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Change in polymer scaling laws due to disorder

V Blavats'ka[1], Ch von Ferber[2] and Yu Holovatch[3]

[1] Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 79011 Lviv, Ukraine
[2] Physikalisches Institut, Theoretische Polymerphysik, Universität Freiburg, 79104 Freiburg, Germany
[3] Institut für Theoretische Physik, Johannes Kepler Univetsität Linz, 4040 Linz, Austria

E-mail: viktoria@ph.icmp.lviv.ua, ferber@physik.uni-freiburg.de and hol@ph.icmp.lviv.ua

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Abstract

We study the scaling properties of polymer macromolecules in media with defects that are correlated or belong to some porous or spongelike structure. To this end, we use the model of self-avoiding walks on a randomly diluted lattice with long-range-correlated quenched disorder. We apply the field-theoretical renormalization group refined by the resummation technique and perform calculations directly in three dimensions up to the two-loop approximation. The scaling behaviour of polymers in media with long-range-correlated disorder is found to be governed by a new set of exponents.

Long flexible polymer chains in good solvent possess a number of properties that are universal, i.e. independent of the details of their chemical microstructure. These universal scaling properties are perfectly described within a model of self-avoiding walks (SAWs) on a regular lattice [1, 2]. The limit of a SAW with an infinite number of steps may be mapped to a formal $m \to 0$ limit of the m-vector model at its critical point. In particular, the average square end-to-end distance $\langle R^2 \rangle$, and the number of configurations Z_N of a SAW with N steps on a regular lattice, scale in the asymptotic limit $N \to \infty$ as

$$\langle R^2 \rangle \sim N^{2\nu}, \qquad Z_N \sim z^N N^{\gamma-1} \tag{1}$$

where ν and γ are the universal correlation length and susceptibility exponents for the $m = 0$ model that only depend on the space dimensionality d, and z is a nonuniversal fugacity. For $d = 3$ the exponents read [3] $\nu = 0.5882 \pm 0.0011$ and $\gamma = 1.1596 \pm 0.0020$.

In this study, we are interested in the scaling laws that govern the behaviour of polymers in disordered media when the defects are correlated or belong to some porous or spongelike structure. In magnetic systems, the presence of pointlike uncorrelated (or short-range-correlated) quenched disorder has a nontrivial effect on their critical behaviour only if the specific heat critical exponent α is positive [4] (the so-called Harris criterion).

However, although the critical exponent α of a SAW on a $d = 3$ pure lattice is positive ($\alpha(d = 3) = 0.235 \pm 0.003$) [3], a weak quenched short-range-correlated disorder does not alter the SAW critical exponents. This statement was proven by Harris [5] and confirmed later by renormalization group (RG) results [6].

Weinrib and Halperin [7] introduced a model with 'random-temperature' disorder, arising from a small density of impurities, causing random variations in the local phase transition temperature $T_c(\vec{x})$. The fluctuations in $T_c(\vec{x})$ are characterized by a correlation function, that falls off according to a power law: $\sim x^{-a}$ at large distances x, where a is a constant. The m-vector model of this type of disorder has been studied by two complementary RG approaches: first using a double expansion in the parameters $\varepsilon = 4-d, \delta = 4-a$ in the linear approximation [7], and more recently in the fixed d, a technique for $d = 3$ and different values of correlation parameter a in a two-loop approximation [8]. Both approaches qualitatively confirmed that long-range-correlated disorder leads to new universality behaviour for these magnetic systems.

In a previous publication [9] we have addressed the same question for the asymptotic behaviour of polymers. Our linear approximation of the double ε, δ-expansion indicates qualitatively the existence of a new RG fixed point for long-range-correlated disorder. Here, we present a two-loop approximation using the fixed a, d technique that confirms the qualitative picture and results in physically meaningful values for the fixed point and exponents. The critical behaviour of a SAW in a medium with long-range-correlated disorder is described by an effective Hamiltonian with two couplings, that is derived by the replica method for averaging the quenched disorder. It reads [9]

$$H_{eff} = \sum_{k}\sum_{\alpha}^{n}(\mu_0^2 + k^2)(\vec{\phi}_k^{\alpha})^2 + \frac{u_0}{4!}\sum_{\alpha}^{n}\sum_{k_1k_2k_3k_4}\delta(k_1+k_2+k_3+k_4)\vec{\phi}_{k_1}^{\alpha}\vec{\phi}_{k_2}^{\alpha}\vec{\phi}_{k_3}^{\alpha}\vec{\phi}_{k_4}^{\alpha} - \frac{w_0}{4!} \times \sum_{\alpha\beta}^{n}\sum_{kk_1k_2k_3k_4} f(k)\delta(k_1+k_2+k)\delta(k_3+k_4-k)\vec{\phi}_{k_1}^{\alpha}\vec{\phi}_{k_2}^{\alpha}\vec{\phi}_{k_3}^{\beta}\vec{\phi}_{k_4}^{\beta}, \qquad m, n \to 0. \tag{2}$$

