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On the number of intersections of self-repelling polymer chains

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Abstract. We give a detailed analysis of the intersection properties of polymers. Using the renormalization group we provide a full crossover function for the dependence of the number of intersections in a single polymer on chain length and excluded volume strength. We compare our results with Monte-Carlo data and with exact calculations for a random walk, finding good agreement in all respects. Restricting to the vicinity of the eight ternary fixed points we also calculate the number of intersections between two chains placed at a fixed distance, including the two halves of a block-copolymer. The analysis of these systems confirms the interpretation of the different contributions to the number of intersections in a single chain. Due to the highly nontrivial character of the correlations in a polymer chain the correction exponents in both cases however are different. None of the results can be extracted from any Flory-type estimate.

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1 Introduction

For a polymer in solution, modeled as a self-repelling random walk, the number of intersections is a measure of the internal energy of the chain. As such it is of considerable interest for the thermodynamics of dilute solutions. Furthermore it has been used in heuristic approaches to the swelling of a single macromolecule and it is relevant for problems like network formation or intramolecular reactions. In the present contribution we use renormalization group methods to analyze the number of intersections within a single macromolecule as function of the chain length or of the excluded volume strength. We generalize the discussion to the intersections either of two macromolecules placed at a fixed distance of each other, or of the two blocks of a copolymer. The latter problem contains the number of intersections among the two halves of a single macromolecule as a special case.

For a noninteracting chain of length (polymerization index) n the number of intersections $\sigma(n,0)$ is well known [1]:

$$\sigma(n;0) = a_0 n + b_0 n^{\epsilon/2} + c_0 + o(n^0). \tag{1.1}$$

Here $\epsilon = 4 - d$, where d is the spatial dimension of the system. The result holds for $2 < d < 4$. Some time ago a similar result has been shown to hold for a self-repelling chain in the excluded volume limit [2,3]:

$$\sigma(n;u^*) = a_* n + b_* n^{-\nu\omega} + c_* + o(n^{-\nu\omega}). \tag{1.2}$$

Here ν or ω are standard critical exponents,

$$\begin{aligned}\nu &= \frac{1}{2} + \frac{\epsilon}{16} + \mathcal{O}(\epsilon^2) \overset{d=3}{=} 0.588\\ \omega &= \epsilon - \frac{21}{32}\epsilon^2 + \mathcal{O}(\epsilon^3) \overset{d=3}{=} 0.80.\end{aligned} \tag{1.3}$$

In equations (1.1, 1.2) only the exponents are universal. The coefficients a_0, a_*, b_0 *etc.* depend on the microstructure of the model.

Comparing equation (1.1) to equation (1.2) we immediately note a change in the character of the leading correction. While in the noninteracting case it diverges $\sim n^{\epsilon/2}$, it stays finite $\sim n^0$ for an excluded volume chain. Indeed, the contribution $\sim n^{\epsilon/2}$ corresponds to the subleading correction $\sim n^{-\nu\omega}$ in the latter case. This is a direct consequence of the behaviour of the renormalized excluded volume coupling u. While $u > 0$ is a relevant perturbation at the noninteracting (Gaussian) fixed point $u = 0$, the deviation $u - u^*$ is irrelevant at the excluded volume fixed point $u = u^*$. It is one subject of this work to calculate the universal scaling function $H(u)$ that describes this crossover among the asymptotic laws (Eqs. (1.1, 1.2)). The calculation is restricted to one loop order of renormalized perturbation theory, and to test our results we measured the number of intersections in a Domb-Joyce model on a simple cubic lattice *via* Monte-Carlo simulations. We find good agreement among the numerical or analytical results.

The structure of equation (1.2) deserves special interest. It is dominated by an "extensive" term $\sim n$, which, as the corresponding term in equation (1.1), is due to backfolding of short parts, summed along the chain. It thus is a

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fairly trivial effect. The constant contribution can be seen as an endeffect, and only the subleading correction $\sim n^{-\nu\omega}$ represents intersections among segments spaced along the chain infinitely far in the limit $n \to \infty$. This illustrates the efficiency of excluded volume swelling in suppressing nontrivial intrachain contacts. To support that interpretation we quote the number of intersections found for two related problems.

Firstly we may count the number of intersections among the two halves of a chain. This is a special case of a block-copolymer problem. At the excluded volume fixed point we find

$$\sigma_{\mathrm{co}}(n;\mathrm{S}) = b_{\mathrm{co}}(\mathrm{S}) n^{-\nu\omega_{12}(\mathrm{S})} + c_{\mathrm{co}}(\mathrm{S}) + o(n^{-\nu\omega_{12}(\mathrm{S})}), \quad (1.4)$$

where the argument S refers to the fully symmetrical situation considered (both blocks are identical). As expected the extensive term is absent since only backfolding near the central segment counts. The leading contribution $\sim c_{\mathrm{co}}(\mathrm{S})$ arises from this effect. Segments farther spaced along the chain contribute a correction only, which again vanishes for $n \to \infty$. The exponent

$$\omega_{12}(\mathrm{S}) = \frac{\epsilon}{2} - \frac{19}{64}\epsilon^2 + \mathcal{O}(\epsilon^3) \overset{d=3}{=} 0.40 \quad (1.5)$$

differs from ω (Eq. (1.3)), which illustrates the highly nontrivial character of the correlations within an excluded volume chain: even for given chemical distance $|j-i|$ of two segments i, j, their intersection probability crucially depends on their position along the chain.

We finally consider two identical chains of single-chain radius of gyration R_{g}, placed at mutual end-to-end distance R. In that configuration also the constant contribution is eliminated, the number of intersections obeying the scaling law

$$\sigma_2(n, R; \mathrm{S}) = b_2(\mathrm{S}) n^{-\nu\omega_{12}(\mathrm{S})} \bar{\sigma}_2(R/R_{\mathrm{g}}; \mathrm{S}) + o(n^{-\nu\omega_{12}(\mathrm{S})}). \quad (1.6)$$

For fixed $R/R_{\mathrm{g}} > 0$ the two chains in the limit $n \to \infty$ carefully rearrange so as not to intersect each other. This is consistent with the previous finding that the free energy excess of two interpenetrating coils stays finite even for $n \to \infty$ [4]. It is a remarkable result showing that in the limit of long chains even weak repulsion leads to strict mutual avoidance.

Technically the sequence of results (Eqs. (1.2, 1.4, 1.6)) reflects the renormalization properties of the quantities considered. Additive renormalization leads to an extensive contribution (Eq. (1.2)). The need of an explicit multiplicative renormalization gives rise to the constant contributions. Finally the implicit multiplicative renormalization of the coupling yields corrections of order $n^{-\nu\omega}$ or $n^{-\nu\omega_{12}(\mathrm{S})}$. All these results differ considerably from estimates based on simple smoothed density models [1] which involve some grain of truth only for noninteracting (θ-) conditions.

In the sequel we present the detailed derivation of these results, extending the discussion of the copolymer or the two polymer case also to other fixed points describing for instance the interaction of a θ-chain with an excluded volume chain. In the sense of a short distance expansion we also consider how the result equation (1.6) reduces to the copolymer result equation (1.4) in the limit $R/R_{\mathrm{g}} \to 0$.

We should note that in this work we consider only the effect of two body interactions, but ignore three body interactions which in $d = 3$ induce logarithmic corrections at the θ-point. Crossings of higher order in a noninteracting chain, which are related to many body interactions have been discussed by Duplantier [5].

This paper is organized as follows: in Section 2 we define the model and recall results from renormalization theory. Section 3 is devoted to the intersections within a single chain. We calculate the crossover among the θ- or excluded volume limits, and we compare to Monte-Carlo data. The copolymer or two interpenetrating polymers are discussed in Section 4, where we concentrate on the fixed point behaviour. Section 5 summarizes our results. Expressions for the partition functions needed in the analysis are derived in appendices.

2 The model and standard results from renormalization theory

In our analytical calculations we use the "spring and bead model" which represents the polymer as a discrete chain in a continuous, d-dimensional embedding space. For a chain of length n the configuration is fixed by the endpoints $\mathbf{r}_0, ..., \mathbf{r}_n \in \mathbb{R}^{\mathrm{d}}$ of the n segments. The corresponding statistical weight is given as ($k_{\mathrm{B}}T = 1$)

$$\mathrm{e}^{-\mathcal{H}} = \mathrm{e}^{-\frac{1}{4l^2}\sum_{j=1}^{n}(\mathbf{r}_j - \mathbf{r}_{j-1})^2} \times \prod_{(i,j)}{}' \left[1 - (4\pi l^2)^{d/2} \beta_{\mathrm{e}} \delta^{\mathrm{d}}(\mathbf{r}_i - \mathbf{r}_j)\right]. \quad (2.1)$$

The Hamiltonian consists of a Gaussian part where l determines the effective length of one segment and a product of δ-functions which model the repulsive interaction among the segments. The dimensionless coupling constant $\beta_{\mathrm{e}} \geq 0$ measures the strength of repulsion. In an expansion of the product $\prod'$ over all segment pairs (i, j) in equation (2.1) we omit all terms where one segment coordinate occurs more than once. On a technical level this avoids artificial divergencies due to products of δ-functions while physically this restriction is consistent with the neglect of m-body interactions with $m \geq 3$. In the limit of long chains the three microscopic parameters n, l, β_{e} are known to be sufficient to describe the universal properties of self-repelling chains. It should be noted that starting from a discrete chain model is essential for an unambiguous definition of the number of intersections, which is an illdefined object for a continuos chain.

The partition function $\mathcal{Z}$ is defined as

$$\mathcal{Z}(n, l, \beta_{\mathrm{e}}) := \int_{\Omega} \mathcal{D}[\mathbf{r}] \mathrm{e}^{-\mathcal{H}}, \quad (2.2)$$

where

$$\mathcal{D}[\mathbf{r}] := \prod_{j=0}^{n} \frac{\mathrm{d}^d r_j}{(4\pi l^2)^{d/2}} \tag{2.3}$$

and $\Omega \to \infty$ is the system volume. Any explicit calculation of physical quantities has to be carried out perturbatively (*cf.* Append. A), where it turns out that the expansion parameter is given as $z := \beta_\mathrm{e} n^{\epsilon/2}$. In the limit of long chains, $n \to \infty$ with $\beta_\mathrm{e} > 0$ fixed, any bare perturbation theory thus breaks down.

