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Examination of the $1/d$ expansion method from exact enumeration for a self-interacting self-avoiding walk

Takao Ishinabe[†], Jack F Douglas[‡], Adolfo M Nemirovsky[§]|| and Karl F Freed[¶]

[†] Faculty of Engineering, Yamagata University, Yonezawa 992, Japan

[‡] Polymer Division, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

[§] Departamento de Estructura y Constituyentes de la Materia, Universidad de Barcelona, Barcelona E-08028, Spain

[¶] James Franck Institute, University of Chicago, Chicago IL 60637, USA

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Abstract. The $1/d$ expansion method for polymer chains is examined by comparing these expansions for several thermodynamic and structural quantities with the results of standard series analysis of exact enumeration data. The comparisons cover a wide range of spatial dimensions d , including non-integer ones, and are performed for particular values of interaction energy. Good agreement is generally found for $d > 4$, whereas discrepancies become conspicuous as d decreases to $d = 2$. Reasonable values are obtained for the exponents ν and γ in $d = 2 - 4$ by applying the coherent-anomaly method of Suzuki to our $1/d$ expansions through fifth order in d^{-1} .

1. Introduction

Polymers in dilute solutions can be reasonably modelled by lattice self-avoiding walks (SAW) with nearest-neighbour interactions [1]. Consequently, the lattice model of 'polymers' has been extensively investigated using both analytical and numerical methods (see e.g. [2]). The geometrical properties of SAW can also be described in terms of a 'critical phenomena' formulation. Specifically, SAW is related to the $N=0$ limit [3] of the classical N -vector model and for this reason the geometrical properties of SAW attract a much broader interest.

Fisher and Gaunt [4] first established the formal $1/d$ expansion method for SAW on a d -dimensional lattice along with that for the Ising model ($N=1$). They derive expansions in power of d^{-1} for both the number C_n of n -step SAW and the connectivity constant μ through fifth order in the large- n limit by exploiting information from exact enumeration of SAW for small n . The validity of such expansion series is rigorously shown by Kesten [5] in high dimensions. The corresponding expansion of μ for neighbour-avoiding walks (NAW) is given by Gaunt *et al* [6] through $O(d^{-3})$. Further extension to the general N -vector model and for a model for random branch polymers are provided by Gerber and Fisher [7] and Gaunt *et al* [8], respectively, while Gaunt

|| Present address: Taligent Inc, 10725 N De Anza Blvd, Cupertino, CA 95014, USA.

[9] has obtained the $1/d$ expansion of the free energy amplitude for SAW through $O(d^{-5})$.

Recently, we have developed a more general $1/d$ expansion method for SAW having nearest-neighbour contact energy ω . This method employs input information from the lattice cluster theory [10] and has been used to provide $1/d$ expansions of the partition function [11] and the mean-square end-to-end distance [12] of SAW through $O(d^{-5})$. The new feature of this work is the fact that these expansions are obtained with the full ω -dependence for any d (including non-integer ones) using exact enumeration data for n up to eleven in $d=2-6$.

This paper uses the expansion of the free energy from [11] to derive $1/d$ expansions for the internal energy and the specific heat that are valid in the large- n limit and that are complete functions of temperature (i.e. of ω). These quantities, together with the respective amplitudes A_C and A_R of the free energy and the end-to-end distance, are compared with results from standard series analysis of the exact enumeration data over a wide range of dimensions d for the three representative cases of SAW, NAW and θ' chains near the theta point. (The precise definition of θ' chains is provided in the next section). Moreover, we estimate the critical exponents γ and ν for SAW and θ' chains in some selected dimensions d by combining the respective $1/d$ expansions for A_C , A_R and μ with the coherent anomaly method (CAM) of Suzuki [13].