Here, $\vec{\phi}_k^{\alpha}$ is the α replica of the n-fold replicated m-component vector field for d-dimensional momentum k; $u_0 > 0$, $w_0 > 0$ and μ_0 are respectively the bare coupling constants and the bare mass; both the polymer ($m = 0$) and the replica ($n = 0$) limits are implied. The coefficient of w_0 describes the effective coupling of replicas due to the disorder. For small k, the function $f(k)$ behaves as $f(k) = |k|^{a-d}$, which stems from the Fourier transform of the large-x behaviour (x^{-a}) of the disorder correlations. Power counting implies that this term is irrelevant in the RG sense for $a \geqslant d$. The above-mentioned linear ε–δ expansion finds the stable RG fixed point in this unphysical region. A similar picture is found in the linear ε, δ approximation also for the model of a magnet with long-range-correlated disorder [7,9]. In the latter case, the reason could be traced to the complicated symmetry of the effective Hamiltonian and the unknown asymptotic properties of the resulting series [8,11]. Our present approach, which relies on the higher-order (two-loop) perturbation theory expansions refined by the resummation technique, yields physically meaningful results for $a < d$. In the field-theoretical RG approach [2], the change of the renormalized couplings u, w under renormalization defines a flow in parametric space, governed by corresponding β-functions $\beta_u(u, w)$, $\beta_w(u, w)$. The fixed points u^*, w^* of this flow are the solutions of the system of equations $\beta_u(u^*, w^*) = 0$, $\beta_w(u^*, w^*) = 0$. Using the notation v_1, v_2 for the couplings u, w the fixed point is defined as stable if the stability matrix $B_{ij} = \partial\beta_{v_i}/\partial v_j$ eigenvalues λ_i have positive real parts.

The RG functions of the model in equation (2), as listed in [9], are possibly divergent series with zero radius of convergence [10], familiar to the theory of critical phenomena. If the series

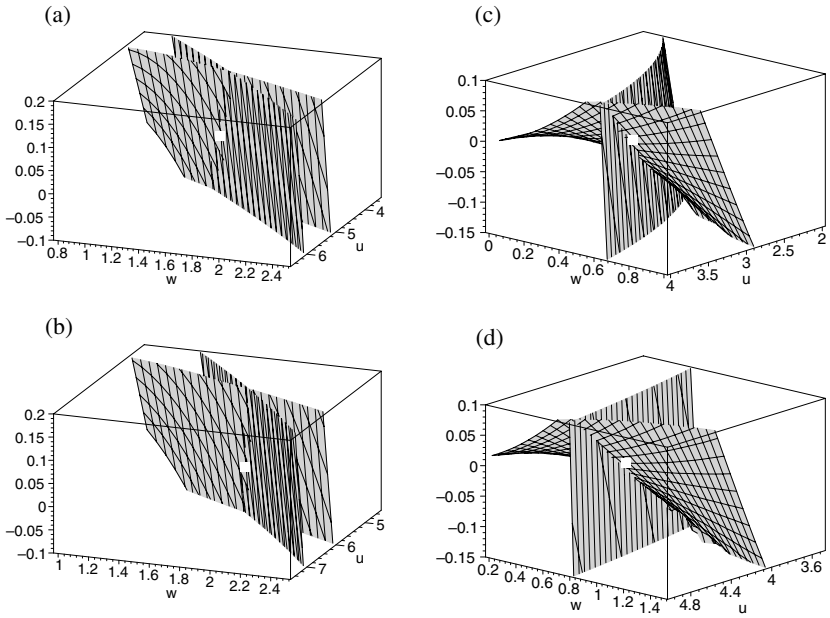

Figure 1. The resummed β-functions in the two-loop approximation for $d = 3$. (a), (b) the Chisholm–Borel resummation; (c), (d) the subsequent resummation. (a), (c) $a = 2.9$; (b), (d) $a = 2.7$. The LR stable fixed point is shown by an open square.

are asymptotic, then the situation is, at least in principle, controllable: in this case a good estimate for the sum of the series is obtained by keeping a certain number of the first terms ('optimal truncation') or applying an appropriate Borel resummation procedure [10].

