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LETTER TO THE EDITOR

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Abstract. A Monte Carlo renormalisation-group method for polymers is developed and applied to the freely jointed polymer model with excluded volume potential. Both the exponent and the amplitude of the end-to-end correlation length are obtained.

Recently Monte Carlo (MC) simulation and renormalisation group (RG) analysis have been successfully combined in investigating the critical properties of Ising and Potts models (Ma 1976, Swendsen 1979). In this Letter a MCRG method for polymer models is presented which uses a block transformation technique based on de Gennes' suggestion of renormalisation along the chemical sequence of the chain (de Gennes 1977). The MCRG approach provides several advantages in comparison with ordinary MC simulations and RG investigations. The correlation length exponent is estimated to be $\nu = 0{\cdot}589 \pm 0{\cdot}003$, which is in good agreement with field theoretical RG calculations (Le Guillou and Zinn-Justin 1977). Critical amplitudes and crossover scaling functions of the end-to-end correlation length and related quantities are accessible. Moreover, the MCRG method proposed here is general and is not restricted to a certain class of polymer models. Thus attractive interactions, which often play an essential role in polymer problems, as well as steric constraints of the chemical structure may be included in the MCRG calculations.

The MCRG method for polymers will be illustrated by an application to the 'pearl-necklace' model. This polymer model consists of $N_0 + 1$ hard spheres of diameter h_0 indexed from 1 to $N_0 + 1$, which are connected by N_0 bonds of length l_0. The angles between neighbouring bonds are not restricted. The quantity in which we are interested here is the end-to-end correlation length

$$R(l_0, h_0, N_0) = \langle (\mathbf{r}_1 - \mathbf{r}_{N_0+1})^2 \rangle^{1/2} \tag{1}$$

where $\mathbf{r}_i$ are the coordinates of the ith sphere and the brackets $\langle \ldots \rangle$ denote the average over all possible configurations $\{\mathbf{r}_1, \ldots, \mathbf{r}_{N+1}\}$. The scaling law for the correlation length may be written (Riedel 1972, de Gennes 1975, Daoud and Jannink 1976)

$$R(l_0, h_0, N_0) = l_0 N_0^{\nu_t} f[N_0(h_0/l_0)^{d/\phi_t}] \tag{2}$$

where d is the dimension, ν_t is the tricritical exponent and ϕ_t the corresponding crossover exponent. For potentials with a repulsive part only, as in our case, the tricritical exponents reduce to their mean field values $\nu_t = \nu_{MF} = \frac{1}{2}$ for all dimensions d. In the critical domain $N \to \infty$, we recover the critical scaling law

$$f(x) = Ax^{\nu - \nu_t} \qquad (x > 0; \nu_t = \nu_{MF} = \tfrac{1}{2}). \tag{3}$$

The value $\nu = 0 \cdot 588 \pm 0 \cdot 001$ for $d = 3$ has been obtained using field theoretical renormalisation-group methods (Le Guillou and Zinn-Justin 1977). For $h_0 = 0$, f is independent of N, and $f = 1$ in the pearl-necklace model (see e.g. Flory 1969). From (2) and (3) we have

$$R(l_0, h_0, N_0) = A l_0 \delta_0^c N^\nu \qquad (N \to \infty, \delta_0 > 0) \qquad (4a)$$

$$c = d(\nu - \nu_{MF})/\phi_{MF} \qquad (\nu_{MF} = \phi_{MF} = \tfrac{1}{2}) \qquad (4b)$$

$$\delta_0 = h_0/l_0. \qquad (4c)$$

A similar law with $\nu = \tfrac{3}{5}$ was obtained without using scaling ideas by Flory (1949) and Edwards (1965).

The usual presentation of renormalisation groups is based on a thinning of the number of degrees of freedom in momentum space or in real space. These techniques can, of course, be applied to polymers using the $n = 0$ theorem (de Gennes 1972, Hilhorst 1977). However, to establish the MCRG method for polymers we have proceeded in a different way, following de Gennes' suggestion (1977) which is based on the one-dimensional structure of the chain. The idea is shown in figure 1. We start with N_0 bonds of length l_0 and sphere diameter h_0. As in block transformation techniques in spin systems (see e.g. Kadanoff 1976) we group the bonds in N_0/s consecutive 'block bonds', each composed of s original bonds (s is the scale factor). The length l_1 of the block bonds is identified as the average correlation length of s original bonds

$$l_1 = \langle (\boldsymbol{r}_j - \boldsymbol{r}_{j+s})^2 \rangle^{1/2} \qquad (5)$$

which is estimated from a MC simulation. j was chosen so that l_1 was a representative average correlation length which did not exhibit a significant dependence on the finite system size N_0 (details will be published elsewhere). For details of the MC simulation
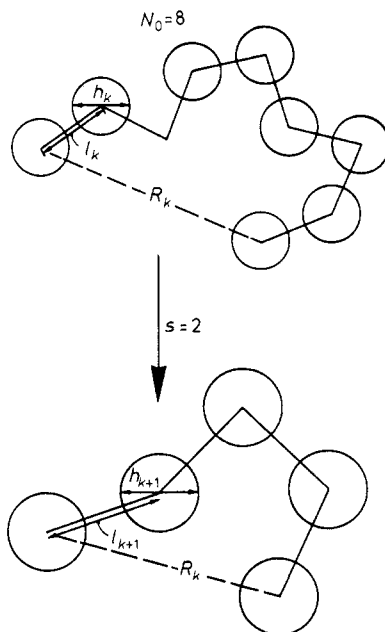

Figure 1. Illustration of the block-transformation technique in the pearl-necklace model.

method we refer to the article of Baumgärtner and Binder (1979). But it should be noted that the MCRG principle is independent of the particular MC method.