2. $1/d$ expansion

We consider the Orr model [1] of a polymer chain in dilute solutions. The partition function of the chain with nearest-neighbour interaction energy ε_{nn} is represented by

$$C_n(\omega) = \sum_{m=0} C_{n,m} e^{m\omega} \quad (1)$$

where $\omega = -\varepsilon_{nn}/kT$ and $C_{n,m}$ is the number of n -step SAW with m non-bonded nearest neighbours on a d -dimensional hypercubic lattice. In general, $C_{n,m}$ may be expressed as [11]

$$C_{n,m} = \sum_{l=1}^n 2^l \binom{d}{l} p_{n,m}^{(l)} \quad (2)$$

with the full dimensionality dependence present in the binomial factor. The d -independent positive integers $\{p_{n,m}^{(l)}\}$ may be obtained using exact enumeration data for $C_{n,m}$. Values of $\{p_{n,m}^{(l)}\}$ for $n \leq 11$ and methods for determining the $\{p_{n,m}^{(l)}\}$ are given in [11]. It should be noted that once the $\{p_{n,m}^{(l)}\}$ are evaluated, (2) yields a set of $C_{n,m}$ for $n \leq 11$ that are valid for any d , even for non-integer dimensionalities.

By analogy with the SAW, theta, etc. limits, we introduce interaction-dependent crossover scaling assumption

$$C_n(\omega) \cong A_C(\omega) n^{\gamma(\omega)-1} \mu(\omega)^n \quad (3)$$

and define the reduced free energy by

$$F^*(\omega) \equiv \log \mu(\omega) = \lim_{n \rightarrow \infty} n^{-1} \log C_n(\omega). \quad (4)$$

Setting $\gamma=1$ in (3) and $f=e^\omega-1$ and using results from [11] generate the $1/d$ expansion from (4)

$$\begin{aligned}
 F^*(f) = & \log \sigma + f\sigma^{-1} - (1 - f - \frac{3}{2}f^2)\sigma^{-2} - (2 - 7f - 11f^2 - 5\frac{1}{3}f^3)\sigma^{-3} \\
 & - (11\frac{1}{2} - 35f - 58\frac{1}{2}f^2 - 56f^3 - 25\frac{3}{4}f^4 - 3f^5)\sigma^{-4} \\
 & - (64 - 250f - 251f^2 - 532f^3 - 379f^4 - 125\frac{1}{5}f^5 - 14f^6)\sigma^{-5} - \dots \quad (5)
 \end{aligned}$$

and the expansion for the free energy amplitude

$$\begin{aligned}
 A_C(f) = & (1 + \sigma^{-1})[1 - 2f\sigma^{-1} + (3 - 8f - 6f^2)\sigma^{-2} + (13 - 70f - 75f^2 - 28f^3)\sigma^{-3} \\
 & + (107 - 588f - 685f^2 - 456f^3 - 161f^4 - 18f^5)\sigma^{-4} \\
 & + (895 - 5818f - 5192f^2 - 6018f^3 - 3417f^4 - 988f^5 - 122f^6)\sigma^{-5} + \dots] \quad (6)
 \end{aligned}$$

where $\sigma=2d-1$. Similarly, the amplitude for the mean-square end-to-end distance R_n^2 is obtained from [12] as

$$\begin{aligned}
 A_R(f) = & 1 + (2 - 2f)\sigma^{-1} + (6 - 14f - 4f^2)\sigma^{-2} + (28 - 102f - 68f^2 - 22f^3)\sigma^{-3} \\
 & + (180 - 832f - 712f^2 - 412f^3 - 134f^4 + 23f^5)\sigma^{-4} \\
 & + (1382 - 6700f - 10\,142f^2 - 12\,312f^3 - 16\,658f^4 \\
 & - 11\,654f^5 - 1441f^6)\sigma^{-5} + \dots \quad (7)
 \end{aligned}$$

using the assumed form

$$R_n^2(f) \cong A_R(f)n^{2\nu(f)} \quad (8)$$

with $\nu = \frac{1}{2}$.

