



HAL
open science

Polymer chain in annealed random media

A. Baumgärtner, B.K. Chakrabarti

► **To cite this version:**

A. Baumgärtner, B.K. Chakrabarti. Polymer chain in annealed random media. Journal de Physique, 1990, 51 (16), pp.1679-1682. <10.1051/jphys:0199000510160167900>. <jpa-00212478>

HAL Id: jpa-00212478

<https://hal.science/jpa-00212478v1>

Submitted on 4 Feb 2008

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



HAL Authorization

Classification
Physics Abstracts
 05.40 — 72.90 — 64.70

Short Communication

Polymer chain in annealed random media

A. Baumgärtner⁽¹⁾ and B.K. Chakrabarti⁽²⁾

⁽¹⁾ Institut für Festkörperforschung, Forschungszentrum Jülich, D-5170 Jülich, F.R.G.

⁽²⁾ HLRZ, Forschungszentrum Jülich, D-5170 Jülich, F.R.G. and Sha Institute of Nuclear Physics, Calcutta 700009, India

(Received June 1st 1990, accepted June 7, 1990)

Abstract. — Self-avoiding polymer chains trapped in annealed random media have been investigated by Monte Carlo methods. It is found that the configurational characteristics of a polymer are *not affected* by the media and are *independent* of the concentration of the impurities. This is in agreement with an early conjecture, but in disagreement with recent analytical results.

1. Introduction.

The question on the effect of *quenched* disorder on the statistics of self-avoiding walks (SAW) has been quite stormy [1, 2]. Compared to that, the apparently much more simpler question on the effect of *annealed* impurities on the statistics of SAWs has been addressed only very recently [3, 4, 5].

Consider the problem of a SAW on a lattice with missing bonds (say) at a given concentration. Assume the remaining bonds to be in thermal equilibrium with the chain.

One would not, in fact, expect any effect of annealed disorder on the SAW statistics for any amount of disorder. Denoting by R_N the average end-to-end distance of an N stepped SAW,

$$R_N^2 = \frac{\sum_{(c)} r_N^2(c) P_c}{\sum_{(c)} P_c} \tag{1}$$

where (c) denotes all possible SAW configurations on the (perfect) lattice, and $r_N^2(c)$ denotes the end-to-end distance of the N step SAW for the c -th SAW configuration and $P_c = 1$ if the c -configuration of the SAW is possible on the dilute lattice; $P_c = 0$ otherwise. $P_c = P_1 P_2 P_3 \dots P_N$, where P_i are the occupation operators ($P_i = 1$ or 0) of the bonds of the lattice through which the SAW configuration c (on the perfect lattice) passes. For annealed impurities, the averaged

end-to-end size of the SAW could be given by

$$\langle R_N^2(p) \rangle = \frac{\langle \sum_{(c)} r_N^2(c) P_c \rangle}{\langle \sum_{(c)} P_c \rangle} = \frac{p^N \sum_{(c)} r_N^2(c)}{p^N \sum_{(c)} 1} = \langle R_N^2(1) \rangle \quad (2)$$

since $\langle P_c \rangle = p^N$, where p is the average occupation concentration of bonds, because a SAW never visits the same bond more than once. The SAW chain size should thus remain completely unchanged for any amount of lattice disorder. Note, that the above independent disorder average for the numerator and denominator is perhaps possible for annealed disorder only, and was in fact wrongly [6, 2] applied to the quenched disorder case [7].