The renormalised coupling constant h_1 is estimated using the invariance condition

$$R(l_0, h_0, N_0) = R(l_1, h_1, N_0/s) \tag{6}$$

which is analogous to the usual renormalisation-group approach in which the RG transformation leaves the free energy unchanged (see e.g. Kadanoff 1976). In practice h_1 is estimated by MC simulation. For various trial values $h_1^{(1)}, h_1^{(2)}, \ldots$ the end-to-end correlation lengths $R(l_1, h_1^{(1)}, N_0/s)$, $R(l_1, h_1^{(2)}, N_0/s), \ldots$ are calculated. By comparing with $R(l_0, h_0, N_0)$ as given by equation (6) a value for h_1 is obtained.

We iterate the process, starting with N_0 bonds of length l_k and coupling constant h_k and going to a transformed set of variables $\{l_{k+1}, h_{k+1}\}$. When the process has been repeated a sufficient number of times the large block-bonds have the asymptotic behaviour

$$l_k \simeq A l_0 \delta_k^c s^{\nu k} \qquad (k \gg 1) \tag{7}$$

according to equation $(4a)$ and

$$l_{k+1}/l_k \simeq s^\nu (\delta_k/\delta_{k+1})^c \qquad (k \gg 1) \tag{8}$$

on using equations $(4a)$ and (6). Clearly the fixed point of the transformation (8) is given by

$$l_{k+1}/l_k = s^\nu \qquad (k \to \infty) \tag{9}$$

with

$$\delta_k \to \delta_{k+1} \to \delta^* \qquad (k \to \infty). \tag{10}$$

The fixed point has the following physical interpretation. Let us apply the RG transformation at the fixed point $\delta_0 = \delta^*$. Then the transformation leaves the coupling constant unchanged, i.e. $\delta_k = \delta^*$ for all k. On the other hand equation (8) tells us that in this case

$$l_{k+1} = l_k s^\nu = l_0 s^{\nu(k+1)} \qquad (\delta_0 = \delta^*). \tag{11}$$

A comparison of equation (7) and equation (11) (with $\delta_k = \delta^*$) yields

$$A = (1/\delta^*)^c. \tag{12}$$

This result suggests that in general in the pearl-necklace model the end-to-end correlation length follows the law

$$R(l, h, N) = l(\delta/\delta^*)^c N^\nu \qquad (N \gg 1). \tag{13}$$

This is supported by an analysis of recent MC simulations on the same model (Bruns 1977), which will be reported elsewhere.

In figure 2 the flow lines representing the iteration process $\{l_k, \delta_k\} \to \{l_{k+1}, \delta_{k+1}\}$ for $k = 0, 1, 2, \ldots$ in the pearl-necklace model for $d = 3$ dimensions are shown. We used a transformation with scale factor $s = 2$ applied to chains of lengths $N_0 = 8$ and $N_0 = 16$. According to equations (8)–(10) the exponent ν is the value of $\ln(l_{k+1}/l_k)/\ln 2$ for $\ln(\delta_k/\delta_{k+1}) = 0$. We estimate $\nu = 0.589 \pm 0.003$ (compare lower part of figure 2). In the same manner the fixed point value δ^* was estimated as $\delta^* = 0.530 \pm 0.003$ (compare upper part of figure 2). It should be noted that the crossover exponent ϕ_{MF} defined by equation $(4b)$ may be obtained from the slope at the fixed point according to
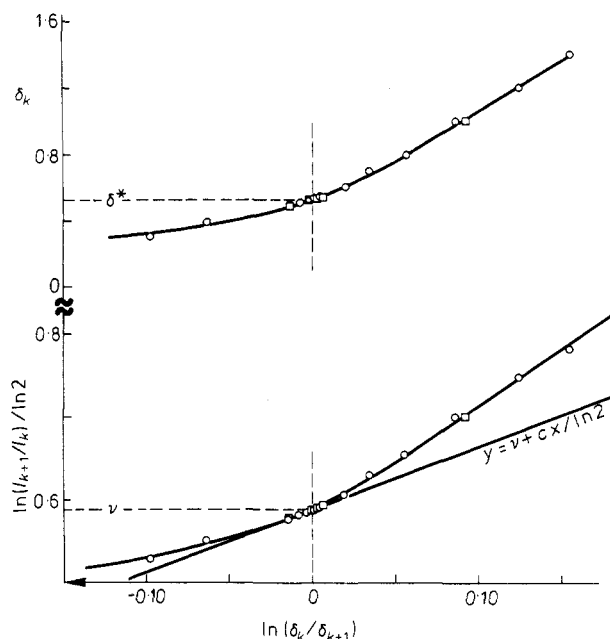
Figure 2. The renormalised coupling constant δ_k and bond length $\ln (l_{k+1}/l_k)$ plotted against $\ln (\delta_k/\delta_{k+1})$. These results were obtained with scale factor $s = 2$ for chains of lengths $N_0 = 8$ and $N_0 = 16$. The slope of $\ln (l_{k+1}/l_k)/\ln 2$ is indicated by the line $y = \nu + cx/\ln 2$, where $\nu = 0.589$ and $c = 0.762$. $\bigcirc$ $N_0 = 8$; $\square$ $N_0 = 16$.

equation (8) (lower part of figure 2). As expected the result is consistent with the prediction $\phi_{MF} = \frac{1}{2}$.

In practice the same flow lines are obtained irrespective of the initial values δ_0 and l_0. The full curves in figure 2 also yield corrections to the leading asymptotic law (4a). These corrections and applications of the MCRG method to other systems will be discussed elsewhere.

I would like to thank Professor K Binder for many valuable discussions and suggestions.

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