Two-variable quasi-scaling for three-dimensional lattice polymers in a poor solvent regime

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Abstract. The context of the renormalization group applied to the lattice polymer statistical mechanics with the nearest-neighbour triplet interaction in addition to the usual nearest-neighbour pair interaction yields a two-variable quasi-scaling relation. It asserts that a reduced moment is described by two arbitrary reduced moments. The validity of the two-variable quasi-scaling has been examined for lattice polymers with polymerization degree up to 1000 in the poor solvent regime and was confirmed. It is well known that single-variable scaling fails in this solvent regime. Linear relations connecting three reduced moments which are valid near the respective Gaussian points and considered to be universal are presented. The results, however, are not consistent with the premise employed in the continuous polymer model. The working RG is nonlinear. The consistency may be attained by polymers with polymerization degree much larger than 1000 for which the linearized RG will work. Our basic equation involves no particular reference point such as the Θ-point. This is in contrast to previous scaling simulations and experiments.

1. Introduction

In addressing finite polymer statistical mechanics, the concept of scaling, which is essentially appropriate for infinite polymers, should be replaced by that of quasi-scaling (Watanabe *et al* 1990). This paper demonstrates that the statistical mechanics of three-dimensional finite lattice polymers (with excluded volume and not shorter than 225 in chain length) in the poor solvent regime better obeys *two-variable* quasi-scaling rather than *single-variable* quasi-scaling. The intra-chain interaction includes, in addition to the nearest-neighbour pair interaction, the nearest-neighbour triplet interaction. Here, the latter means that an arrangement in which a chain element is the nearest neighbour of two non-bonded chain elements contributes some amount of energy (figure 1). The introduction of the new interaction into the lattice polymer model may
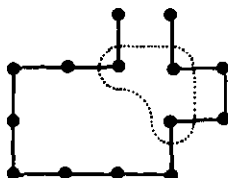
Figure 1. Illustration of the nearest-neighbour triplet interaction. A configuration in which an element neighbouring two arbitrary non-bonded elements contributes an energy ε_3 in addition to the pair interaction energy ε_2.

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be viewed as an artifice of the polymer renormalization group (RG) to rescue the failure of *single-variable* scaling for lattice polymers in the poor solvent regime (e.g. Kremer *et al* 1982, Okamoto 1988). The theoretical continuous polymer model considers a polymer chain to be a Gaussian chain with two- and three-body δ-function like interaction (see the appendix). We should recall that the operation of an RG on a continuous polymer with only two-body interaction yields the three-body term. (Oono and Freed 1981). Such may occur for lattice polymers.

Controlling the nearest-neighbour triplet interaction in lattice polymers will also help us to study the meaning of the difference in the scaling behaviours between the two polymer models and the logarithmic correction (e.g. Freed 1987, Duplantier 1987) in the future. The study of how one might connect the two polymer models has also attracted the interest of theorists (e.g. Freed 1985).

The two-variable quasi-scaling for lattice polymers asserts that a reduced moment (see (2.3) below) is described by two arbitrary reduced moments. Watanabe *et al* (1990) confirmed the quasi-scaling through numerical experiments by using relatively short polymers. Because of the chain length limitation, however, their data around the Gaussian points were rather scarce. (The Gaussian point is the point from the Gaussian chains in a three-dimensional reduced moment space.) We should notice that the behaviour around Gaussian points must be a key to understanding the relations between the two polymer models.

In this paper the lattice polymer simulation is performed through the inversely restricted sampling method (Rosenbluth and Rosenbluth 1955, Mazur and McCrackin 1968). It allows us to handle chains of considerable length near the Θ-point (McCrackin *et al* 1973) where the inter-chain excluded volume effectively vanishes. With high certainty, the Gaussian points lie in the respective master surfaces (or more correctly, master shells). Several numerical formulae connecting three reduced moments, which are valid near the Gaussian points and considered to be universal, are presented.

Our lattice polymer RG based on the intra-chain correlation works nonlinearly. This is in contrast with the RG based on the inter-chain correlation (Okamoto 1988, Yato and Okamoto 1990). We should be careful in comparing the single lattice polymer statistical mechanics with theoretical ones from the linearized RG.

Our basic equation involves no specific reference point such as the Θ-point. We made analysis only through direct comparison of measured reduced moments. This is in contrast with previous simulations (e.g. Curro and Schaefer 1980, Kremer *et al* 1982, Okamoto 1988) and experiments (e.g. Miyaki and Fujita 1981, Perzynski *et al* 1982, Park *et al* 1987), in which polymer scaling was studied by a scaling variable constructed by chain length and the distance from the Θ-point.