Annealed impurities being in thermal equilibrium with the heat bath, are quite often "constrained"; e.g., their total number may be given by an (analytic) function of the heat bath parameters or may be kept fixed. There is considerable literature on the effect of such commonly encountered constrained-annealed impurities on magnetic systems (n -vector magnetic model in general) [8-10]. Essentially, a long range ϕ^4 term (with slightly different momentum conservation rule) appears [10], apart from some renormalisation (reduction) of the usual ϕ^4 term (standard excluded volume term in the $n \rightarrow 0$ limit):

$$H = \sum_{\alpha=1}^n \sum_q (r + q^2) \phi_q^\alpha \phi_{-q}^\alpha + u \sum_{\alpha, \beta=1}^n \sum_{q_1 q_2 q_3 q_4} \phi_{q_1}^\alpha \phi_{q_2}^\alpha \phi_{q_3}^\beta \phi_{q_4}^\beta \delta(q_1 + q_2 + q_3 + q_4) \quad (3)$$

$$+ v \sum_{\alpha, \beta=1}^n \sum_{q_1 q_2 q_3 q_4} \phi_{q_1}^\alpha \phi_{q_2}^\alpha \phi_{q_3}^\beta \phi_{q_4}^\beta \delta(q_1 + q_2) \delta(q_3 + q_4)$$

This new v term, arising from constrained-annealed impurities, is responsible for a crossover to Fisher renormalised critical behavior ($\nu \rightarrow \nu/(1 - \alpha)$) for the general n -vector model, when $\alpha (= 2 - d\nu)$ of the nonrandom model ($v = 0$) is positive. This Fisher renormalised critical behavior due to annealed impurities, which is so commonly observed in magnetic systems (for anisotropic or Ising-like magnets $n = 1$, say), is, of course, unrealisable in the SAW limit $n \rightarrow 0$, where the renormalised size exponent ν may become greater than unity, which is meaningless [4]. This is, however, circumvented [5] because of the appearance of a collapsed ($\nu = 1/d$) phase described by a "discontinuity" fixed point, when one notices that the Fisher renormalised fixed point (being a long range interaction fixed point) is of order $1/n$ and runs away to infinity as $n \rightarrow 0$ in the SAW limit. Thirumalai [3] argued that annealed impurities will renormalise, and hence decrease, the u term in (3) and could eventually (for impurity densities beyond a critical value p_c), make a crossover to a Gaussian chain behaviour. Duplantier [4], extended the calculations and argued that higher order (ϕ^3 order) terms would also appear due to annealed impurities and under such cases a tricritical θ -point behaviour will be observed at p_c (where $u = 0$) and collapse would occur beyond that point ($p < p_c$, where u is negative). However, if such nontrivial (averaging) effects are introduced by some kind of annealed impurities (which do not permit the straightforward averaging in Eq.(2)) then, the crucial term, would be the v -term (not considered in Refs. [3] and [4]) which introduces the Fisher renormalised fixed point for usual n -vector magnets ($n > 0$). The fixed point, of course, runs away to give a "discontinuity" fixed point in the SAW ($n \rightarrow 0$) limit, giving [5] a collapsed phase ($\nu = 1/d$) for any amount of impurities ($p < 1$). In what follows, we did not see any such nontrivial effects on the SAW statistics, due to the (simplest) kind of annealed impurities considered in our simulations.

2. Model, simulation technique and results.

As a model for a polymer chain, we consider a self-avoiding walk on the cubic lattice. Ensembles of chain conformations are generated by randomly applying kink-jump and reptation algorithms during the simulations (for details see e.g. [11]). A local kink-jump is performed by changing the coordinate of the $k -$ th polymer segment at \mathbf{r}_k to $\mathbf{r}'_k = \mathbf{r}_{k+1} + \mathbf{r}_{k-1} - \mathbf{r}_k$. A configurational change according to the reptation algorithm is obtained by clipping one of the two segments at the ends of the chain and attaching at the other end a new segment pointing in a randomly chosen direction on the cubic lattice. Any attempt violating the self-avoidance is rejected.

But even if this attempt is successful with respect to self-avoidance, this attempt has to be rejected if the new site \mathbf{r}'_k is occupied by an impurity. The occupation of \mathbf{r}'_k by an impurity at each attempted configurational change of the polymer occurs in $\eta < p$, where $0 < \eta < 1$ is a random number determined anew whenever the polymer attempts to occupy this site, and $0 \leq p \leq 1$ is the concentration of the impurities. This fulfills the requirement that the (annealed) impurities are in “thermal” equilibrium with the polymer chain. However, unlike in cases where the total number of such impurities could be kept fixed or constrained, we believe the annealed impurities in our model are “unconstrained”.