Defining the reduced internal energy E^* and specific heat C^* by $E^* = \partial F^* / \partial \omega$ and $C^* = \partial^2 F^* / \partial \omega^2$, we have from (5)

$$\begin{aligned}
 E^*(f) = & (1 + f)\sigma^{-1} + (1 + 4f + 3f^2)\sigma^{-2} + (7 + 29f + 38f^2 + 16f^3)\sigma^{-3} \\
 & + (35 + 152f + 285f^2 + 271f^3 + 118f^4 + 15f^5)\sigma^{-4} \\
 & + (250 + 752f + 2098f^2 + 3112f^3 + 2142f^4 + 626f^5)\sigma^{-5} + \dots \quad (9)
 \end{aligned}$$

and

$$\begin{aligned}
 C^*(f) = & (1 + f)\sigma^{-1} + (4 + 10f + 6f^2)\sigma^{-2} + (29 + 105f + 124f^2 + 48f^3)\sigma^{-3} \\
 & + (152 + 722f + 1383f^2 + 1285f^3 + 547f^4 + 75f^5)\sigma^{-4} \\
 & + (752 + 4948f + 13\,532f^2 + 17\,904f^3 + 13\,698f^4 + 5130f^5)\sigma^{-5} + \dots \quad (10)
 \end{aligned}$$

Values of F^* , A_C , A_R , E^* and C^* for SAW and NAW are determined by substituting $f=0$ and $f=-1$, respectively, into these equations (of course, $E^* = C^* = 0$ for NAW). The $f=0$ limit of (5) reproduces the $1/d$ expansion of μ_{SAW} given by Fisher and Gaunt [4]; the $f=-1$ case is consistent with that of μ_{NAW} by Gaunt *et al* [6] through $O(d^{-3})$, and the $f=0$ limit of $A_C(f)$ agrees with the result of Gaunt [9]. We continue to restrict attention to SAW, NAW and θ' chains, where the latter is defined by having $f = \sigma^{-1}$ so that the θ' state is near to the theta point $\omega_\theta = 1/(\sigma-1)$ of the lattice model [14] in the large- d limit.

Table 1. Values of $C_{n,m}$ for SAW on the simple cubic lattice.

m	$C_{12,m}$	$C_{13,m}$	$C_{14,m}$	$C_{15,m}$	$C_{16,m}$
0	45 054 630	184 400 910	755 930 958	3089 851 782	12 645 783 414
1	57 525 552	256 574 352	1137 418 464	5001 796 944	21 899 428 128
2	44 547 912	214 532 136	1019 264 736	4783 813 296	22 238 211 480
3	27 853 008	143 817 120	726 606 720	3613 467 552	17 708 666 496
4	14 169 312	79 878 144	431 661 240	2283 391 464	11 811 895 992
5	6 441 456	38 486 304	224 538 960	1273 428 048	6 950 393 088
6	2 418 264	17 723 064	106 521 864	639 155 304	3 711 295 944
7	651 648	6 191 616	46 237 488	306 732 000	1 836 897 600
8	161 856	1 957 344	15 062 256	124 409 592	841 657 896
9	19 104	289 392	4 666 368	43 422 984	324 331 728
10		124 128	817 920	11 892 576	114 649 920
11			184 704	3 458 688	29 830 656
12				223 392	8 132 640
13				102 432	569 856
14					131 136
C_n	198 842 742	943 974 510	4468 911 678	21 175 146 054	100 121 875 974

3. Series analysis

Exact values of $C_{n,m}$ ($n \leq 11$) from (2) are also used to estimate $F^*(f)$, $E^*(f)$, $C^*(f)$ and $A_C(f)$ over a wide range of d for SAW ($f=0$), NAW ($f=-1$), and θ' chains by using a standard series analysis method (see e.g. [15]). The treatment of $A_R(f)$ exploits the unnormalized square end-to-end distance $r_{n,m}^2$ for SAW as expressed in a similar form to (2),

$$r_{n,m}^2 = \sum_{\lambda=1}^n 2^\lambda \lambda! \binom{d}{\lambda} q_{n,m}^{(\lambda)} \quad (11)$$

where the integer coefficients $q_{n,m}^{(\lambda)}$ ($n \leq 11$) are presented in [12]. The mean-square distance R_n^2 may be obtained from

$$R_n^2 = \left(\sum_{m=0}^n r_{n,m}^2 e^{mw} \right) / C_n(\omega) \quad (12)$$

for any d and f . The analysis in $d=2$ and 3 uses our exact enumeration data of $C_{n,m}$ and $r_{n,m}^2$ for $n \leq 22$ and 16, respectively. The new terms (with $n=12-16$) for $C_{n,m}$ and $D_{n,m}$ ($=r_{n,m}^2$) in $d=3$ are listed in tables 1 and 2 for convenience. Rapaport [16] has obtained $C_{n,m}$ for $n \leq 13$.