2. The concept of polymer two-variable quasi-scaling

We consider that the essentials of the lattice polymer RG are contained in the following premise (Okamoto 1988). A two-point correlation function $\Gamma(1/n, \eta, \xi; r)$ defined for a polymer ensemble before an RG operation is connected with a two-point correlation function $\Gamma(1/n', \eta', \xi'; r)$ for the ensemble after the operation by

$$\Gamma(1/n, \eta, \xi; r) = \lambda^a \Gamma(1/n', \eta', \xi'; r') \tag{2.1}$$

with $r = \lambda r'$.

In the above, r is the vector distance between the two points involved in the correlation, n is the number of elements in a chain, η and ξ are the parameters signifying the nearest-neighbour pair and triplet interaction respectively, λ is the coarse graining ratio and the primed quantities are for the ensemble after the RG operation. The exponent a should be appropriately chosen. To proceed, we convert (2.1) into a more convenient form in which the discreteness of lattices is averaged out. For an intra-chain correlation, we define the mth moment by

$$\langle r^m \rangle_\Gamma \equiv \int d^d r \, r^m \Gamma(1/n, \eta, \xi, r). \tag{2.2}$$

Equation (2.1) asserts that a reduced moment $M_\Gamma^{m,n}$

$$M_\Gamma^{m,n} \equiv \langle r^m \rangle_\Gamma / \langle r^n \rangle_\Gamma^{m/n} \tag{2.3}$$

is invariant under an RG operation. That is

$$M_\Gamma^{m,n} = M_{\Gamma'}^{m,n}. \tag{2.4}$$

In considering the radius of gyration reduced moments (see (3.1*b*) below), we have to reinterpret the two-point correlation appropriately. Consider a flow line in the three-dimensional parameter space spanned by $1/n$, η and ξ. Since a reduced moment is held constant along a flow line, and since a flow line in the parameter space can be specified by assigning specified values to two arbitrary reference reduced moments M_{ref1} and M_{ref2}, we have

$$M_\Gamma^{m,n} = M_\Gamma^{m,n}(M_{\text{ref1}}, M_{\text{ref2}}). \tag{2.5}$$

Equation (2.5) asserts the existence of a master surface in a space spanned by $M_\Gamma^{m,n}$, M_{ref1} and M_{ref2}, containing points from polymers with various $1/n$, η, and ξ. For finite polymers, however, (2.5) does not hold strictly. The points from polymers with a fixed $1/n$ but with various η and ξ will make a surface in the reduced moment space. Likewise, the points polymers with another $1/n$ will make another surface. The two surfaces are different. The usual scaling concept considers that each surface asymptotes to that for an infinite polymer. As for finite polymers, one must admit some small but finite deviations from (2.5). The concepts of scaling and master surface should be replaced by those of quasi-scaling and master shell, respectively. The thickness of the master shell is arbitrary, but we assume it to be of the same order as the experimental resolution.

3. Procedure

A polymer chain is simulated by a self-avoiding chain of n elements each occupying contiguous lattice sites ($n$mer) in a simple cubic (SC) lattice. A nearest-neighbour non-bonded element pair contributes an energy ε_2 to the conformation. In the same way, a nearest-neighbour non-bonded element triplet (figure 1) contributes an energy ε_3. The interaction parameters η and ξ are, respectively, defined by $\eta = \exp(-\beta\varepsilon_2)$ and $\xi \equiv \exp(-\beta\varepsilon_3)$. A solvent condition is specified by a combination of η and ξ.

Mean square end-to-end distances, radii of gyration, quasi-radii of gyration and mid-$\frac{1}{3}$-internal distances (see figure 2), as well as their even-order reduced moments,
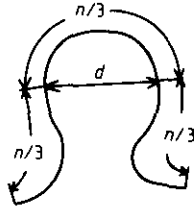
Figure 2. Illustration of the mid-$\frac{1}{3}$-internal distance d.

were determined for polymers with n up to 1000. The lattice polymers were generated by the Monte Carlo technique of inversely restricted sampling (Rosenbluth and Rosenbluth 1955, Mazur and McCrackin 1968). This sampling method allows us to handle considerably longer chains but is effective only near the Θ-point (McCrackin *et al* 1973). Yato and Okamoto (1990) have obtained a few series of the Θ-point solvent conditions. By referring to this, we have chosen the solvent conditions which are to be investigated here (table 1). Table 2 lists the number of samples generated.