The well established solution to this problem is provided by renormalization (see *e.g.* [6], or, for the field theoretic language as used here: [7]). Renormalization maps the "critical" system (n, l, β_e), $n \gg 1$, to an uncritical theory expressed in renormalized parameters $(n_\mathrm{R}, l_\mathrm{R}, u)$. In the renormalized theory a perturbative calculation is feasible since n_R can be chosen to be of order 1. In concrete terms renormalization implies the existence of a mapping

$$\beta_\mathrm{e} = \lambda^{\epsilon} u Z_u(u, \lambda), \tag{2.4}$$

$$n = \lambda^{-2} n_\mathrm{R} Z_n(u, \lambda), \tag{2.5}$$

where the renormalization factors Z_u and Z_n have to be chosen such that any perturbative expression of any observable expressed in renormalized parameters $(n_\mathrm{R}, l_\mathrm{R}, u)$ for long chains is independent of

$$\lambda := \frac{l}{l_\mathrm{R}}, \tag{2.6}$$

up to negligible corrections. The renormalization factors are given as power series in u, with coefficients that depend on λ^{ϵ}. For quantities like the partition function which are not normalized, we need further additive or multiplicative renormalizations, which introduce a critical chemical potential $\mu_\mathrm{s}^*(\beta_\mathrm{e})$ or an additional renormalization factor $Z(u, \lambda)$ respectively. It has been proved that the three renormalization factors Z, Z_u, Z_n together with $\mu_\mathrm{s}^*(\beta_\mathrm{e})$ are sufficient to absorb the whole dependence on λ (up to order λ^2) in any physical quantity to any order perturbation theory. The relation among the bare and the renormalized partition function, in particular, reads

$$\mathcal{Z}(n, l, \beta_\mathrm{e}) = \frac{\Omega}{(4\pi l^2)^{d/2}} \mathrm{e}^{\mu_\mathrm{s}^*(\beta_\mathrm{e})\, n} \frac{Z(u, \lambda)}{Z_n(u, \lambda)} \times \mathcal{Z}_\mathrm{R}(n_\mathrm{R}, u) \left(1 + \mathcal{O}(\lambda^2)\right), \tag{2.7}$$

where $\mathcal{Z}_\mathrm{R}$ is independent of λ. For convenience a factor of the volume has been extracted.

In the renormalized theory all explicit reference to λ is eliminated, the renormalized theory being scale invariant. Renormalization thus constructs a one-parameter family of renormalized theories, all equivalent to the original bare theory. The renormalization group flow equations give the change of the renormalized parameters under a change of l_R or λ, equivalently, for a given fixed bare theory. In particular the flow of the renormalized coupling u is governed by a simple first order differential equation

$$\lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} u =: W(u). \tag{2.8}$$

The Wilson function $W(u)$ is independent of λ. Equation (2.8) shows two fixed points, *i.e.* zeros of $W(u)$, an unstable "Gaussian" fixed point $u = 0$ and a stable nontrivial fixed point $u = u^*$. The "correction to scaling exponent" ω describes the flow of u near $u = u^*$:

$$\omega := \left. \frac{\mathrm{d}W}{\mathrm{d}u} \right|_{u=u^*}. \tag{2.9}$$

From the renormalization factors we can construct two further flow equations

$$\lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln Z_n(u, \lambda) =: 2 - 1/\nu(u), \tag{2.10}$$

$$\lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln Z(u, \lambda) =: \eta(u). \tag{2.11}$$

As in equation (2.8) the right hand sides are independent of λ. At the nontrivial fixed point we obtain the well known critical exponents $\nu = \nu(u^*)$ and $\eta = \eta(u^*)$.

The at present most accurate form for the functions $W(u), \nu(u)$, and $\eta(u)$ defined above can be found in [8], where perturbation expansions evaluated to the order u^5 resp. u^6 are resummed. Rewriting the results within our scheme we get in $d = 3$

$$W(u) = -u(1-f)(1+0.824f)/(1+1.280f) \tag{2.12}$$

$$\nu(u) = 1/(2-0.364f+0.166f^2-0.174f^3+0.073f^4) \tag{2.13}$$

$$\eta(u) = 0.033f^2-0.002f^3 \tag{2.14}$$

with

$$f := u/u^* \tag{2.15}$$

and

$$u^* = 0.364. \tag{2.16}$$

(note that the coupling u of [8] corresponds to $u/8$ in our notation. Furthermore we have slightly corrected the parametrization of $\nu(u)$, so as to reproduce the now well established fixed point value $\nu = 0.588$ instead of the value $\nu = 0.59$ used in [8]). As numerical values for the critical exponents we in the following will use

$$\omega = 0.80, \nu = 0.588, \eta = 0.03. \tag{2.17}$$

Integrating equations (2.8, 2.10) we obtain the final form of the Renormalization Group (RG) mapping in three dimensions:

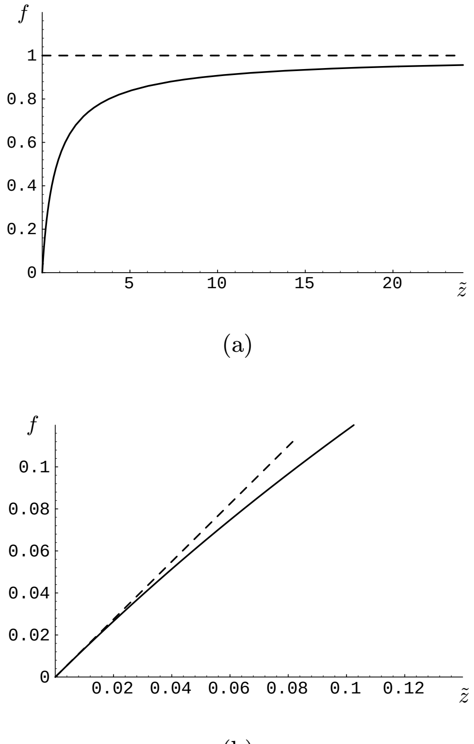
$$l_\mathrm{R} = f|1-f|^{-1/\omega} H_u(f) s_l l, \tag{2.18}$$

$$n_\mathrm{R} = f^{-2}|1-f|^{1/\nu\omega} H_n(f) s_n n. \tag{2.19}$$

The two functions $H_u(f)$ und $H_n(f)$ are regular in f,

$$H_u(f) = (1+0.824f)^{0.25} \tag{2.20}$$

$$H_n(f) = (1+0.824f)^{-0.789} \times \exp\left(0.228f - 0.206f^2 + 0.038f^3\right). \tag{2.21}$$



(a)

(b)

Fig. 1. (a) Flow of the coupling $f = u(\tilde{z})/u^*$ in three dimensions. (b) Flow of the coupling $f = u(\tilde{z})/u^*$ in three dimensions in the limit of small $\tilde{z}$.

The parameters s_l, s_n depend on the starting value $u(\lambda = 1)$ of the integration, which in turn is taken to be an analytic function of β_e. Equations (2.18–2.21) therefore identify the family of renormalized theories equivalent to a given bare theory. The bare parameters and thus the microstructure dependence are absorbed into $s_l l$ or s_n. To switch to a more familiar notation we introduce a "z-parameter"

$$\tilde{z} := (s_n n)^{\epsilon/2} =: \tilde{v}(\beta_e) n^{\epsilon/2}. \tag{2.22}$$

Figure 1a shows the flow diagram as calculated from equation (2.19) with $n_R = 0.53 = \mathcal{O}(1)$ (*cf.* Append. A). Near the Gaussian fixed point we have a proportionality $u(\tilde{z}) \sim \tilde{z}$ (see Fig. 1b).

3 Mean number of contacts in a single polymer chain

In a naive estimate of the number of contacts in a self-repelling chain one replaces the chain by a cloud of segments of volume $\sim l^d$ which are randomly distributed in a volume $R_g^d \sim (l\, n^{\nu_{\text{eff}}})^d$. Here $\nu_{\text{eff}} = 1/2$ at the Gaussian fixed point $u = 0$ (*i.e.* random walk) and $\nu_{\text{eff}} = \nu$ at the nontrivial fixed point $u = u^*$. This approximation results in the Flory-type estimate

$$\sigma(n) \sim n^2 \left(\frac{l}{R_g}\right)^d \sim n^{2-\nu_{\text{eff}} d}, \tag{3.1}$$

so that [1]

$$\sigma(n) \sim \begin{cases} n^{1/2} & \text{at } u = 0 \\ n^{0.236} & \text{at } u = u^* \end{cases} \ (d = 3). \tag{3.2}$$

Since this estimate completely neglects the chain connectedness, equations (3.1, 3.2) at best can be correct for contacts between segments which are well separated along the chain. Such segments might not notice their connectedness anymore. Nevertheless, in the case of nonvanishing self-repulsion even segments spaced far along the chain influence each other. The self-repulsion builds up correlations which invalidate the result equation (3.2) for $u > 0$. A correct treatment of this problem will be presented next.

3.1 Analytical results

A measure of the probability of intersection of two segments i and j in our model is given by $(4\pi l^2)^{d/2} \langle\!\langle \delta^d(\mathbf{r}_j - \mathbf{r}_i) \rangle\!\rangle$, where the numerical factor $(4\pi)^{d/2}$ is introduced for convenience. The angular brackets denote the statistical average $\langle ... \rangle = \int_\Omega \mathcal{D}[\mathbf{r}] \ ... \ \mathrm{e}^{-\mathcal{H}}/\mathcal{Z}$. We thus find for the mean number of intersections in a self-repelling chain

$$\sigma(n) = \sum_{0 \le i < j \le n} (4\pi l^2)^{d/2} \left\langle \delta^d(\mathbf{r}_j - \mathbf{r}_i) \right\rangle \tag{3.3}$$

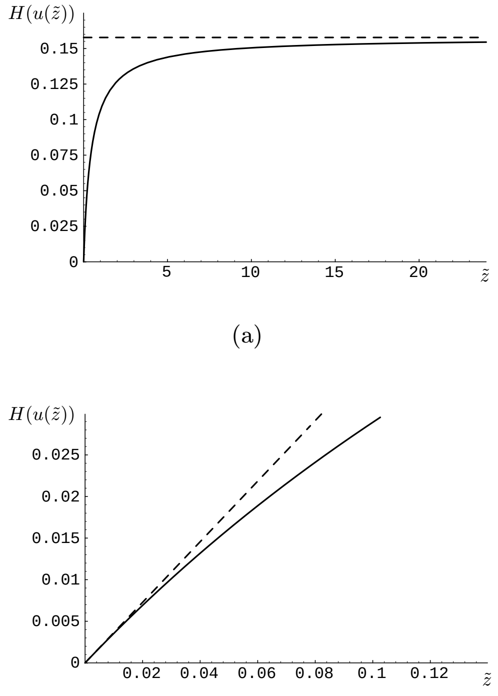
$$= -\frac{\partial}{\partial \beta_e} \ln \mathcal{Z}(n, l, \beta_e). \tag{3.4}$$

We now express $\mathcal{Z}$ by its renormalized counterpart *via* equation (2.7). Two words of caution seem to be appropriate: firstly the RG-mappings equations (2.4, 2.5) determine only two of the three renormalized parameters as functions of n, l, and β_e, giving a one parameter family of renormalized theories as pointed out above. Thus in taking the derivative one renormalized parameter has to be kept fixed. In the following we will choose l_R as fixed. Secondly we carefully have to keep track of the nonuniversal content of the theory. This amounts to taking all renormalization factors as explicitly dependent on $\lambda = l/l_R$ (cut-off regularization). Proceeding as described we obtain

$$\begin{aligned} \sigma(n) = &-\frac{\mathrm{d}}{\mathrm{d}\beta_e} \mu_s^*(\beta_e)\, n \\ &- \frac{\partial}{\partial \beta_e} u(\beta_e, \lambda) \left[\frac{\partial}{\partial u} \ln \frac{Z(u, \lambda)}{Z_n(u, \lambda)} + \frac{\partial}{\partial u} \ln \mathcal{Z}_R(u, n_R)\right] \\ &- \frac{\partial}{\partial \beta_e} n_R(\beta_e, \lambda, n) \frac{\partial}{\partial n_R} \ln \mathcal{Z}_R(u, n_R). \end{aligned} \tag{3.5}$$