The outline of our series analysis is as follows: first form the ratios of alternate terms

$$\mu_n = (C_n / C_{n-2})^{1/2} \quad (13)$$

for the estimation of F^* ($= \log \mu$). Then, construct the Neville tables for their linear, quadratic and cubic extrapolants [15]

$$\mu_n^{(r)} = [n\mu_n^{(r-1)} - (n-2r)\mu_{n-2}^{(r-1)}] / 2r \quad (14)$$

for $r=1-3$ with $\mu_n^{(0)} \equiv \mu_n$. Subsequently, we estimate μ by plotting these extrapolants against n^{-1} and extrapolating to $n \rightarrow \infty$ in view of the curvature of convergence as a whole and damping oscillations with decreasing n^{-1} as shown in [17]. For example, we

Table 2. Values of $D_{n,m}$ for SAW on the simple cubic lattice.

m	$D_{12,m}$	$D_{13,m}$	$D_{14,m}$	$D_{15,m}$	$D_{16,m}$
0	1369 313 472	6236 190 462	28 141 065 048	125 990 905 734	560 238 622 848
1	1356 637 248	6878 260 464	34 203 387 648	167 320 375 440	807 175 365 792
2	821 558 208	4592 156 328	24 931 816 032	132 114 193 584	685 904 382 528
3	397 535 616	2439 747 744	14 387 859 552	82 113 708 192	456 105 866 688
4	150 472 128	1039 084 992	6 748 126 608	41 841 510 504	250 070 912 544
5	51 006 240	387 787 104	2 782 259 232	18 765 400 272	120 542 909 856
6	15 270 528	135 730 680	1 047 296 688	7 625 474 760	52 866 411 456
7	3 802 176	39 930 432	369 018 048	2 941 221 888	21 613 713 120
8	627 072	9 907 200	101 862 816	968 931 960	8 092 857 984
9	98 496	1 403 856	25 722 240	285 963 816	2 652 089 856
10		426 432	4 625 280	66 601 248	795 054 144
11			757 440	16 819 968	191 363 712
12				781 536	41 013 696
13				371 328	3 506 112
14					518 976
D_n	4166 321 184	21 760 625 694	112 743 796 632	580 052 260 230	2966 294 589 312

find $\mu = 5.746 \pm 0.008$ for SAW in $d = 3.5$. The values of F^* thus estimated for SAW, NAW and θ' chains are represented in figure 1 as a function of d over the range $d = 2-6$ and including non-integer d . The estimates in the range $2 < d < 3$ are ill-behaved, especially for NAW. The corresponding $1/d$ expansions (5) are depicted by solid curves. Excellent agreement with the series analysis is generally found for $d > 4$, whereas deviations become conspicuous, as expected, with decreasing d for SAW and NAW.

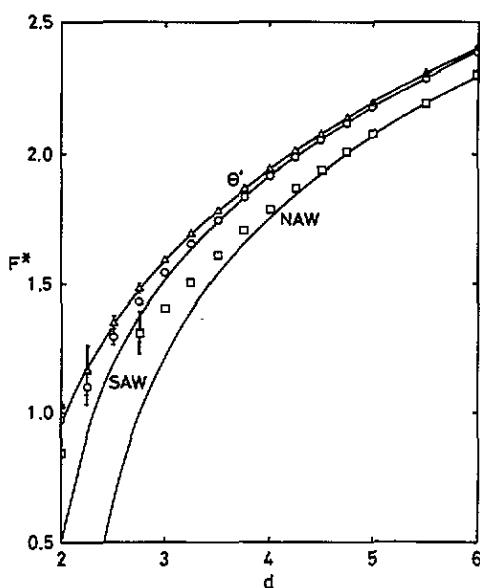


Figure 1. The d dependence of the reduced free energy F^* as estimated by series extrapolation methods for SAW (\circ), NAW (\square) and θ' chains (\triangle). Solid curves indicate the corresponding $1/d$ expansions.