The quantities mentioned above were calculated respectively by using the relations

$$\langle h^{2k}\rangle = (1/Q)\sum_j (r_n(j) - r_1(j))^{2k} p_j^{-1} \exp(-\beta w(j)) \tag{3.1a}$$

$$\langle r^{2k}\rangle = (1/Q)n^{-k}\sum_j \left(\sum_i s_i(j)^2\right)^k p_j^{-1} \exp(-\beta w(j)) \tag{3.1b}$$

$$\langle s^{2k}\rangle = (1/Q)n^{-k}\sum_j \sum_i s_i(j)^{2k} p_j^{-1} \exp(-\beta w(j)) \tag{3.1c}$$

$$\langle d^{2k}\rangle = (1/Q)\sum_j (r_{2n/3}(j) - r_{n/3}(j))^{2k} p_j^{-1} \exp(-\beta w(j)) \tag{3.1d}$$

$$Q = \sum_j p_j^{-1} \exp(-\beta w(j)) \tag{3.1e}$$

$$M_x^{m,n} = \langle x^m\rangle/\langle x^n\rangle^{m/n} \tag{3.1f}$$

with $x \in \{h, r, s, d\}$.

Table 1. The solvent conditions (η, ξ) investigated. The values of η were in the range from $\eta_{\min}$ to $\eta_{\max}$ with an interval of 0.005.

ξ	$\eta_{\min}$	$\eta_{\max}$
1.0	1.270	1.360
1.037	1.210	1.260
1.05	1.185	1.205

Table 2. The number of elements in a chain n and the number of samples generated N_s.

n	225	340	500	750	1000
N_s	102 000	99 500	96 000	90 500	85 000

In the above, $r_i(j)$ is the position vector of the ith element, $s_i(j)$ is the distance of the ith element measured from the mass centre, p_j is the generating probability (Mazur and McCrackin 1968), and $w(j)$ is the energy of the jth sample.

4. Results

4.1. Single-variable quasi-scaling

As a preliminary, we briefly illustrate the success and the failure of the single-variable quasi-scaling in terms of the reduced moments. If polymer chains, with only the nearest-neighbour pair interaction, obey a relation similar to (2.1), the quasi-scaling is

$$M_\Gamma^{m,n} = M_\Gamma^{m,n}(M_{ref}). \tag{4.1}$$

This claims that any reduced moment $M_\Gamma^{m,n}$ is described solely by an arbitrary reference reduced moment M_{ref}. If so, plotting of $M_\Gamma^{m,n}$ against M_{ref} for polymers with various $1/n$ and η but with a fixed ξ $(=1)$, will form a single curve. Freed (1987) emphasized the importance of studies of this kind. The quasi-scaling (4.1) for finite lattice polymers is successful in the good solvent regime, but fails in the solvent regime investigated in this study. Figure 3 demonstrates an example in which the 100-mer and 31-mer points are obtained from Watanabe *et al* (1990).
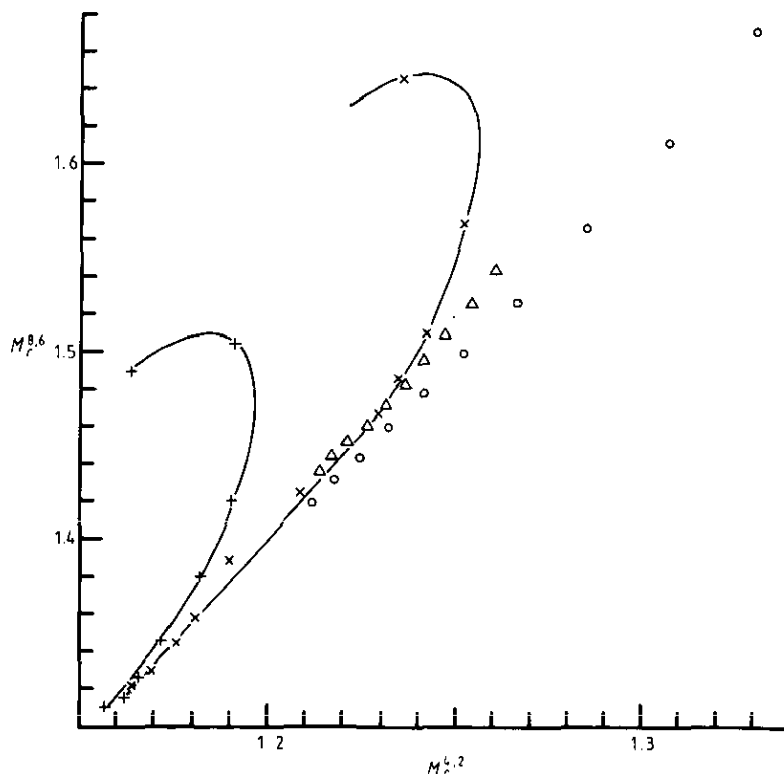

Figure 3. Plots of $M_r^{8,6}$ against $M_r^{4,2}$ for polymers with various n, η and a fixed $\xi(=1.0)$. Symbols $(+)$, $(\times)$, $(\triangle)$ and $(\bigcirc)$ are for polymers with $n = 31, 100, 340$ and 1000, respectively. The points of the 31-mer and the 100-mer are from Watanabe *et al* (1990).