To rewrite the partial derivatives with respect to β_e we make use of equations (2.4, 2.5) to find

$$\frac{\partial}{\partial \beta_e} n_R(\beta_e, \lambda, n) = -n_R \frac{\partial}{\partial u} \ln Z_n(u, \lambda) \frac{\partial}{\partial \beta_e} u(\beta_e, \lambda) \tag{3.6}$$



(a)

(b)

Fig. 2. (a) The scaling function $H(u(\tilde{z}))$ in three dimensions. Dashed: the asymptote $\gamma - 1 \approx 0.16$. (b) The scaling function $H(u(\tilde{z}))$ in three dimensions in the limit of small $\tilde{z}$. Dashed: the Gaussian asymptote $\sim \tilde{z} \sim n^{1/2}$.

and

$$\frac{\partial}{\partial \beta_{\mathrm{e}}} u(\beta_{\mathrm{e}}, \lambda) = -\frac{W(u)}{\epsilon \beta_{\mathrm{e}}} \left(1 + \frac{\lambda}{\epsilon} \frac{\partial}{\partial \lambda} \ln Z_u(u, \lambda) \right)^{-1}. \tag{3.7}$$

(In the sequel we frequently have to transform partial derivatives as above. More complicated examples are presented in more detail in Append. C). Furthermore the partial derivative of $\ln \mathcal{Z}_{\mathrm{R}}$ with respect to n_{R} in the last line of equation (3.5) can be replaced by a partial derivative of $\ln \mathcal{Z}_{\mathrm{R}}$ with respect to u by means of the RG equation for $\mathcal{Z}_{\mathrm{R}}$ (Eq. (A.8)), which results from taking the logarithmic derivative $\mathrm{d}/\mathrm{d} \ln l_{\mathrm{R}}$ of equation (2.7), keeping all bare parameters fixed. After some algebra we arrive at our final expression for the mean number of contacts:

$$\sigma(n) = an + c - bH(u). \tag{3.8}$$

The scaling function $H(u)$ which contains the universal part of the observable $\sigma(n)$ is found as

$$H(u) = \gamma(u) - 1 - \nu(u) W(u) \frac{\partial}{\partial u} \ln \mathcal{Z}_{\mathrm{R}}(u, n_{\mathrm{R}}) \tag{3.9}$$

where

$$\gamma(u) := \nu(u)(2 - \eta(u)). \tag{3.10}$$

At the fixed point equation (3.10) reduces to a well known scaling relation. The whole dependence of $\sigma(n)$ on microstructure is included in the three nonuniversal constants a, b, and c which can be written as

$$a = -\frac{\mathrm{d}}{\mathrm{d}\beta_{\mathrm{e}}} \mu_{\mathrm{s}}^*(\beta_{\mathrm{e}}) \tag{3.11}$$

$$b = \frac{2}{\epsilon \beta_{\mathrm{e}}} \left\{ 1 - \beta_{\mathrm{e}} \frac{\partial}{\partial \beta_{\mathrm{e}}} \bigg|_u \ln(Z_u Z_n^{\epsilon/2}) \right\} \tag{3.12}$$

$$c = -\frac{\partial}{\partial \beta_{\mathrm{e}}} \bigg|_u \ln(Z/Z_n). \tag{3.13}$$

All the three constants are functions of β_{e} only. This is obvious for a. Regarding b and c it can easily be proved by an integration of equations (2.8, 2.10, 2.11) which for all the renormalization factors yields the general structure

$$Z_a(u, \lambda) = Z_a(u(1), 1) \frac{h_a(u)}{h_a(u(1))}, \tag{3.14}$$

where the precise form of the functions $h_a(u)$ depends on the right hand side of equations (2.8, 2.10, 2.11). The derivatives in equations (3.12, 3.13) act only on the dependence on the starting point of integration, $u(1)$, which depends only on β_{e} (*cf.* Eq. (2.4)).

The interpretation of our result (Eq. (3.8)) is as follows: the "extensive" term an that arises from the additive renormalization has its origin in contacts between segments which are spaced closely along the chain, such contacts beeing the origin of $\mu_{\mathrm{s}}^*(\beta_{\mathrm{e}})$. Together with the constant c which might be interpreted as an endeffect it yields that contribution to the mean number of contacts that is due to chain connectedness. This part is ignored in the estimate equation (3.2). All the contribution of contacts between widely seperated segments should be described by the scaling function $H(u)$. We first discuss the behaviour close to the fixed points. Inserting the general results of Section 2 for the flow of the coupling we obtain with $\gamma := \gamma(u^*)$:

$$H(u(\tilde{z})) = \begin{cases} \text{const.}\, n^{\epsilon/2} & \text{for } u \simeq 0 \\ \gamma - 1 + \text{const.}\, n^{-\nu\omega} & \text{for } u \simeq u^*. \end{cases} \tag{3.15}$$

Thus the naive estimate equation (3.2) is correct at the Gaussian fixed point. However, for nonvanishing repulsion the mean number of contacts of segments spaced far along the chain tends to zero (if we absorb $\gamma - 1$ into the constant c) instead of diverging [1]. Formally the vanishing contribution $\sim n^{-\nu\omega} \sim (u - u^*)$ is nothing else than the usual "corrections to scaling". Physically the segments arrange such that the mean number of intersections after a subtraction of the extensive part an stays finite in the limit $n \to \infty$. We should note that the asymptotic behaviour of the mean number of contacts at $u = u^*$, $\sigma(n) = \tilde{a}n + \tilde{c} + \mathcal{O}(n^{-\nu\omega})$, has been derived with field theoretic methods some time ago [2,3].

Des Cloizeaux in later work tries to calculate $\sigma(n)$ by direct summation of equation (3.3). Using an asymptotic formula for the intersection probability of two segments

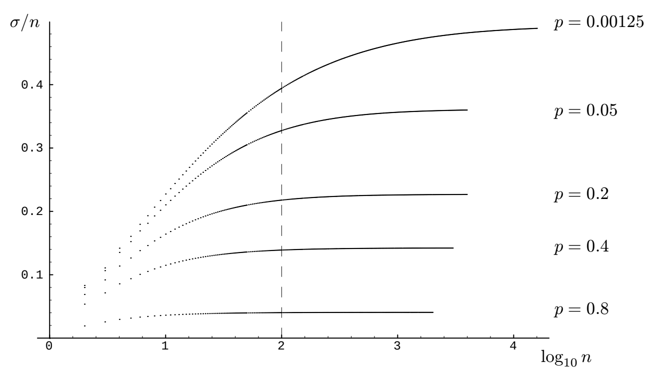


Fig. 3. Monte-Carlo results for σ in the Domb-Joyce model. On the right of the dashed line we expect universality.

well inside the chain he finds at the nontrivial fixed point [9,10]:

$$\sum_{0\le i<j\le n} \left\langle \delta^{\mathrm{d}}(\mathbf{r}_j-\mathbf{r}_i)\right\rangle \sim \bar{a}n + \bar{c} + \mathcal{O}(n^{2-\nu(d+\Theta_2)}). \quad (3.16)$$

Thus the leading behaviour in the critical limit of long chains, $\sigma(n) \approx \bar{a}n + \bar{c}$, is recovered but the correction exponent $2 - \nu(d + \Theta_2) \approx -0.18$ in $d = 3$ differs from the correct value $-\nu\omega \approx -0.47$. This is related to the dependence of the intersection probability on the positions of the segments along the chain, as will be further discussed at the end of Section 4.2.1.

Leaving the fixed point regime we now evaluate the crossover from Θ- to excluded volume-conditions. In Figures 2a, 2b we show the one loop result for the universal scaling function $H(u(\tilde{z}))$ (*cf.* Eqs. (3.9, 3.10, A.9))

$$H(u) = \gamma(u) - 1 - 0.456\nu(u)W(u), \quad (3.17)$$

where $u = u(\tilde{z})$ as in Figure 1. The surprising similarity between Figures 1 and 2 is easily understood: for the renormalized chain with $n_{\mathrm{R}} = \mathcal{O}(1)$ we should expect the Flory-type argument to be valid. Thus the interaction energy can be estimated as $E_{\mathrm{I}} \sim u n_{\mathrm{R}}^2 (l_{\mathrm{R}}/R_{\mathrm{g}})^3 \sim u$, where $R_{\mathrm{g}}^2 \sim n_{\mathrm{R}} l_{\mathrm{R}}^2$. Comparing to $E_{\mathrm{I}} \sim H(u(\tilde{z}))$ we find $H(u) \sim u$.

3.2 Comparison with Monte-Carlo data

A convenient model to examine the universal properties of self-repelling (not just self-avoiding) walks in computer simulations is provided by the Domb-Joyce model [11]. In this model every random walk configuration on the lattice is weighted by $(1-p)^{\sigma}$, where σ stands for the number of contacts in this configuration. An m-body contact is counted as $\frac{m(m-1)}{2}$ interacting pairs. The parameter p with $0 \le p \le 1$ serves as a measure of the strength of self-repulsion. The model interpolates among a random walk ($p = 0$) and a self-avoiding walk ($p = 1$).

An extensive Monte-Carlo simulation of chains in the Domb-Joyce model on a simple cubic lattice has been carried through by Grassberger (see [12] for a detailed description of the method). Selected results for the mean number of contacts are shown in Figure 3, covering a range of repulsion strength from $p = 0.8$ to $p = 1.25 \times 10^{-3}$ and chain lengths up to $n \approx 15\,000$.

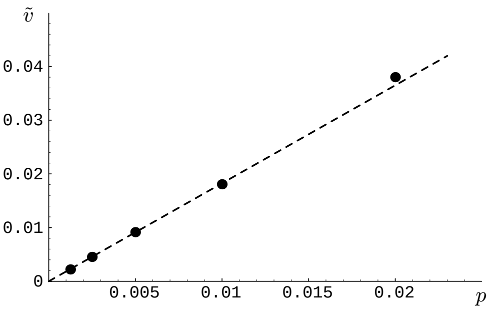


Fig. 4. The nonuniversal parameter $\tilde{v}$ in the Domb-Joyce model [12].

To compare these results with our theory we first of all note that universal behavior is to be expected only for sufficiently long chains, say $n \gtrsim 100$. Moreover the nontrivial part of our theoretical result is given by the scaling function $H(u)$, which is only a correction to the leading proportionality $\sigma(n) \sim n$. A short glance at Figure 3 reveals that for large self-repulsion the mean number of contacts for long chains is completely dominated by the leading term an, in full agreement with equation (1.2). In the following we therefore restrict ourselves to the data for $p \le 0.02$.

Fitting the Monte-Carlo results to equation (3.8) we in principle have four free parameters for each value of p, *viz.* a,b,c, and $\tilde{v}$. However the coupling $\tilde{v}$ has been independently determined by fitting Monte-Carlo data for the end-to-end distance to the one loop approximation of our theory [12]. The relevant results are shown in Figure 4. A linear regression through the three smallest values yields in the limit of vanishing self-repulsion

$$\tilde{v} = 1.82\,p \qquad \text{for} \quad p \ll 1. \quad (3.18)$$

In view of the rescaling $z = 0.15\tilde{z}$ according to [13] equation (3.18) lies well within the range of previous work [14], which uses the variable $z = (3/2\pi)^{3/2}\,p\,n^{1/2}$, resulting in $\tilde{v} = 2.20\,p$.