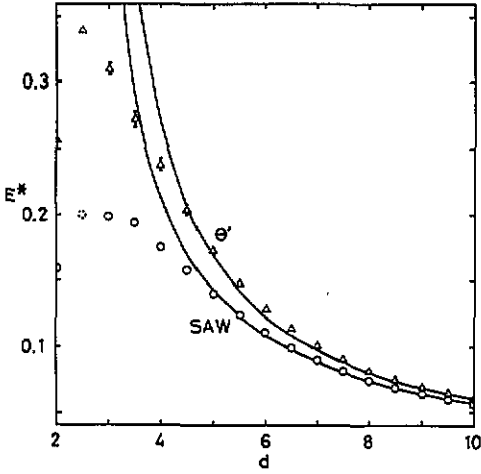


Figure 2. Same as in figure 1 but for the reduced internal energy E_n^* and SAW and θ' chains.

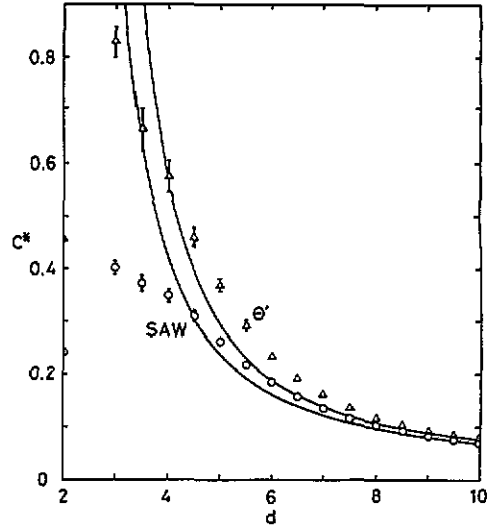


Figure 3. Same as in figure 2 but for the reduced specific heat C_n^* .

The reduced internal energy E_n^* and the specific heat C_n^* of finite chains may be written from (1) as

$$E_n^* = \langle m \rangle / n \tag{15}$$

and

$$C_n^* = (\langle m^2 \rangle - \langle m \rangle^2) / n \tag{16}$$

with averages defined by

$$\langle \dots \rangle = \left[\sum_m (\dots) C_{n,m} e^{m\omega} \right] / C_n(\omega). \tag{17}$$

We estimate E^* and C^* for infinite chains by plotting the r th extrapolants ($r=1-3$) of E_n^* and C_n^* against n^{-1} in the same manner as described above for F^* . Values of E^* have already been estimated from the exact enumeration of SAW on square and tetrahedral lattices [18]. Figures 2 and 3 display the estimates of E^* and C^* for SAW and θ' chains as functions of d together with the respective $1/d$ expansions from (9) and (10). These figures exhibit a deteriorating agreement between results of series analysis and the $1/d$ expansion as d decreases, especially for SAW. A noticeable maximum is present in the series analysis results near $d=3$, whereas the $1/d$ expansions show a rapid increase as d decreases. The maximum is sharper for θ' chains than SAW for both E^* and C^* .

The estimation of A_C is carried out by first estimating γ from the extrapolants $\gamma_n^{(r)} = n(\mu_n / \mu_n^{(r)} - 1) + 1$ as before. Then, A_C is estimated using Neville tables of the extrapolants $A_C = C_n / (\mu_n^{r-1})$. Similarly, we estimate $A_R (= R_n^2 / n^{2\nu})$ after determining ν by using the ratio method and Neville tables. The logarithmic correction [19, 20] $(\log n)^{1/4}$ is included when evaluating these estimations for SAW and NAW in $d=4$. The

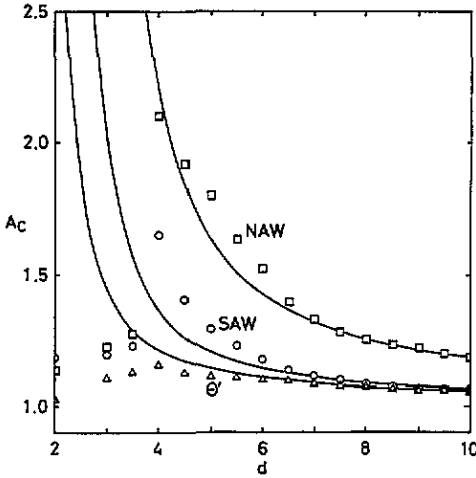


Figure 4. Same as in figure 1 but for A_C .