The study by Kremer *et al* (1982) of tetrahedral lattice polymers using the scaling variable of an explicit combination of n and η also found the failure of the single-variable scaling for prefactors in the poor solvent regime. The failure of scaling for multi-chain systems in the poor solvent regime has also been reported (Okamoto 1988).

4.2. Two-variable quasi-scaling

The above failure and the expected generation of the three-body term by an operation of the RG mentioned earlier urges us to study the two-variable quasi-scaling (2.5) for polymers with the nearest-neighbour pair and triplet interactions. The study requires plotting in a three-dimensional reduced moment space. To envision it, their cross sections in planes of constant $M_r^{m,n}$ were constructed from the available discrete data through interpolation. The reduced moments of order $\{4, 2\}$, $\{6, 4\}$ and $\{8, 6\}$ were evaluated for η and ξ listed in table 1. Although in the following our results are illustrated only graphically, all the numerical reduced moment data have been deposited with the British Library Document Supply Centre as Supplementary Publication No SUP 70041 (12 pages).

We examined the cross sectional plottings with respect to possible combinations of the twelve reduced moments. Figures 4–10 show arbitrary examples such as $M_h^{4,2}$ against $(M_r^{6,4}, M_r^{4,2})$ etc. Each figure contains the cross section in its Gaussian plane. (The Gaussiaan plane is that which contains the Gaussian point and crosses the $M_r^{m,n}$ axis perpendicularly.) Figures 6(b) and 8(b) contain the Bruns point which represents the reduced moments at the Θ-point for infinite SC polymers with ξ equal to unity. Bruns obtained them through extrapolation using a polynomial of $1/\sqrt{n}$ (Bruns 1984).
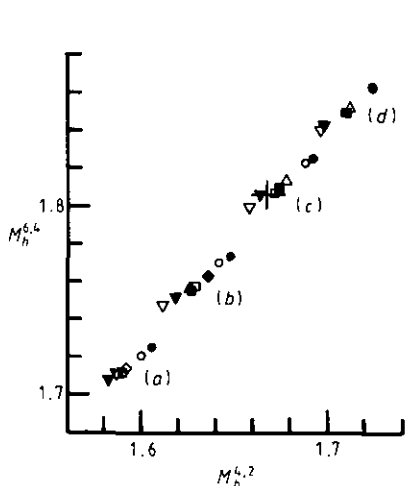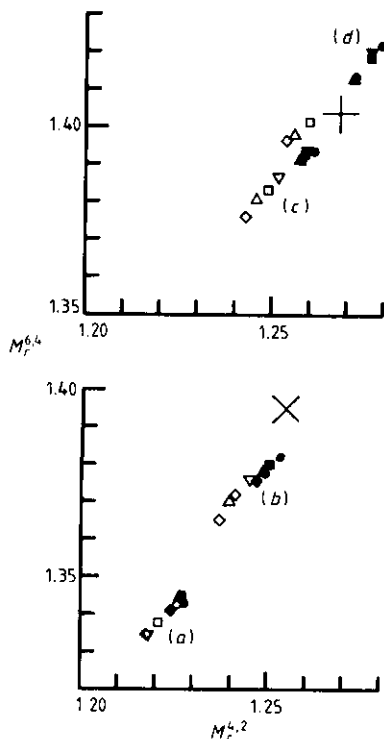