However, there is no proof of the Borel summability of the RG series for disordered models [11]. Moreover, their summability has been seriously questioned recently [12, 13]. Nonetheless the Borel-based resummation technique applied to the RG series of disordered models usually provides reliable data [11]. Here, we apply several methods of resummation in order to obtain quantitative results for the problem under consideration and to check the stability of these results. A simple two-variable Chisholm–Borel resummation technique [14] turns out to be the most effective one for our problem. Applying it to the two-loop series for the RG β-functions we obtain for $a < 3$ together with the familiar fixed points describing Gaussian chains ($u^* = w^* = 0$) and SAWs in media without defects ($u^* \neq 0$, $w^* = 0$) the stable 'long-range' (LR) fixed point $u^* \neq 0$, $w^* \neq 0$ describing polymers in long-range-correlated disorder (see the left-hand column in figure 1). This leads to the conclusion that, for certain values of $a < d$ the polymer scaling is influenced by disorder. Then, at some value $a = a_{\mathrm{marg}}$ the LR fixed point becomes unstable, which in its turn suggests the collapse of the polymer chain in a medium with too strong correlated disorder.

Secondly, we apply the method of subsequent resummation, developed in the context of the $d = 0$-dimensional diluted Ising model in [13] and successfully used for the $d = 3$ case in [15]. Here, the summation is carried out first in the coupling u and subsequently in w. While we do not expect any high accuracy from this method, as the applicability has not been proven for our problem, again the presence of a stable fixed point LR for $a_{\mathrm{marg}} \leqslant a < d$ confirms the stability of a new type of critical behaviour (see the right-hand column of figure 1). Note, however, that the subsequent resummation method was especially devised [15] to analyse the behaviour of the β-functions in the vicinity of a mixed fixed point ($u \neq 0$, $w \neq 0$) and it does

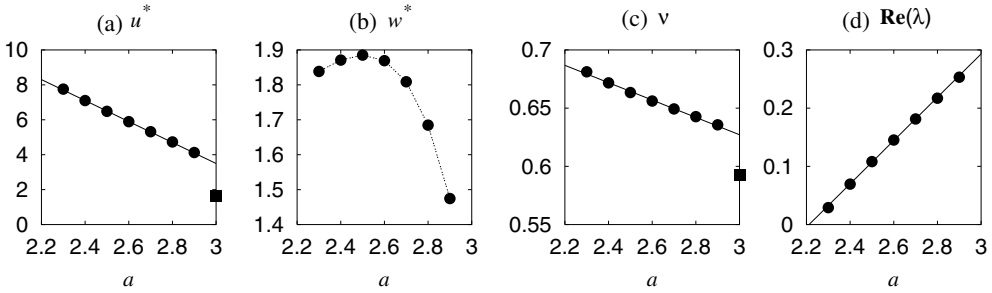

Figure 2. (a), (b) Fixed-point coordinates u^*, w^*, (c) exponent ν and (d) real part of $\lambda_{1,2}$ plotted as functions of the disorder parameter a. Circles, LR fixed-point values; squares, unperturbed fixed-point values; lines are guides to the eye.

not allow us to analyse the full RG flow. That is why we have chosen the Chisholm–Borel resummation method to derive numerical results in our approach.

The values of the Chisholm–Borel resummed stable fixed-point coordinates and the stability matrix eigenvalues along with the numerical values for critical exponent ν are shown in figure 2. Departing from the value $a = d = 3$ downward to 2 one notices a major increase of the value of the coupling u, so the results are expected to be more reliable for a close to 3. Our numerical results for the LR fixed-point values of the coupling u^* and the exponent ν do not extrapolate to the unperturbed fixed-point values. Moreover, the real part of the stability eigenvalues seems to vanish near $a = 2.2$.

In summary, our results confirm that in a medium with long-range-correlated quenched disorder the swelling of the polymer coil at $d = 3$ is governed by a distinct exponent ν that increases when the correlation of the disorder is increased (i.e. a decreases). A crossover to the collapse of the polymer is predicted when the correlation is too strong, i.e. a is below some marginal value $a_{\mathrm{marg}} \geqslant 2$.

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