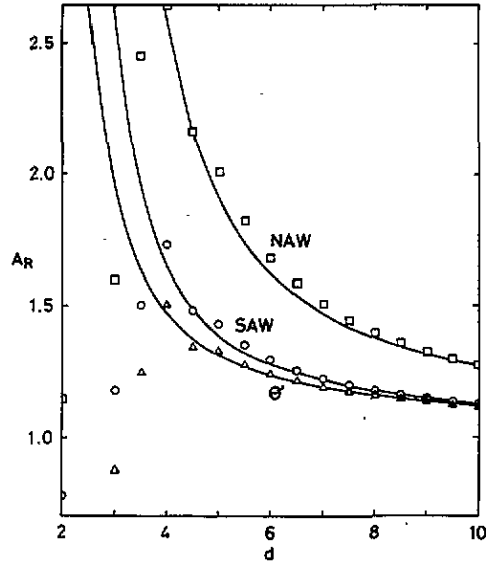


Figure 5. Same as figure 4 but for A_R .

computations of γ and ν are described elsewhere [21]. Figures 4 and 5 present the calculated amplitudes A_C and A_R . The $1/d$ expansions for SAW, NAW and θ' chains are consistent with the series extrapolations for $d > 5$, but a striking discrepancy between them again appears in both figures 4 and 5, with decreasing d . The A_C and A_R from exact enumerations exhibit maxima which become more prominent in passing from θ' chains to SAW and then to NAW, while the $1/d$ expansions again become divergent as d decreases.

4. Estimation of γ and ν from CAM theory

The $1/d$ expansions of A_C and A_R appear to diverge for small d with increasing order of the expansions. This suggests [22] that γ and ν may be estimated by applying CAM theory [13] to our mean-field approximation $1/d$ expansions. The CAM theory estimation of γ for SAW in $d=2$ and 3 has been performed by Hu and Suzuki [23], exploiting the finite-order-restricted walk approximation, and we now apply this method to obtain γ and ν for SAW and θ' chains.

The CAM theory requires use of analogies between polymers and critical phenomena, and it is useful to explain the method using the latter language. The Ising model susceptibility χ near the critical point T_c is written as

$$\chi \sim \varepsilon^{-\gamma} \tag{18}$$

with $\varepsilon = (T - T_c)/T_c$. The CAM theory states that

$$\chi \cong \bar{\chi}(\bar{T}_c) \bar{\varepsilon}^{-1} \tag{19}$$

where $\bar{\varepsilon} = (T - \bar{T}_c)/\bar{T}_c$, \bar{T}_c is the mean-field value of T_c , and $\bar{\chi}(\bar{T}_c)$ represents the mean-field approximation to χ which is given by

$$\bar{\chi}(\bar{T}_c) \sim 1/(\bar{T}_c - T_c)^{\gamma-1}. \tag{20}$$

It should be noted that $\bar{\chi}(\bar{T}_c) \rightarrow \infty$ as $\bar{T}_c \rightarrow T_c$.

Introducing the mean-field value $\gamma=1$ in (3), the generating function of C_n for SAW ($f=0$) is given by

$$\chi_0 = 1 + \sum_{n=1}^{\infty} C_n x^n \cong A_C(\sigma)(1-\mu x)^{-1} \quad (21)$$

where μ is the connectivity constant for SAW. Since μ for polymers corresponds to T_c for the Ising model [4], the comparison between (19) and (21) yields

$$A_C(\bar{\mu}) \sim (\bar{\mu} - \mu)^{-\psi} \quad (22)$$

where $\psi = \gamma - 1$, $\bar{\mu}$ is the mean-field value of μ , and we may regard σ in (6) as $\bar{\mu}$, i.e. $\sigma = \bar{\mu}$.

