# A new renormalisation-group weight function for linear polymers



1985 J. Phys. A: Math. Gen. 18 551

(http://iopscience.iop.org/0305-4470/18/3/028)

J. Phys. A: Math. Gen. **18** (1985) 551-555. Printed in Great Britain

COMMENT

# A new renormalisation-group weight function for linear polymers

N-C Chao†

Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA

Received 9 August 1984

**Abstract.** We propose a true centre rule weight function for treating linear polymers with a cell position-space renormalisation group (PSRG). For a cell-to-cell PSRG, our preliminary results for small cells give the critical fugacity per monomer $K^* = 0.3886$ and the critical exponent $\nu = 0.7471$. Accurate results are also obtained for $\nu$ with a cell-to-bond PSRG.

Polymers are macromolecules formed by monomers with a typical number of about $10^4$. Statistical mechanics is therefore highly appropriate for studying such systems. In particular, the lattice statistical model of a self-avoiding walk (SAW) seems able to take account of the essential features of a linear polymer including the excluded-volume effect. The SAW problem is characterised by a starting point for all walks, which are free to go in any direction subject only to the constraint that such a walk does not intersect itself.

One of the most interesting statistical aspects for polymers is the analogy between polymerisation and the ordinary thermal critical phenomena. For a linear polymer in dilute solution, it is well known that the dependence of the mean end-to-end distance $\xi$ on the molecular weight $M$ is characterised by a critical exponent $\nu$, i.e., $\xi \sim M^{\nu}$ as $M \to \infty$. For simplicity, we will consider a linear polymer as described by only one parameter $K$ which is the fugacity per monomer. It can then be argued that the parameter $M^{-1}$ corresponds to $|K - K_c|$, where $K_c$ is the fugacity per monomer for the system to be at criticality (see Redner and Reynolds 1981).

Several approaches have been employed to evaluate $\nu$ (see Stanley *et al* 1982). Here we are interested in a cell position-space renormalisation group (PSRG). Within a renormalisation group scheme, the invariance of the characteristic quantity $\xi \to \infty$ upon repeated length rescaling of the system corresponds to a fixed point at criticality. A cell PSRG has been carried out by de Queiroz and Chaves (1980) using a modified scheme of Reynolds *et al* (1977) for bond percolation and incorporating the characteristics of non-intersection as well as a fixed starting point for the paths. This scheme is generally referred to as the corner rule. Subsequently, Redner and Reynolds (1981) have carried out a thorough investigation for different weight functions, such as the centre rule, transfer matrix, multicells, equal averaging and toroidal rule and have obtained very impressive results. In particular, the toroidal rule gives $K_c = 0.3791 \pm 0.0001$ and $\nu = 0.756 \pm 0.004$ on the square lattice compared with $K_c = 0.379003 \pm 0.000015$ of Sykes *et al* (1972) and the classical value $\nu = 0.75$ predicted by

† On leave from Universidade Federal do Rio Grande do Norte, Departamento de Física, Natal, Rio Grande do Norte, Brasil.

0305-4470/85/030551+05$02.25  

the Flory theory (Flory 1953). Furthermore, it appears that if the estimates of the toroidal rule are correct, then the classical value in two dimensions can be excluded. However, since the toroidal rule still has some defects (Redner and Reynolds 1981), it is worthwhile investigating other weight functions which may give an independent check on these estimates.

To perform a PSRG calculation for a SAW on the square lattice, we first partition the lattice into cells of size $b$ in the same manner as is done for bond percolation by Reynolds *et al* (1977); thus the $b=1$ cell, the elementary cell, is just two bonds connected perpendicular to each other, the $b=2$ cell can be formed by joining $2\times2$ elementary cells into a square and so on. For $b$ even, we choose the site at the centre of the cell as the starting point (the origin) for all SAWs; whereas for $b$ odd, each of the four corners of the square at the centre of the cell can be chosen as the origin and a consistent choice of the origin should be made for all cells. The families of cells with $b$ even and odd are therefore slightly different due to the location of the origin. Our choice of the origin seems more natural compared to the corner rule of de Queiroz and Chaves (1980) and the centre rule of Redner and Reynolds (1981, hereafter referred to as the edge-centred rule), for which the origin is chosen at a corner and at the centre of an edge respectively. A spanning SAW is defined as a path that traverses a cell from one edge to the opposite edge via the origin. Each spanning path actually consists of two non-intersecting SAWs starting from the origin. Effectively, we consider only the SAWs that can reach one edge and still allow the existence of a SAW to reach the opposite edge. However, this is already a great improvement compared to, for example, the corner rule and the edge-centred rule, which take into account, respectively, only the SAWs that are confined to a wedge-shaped region with opening angle $\frac{1}{2}\pi$ and to a half-plane. Furthermore, in order to eliminate any ramified configurations that may occur at the 'interfacing' when cells are connected, we choose to delete all the bonds on the edge that spans the traversing SAWs. This is an improvement over all the weight functions used before, including the toroidal rule. Therefore, apart from the fixed origin, our cells are the same as those of Reynolds *et al* (1977) for bond percolation and also have similar connectivity properties. Just as in bond percolation, a spanning path for a SAW on one cell does not always connect to another on the other cell when two cells are connected. However, the connectivity problem can be treated better with our centre rule than the corner rule and edge-centred rule, for which most of the spanning SAWs do not terminate at the starting point on the next cell. Moreover, Reynolds *et al* (1980) have argued that the error due to approximation in the PSRG for percolation should vanish in the large-cell limit; such arguments may also apply to our centre rule.