Having fixed $\tilde{v}$ we perform a least square fit to the Monte-Carlo data in the range $n \ge 100$. The resulting curves for the smallest resp. the largest value of p we considered are shown in Figure 5. The agreement for the other values of p is of the same quality. Remarkable is the likewise good fit even in the supposed nonuniversal range $n < 100$. Recall that the data with $n < 100$ has not been taken into account in the fit procedure.

The results for the fit parameters, *i.e.* the nonuniversal constants a, b, and c, are shown in Figures 6 and 7. Nonuniversal constants can not be calculated reliably by perturbative methods. Clearly on a microscopic level our "spring and bead model" has little to do with the Domb-Joyce model. We note however that according to the basic assumptions of the method the initial values used in integrating the flow equations should be analytic functions of

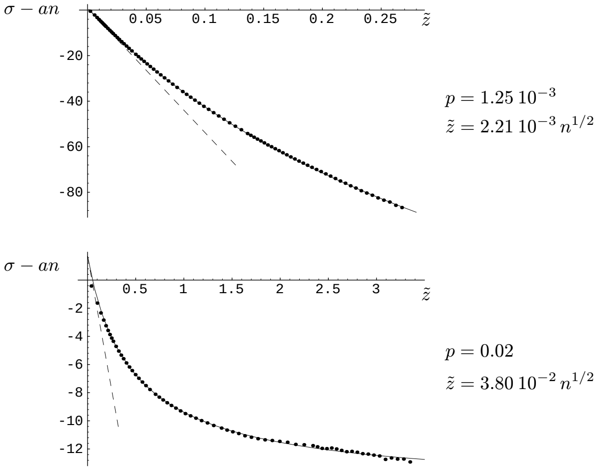


Fig. 5. Monte-Carlo results and corresponding fits obtained with equation (3.8). Dashed: random walk (Eq. (1.1)).

β_e. Since in turn $\beta_e \sim p$, $p \ll 1$, we for instance conclude from equation (3.12) for small self-repulsion: $b \sim 1/p$. This proportionality is obviously confirmed by Figure 6. A linear fit through the three smallest points yields

$$1/b = 0.53\,p \qquad \text{for} \quad p \ll 1. \tag{3.19}$$

We further may compare our results with exact expressions in the case of a random walk ($p = 0$). In analogy to equation (3.3) we have for the mean number of intersections in a random walk on a simple cubic lattice ($\mathbf{r}_k \in \mathbb{Z}^d$)

$$\sigma^{\mathrm{RW}}(n) = \sum_{0 \le i < j \le n} \left\langle \delta_{\mathbf{r}_j \mathbf{r}_i} \right\rangle \tag{3.20}$$

$$= n \sum_{k=1}^{n} P_k(0) + \sum_{k=1}^{n} P_k(0) - \sum_{k=1}^{n} k P_k(0). \tag{3.21}$$

Here $P_k(0) = \langle \delta_{\mathbf{r}_k \mathbf{r}_0} \rangle$ denotes the probability that the random walk returns to its starting point after k steps (note that $P_k(0) = 0$ if k is odd). By means of an asymptotic expansion for $P_{2k}(0)$ in $d = 3$ as given in [15],

$$P_{2k}(0) = 2\left(\frac{3}{2\pi}\right)^{3/2} (2k)^{-3/2} \left[1 - \frac{3}{8}k^{-1} + \frac{13}{128}k^{-2} + \mathcal{O}(k^{-3})\right], \tag{3.22}$$

we find

$$\begin{aligned} \sigma^{\mathrm{RW}}(n) = {} & n(P(1)-1) + P(1) - 1 - \hat{c} \\ & - \left(\frac{3}{2\pi}\right)^{3/2} \Bigg\{ (n+1)\left[2\hat{n}^{-1/2} + \frac{1}{2}\hat{n}^{-3/2} - \frac{7}{80}\hat{n}^{-5/2}\right] \\ & + 2\,\hat{n}^{1/2} + \frac{1}{2}\hat{n}^{-1/2} + \frac{5}{16}\hat{n}^{-3/2} \Bigg\} + \mathcal{O}(n^{-5/2}). \end{aligned} \tag{3.23}$$

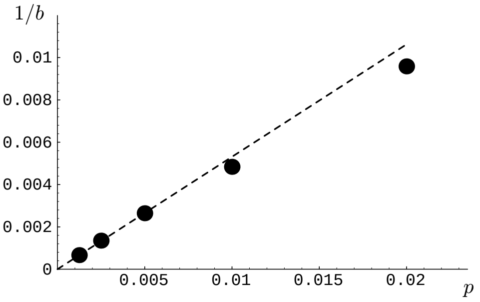


Fig. 6. The nonuniversal constant $1/b$.

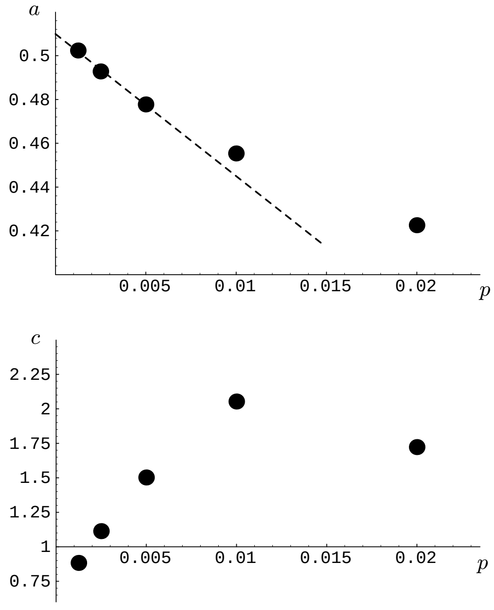


Fig. 7. The nonuniversal constants a and c.

Here

$$\hat{n} = \begin{cases} n+2 \text{ if } n \text{ even} \\ n+1 \text{ if } n \text{ odd} \end{cases} \tag{3.24}$$

represents odd-even effects and

$$P(1) = \sum_{k=0}^{\infty} P_k(0) \tag{3.25}$$

$$\hat{c} = \lim_{n \to \infty} \left[\sum_{k=1}^{n} k P_k(0) - 2\left(\frac{3}{2\pi}\right)^{3/2} n^{1/2} \right]. \tag{3.26}$$

$P(1)$ is known exactly [16],

$$P(1) = \left(\frac{12}{\pi^2}\right)\left(18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6}\right)\left[K\left(k_-\right)\right]^2 \approx 1.516, \tag{3.27}$$

where $k_- = (2 - \sqrt{3})(\sqrt{3} - \sqrt{2})$ and $K(k)$ stands for the complete elliptic integral of the first kind. $\hat{c}$ may be calculated using the approximation (3.22),

$$\hat{c} \approx 2^{-1/2}\left(\frac{3}{2\pi}\right)^{3/2}\left[2\zeta(\frac{1}{2})-\frac{3}{4}\zeta(\frac{3}{2})+\frac{13}{64}\zeta(\frac{5}{2})\right] \approx -1.075. \tag{3.28}$$

Then in the limit of long chains we extract from equation (3.23) the asymptotic behavior

$$\sigma^{\mathrm{RW}}(n) = a_{\mathrm{RW}}n - b_{\mathrm{RW}}n^{1/2} + c_{\mathrm{RW}}, \tag{3.29}$$

with

$$a_{\mathrm{RW}} = P(1) - 1 \approx 0.516 \tag{3.30}$$

$$b_{\mathrm{RW}} = 4\left(\frac{3}{2\pi}\right)^{3/2} \approx 1.320 \tag{3.31}$$

$$c_{\mathrm{RW}} = P(1) - 1 - \hat{c} \approx 1.591. \tag{3.32}$$

As can be seen in Figure 8 the approximate formula (Eq. (3.23)) is excellent even for small values of the number of steps n. The solid curve shown there interpolates smoothly among the discrete values calculated with equation (3.23), whereas the points represent the exact values of $\sigma^{\mathrm{RW}}(n)$. The latter are calculated with equation (3.21) by making use of the exact values for $P_k(0)$ as cited in [15]. The dashed curve given by equation (3.29) obviously serves as a good approximation only for larger values of n.

These results concerning the random walk will now be compared with those obtained from the Monte-Carlo calculations, extrapolated to $p = 0$. The value for $a(0)$ can be read from a linear regression through the smallest three values plotted in Figure 7. With regard to b we however first have to analyze equation (3.8) in the Gaussian limit $\tilde{z} \to 0$. Defining $b_{\mathrm{G}}(0)$, which corresponds to b_{RW}, by

$$bH(u(\tilde{z})) \overset{\tilde{z}\to 0}{\longrightarrow} b_{\mathrm{G}}(0)n^{1/2}, \tag{3.33}$$

we obtain

$$b_{\mathrm{G}}(0) = u^* b\tilde{v}. \tag{3.34}$$

Inserting equations (2.16, 3.18, 3.19) we therefore find $b_{\mathrm{G}}(0) \approx 1.25$. Concerning c we note that it only yields a correction of $\mathcal{O}(10^{-2}) - \mathcal{O}(10^{-4})$ to the leading terms. Thus its value cannot be extracted from Figure 7 with high precision. Collecting all values we have in comparison with equations (3.30) to (3.32)

$$a(0) \approx 0.51 \tag{3.35}$$

$$b_{\mathrm{G}}(0) \approx 1.25 \tag{3.36}$$

$$c(0) \approx \mathcal{O}(1). \tag{3.37}$$

These results for the nonuniversal parameters in the limit of vanishing repulsion agree reasonably well with equations (3.30) to (3.32).

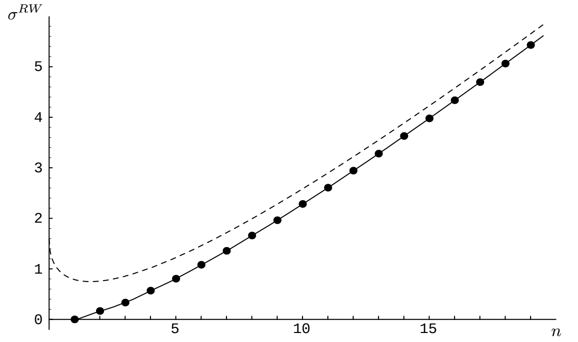


Fig. 8. Exact values for $\sigma^{\mathrm{RW}}(n)$ plotted with approximations according to equation (3.23) (solid curve) resp. equation (3.29) (dashed curve).

4 Mean number of contacts between two mutually repelling chains

As discussed above the number of intersections within a single chain is dominated by nonuniversal short range effects. To suppress these contributions we have to consider the intersections of two separate chains occupying the same volume. The latter constraint most easily is incorporated by fixing the distance R among a pair of chain ends. For general $R/R_{\mathrm{g}} > 0$ the number of intersections then is given by a scaling function analogous to the subleading contribution $H(u)$ discussed in the previous section. For $R \to 0$ we actually count the intersections of the two parts of a copolymer and we recover the nonuniversal constant contribution $\sim c$.