Figure 4. Cross sections of $M_h^{8,6}$ against $(M_h^{6,4}, M_h^{4,2})$ for polymers with various n, η and ξ in the planes of $M_h^{8,6} = (a)$ 1.800; (b) 1.850; (c) 1.908 ($M_h^{8,6}$ value for the Gaussian chain); and (d) 1.950. Symbols ($\Diamond$), ($\triangle$), ($\square$), (∇) and ($\bigcirc$) are for polymers with $\xi = 1$ and $n = 225$, 340, 500, 750 and 1000, respectively. Symbols ($\blacklozenge$), ($\blacktriangle$), ($\blacksquare$), ($\blacktriangledown$) and ($\bullet$) are for polymers with $\xi = 1.05$ and $n = 225$, 340, 500, 750 and 1000, respectively. ($+$) marks the Gaussian point.
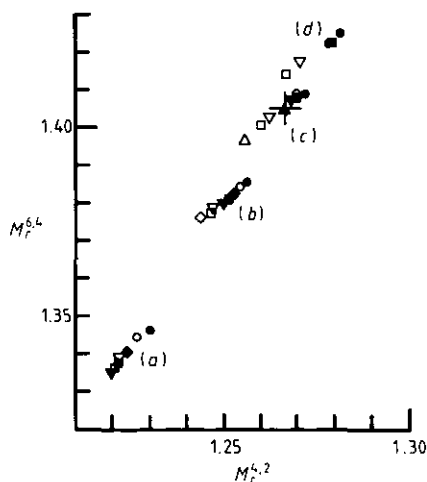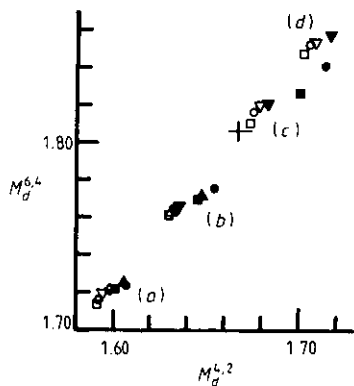
Figure 5. Cross sections of $M_r^{8,6}$ against $(M_r^{6,4}, M_r^{4,2})$ for polymers with various n, η and ξ in the planes of $M_r^{8,6} = (a)$ 1.420; (b) 1.500; (c) 1.533 ($M_r^{8,6}$ value for the Gaussian chain); and (d) 1.550. For the symbols, see the legend to figure 4.
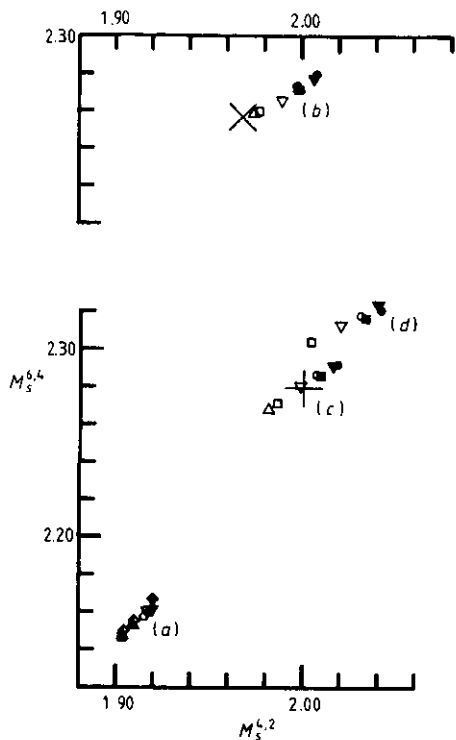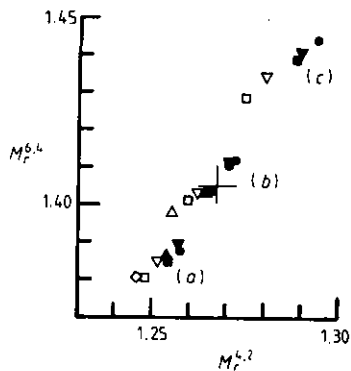
Figure 6. Cross sections of $M_s^{8,6}$ against ($M_s^{6,4}$, $M_s^{4,2}$) for polymers with various n, η and ξ in the planes of $M_s^{8,6} = (a)$ 2.300; (b) 2.425 ($M_s^{8,6}$ value at the Bruns (1984) point); (c) 2.446 ($M_r^{8,6}$ value for the Gaussian chain); and (d) 2.480. For the symbols, see the legend to figure 4. ($\times$) marks the Bruns point (see the text).

Figure 8. Cross sections of $M_h^{4,2}$ against ($M_r^{6,4}$, $M_r^{4,2}$) for polymers with various n, η, and ξ in the planes of $M_h^{4,2} = (a)$ 1.600; (b) 1.650; (c) 1.667 ($M_h^{4,2}$ value for the Gaussian chain); and (d) 1.70. For the symbols, see the legends to figures 4 and 6.

Figure 7. Cross sections of $M_d^{8,6}$ against ($M_d^{6,4}$, $M_d^{4,2}$) for polymers with various n, η, and ξ in the planes of $M_d^{8,6} = (a)$ 1.800; (b) 1.850; (c) 1.908 ($M_r^{8,6}$ value for the Gaussian chain); and (d) 1.950. For the symbols, see the legend to figure 4.