The rest of the PSRG procedure is the same as that used in the previous SAW calculations, except that we may be allowed to consider only the cell-to-cell PSRG for each of the two families of cells separately. Nevertheless, we will first try a cell-to-bond PSRG. We sum the statistical weights for all spanning paths of SAWs that traverse a cell of size $b$ in the top–bottom direction via the origin to obtain a polynomial $G_b(K)$, which is then renormalised to a vertical bond with fugacity $K'$ to yield a recursion relation $K'=G_b(K)$. From this recursion relation, we obtain the non-trivial fixed point $K^*$ and the critical exponent $\nu$ through the formula (see Stanley *et al* 1982)

$$\nu=\ln b/\ln\lambda, \tag{1}$$

with $\lambda=(\mathrm{d}G_b(K)/\mathrm{d}K)|_{K^*}$. For the sake of convenience, cells are represented by graphs such as those in figure 1, where $(a)$–$(c)$ are graphs corresponding to the $b=2$–4

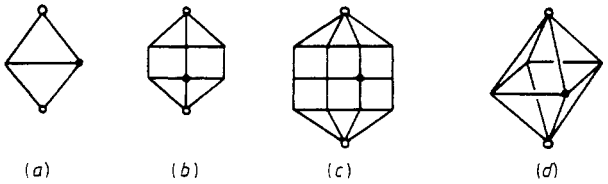


**Figure 1.** Graphs representing some cells on square and simple cubic lattices. The graphs $(a)$-$(c)$ represent the $b = 2$-4 cells on the square lattice, while the graph $(d)$ represents the $b = 2$ cell on the simple cubic lattice. Open circles indicate terminals and full circles indicate the starting points for spanning SAWs.

cells on a square lattice and $(d)$ corresponds to the $b = 2$ cell on a simple cubic lattice. For the square lattice, the graph in figure 1$(a)$ for the $b = 2$ cell can be spanned by three paths, one is a two-step walk and two are three-step walks. Thus, we obtain

$$G_2(K) = 2K^3 + K^2, \tag{2}$$

which when renormalised to $K'$ leads to a recursion relation having a non-trivial fixed point $K^* = 0.5$. The critical exponent calculated from (1) gives $\nu = 0.7565$. Although the value for $K^*$ is too large, $\nu$ is surprisingly accurate.

The graph shown in figure 1$(b)$ for the $b = 3$ cell can be broken into nine graphs illustrated in figure 2 according to the specific combination of bonds originating from the starting point. Each graph in figure 2 has been simplified by deleting the bonds

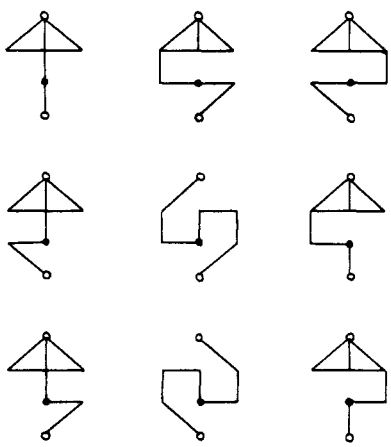

**Figure 2.** Graphs separated from figure 1$(b)$ according to specific combination of bonds originating from the starting point. Inaccessible bonds for SAWs are deleted for clarity.

which are inaccessible to a SAW in that graph. Since seven of these graphs have three spanning SAWs, these nine graphs are spanned by 23 SAWs, which can easily be obtained and summed to give

$$G_3(K) = 4K^7 + 4K^6 + 8K^5 + 6K^4 + K^3. \tag{3}$$

Renormalising $G_3(K)$ into a single bond and using (1), we obtain $K^* = 0.4275$ and $\nu = 0.7566$. The value for $\nu$ seems to be slightly worse than for the $b = 2$ case, but we recall that they belong to a different family of cells. Another choice of the origin can be made for the $b = 3$ cell. The corresponding graph is similar to that of figure 1$(b)$

with the origin displaced to the right. From this graph, we obtain $K^* = 0.4847$ and $\nu = 0.7508$.