To carry through that program we use the standard extension of the model to a "ternary" system [17,18]. The two polymers ($a = 1, 2$) interact *via* three couplings $\beta_{ab} = \beta_{ba}; a, b = 1, 2$; representing the intrachain ($a = b$) resp. interchain ($a \neq b$) repulsion. The Hamiltonian is given as

$$\mathcal{H}_{12} = \sum_{a=1}^{2}\frac{1}{4l^2}\sum_{j=1}^{n_a}\left(\mathbf{r}_j^{(a)} - \mathbf{r}_{j-1}^{(a)}\right)^2 + \mathcal{H}_I, \tag{4.1}$$

where

$$\mathrm{e}^{-\mathcal{H}_I} = \prod{}' \left[1 - (4\pi l^2)^{d/2}\beta_{ab}\delta^{\mathrm{d}}(\mathbf{r}_i^{(a)} - \mathbf{r}_j^{(b)})\right]. \tag{4.2}$$

The product extends over all different pairs of segments, subject to the same restriction as in equation (2.1). Note that with an appropriate choice of β_{ab} we describe the interaction between two Gaussian ($\beta_{11} = \beta_{22} = 0$) or self-repelling ($\beta_{11} > 0, \beta_{22} > 0$) chains as well as the case of one Gaussian and one self-repelling chain.

Renormalizing this model we note that the "binary" parameters n_a, l, β_{aa} renormalize in the same way as in the single chain case, *cf.* equations (2.4, 2.5). Only the mixed coupling β_{12} requires a new renormalization factor $Z_u^{(12)}$:

$$\beta_{12} = \lambda^{\epsilon}u_{12}Z_u^{(12)}(u_{12}, u_{11}, u_{22}, \lambda). \tag{4.3}$$

Table 1. The eight ternary fixed points [19].

Fixed point	u_{11}	u_{22}	u_{12}	Fixed point	u_{11}	u_{22}	u_{12}
G_0	0	0	0	G	0	0	$u^*_{12}(\mathrm{G})$
U_0	u^*	0	0	U	u^*	0	$u^*_{12}(\mathrm{U})$
U_0'	0	u^*	0	U’	0	u^*	
S_0	u^*	u^*	0	S	u^*	u^*	u^*

Table 2. Fixed point values of the mixed coupling [18].

	ϵ-expansion	$d = 3$, resummed
$f^*_{12}(\mathrm{G})$	$2\left(1 - \frac{5}{32}\epsilon + \mathcal{O}(\epsilon^2)\right)$	1.867
$f^*_{12}(\mathrm{U})$	$\frac{3}{2}\left(1 - \frac{1}{48}\epsilon + \mathcal{O}(\epsilon^2)\right)$	1.449
$f^*_{12}(\mathrm{S})$	1	1

The corresponding Wilson function

$$W_{12}(u_{12}, u_{11}, u_{22}) := \lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} u_{12} \tag{4.4}$$

depends on all the three couplings, which gives rise to a rich flow diagram [19]. The eight fixed points G_0, U_0, U_0', S_0; G, U, U$'$, S of the flow are listed in Table 1. The fixed point values of the normalized mixed coupling

$$f_{12} := \frac{u_{12}}{u^*} \tag{4.5}$$

can be found in Table 2.

The constrained partition function of a two chain system with fixed mutual end-to-end distance R is defined as

$$\mathcal{Z}^{(12)}(R) = \Omega \int_\Omega \mathcal{D}[\mathbf{r}^{(1)}]\mathcal{D}[\mathbf{r}^{(2)}]\delta^{\mathrm{d}}(\mathbf{r}_0^{(2)} - \mathbf{r}_0^{(1)} - \mathbf{R})\, \mathrm{e}^{-\mathcal{H}_{12}}. \tag{4.6}$$

If the chains do not interact with each other, the two chain partition function factorizes. This is the case for vanishing mixed coupling,

$$\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} \equiv 1 \qquad \text{for} \quad \beta_{12} = 0, \tag{4.7}$$

as well as for infinite distance

$$\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} \overset{R\to\infty}{\longrightarrow} 1. \tag{4.8}$$

Here $\mathcal{Z}^{(1)}, \mathcal{Z}^{(2)}$ denote the partition functions of the isolated chains.

The limiting behaviour (Eq. (4.8)) also must hold for the renormalized partition function. Thus $\mathcal{Z}^{(12)}(R)/\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}$ for $R/R_{\mathrm{g}} > 0$ is renormalized with no explicit multiplicative Z-factor

$$\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} = \left(\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}}\right)_{\mathrm{R}}, \tag{4.9}$$

and renormalization simply amounts to replacing the bare parameters by their renormalized counterparts (*via* Eqs. (2.4, 2.5, 4.3), *cf.* Append. B.2). However, in the limit $R \to 0$ we obtain the partition function of a copolymer,

$$\mathcal{Z}_{\mathrm{co}} := \mathcal{Z}^{(12)}(0), \tag{4.10}$$

which shows new singularities. These have to be absorbed into a new renormalization factor $Z_2^{(12)}(u_{12}, u_{11}, u_{22}, \lambda)$:

$$\frac{\mathcal{Z}_{\mathrm{co}}}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} = \left[Z_2^{(12)}\right]^{-1} \frac{\mathcal{Z}_{\mathrm{co,R}}}{\mathcal{Z}_{\mathrm{R}}^{(1)}\mathcal{Z}_{\mathrm{R}}^{(2)}} \cdot \tag{4.11}$$

Turning now to the mean number of contacts between the two chains we in complete analogy with equation (3.4) find

$$\sigma_2(R) = -\frac{\partial}{\partial\beta_{12}} \ln \mathcal{Z}^{(12)}(R). \tag{4.12}$$

In taking the partitial derivative with respect β_{12} one has to keep all the other bare parameters $\{n_1, n_2, \beta_{11}, \beta_{22}, l\}$ as well as R fixed.

For a renormalized formulation we as before keep l_{R} fixed. All dependence on β_{12} is contained in u_{12} only. For convenience we normalize $\mathcal{Z}^{(12)}(R)$ with the partition functions $\mathcal{Z}^{(a)}$ of the isolated chains, which are independent of β_{12}. We thus obtain

$$\sigma_2(R) = \left[\frac{\partial\beta_{12}}{\partial u_{12}}\right]^{-1} \left[-\frac{\partial}{\partial u_{12}} \ln\left(\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}}\right)_{\mathrm{R}}\right] \quad (R > 0), \tag{4.13}$$

or

$$\sigma_{\mathrm{co}} := \sigma_2(0) = \left[\frac{\partial\beta_{12}}{\partial u_{12}}\right]^{-1} \left\{-\frac{\partial}{\partial u_{12}} \ln\left[\left(Z_2^{(12)}\right)^{-1} \frac{\mathcal{Z}_{\mathrm{co,R}}}{\mathcal{Z}_{\mathrm{R}}^{(1)}\mathcal{Z}_{\mathrm{R}}^{(2)}}\right]\right\} \tag{4.14}$$

in the copolymer case. To proceed we now first analyze the partition functions, essentially recalling results of Witten and Prentis [20].

4.1 The partition function

4.1.1 The copolymer

To analyze the scaling behaviour of the normalized copolymer partition function (Eq. (4.11)) we use the flow equation for the renormalization factor $Z_2^{(12)}$,

$$\lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln Z_2^{(12)} =: \eta_2^{(12)}(u_{12}, u_{11}, u_{22}), \tag{4.15}$$

where

$$\eta_2^{(12)}(u_{12}, u_{11}, u_{22}) = -u_{12}\left[1 - \frac{1}{2}(u_{12} + u_{11} + u_{22}) + \mathcal{O}(u_{ab}^2)\right]. \tag{4.16}$$

Integrating equation (4.15) at a fixed point $P \in \{\mathrm{G}_0, \mathrm{U}_0, \mathrm{U}'_0, \mathrm{S}_0; \mathrm{G}, \mathrm{U}, \mathrm{U}', \mathrm{S}\}$ we obtain

$$Z_2^{(12)} \sim \lambda^{\eta_2^{(12)}(P)}. \tag{4.17}$$

Resummed values for $\eta_2^{(12)}(P)$, based on a higher order calculation, are given in Table 3. Note that for $u_{12} = 0$ we trivially have

$$\eta_2^{(12)}(\mathrm{G}_0) = \eta_2^{(12)}(\mathrm{U}_0) = \eta_2^{(12)}(\mathrm{S}_0) = 0, \tag{4.18}$$

where G_0 *etc.* identify the fixed points as given in Table 1. Note further that at S, the symmetric fixed point, $\mathcal{Z}_{\mathrm{co}}$ corresponds to the partition function of a single chain of length $n_1 + n_2$, which yields the scaling relation

$$\eta_2^{(12)}(\mathrm{S}) = \frac{1}{\nu}(1-\gamma). \tag{4.19}$$

Inserting equation (4.17) into equation (4.11) we have

$$\frac{\mathcal{Z}_{\mathrm{co}}}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} \sim \left(\frac{l}{l_{\mathrm{R}}}\right)^{-\eta_2^{(12)}(P)} \frac{\mathcal{Z}_{\mathrm{co,R}}}{\mathcal{Z}_{\mathrm{R}}^{(1)}\mathcal{Z}_{\mathrm{R}}^{(2)}}\,. \tag{4.20}$$

For problems concerning a single homopolymer (*cf.* Sect. 3) we now could choose $n_{\mathrm{R}} = \mathcal{O}(1)$ resulting in $l_{\mathrm{R}} \sim n_{\mathrm{R}}^{-1/2} R_{\mathrm{g}} \sim R_{\mathrm{g}}$ since in that case R_{g} is the only relevant length scale. In the copolymer case we however deal with two macroscopic lengths $R_{\mathrm{g}a}^2 \sim n_{a\mathrm{R}} l_{\mathrm{R}}^2$, $a = 1, 2$, the radii of gyration of the two blocks. l_{R} thus should be some symmetric mean of the two scales, which however is not easily identified *a priori*. Some hint can be taken from the ϵ-expansion. Equations (A.7, B.5) yield

$$\frac{\mathcal{Z}_{\mathrm{co,R}}}{\mathcal{Z}_{\mathrm{R}}^{(1)}\mathcal{Z}_{\mathrm{R}}^{(2)}} = 1 + \frac{\epsilon}{4} f_{12}^{*}(P)\left[\frac{1}{2}\ln\left(\frac{n_{1\mathrm{R}}+n_{2\mathrm{R}}}{n_{1\mathrm{R}}n_{2\mathrm{R}}}\right) - \frac{1}{2}\right] + \mathcal{O}(\epsilon^2). \tag{4.21}$$

With equation (4.16) this equivalently can be written as

$$\frac{\mathcal{Z}_{\mathrm{co,R}}}{\mathcal{Z}_{\mathrm{R}}^{(1)}\mathcal{Z}_{\mathrm{R}}^{(2)}} = \left(\frac{1}{n_{1\mathrm{R}}} + \frac{1}{n_{2\mathrm{R}}}\right)^{-\frac{1}{2}\eta_2^{(12)}(P)} \left\{1 - \frac{1}{8} f_{12}^{*}(P)\epsilon + \mathcal{O}(\epsilon^2)\right\}, \tag{4.22}$$

resulting in

$$\frac{\mathcal{Z}_{\mathrm{co}}}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} \sim \left[\frac{l^2}{R_{\mathrm{g}1}^2} + \frac{l^2}{R_{\mathrm{g}2}^2}\right]^{-\frac{1}{2}\eta_2^{(12)}(P)} \tag{4.23}$$

as scaling behaviour at the fixed point P. The smaller of the two radii of gyration determines the scaling. Equation (4.20) reproduces this result, provided we fix l_{R} by the condition $1/n_{1\mathrm{R}} + 1/n_{2\mathrm{R}} = \mathcal{O}(1)$.