We have estimated the mean square radius of gyration $\langle S^2 \rangle$, the mean square end-to-end distance $\langle R^2 \rangle$, the number of nearest-neighbor contacts per bead E/N , and the corresponding “specific heat” C

$$C/N = \langle \left(\frac{E}{N} \right)^2 \rangle - \langle \frac{E}{N} \rangle^2 \tag{4}$$

where N is the chain length.

Simulations have been performed for $0 \leq p \leq 0.95$ for $N = 300$ and $N = 600$. We found that the configurational characteristics are *not affected* by the annealed impurities and are *independent* of p . The results are given below.

$\langle S^2 \rangle N^{-1.18}$	$\langle R^2 \rangle N^{-1.18}$	E/N	C
0.183(3)	1.16(3)	0.197(2)	0.39(2)

The numbers in brackets denote the statistical error.

No significant indication of any crossover in the SAW critical behaviour, as predicted by the analytic theories [3-5], could be observed. The “specific heat” doesn’t exhibit any anomaly, as would be expected at a θ -point [4] . Since critical behaviour of the specific heat has been observed in numerous simulations (see e.g. [12]) of the “classical” collapse transition, we must conclude that, at least for the present model of self-avoiding polymers in annealed random medium, a θ -point does *not* exist.

Since we have not observed any effect of the impurities, one might distrust the simulations. Therefore we have performed some preliminary simulations of polymers with weaker self-avoidance (Domb-Joyce polymer model [13]), which in fact yield evidence of an influence of annealed impurities on the configurational properties of a polymer chain. This situation might be of interest and deserves further investigations.

3. Conclusions.

All these observations seem to confirm that any amount of (“unconstrained”) annealed impurities do not affect the critical behaviour of “strict” self-avoiding polymer chains, as conjectured originally by Harris [7] (wrongly applied to the quenched disorder case), due to the cancellation of the disorder effects on the average polymer size as discussed in equation (2). In such cases, presumably, no v term, in Hamiltonian (3), arises and no Fisher renormalised fixed point appears. [5] Our observations do not indicate any tricritical θ -point and collapse behaviour [4] for polymer chains in random media with annealed impurities.

Acknowledgement.

We are grateful to Professor D. Stauffer for a critical reading of the manuscript and for some useful comments.

References

- [1] LEE S.B., NAKANISHI H., *Phys. Rev. Lett.* **61** (1988) 2022.
- [2] MEIR Y., HARRIS A.B., *Phys. Rev. Lett.* **63** (1989) 2819.
- [3] THIRUMALAI D., *Phys. Rev. A* **37** (1988) 269.
- [4] DUPLANTIER B., *Phys. Rev. A* **38** (1988) 3647.
- [5] BHATTACHARJEE S.M., CHAKRABARTI B.K., *preprint 1990*.
- [6] LYKLEMA J.W., KREMER K., *Z. Phys. B* **55** (1984) 41.
- [7] HARRIS A.B., *Z. Phys. B* **49** (1983) 347.
- [8] FISHER M.E., *Phys. Rev.* **176** (1968) 257.
- [9] STINCHCOMBE R.B., in *Phase Transition and Critical Phenomena*, vol.7, C. Domb and J.L. Lebowitz Eds. (Academic Press, N.Y., 1983) p.151.
- [10] see e.g., J. SAK, *Phys. Rev. B* **10** (1974) 3957;
BRUNO J., SAK J., *Phys. Rev. B* **22** (1980) 3302.
- [11] BAUMGÄRTNER A., in *Monte Carlo Methods in Statistical Physics*, K. Binder Ed. (Springer, Berlin, 1984).
- [12] BAUMGÄRTNER A., *J. Phys. France* **43** (1982) 1407.
- [13] DOMB C., JOYCE G.S., *J. Phys. C* **5** (1972) 956.

Cet article a été imprimé avec le Macro Package "Editions de Physique Avril 1990".