We have evaluated $G_4(K)$ using figure 1(*c*) which corresponds to the $b = 4$ cell. The result is

$$G_4(K) = 14K^{13} + 40K^{12} + 52K^{11} + 56K^{10} + 56K^9 + 45K^8 + 38K^7 + 24K^6 + 8K^5 + K^4.$$

Renormalisation of $G_4(K)$ leads to $K^* = 0.4147$ and $\nu = 0.7526$ which are less than the corresponding values for the $b = 2$ case and seem to converge rapidly. Our value for $\nu$ calculated using the $b = 4$ cell is already less than the extrapolated value $\nu = 0.756$ of Redner and Reynolds (1981). Thus, if the trend continues, $\nu$ should converge to a smaller value. However, the results of our cell-to-bond PSRG may not be reliable.

We now perform a cell-to-cell PSRG by setting $G_4(K) = G_2(K')$ to yield a recursion relation which has a non-trivial fixed point $K^* = 0.3886$. The critical exponent calculated from the formula $\nu = \ln 2/\ln \lambda$ with $\lambda = [(\mathrm{d}G_4(K)/\mathrm{d}K)/(\mathrm{d}G_2(K)/\mathrm{d}K)]_{K^*}$ gives $\nu = 0.7471$. Our $K^*$ value is greater than the $K_c$ value of Sykes *et al* (1972) by 2.5% and $\nu$ is less than the classical value 0.75 by only 0.4%.

Our centre rule can readily be applied to other lattice animals and lattice statistical problems as well as kinetic aggregation models which are characterised by an origin. Also, extension to the three-dimensional system is straightforward. For a simple cubic lattice, for example, the spanning SAWs that traverse the $b = 2$ cell can be obtained by inspecting figure 1(*d*) to give

$$G_2(K) = 8K^5 + 6K^4 + 4K^3 + K^2, \tag{5}$$

which when renormalised to a single bond leads to $K^* = 0.3184$ and $\nu = 0.6235$. These results are comparable to the existing ones: $K_c = 0.2135$ (Watts 1975), $\nu = 0.6$ (Flory 1953), $\nu = 0.588$ (le Guillou and Zinn-Justin 1980) and $\nu = 0.595$ (Alexandrowicz 1983). The corner rule has been applied to the simple cubic lattice by Family (1981) who obtained $K^* = 0.297$ and $\nu = 0.588$ for the $b = 2$ case. However, the results for $b = 3$ lead to $\nu = 0.581$ which seems too small, although $K^* = 0.276$ is still reasonable (Family 1981, Stanley *et al* 1982). It is therefore interesting to see if there is a systematic improvement for $K^*$ and $\nu$ for larger cells using both the cell-to-bond and the cell-to-cell PSRGs with our weight function.

In conclusion, we have proposed a true centre-rule weight function for a PSRG approach to the SAW problem. Our centre rule seems to be more natural and straightforward and gives good results with little effort. Also, it seems questionable whether our centre rule can lead to a $\nu$ value for the square lattice that conforms to the estimated value of Redner and Reynolds (1981) using the toroidal rule. Therefore, we believe that a definite value for $\nu$ in two dimensions still remains to be obtained and more work using our weight function as well as other plausible weight functions is needed.

I would like to thank Professor F Y Wu for his kind invitation to visit the Northeastern University where this work was completed. The financial support from the Brazilian Conselho Nacional de Desenviolvimento Científico Tecnológico (CNPq) is gratefully acknowledged.

## References

Alexandrowicz Z 1983 *Phys. Rev. Lett.* **50** 736
de Queiroz S L A and Chaves C M 1980 *Z. Phys.* B **40** 99

Family F 1981 *J. Physique* **42** L189
Flory P J 1953 *Principles of Polymer Chemistry* (Ithaca: Cornell UP)
le Guillou J C and Zinn-Justin J 1980 *Phys. Rev.* B **21** 3976
Redner S and Reynolds P J 1981 *J. Phys. A: Math. Gen.* **14** 2679
Reynolds P J, Klein W and Stanley H E 1977 *J. Phys. C: Solid State Phys.* **10** L167
Reynolds P J, Stanley H E and Klein W 1980 *Phys. Rev.* B **21** 1223
Stanley H E, Reynolds P J, Redner S and Family F 1982 in *Real-space renormalization* ed T Burkhard and J W J van Leeuwen (Heidelberg: Springer)
Sykes M F, Guttman A J, Watts M G and Roberts P D 1972 *J. Phys. A: Math. Gen.* **5** 653
Watts M G 1975 *J. Phys. A: Math. Gen.* **8** 61