From Table 3 we note the relation $-\eta_2^{(12)}(\mathrm{S}) < -\eta_2^{(12)}(\mathrm{U}) < -\eta_2^{(12)}(\mathrm{G})$, so that the normalized partition function $\mathcal{Z}_{\mathrm{co}}/\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}$ in the critical limit $n_a \to \infty$ decreases most rapidly at the fixed point G. This is easily understood: assuming true self-avoidance between the two copolymer blocks the normalized partiton function can be interpreted as the probability that the blocks do not intersect [22]. Now at the fixed point S we deal with intersections between two geometrical objects of Haussdorff dimension $d_{\mathrm{H}} = 1/\nu \approx 1.7$, at U we have one block with $d_{\mathrm{H}} = 1/\nu$, the other with $d_{\mathrm{H}} = 2$, whereas at G both are of dimension $d_{\mathrm{H}} = 2$. But the greater the Haussdorff dimension the more "compact" the geometrical objects is, *i.e.* the probability that the two blocks do not intersect is smallest at G. At U one block of the copolymer is more "diluted", the probability of non-intersection increases. Finally at S the normalized partition function $\mathcal{Z}_{\mathrm{co}}/\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}$ vanishes most slowly.

Table 3. The exponent $\eta_2^{(12)}(P)$ [21]. Note that $\eta_2^{(12)}(\mathrm{G})$ in ϵ-expansion can also be found in [22], called 2ζ there.

	ϵ-expansion	$d = 3$, resummed
$\eta_2^{(12)}(\mathrm{G})$	$-\frac{1}{2}\epsilon - \frac{1}{8}\epsilon^2 + \mathcal{O}(\epsilon^3)$	-0.56
$\eta_2^{(12)}(\mathrm{U})$	$-\frac{3}{8}\epsilon - \frac{31}{256}\epsilon^2 + \mathcal{O}(\epsilon^3)$	-0.43
$\eta_2^{(12)}(\mathrm{S})$	$-\frac{1}{4}\epsilon - \frac{9}{128}\epsilon^2 + \mathcal{O}(\epsilon^3)$	-0.27

4.1.2 Finite distance between the endpoints of the chains

For reasons of simplicity we in the following mostly restrict ourselves to the symmetric case $n_{1\mathrm{R}} = n_{2\mathrm{R}} =: n_{\mathrm{R}}$, $u_{11} = u_{22} =: u$. Equation (4.8) ensures that the normalized partition function is a universal scaling function which thus can depend on dimensionless ratios of macroscopic quantities only. Since here the only relevant length scales are R and $R_{\mathrm{g}} := R_{\mathrm{g}1} = R_{\mathrm{g}2}$ we have

$$\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} = \Phi\left(R/R_{\mathrm{g}}\right). \tag{4.24}$$

With the notation

$$x_{\mathrm{g}} := \sqrt{\frac{d}{12}}\,\frac{R}{R_{\mathrm{g}}}, \tag{4.25}$$

the tree approximation of $\mathcal{Z}^{(12)}(R)/\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}$ at the fixed point P yields in ϵ-expansion (*cf.* Eqs. (B.17, B.19))

$$\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} = 1 - \frac{\epsilon}{4} f_{12}^{*}(P)\left[\frac{1-\mathrm{e}^{-\frac{1}{2}x_{\mathrm{g}}^2}}{x_{\mathrm{g}}^2}\mathrm{e}^{-\frac{1}{2}x_{\mathrm{g}}^2} - Ei\left(-x_{\mathrm{g}}^2\right) + \frac{1}{2}Ei\left(-x_{\mathrm{g}}^2/2\right)\right] + \mathcal{O}(\epsilon^2). \tag{4.26}$$

$Ei(-z)$ denotes the Exponential-integral, which diverges logarithmically for $z \to 0$ [23]:

$$Ei(-z) = \ln z + \gamma_{\mathrm{Eu}} - \int_0^z \frac{1-\mathrm{e}^{-t}}{t}\,\mathrm{d}t. \tag{4.27}$$

Note that the tree approximation (Eq. (4.26)) corresponds to the one loop result (Eq. (B.5)) in the copolymer case since for the copolymer the external Fourier transformation in equation (B.6) converts into an internal loop integration.

While equation (4.26) for $R/R_{\rm g} \gg 1$ yields the correct behaviour $\mathcal{Z}^{(12)}(R) \to \mathcal{Z}^{(1)}\mathcal{Z}^{(2)}$ (Eq. (4.8)) we in the limit $R/R_{\rm g} \ll 1$ again have to exponentiate the logarithmic divergence. By simple scaling arguments (see *e.g.* [24]) we can predict the expected behaviour in that limit. On the one hand $\mathcal{Z}^{(12)}(R)$ for small R ($R = \mathcal{O}(l)$) should smoothly match the copolymer result, *i.e.*

$$\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} \overset{R/R_{\rm g}\to 0}{\approx} \left[Z_2^{(12)}\right]^{-1} \frac{\mathcal{Z}_{\rm co,R}}{\mathcal{Z}_{\rm R}^{(1)}\mathcal{Z}_{\rm R}^{(2)}} \sim \left(\frac{l}{R_{\rm g}}\right)^{-\eta_2^{(12)}(P)}. \tag{4.28}$$

On the other hand $\mathcal{Z}^{(12)}(R)/\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}$ is a function of $R/R_{\rm g}$ only (*cf.* Eq. (4.24)). Fulfilling both requirements we obtain

$$\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} \sim \left(\frac{R}{R_{\rm g}}\right)^{-\eta_2^{(12)}(P)} \qquad \text{for} \quad R \ll R_{\rm g}. \tag{4.29}$$

The more rigorous field theoretic argument which leads to the same result is based on a short-distance-expansion [7]. If we restrict this expansion to the leading term it implies the existence of a function $C(x)$, $x := R/l_{\rm R} \sim x_{\rm g}$, with

$$\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} \overset{R/l_{\rm R}\to 0}{=} C(x)\, \frac{\mathcal{Z}_{\rm co,R}}{\mathcal{Z}_{\rm R}^{(1)}\mathcal{Z}_{\rm R}^{(2)}}\,. \tag{4.30}$$

By taking the derivative $\lambda\, {\rm d}/{\rm d}\lambda$ we obtain, using equations (4.11) and (4.15),

$$\lambda \frac{\rm d}{{\rm d}\lambda} \ln C(x) = -\eta_2^{(12)}. \tag{4.31}$$

Integration of this equation at a fixed point confirms equation (4.29).

In the limit $x_{\rm g} \ll 1$ the appropriate form of equation (4.26) therefore reads

$$\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} = \left(2\,x_{\rm g}^2\right)^{-\frac{1}{2}\eta_2^{(12)}(P)} \Bigg\{1 - \frac{\epsilon}{4} f_{12}^*(P) \times \left[\frac{1-{\rm e}^{-\frac{1}{2}x_{\rm g}^2}}{x_{\rm g}^2}{\rm e}^{-\frac{1}{2}x_{\rm g}^2} - Ei\left(-x_{\rm g}^2\right) + \frac{1}{2}Ei\left(-x_{\rm g}^2/2\right) + \frac{1}{2}\ln\left(2x_{\rm g}^2\right)\right] + \mathcal{O}(\epsilon^2)\Bigg\}. \tag{4.32}$$

The asymptotic power law (Eq. (4.29)) takes the form

$$\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} = \hat{A}^{(12)}(P) {x_{\rm g}}^{-\eta_2^{(12)}(P)} \qquad \text{for} \quad l \ll R \ll R_{\rm g}, \tag{4.33}$$

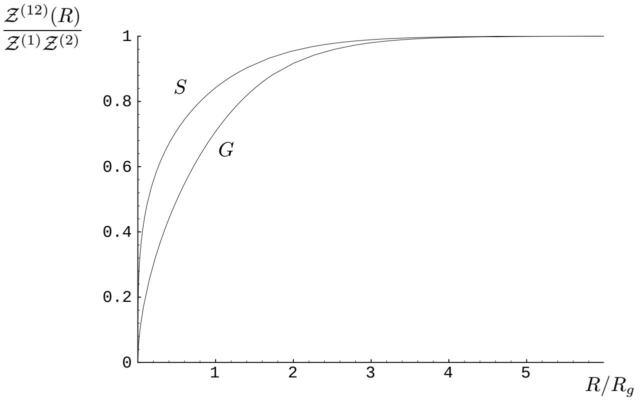


Fig. 9. The scaling function $\mathcal{Z}^{(12)}(R)/\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}$ at the fixed points G and S.

with the universal amplitude

$$\hat{A}^{(12)}(P) = 1 - \frac{1}{8} f_{12}^*(P)\,(1 - \gamma_{\rm Eu} - \ln 2)\,\epsilon + \mathcal{O}(\epsilon^2). \tag{4.34}$$

It should be mentioned that for the general case of $R_{\rm g1} \neq R_{\rm g2}$ a similar analysis of the tree term yields

$$\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} \sim \left(\frac{R^2}{R_{\rm g1}^2} + \frac{R^2}{R_{\rm g2}^2}\right)^{-\frac{1}{2}\eta_2^{(12)}(P)} \qquad \text{for} \quad R \ll \min\{R_{\rm g1}, R_{\rm g2}\}. \tag{4.35}$$

At the symmetric fixed point S this result is consistent with the scaling considerations of [20].

Since equations (4.26, 4.32) match smoothly in the intermediate regime $R/R_{\rm g} \approx \mathcal{O}(1)$ we thus have constructed a universal function (*cf.* Eq. (4.24)) in tree approximation for all values of $R/R_{\rm g}$. For $d = 3$ it is shown in Figure 9. Consistent with the discussion given at the end of Section 4.1.1 the scaling function at fixed point S for all R is larger than at fixed point G.

4.2 Mutual intersections

We now turn to the number of intersections as given by equation (4.13) or (4.14), respectively. The behaviour of $\partial\beta_{12}/\partial u_{12}$ in equations (4.13, 4.14) close to fixed point P is determined by a “correction to scaling exponent” $\omega_{12}(P)$ (*cf.* Tab. 4), defined as the fixed point value of

$$\omega_{12}(u_{12}, u_{11}, u_{22}) := \frac{\partial}{\partial u_{12}} W_{12}(u_{12}, u_{11}, u_{22}). \tag{4.36}$$

Indeed, a straightforward calculation yields (*cf.* Append. C)

$$\lambda \frac{\rm d}{{\rm d}\lambda} \ln \left[\frac{\partial \beta_{12}}{\partial u_{12}}\right]^{-1} = \omega_{12}(u_{12}, u_{11}, u_{22}), \tag{4.37}$$

Table 4. Mixed “correction to scaling exponent” $\omega_{12}(\mathrm{P})$ [19].