Figure 9. Cross sections of $M_s^{6,4}$ against ($M_r^{6,4}$, $M_r^{4,2}$) for polymers with various n, η, and ξ in the planes of (a) $M_s^{6,4} = 2.240$; (b) 2.278 ($M_r^{6,4}$ value for the Gaussian chain); and (c) 2.320. For the symbols, see the legend to figure 4.
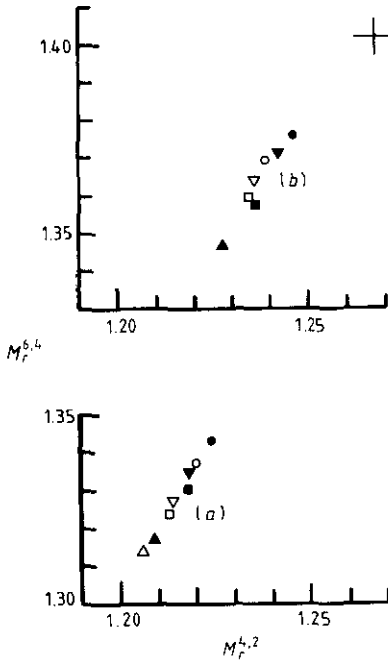
Figure 10. Cross sections of $M_d^{4,2}$ against $(M_r^{6,4}, M_r^{4,2})$ for polymers with various n, η, and ξ in the planes of $M_d^{4,2} = (a)$ 1.550; and (b) 1.667 $(M_h^{4,2}$ value for the Gaussian chain). For the symbols, see the legend to figure 4.

All figures, including non-demonstrated ones, show that points from polymers with various $1/n$, η and ξ falls on a single curve and that the Gaussian point lies in the respective master shell. By virtue of using longer chains in this work, the situations near the Gaussian points are much clearer than those in Watanabe *et al* (1990). (Compare the plot of $M_s^{6,4}$ against $(M_r^{6,4}, M_r^{4,2})$ in this work with that in Watanabe *et al.*) The quasi-scaling (2.5) is thus confirmed. The Bruns points do not always lie in the respective master shells.
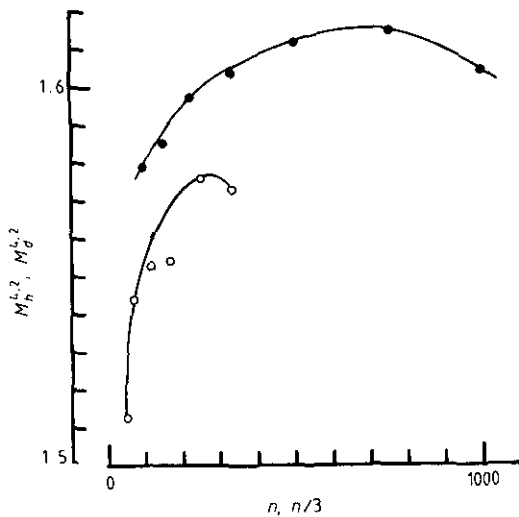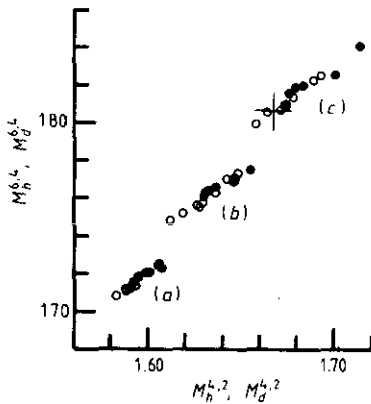

Figure 11. Comparison of $M_h^{4,2}$ against $n(\bullet)$ with $M_d^{4,2}$ against $n/3(\bigcirc)$ for polymers with $\xi = 1$ and $\eta = 1.30$.

Figure 12. Illustration showing the overlapping of $M_h^{8,6}$ against $(M_h^{6,4}, M_h^{4,2})$ and $M_d^{8,6}$ against $(M_d^{6,4}, M_d^{4,2})$. The cross sections in the planes of $M_h^{8,6} = M_d^{8,6} = (a)$ 1.800; (b) 1.850; and (c) 1.908 ($M_h^{8,6}$ value for the Gaussian chain). ($\bigcirc$) represents points from the end-to-end reduced moments; ($\bullet$) represents points from mid-$\frac{1}{3}$ internal distance reduced moments.

