

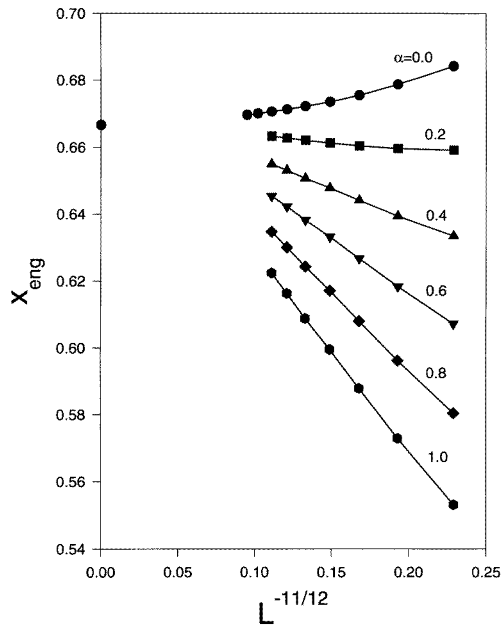

Figure 4. Data for the scaling dimension x_{eng} of type 1 walks from equation (5) with $\alpha = 0, 0.2, \ldots, 1$ and $L \leqslant 13$ for $\alpha = 0$, $L \leqslant 11$ for $\alpha > 0$. The exact result $2/3$ for the SAW ($\alpha = 0$) is indicated on the vertical $L = \infty$ axis.

Table 3. Estimates of K_{c}, x_{mag} and x_{eng} for type 1 and type 2 hybrid walks. For type 1 walks both intersections and collisions have weight α. For type 2 walks the weights are α and 1, respectively. The results were obtained from iterated power-law fits to the finite-size data, using finite-size exponents $-9/4$ and -2. For $\alpha = 0$ more accurate extrapolations are quoted in the text. The uncertainty in the last decimal places, shown in parentheses, is five times the difference of the two extrapolations using the largest available system sizes. This usually gives a reasonable estimate, but underestimates the uncertainty if there is an extremum near the largest system sizes (e.g. in the case of x_{eng} for $\alpha = 1$).

Type	L_{max}	α	K_{c}	x_{mag}	x_{eng}
1	13	0.0	0.379 03(2)	0.1042(4)	0.666(1)
1	11	0.2	0.376 89(2)	0.1044(9)	0.667(0)
1	11	0.4	0.374 70(2)	0.1046(8)	0.668(1)
1	11	0.6	0.372 42(2)	0.1049(12)	0.669(2)
1	11	0.8	0.370 04(1)	0.1054(19)	0.670(1)
1, 2	11	1.0	0.367 57(1)	0.1062(29)	0.671(1)
2	10	0.8	0.368 72(2)	0.1063(31)	0.670(3)
2	10	0.6	0.369 88(2)	0.1059(24)	0.670(2)
2	10	0.4	0.371 05(2)	0.1055(16)	0.669(1)
2	10	0.2	0.372 23(2)	0.1052(7)	0.669(1)
2	10	0.0	0.373 43(2)	0.1048(5)	0.669(2)

To obtain additional information on the universality class of trail-like models, we have also investigated a second type of hybrid model, which interpolates between the trail model and another SAW-like model, in which ‘collisions’ between walk segments are allowed. In type 2 walks the weights of collisions and intersections are 1 and α, respectively, whereas both weights equal α for type 1 walks. For both types of walk we have determined the critical bond fugacity from equation (2), the magnetic scaling dimension from (4), and the energy scaling dimension from (3) and $x_{\text{eng}} = 2 - y_t$. The results are summarized in table 3. For both models there is good agreement with the SAW universal properties.

Finally we mention a third type of hybrid model, which interpolates between the trail model and the SAW-type branch 1 $O(n = 0)$ model described by Blöte and Nienhuis [11]. The relative distance from the SAW-type model is again denoted α. For $\alpha = 0.25$ and $\alpha = 0.5$ we calculated the magnetic scaling dimension x_{mag} as described above. The results agree within a few times 10^{-4} with the SAW value $5/48$.

In summary, we have carried out transfer-matrix calculations of the connectivity and universal exponents ν and γ of hybrid walks with intersection fugacity α on the square lattice. The cases $\alpha = 0$ and $\alpha = 1$ correspond to SAWs and trails, respectively. Our numerical results strongly support the interpretation that walks with $0 < \alpha \leqslant 1$ belong to the same universality class as self-avoiding walks. As in studies based on exact enumerations, the finite-size corrections for trails are considerably larger than for SAWs. An explanation in terms of an irrelevant variable u with scaling index $y_u = -11/12$ related to the fugacity of intersections is given. It would be interesting to reanalyse the enumerations data for trails [3, 4, 6] taking this irrelevant variable into account.

Finally, we note that Ding and Huang [26], using Monte Carlo simulations, recently confirmed that trails on the honeycomb lattice are in the SAW universality class and found that trails on the square lattice behave differently. We suspect that the difference is due to the large finite-size corrections, not to a different universality class.

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Note added in proof. Since submission of this paper for publication, the exact enumeration of SAWs has been extended from 39 steps [21] to 51 steps (Conway A R and Guttmann A J 1996 *Phys. Rev. Lett.* **77** 5284). Analysis of the longer series provides compelling evidence that the correction to scaling exponent is $\Delta = 3/2$, i.e. $y_u = 2$, consistent with the transfer-matrix results for SAWs discussed above.

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