The correlation length ξ near T_c scales as

$$\xi \sim \varepsilon^{-\nu}. \quad (23)$$

Since ξ and ε correspond to R_n and $1/n$ for SAW [3], respectively, comparing (8) with (23) similarly provides the correspondence

$$A_R(\bar{\mu}) \sim (\bar{\mu} - \mu)^{-\lambda} \quad (24)$$

where $\lambda = 2\nu - 1$.

We may estimate ψ and λ , i.e. γ and ν , for any f by using (6) and (7) provided that the exact μ and some systematic mean-field values μ_n ($n=0, 1, \dots$) in a successive approximation scheme are available. It is known that $\mu = 2.6381$ ($d=2$), 4.6839 ($d=3$) [24] and $\mu = 6.772$ ($d=4$) [19], and likewise, $\mu_0 = 2d$ and $\mu_1 = 2d - 1$ ($=\sigma$) for the random walk and non-reversing random walk, respectively, which represent the 0th and 1st approximations to SAW, respectively.

Inverting equation (22) produces

$$\psi = \log [A_C(\mu_0)/A_C(\mu_1)] / \log (\Delta\mu_0/\Delta\mu_1) \quad (25)$$

where $\Delta\mu_n = \mu_n - \mu$. Thus we have the estimates: $\gamma = 1.75$ ($d=2$), 1.18 ($d=3$), 1.05 ($d=4$) and $2\nu = 1.72$ ($d=2$), 1.20 ($d=3$), and 1.06 ($d=4$). These values are comparable with other estimates [24], $\gamma = 1.163$ and $2\nu = 1.179$ for $d=3$, and the accepted $\gamma = 2\nu = 1$ for $d=4$. However, for $d=2$ they deviate from Nienhuis's analytical values [25] $\gamma = 43/32 = 1.34 \dots$ and $2\nu = 3/2 = 1.5$.

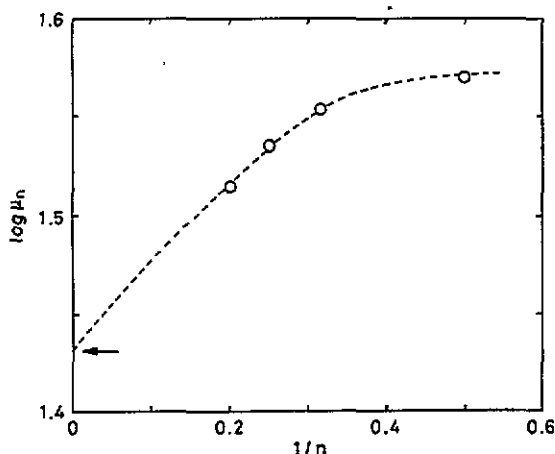


Figure 6. Estimation of μ_∞ for SAW in $d=3$ from the plot of $\log \mu_n$ versus n^{-1} . Arrow provides extrapolation limit.

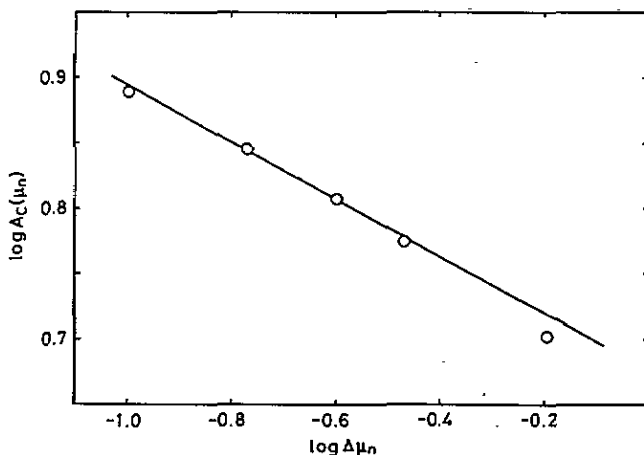


Figure 7. $\log A_C(\mu_n)$ versus $\log \Delta \mu_n$ for SAW in $d=3$.