Fixed point	ω_{12} (P), $\epsilon-$ expansion	$\omega_{12}(P)$, $d=3$, resummed
G_0	$-\epsilon$	-1
U_0	$-\frac{3}{4}\epsilon+\frac{11}{128}\epsilon^2+\mathcal{O}(\epsilon^3)$	-0.70
S_0	$-\frac{1}{2}\epsilon+\frac{11}{64}\epsilon^2+\mathcal{O}(\epsilon^3)$	-0.40
G	$\epsilon-\frac{1}{2}\epsilon^2+\mathcal{O}(\epsilon^3)$	0.82
U	$\frac{3}{4}\epsilon-\frac{47}{128}\epsilon^2+\mathcal{O}(\epsilon^3)$	0.68
S	$\frac{1}{2}\epsilon-\frac{19}{64}\epsilon^2+\mathcal{O}(\epsilon^3)$	0.40

so that integration at a fixed point results in

$$\left[\frac{\partial\beta_{12}}{\partial u_{12}}\right]^{-1}\sim\lambda^{\omega_{12}(P)}. \tag{4.38}$$

More generally, if we keep only the binary couplings at their fixed point value, $u_{aa}\equiv u^*_{aa}\in\{0,u^*\}$, equation (4.37) can be written as

$$\lambda\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln\left[\frac{\partial\beta_{12}}{\partial u_{12}}\right]^{-1}=\frac{1}{W_{12}(u_{12},u^*_{11},u^*_{22})}\lambda\frac{\mathrm{d}}{\mathrm{d}\lambda}W_{12}(u_{12},u^*_{11},u^*_{22}). \tag{4.39}$$

Integrating this equation we obtain

$$\left[\frac{\partial\beta_{12}}{\partial u_{12}}\right]^{-1}\sim W_{12}(u_{12},u^*_{11},u^*_{22}). \tag{4.40}$$

For $u_{12}\to u^*_{12}(P)$ we of course recover equation (4.38) since

$$W_{12}(u_{12},u^*_{11},u^*_{22})\sim(u_{12}-u^*_{12}(P))\sim\lambda^{\omega_{12}(P)}. \tag{4.41}$$

In the further discussion the cases $R=0$ (copolymer) or $R/R_{\mathrm{g}}>0$ again have to be treated separately.

4.2.1 The copolymer

Turning to equation (4.14) we still need to discuss the derivative $\partial\ln Z_2^{(12)}/\partial u_{12}$. Setting $u_{aa}\equiv u^*_{aa}\in\{0,u^*\}$ from the outset we in Appendix C derive

$$\begin{aligned}\frac{\partial}{\partial u_{12}}\ln Z_2^{(12)}=[W_{12}(u_{12},u^*_{11},u^*_{22})]^{-1}\Bigg[&\tilde{c}^{(12)}\omega_{12}(P)\\&+\frac{1}{\omega_{12}(P)}\left(\frac{\partial}{\partial u_{12}}\eta_2^{(12)}\right)_P W_{12}(u_{12},u^*_{11},u^*_{22})\\&+\mathcal{O}\left(u_{12}-u^*_{12}(P)\right)^2\Bigg].\end{aligned} \tag{4.42}$$

Note that $W_{12}(u_{12},u^*_{11},u^*_{22})=\mathcal{O}(u_{12}-u^*_{12}(P))$ (Eq. (4.41)). The nonuniversal constant $\tilde{c}^{(12)}$ depends on the bare couplings β_{ab} only. Denoting the nonuniversal proportionality constants in equations (4.38) resp. (4.40) as $b^{(12)}$ resp. $\bar{b}^{(12)}$ we now can insert equations (4.42, 4.40) into equation (4.14). Neglecting terms of $\mathcal{O}(u_{12}-u^*_{12}(P))^2$ we find for the scaling function of the mean number of contacts between the two halves of a copolymer

$$\begin{aligned}\sigma_{\mathrm{co}}=c^{(12)}-b^{(12)}\lambda^{\omega_{12}(P)}\Bigg[&-\frac{1}{\omega_{12}(P)}\left(\frac{\partial}{\partial u_{12}}\eta_2^{(12)}\right)_P\\&+\left(\frac{\partial}{\partial u_{12}}\ln\frac{\mathcal{Z}_{\mathrm{co,R}}}{\mathcal{Z}^{(1)}_{\mathrm{R}}\mathcal{Z}^{(2)}_{\mathrm{R}}}\right)_P\Bigg].\end{aligned} \tag{4.43}$$

The two nonuniversal constants $b^{(12)}$ and $c^{(12)}:=\bar{b}^{(12)}\tilde{c}^{(12)}\omega_{12}(P)$ absorb the whole dependence of σ_{co} on microstructure.

For an interpretation of equation (4.43) we restrict ourselves to the case $R_{\mathrm{g}1}=R_{\mathrm{g}2}=:R_{\mathrm{g}}$. At the fixed points G_0, U_0, S_0, where the two parts of the copolymer do not mutually interact, the exponent $\omega_{12}(P)$ is negative. Choosing $\lambda\sim l/R_{\mathrm{g}}$ we thus find that the second contribution in equation (4.43) dominates for long chains:

$$\sigma_{\mathrm{co}}\sim\left(\frac{R_{\mathrm{g}}}{l}\right)^{-\omega_{12}(P)}\to\infty\qquad\text{for}\quad P\in\{\mathrm{G}_0,\mathrm{U}_0,\mathrm{S}_0\}. \tag{4.44}$$

This result can be read as the definition of the Hausdorff dimension of the set of intersection points of the two blocks. As pointed out in [19] this interpretation is consistent with the scaling relation

$$-\omega_{12}(P)=\frac{1}{\nu(u^*_{11})}+\frac{1}{\nu(u^*_{22})}-d, \tag{4.45}$$

where $\nu(u^*_{aa})\in(1/2,\nu)$, $a=1,2$, are the exponents governing the radii of the two halves. In [19] equation (4.45) has been proved by field theoretic techniques.

Turning now to those fixed points G, U, S, where the two halves do interact, we obtain a qualitatively different result. $\omega_{12}(P)$ is positive and we find the dominant behaviour

$$\sigma_{\mathrm{co}}\sim\text{const.}\qquad\text{for}\quad P\in\{\mathrm{G},\mathrm{U},\mathrm{S}\}. \tag{4.46}$$

Even in the limit of long chains the number of intersections stays finite and is dominated by segments close to the central link (*cf.* Sect. 4.2.2).

How are these results related to those for a single chain? Comparing equations (4.43, 3.8) we first of all note that for the copolymer the extensive term is absent. This was to be expected since that term counts intersections in small parts of the chain, summed along the chain. Again the constant contribution $c^{(12)}$ can be interpreted as a kind of end effect, this time due to intersections of parts of the copolymer close to the central link (*cf.* Sect. 4.2.2). Of special interest is a comparison of the contributions proportional to $b^{(12)}$ (Eq. (4.43)) or b (Eq. (3.8)). Consider first the Gaussian fixed point $u=0$ which for the copolymer corresponds to G_0. Here we find

$$-\epsilon=\omega_{12}(\mathrm{G}_0), \tag{4.47}$$

so that these contributions scale in the same way. At the nontrivial fixed point which corresponds to fixed point S for the copolymer, we however find different exponents:

$$\omega_{12}(\mathrm{S}) < \omega. \tag{4.48}$$

This difference clearly exhibits some subtleties of the excluded volume problem. As pointed out repeatedly these contributions are due to intersections of segments spaced a large distance along the chain. Being on different halves these segments for the copolymer case generically are deep inside the chain. In the single chain case, however, the two segments though being at distance $|j-i| \gg 1$ in chain coordinate space, still both on scale of the total chain length n can be close to the same chain end. Now it is known that the spatial correlations among segments i, j depend on the position of the interval (i, j) along the chain. Averaging the position of (i, j) along the chain we for the single chain problem find a different subleading exponent than for the copolymer problem, where the central link restricts the shifting of the interval.

These considerations explain the failure of the calculation of [9], mentioned at the end of Section 3.1. The exponent Θ_2 introduced there governs the short distance behaviour of the correlations of two segments deep inside the chain. Equation (3.16) therefore ignores end effects. Indeed, exploiting the relation between the contact exponent Θ_2 and star exponents η_F of star polymers with F legs [25,26], $\Theta_2 = 2\eta_2 - \eta_4$, where η_2 obeys the well known scaling relation $\eta_2 = 1/\nu - 2 + \eta$ and η_4 is connected with $\omega_{12}(\mathrm{S})$ *via* [19] $\eta_4 = 2\eta - \epsilon - \omega_{12}(\mathrm{S})$, we find the scaling relation

$$\nu(d + \Theta_2) - 2 = \nu\omega_{12}(\mathrm{S}). \tag{4.49}$$

The subleading correction in equation (3.16) thus corresponds to the *copolymer* case (Eq. (4.43)).

4.2.2 Finite distance between the endpoints of the chains

For $R \gtrsim R_\mathrm{g}$ we immediately find from equations (4.13, 4.26, 4.38) the tree approximation for the symmetric case,

$$\sigma_2(R) \sim \lambda^{\omega_{12}(P)} \left[\frac{1 - \mathrm{e}^{-\frac{1}{2}x_\mathrm{g}^2}}{x_\mathrm{g}^2} \mathrm{e}^{-\frac{1}{2}x_\mathrm{g}^2} - Ei(-x_\mathrm{g}^2) + \frac{1}{2} Ei(-x_\mathrm{g}^2/2) \right], \tag{4.50}$$

where $\lambda \sim l/R_\mathrm{g}$, as before. In the limit $R \gg R_\mathrm{g}$ equation (4.50) of course yields $\sigma_2(R) \to 0$. Regarding the prefactor $\lambda^{\omega_{12}(P)}$ we just can copy the results of Section 4.2.1.