Care should be paid to the plottings involving $M_d^{m,n}$. In that case, the references $M_{\mathrm{ref}1}$, and $M_{\mathrm{ref}2}$, if ref $\neq d$, should be taken from those of the polymers under the same solvent condition but with the number of elements $n/3$ (e.g. figure 9). Although $M_d^{m,n}$ against $n/3$ and $M_h^{m,n}$ against n behave differently (figure 11), the master shells $M_d^{8,6} = M_d^{8,6}(M_d^{6,4}, M_d^{4,2})$ and $M_h^{8,6} = M_h^{8,6}(M_h^{6,4}, M_h^{4,2})$ overlap with each other (figure 12).

We have to comment on data scattering. Our one numerical run yielded 17 000 samples of 1000-mers and more samples of shorter chains. Five runs were performed. The means of the values of $M_r^{4,2}$ for the 1000-mer at $\eta = 1.236$, $\xi = 1.037$ among the five runs were dispersed from 1.238 and 1.252. The means of $M_h^{4,2}$ were dispersed from 1.600 to 1.660. For the 225-mer, the corresponding dispersions were from 1.227 to 1.230 and from 1.607 to 1.636, respectively. In spite of the dispersion, the points in the cross-sectional plottings, however, were well aligned. This is perhaps because the means of the reduced moments are correlated with each other. In effect, deviations of experimental points from true ones in a reduced moment space are not random, but confined within the master shell.

5. Discussion

5.1. Gaussian point

It appears virtually certain that the Gaussian points always lie in the respective master shells. Approximating a mster shell near the Gaussian point by a plane such as

$$(M_z^{k,l} - G_z^{k,l}) = a_0 + a_1(M_x^{m,n} - G_x^{m,n}) + a_2(M_y^{p,q} - G_y^{p,q}) \tag{5.1}$$

where $G_z^{k,l}$ etc mean the corresponding reduced moment of the Gaussian chains, we estimated the constants in (5.1) by using the least square method and by the multiple regression analysis. At present, only a few reduced moment combinations afforded us numerals of narrow confidence intervals for the 95% confidence coefficient. Table 3 lists those giving the coefficients of determination values larger than 0.920. We estimated them from those experimental points within a distance of 0.05 from the Gaussian point in the reduced moment space.

We compare the lattice polymer statistics with the continuous model polymer (see the appendix). Firstly, while a continuous model polymer is Gaussian irrespective of n for the vanishing strength of the two- and the three-body interactions ($v_2 = 0$, $v_3 = 0$),

Table 3. Numerical values of the coefficients in master planes $(M_z^{k,l} - G_z^{k,l}) = a_0 + a_1(M_x^{m,n} - G_x^{m,n}) + a_2(M_y^{p,q} - G_y^{p,q})$ with confidence intervals for the 95% confidence coefficient and the coefficient of determination R^2. They were evaluated from the experimental points within a distance 0.05 from the Gaussian point in the corresponding reduced moment spaces. The cases in which R^2 was less than 0.92 were omitted.

z	x	y	$\{k, l\}$	$\{m, n\}$	$\{p, q\}$	a_0	a_1	a_2	R^2
h	h	h	$\{8, 6\}$	$\{6, 4\}$	$\{4, 2\}$	0.0031 ± 0.0026	-1.34 ± 0.40	2.17 ± 0.37	0.929
r	r	r	$\{8, 6\}$	$\{6, 4\}$	$\{4, 2\}$	-0.0016 ± 0.0010	-0.87 ± 0.14	1.78 ± 0.14	0.984
s	s	s	$\{8, 6\}$	$\{6, 4\}$	$\{4, 2\}$	-0.0057 ± 0.0019	-1.02 ± 0.23	1.74 ± 0.19	0.961
d	d	d	$\{8, 6\}$	$\{6, 4\}$	$\{4, 2\}$	-0.0073 ± 0.0030	-0.64 ± 0.32	1.57 ± 0.31	0.938
s	r	r	$\{4, 2\}$	$\{6, 4\}$	$\{4, 2\}$	0.0003 ± 0.0010	0.80 ± 0.21	0.92 ± 0.14	0.986
s	r	r	$\{6, 4\}$	$\{6, 4\}$	$\{4, 2\}$	-0.0003 ± 0.0020	-0.54 ± 0.41	2.20 ± 0.29	0.964

we could not find out such particular solvent condition (η_G, ξ_G), at which all lattice polymer reduced moments are Gaussian irrespective of n. This is in contrast with the reported result that the inter-chain interaction effectively vanishes at $\eta = \eta_\Theta$ $(=1.236)$, $\xi = \xi_\Theta$ $(=1.037)$ irrespective of n (Yato and Okamoto 1990) just as the continuous model polymers with $v_2 = 0$ and $v_3 = 0$. Secondly, while the reduced moments $M_R^{m,n}$ of the continuous model polymers near the Θ-point are single-variable scaling, figure 4 shows that this is not the case. The former is a prediction of the $\langle R^{2m} \rangle$ expression of the first-order calculation by Cherayil *et al* (1987) with respect to $z_2 = (2\pi)^{-3/2} v_2 N^{1/2}$ and $z_3 = (2\pi)^{-3} v_3 N$. The z_3 term vanishes in their $M_R^{m,n}$.