It is possible to extract an alternative estimation of γ and ν from the $1/d$ expansion (5). Define the n th order mean-field value μ_n by

$$\mu_n(f) = \sigma \sum_{i=0}^{n-1} a_{i+1}(f) \sigma^{-i} \quad (26)$$

with $\mu_1 = \sigma$. The coefficients a_i may be determined from (5) since $F^*(f) = \log \mu(f)$. Our expansions yield $\mu_n (n \leq 6)$ for SAW and θ' chains as

$$\mu_6(0) = \sigma(1 - \sigma^{-2} - 2\sigma^{-3} - 11\sigma^{-4} - 62\sigma^{-5}) \quad (27a)$$

and

$$\mu_6(\sigma^{-1}) = \sigma(1 - \sigma^{-3} - 3\sigma^{-4} - 18\sigma^{-5}) \quad (27b)$$

respectively. As illustrated in figure 6 for SAW in $d=3$, plotting $\log \mu_n$ against n^{-1} and extrapolating to $n \rightarrow \infty$ determine μ_∞ , which is regarded as μ . Estimates of ψ and λ , i.e. of γ and ν , are likewise obtained by extrapolating plots of $\log A_C(\mu_n)$ and $\log A_R(\mu_n)$ versus $\log \Delta \mu_n$, where $\Delta \mu_n = \mu_n - \mu$. The latter are displayed for $d=3$ in figures 7 and

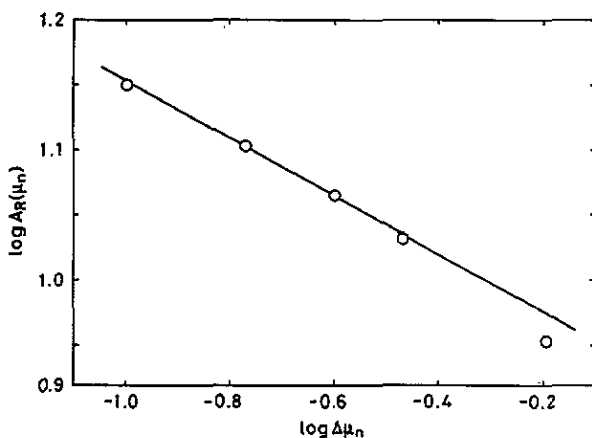


Figure 8. Same as in figure 7 but for A_R .

Table 3. Values of γ and ν for SAW and θ' chains as estimated from CAM theory using (27a) and (27b).

d	γ_{SAW}	$2\nu_{\text{SAW}}$	$\gamma_{\theta'}$	$2\nu_{\theta'}$
3	1.22	1.23	1.026	1.037
3.5	1.06	1.07	1.007	1.011
4	1.018	1.023	1.0017	1.0031

8, respectively. The results thereby obtained for SAW and θ' chains are reproduced in table 3. This estimation method is ineffective for SAW, NAW ($f=-1$) and θ' chains in $d=2$ since the determination of μ_{∞} is difficult. On the other hand, the γ and 2ν for $d=3.5$ are in accord with those from standard series extrapolations of the exact enumeration data [21], $\gamma=1.07\pm 0.015$ and $2\nu=1.07\pm 0.01$, while those for $d=3$ are somewhat larger than expected. The CAM theory estimates for θ' chains are almost consistent with $\gamma=2\nu=1$ at $d=d_c$ (the marginal critical dimension d_c is three for θ chains [26]).

5. Conclusion

Our $1/d$ expansions of the internal energy and specific heat for SAW and θ' chains are shown to be consistent with the results from standard series analysis of exact enumeration data for $d>5$ and including non-integer dimensionalities d . However, the latter exhibit a maximum near $d=3$ for both SAW and θ' chains whereas the former diverge as d decreases. The same tendency is noted for the respective amplitudes A_C and A_R of the free energy and end-to-end distance. The breakdown of the $1/d$ expansion reflects the increased contribution of fluctuation effects which change the critical exponents. A different estimation method for the exponents γ and ν for SAW and θ' chains in various d emerges by applying CAM theory to the $1/d$ expansions of A_C and A_R . These alternative estimates are consistent with the accepted values.

Acknowledgments

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