5.2. Lattice polymer RG and universality

Each $M_x^{m,n}$ against η curve for a fixed ξ has a peak, which gets higher with increasing n, at a solvent condition $(\eta_m(n), \xi_m(n)(=\xi))$ below the Θ-point (see Watanabe *et al* 1990 and their supplementary material). The polymer RG fixed point in the poor solvent regime must be at the solvent condition (η_m^*, ξ_m^*) maximizing the reduced moments of infinite polymers. Unfortunately, because of the biased sample generation inherent in the inversely restricted sampling (Mazur and McCrackin 1973), obtaining reliable reduced moment peak data requires many more samples. An attempt to extrapolate $(\eta_m(n), \xi_m(n))$ to infinite n was abandoned.

Another way to obtain the fixed point solvent condition is based on a plausible assumption that the scaling field at that point is $1/n$. The possible logarithmic correction vanishes at the fixed point solvent condition (Lawrie and Sarbach 1984, Freed 1987, Duplantier 1987). Then, the reduced moments will be independent of n at that solvent condition. We attempted to identify the fixed point by this method, but were unsuccessful. The established quasi-scaling and the failure of the fixed point identification by the latter method suggest that the RG under investigation is nonlinear. Comparison with the continuous model polymer should be done for lattice polymers with enough length n to assure the linearized RG which may be at least a few 1000 in the poor solvent regime. The study of the convergence to the scaling limit for polymers with n less than 1000 should not be guided by theories based on the linearized RG. Previous scaling studies of lattice polymers (Kremer *et al* 1982, Cherayil *et al* 1987) should be re-examined in this sense. The same might be true for the scaling around the good solvent fixed point and for the scaling in SAW (lattice polymers in an athermal solvent).

The study of the convergence to scaling in this regime (e.g. Havlin and Ben-Avraham 1983, Majid *et al* 1983, Rapaport 1985, Kelly *et al* 1987) may be required to take this problem into account.

As mentioned before, the RG relying exclusively on the inter-chain correlation (Okamoto 1988) is linear even in this range of n, and according to Yato and Okamoto (1990) its poor solvent fixed point solvent condition is at $(\eta_\Theta, \xi_\Theta)$. We have to admit that the RG relying on the inter-chain correlation is not consistent with the RG relying on the intra-chain correlation. (This is in contrast with the optimism in Okamoto (1988).) Each RG for finite polymers works well but in its own way. Indeed, this is not a desirable property for a complete RG. At present, we expect that the situation can be improved by polymers with n much longer than 1000 (for SC polymers). This is partly supported by the finding that the Gaussian points always lie in the respective master shells.

The master surfaces found must be universal. The effects of the chain length finiteness and the lattice structure, if any, are negligible for polymers with n not less than 225 in the poor solvent regime. Watanabe *et al* (1990) found that SC and FCC points merged on a single cross section curve. The numerical constants in table 3 should be interpreted as universal.

Appendix

The continuous model considers that a polymer chain is specified by continuous position vector $c(\tau)$ with τ being the contour distance along the chain. Near the Θ-point, its Hamiltonian should involve up to the three-body interaction. After some transformation, it is

$$H(c(\tau))/kT = \tfrac{1}{2} \int d\tau \{dc(\tau)/d\tau\}^2 + (v_2/2!) \int d\tau_2 \int d\tau_1 \, \delta(\{c(\tau_1) - c(\tau_2)\}$$

$$+ (v_3/3!) \int d\tau_3 \int d\tau_2 \int d\tau_1 \, \delta\{c(\tau_1) - c(\tau_2)\}\delta\{c(\tau_2) - c(\tau_3)\} \qquad (A1)$$

where N is the chain length, the cut off, i.e. the constraint $|\tau_1 - \tau_2| \geq a$, applies to the integral in the second term, and the constraints $|\tau_1 - \tau_3|, |\tau_3 - \tau_2|, |\tau_2 - \tau_1| \geq a$ apply to the integral in the third term, and v_2 and v_3 are the strength of the two- and the three-body interaction (e.g. Duplantier 1987, Freed 1987).

Although the polymer Hamiltonian should involve the four- and higher-body interaction terms, they are neglected because the higher-order terms are diminished with negative powers of N.

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