More interesting is the case $R \ll R_\mathrm{g}$. On the one hand we always reach this limit if we look at long chains $R_\mathrm{g} \to \infty$ for finite fixed distance R, on the other hand we expect this limit to be connected with the copolymer case (*cf.* Eq. (4.30)). Due to the logarithmic singularities equation (4.50) can not directly be used to handle the limit $R \ll R_\mathrm{g}$. Instead we exploit the short distance expansion (Eq. (4.30)). Replacing *via* equation (4.11) $\mathcal{Z}_{\mathrm{co,R}}/\mathcal{Z}_\mathrm{R}^{(1)}\mathcal{Z}_\mathrm{R}^{(2)}$ in equation (4.30) by the corresponding unrenormalized quantities we obtain

$$\begin{aligned} 0 =& \lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} \left[\frac{\partial}{\partial \beta_{12}} \ln \frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} \right] \\ =& \left[\frac{\partial}{\partial u_{12}} \ln \left(Z_2^{(12)} C(x) \right) \right] \lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} \left[\frac{\partial u_{12}}{\partial \beta_{12}} \right] \\ &+ \left[\frac{\partial u_{12}}{\partial \beta_{12}} \right] \lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} \left[\frac{\partial}{\partial u_{12}} \ln \left(Z_2^{(12)} C(x) \right) \right]. \end{aligned} \tag{4.51}$$

With equations (4.37, C.6) we can eliminate the derivatives of $Z_2^{(12)}$ to find:

$$\lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} \left[\frac{\partial}{\partial u_{12}} \ln C(x) \right] = -\frac{\partial}{\partial u_{12}} \eta_2^{(12)} - \omega_{12} \left[\frac{\partial}{\partial u_{12}} \ln C(x) \right] \cdot \tag{4.52}$$

Being interested in the fixed point behaviour we set $\{u_{ab}(\lambda) \equiv u_{ab}^*\}$, so that $\lambda\mathrm{d}/\mathrm{d}\lambda \equiv x\mathrm{d}/\mathrm{d}x$. Then integration of equation (4.52) yields

$$-\frac{\partial}{\partial u_{12}} \ln C(x) = \bar{A}^{(12)}(P) x^{-\omega_{12}(P)} + \frac{1}{\omega_{12}(P)} \left(\frac{\partial}{\partial u_{12}} \eta_2^{(12)} \right)_P, \tag{4.53}$$

where $\bar{A}^{(12)}(P)$ is a universal amplitude. Inserting equations (4.9, 4.30, 4.53) into equation (4.13) we obtain, using equation (4.38) and defining a nonuniversal constant $\bar{c}^{(12)} := b^{(12)} \bar{A}^{(12)}(P)$, the final result

$$\begin{aligned} \sigma_2(R) =& \bar{c}^{(12)} \left(\frac{l}{R} \right)^{\omega_{12}(P)} - b^{(12)} \lambda^{\omega_{12}(P)} \\ & \times \left[-\frac{1}{\omega_{12}(P)} \left(\frac{\partial}{\partial u_{12}} \eta_2^{(12)} \right)_P + \left(\frac{\partial}{\partial u_{12}} \ln \frac{\mathcal{Z}_{\mathrm{co,R}}}{\mathcal{Z}_\mathrm{R}^{(1)} \mathcal{Z}_\mathrm{R}^{(2)}} \right)_P \right]. \end{aligned} \tag{4.54}$$

How do we have to interpret this result? Comparing equation (4.54) first with the copolymer result (Eq. (4.43)) we notice that the contributions $\sim \lambda^{\omega_{12}(P)} \sim (l/R_\mathrm{g})^{\omega_{12}(P)}$ in both cases are identical. This is very reasonable since for segments widely spaced along the chains it should not matter how large the distance $R \ll R_\mathrm{g}$ exactly is. Also the dependence on R in the first summand in equation (4.54) is easily understood. While at the fixed points G_0, U_0, S_0 this term in comparison with the diverging contribution $\sim \lambda^{\omega_{12}(P)}$ can be neglected, we at the other three fixed points find

$$\sigma_2(R) = \bar{c}^{(12)} \left(\frac{l}{R} \right)^{\omega_{12}(P)} \quad \text{for } R, l \ll R_\mathrm{g} \text{ and } P \in \{\mathrm{G}, \mathrm{U}, \mathrm{S}\}. \tag{4.55}$$

For macroscopic $R \gg l$ the mean number of intersections thus vanishes in the critical limit. Only if the distance between the chain ends becomes microscopic itself, $R \gtrsim l$, we find that $\sigma_2(R)$ for $R_{\rm g} \gg l$ yields a finite (nonuniversal) value. This confirms the interpretation of the constant $c^{(12)}$ in equation (4.43) as based on intersections between segments near the link.

Finally we confirm these general results with explicit perturbative results up to the order of one loop from Appendix B.2. We find from equation (B.17), where $f := f_{11} \equiv f_{22}$ and $f_{aa} := u_{aa}/u^*$ as in equation (4.5):

$$\begin{aligned}\left[-\frac{\partial}{\partial u_{12}} \ln \frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}}\right] = \hat{T}(x_{\rm g}) + \epsilon \Big[& \hat{L}_0(x_{\rm g}) + f\hat{L}_1(x_{\rm g}) \\ & + f_{12}\left(2\hat{L}_2(x_{\rm g}) + \frac{1}{4}\hat{T}(x_{\rm g})^2\right) \\ & + \frac{1}{2}\ln n_{\rm R}\left(1 - \frac{1}{2}f - f_{12}\right)\hat{T}(x_{\rm g})\Big] \\ & + \mathcal{O}(\epsilon^2). \qquad (4.56)\end{aligned}$$

Inserting equations (4.38, 4.56) into equation (4.13) (note Eq. (4.9)), we note that since $\omega_{12}(P) = -\epsilon[1 - 1/2f^* - f^*_{12}(P)] + \mathcal{O}(\epsilon^2)$ the term $\sim \ln n_{\rm R}$ in equation (4.56) can be reexponentiated to replace $l_{\rm R}^2$ in equation (4.38) by $R_{\rm g}^2 = d/3n_{\rm R}l_{\rm R}^2(1 + \mathcal{O}(\epsilon))$ (*cf.* Eq. (B.15)). We thus obtain

$$\begin{aligned}\sigma_2(R) = \; & b^{(12)}\left(\frac{{\rm d}l^2}{3R_{\rm g}^2}\right)^{\omega_{12}(P)/2} \\ & \times \Big\{\hat{T}(x_{\rm g}) + \epsilon\Big[\hat{L}_0(x_{\rm g}) + f^*\hat{L}_1(x_{\rm g}) \\ & + \; f^*_{12}(P)\left(2\hat{L}_2(x_{\rm g}) + \frac{1}{4}\hat{T}(x_{\rm g})^2\right)\Big] + \mathcal{O}(\epsilon^2)\Big\}. \qquad (4.57)\end{aligned}$$

Equation (4.57) shows that for macroscopic $R, R_{\rm g} \gg l$ the mean number of intersections between the chains explicitly depends on one nonuniversal parameter only. Only if R becomes microscopic itself we obtain a further nonuniversal scale.

Since $\sigma_2(R)$ depends on microstructure *via* one multiplicative constant only, we can define a universal scaling function *e.g.* by

$$D\left(R/R_{\rm g}\right) := -R\frac{\rm d}{{\rm d}R}\ln\sigma_2(R). \qquad (4.58)$$

Note that $D(R/R_{\rm g}) \geq 0$ since $\sigma_2(R)$ is a monotonously decreasing function of R. Inserting equation (4.54) into equation (4.58) we obtain in the short distance limit

$$D\left(R/R_{\rm g}\right) = \frac{\omega_{12}(P)}{1 - A(P)x_{\rm g}^{\omega_{12}(P)}} \qquad \text{for} \quad l \ll R \ll R_{\rm g}, \qquad (4.59)$$

with the universal amplitude

$$A(P) = a_0(P) + a_1(P)\epsilon + a_2(P)\epsilon^2 + ... \qquad (4.60)$$

For $R/R_{\rm g} \to 0$ we have the universal values

$$\begin{cases} D(0) = 0 & \text{for} \quad P \in \{{\rm G}_0, {\rm U}_0, {\rm S}_0\} \\ D(0) = \omega_{12}(P) & \text{for} \quad P \in \{{\rm G}, {\rm U}, {\rm S}\}. \end{cases} \qquad (4.61)$$

Comparing the ϵ-expansion of equation (4.59) with the ϵ-expansion result obtained from inserting equation (4.57) into equation (4.58), we can predict the leading divergence of the tree resp. one loop terms of the perturbation theory as

$$\hat{T}(x_{\rm g}) \overset{x_{\rm g}\to 0}{\sim} -\ln x_{\rm g} \qquad (4.62)$$

$$\hat{L}_0(x_{\rm g}) \overset{x_{\rm g}\to 0}{\sim} -\frac{1}{2}\ln^2 x_{\rm g} \qquad (4.63)$$

$$\hat{L}_1(x_{\rm g}) \overset{x_{\rm g}\to 0}{\sim} \frac{1}{4}\ln^2 x_{\rm g} \qquad (4.64)$$

$$\hat{L}_2(x_{\rm g}) \overset{x_{\rm g}\to 0}{\sim} \frac{1}{8}\ln^2 x_{\rm g}. \qquad (4.65)$$

An explicit calculation in Appendix B.2 shows that equations (4.62–4.65) are indeed fulfilled and the first order approximation of the universal amplitude $A(P)$ in the symmetric case is found from equation (B.20) as

$$A(P) = 1 + \frac{1}{2}\left(1 - \gamma_{\rm Eu} - \ln 2\right)\left(1 - \frac{1}{2}f^* - f^*_{12}(P)\right)\epsilon + \mathcal{O}(\epsilon^2). \qquad (4.66)$$

5 Summary

We have presented a detailed renormalization group analysis of the number of contacts $\sigma(n)$ in a macromolecule. Calculating a one loop crossover function we have been able to describe the dependence of $\sigma(n)$ on chain length n for arbitrary repulsion strength, including the limit of a (Gaussian) Θ-polymer. Close to the nontrivial fixed point we recover the well known result (Eq. (1.2)), establishing that the number of contacts among segments widely spaced along the chain vanishes with the standard "corrections to scaling" exponent ω, unlike contrary statements sometimes found in literature [1,10].

Comparing our crossover function with Monte-Carlo data for the Domb-Joyce model on a simple cubic lattice we find excellent agreement. The Monte-Carlo simulations have been carried through with very low repulsion strength, in particular. Since in this case the excluded volume fixed point is attained for very long chains only, the full crossover function has been necessary to fit the data. Nonuniversal parameters which can not be calculated from any renormalization group treatment have been used as fit parameters. Their values have been checked with exact results for a random walk on a simple cubic lattice.

To confirm the interpretation of the three leading contributions to $\sigma(n)$ we have further calculated the number of intersections σ_2 among two chains with fixed mutual end-to-end distance R, including the copolymer case $R = 0$. Restricting to fixed point behaviour we obtain a scaling behaviour consistent with the single chain case, but with a different correction exponent $\omega_{12}(\mathrm{S})$, known from the theory of ternary polymer systems. This difference is explained by the nontrivial behaviour of spatial correlations among segments on a polymer chain, which do not depend on the mutual chemical distance of the segments alone, but also on their absolute position along the chain.

For finite distance R we obtain a scaling function for the dependence of σ_2 on R/R_g. The connection to the copolymer result in the limit $R/R_\mathrm{g} \to 0$ is derived by a short distance expansion. Taking the logarithmic derivative of $\ln \sigma_2$ with respect to R we have introduced a universal scaling function $D(R/R_\mathrm{g})$. The behaviour of this function in the short distance limit $R/R_\mathrm{g} \to 0$ has been confirmed by an explicit one loop perturbative calculation.

Taken together, our results in much detail show the very complicated structure of internal correlations in self-repelling chains. Simplistic scaling arguments are not capable to exhibit that structure.

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Appendix A: One loop perturbation theory for the partition function of a self-repelling chain

With standard Feynman rules [18,27] a one loop calculation for the bare partition function (Eq. (2.2)) of a single self-repelling chain yields

$$\mathcal{Z} = \frac{\Omega}{(4\pi l^2)^{d/2}} \left[1 - \beta_\mathrm{e} \sum_{0<i<j<n} (j-i)^{-d/2} + \mathcal{O}({\beta_\mathrm{e}}^2) \right]. \tag{A.1}$$

After an additive renormalization introducing the critical chemical potential

$$\mu_\mathrm{s}^*(\beta_\mathrm{e}) = -\beta_\mathrm{e}\zeta(d/2) + \mathcal{O}({\beta_\mathrm{e}}^2) \tag{A.2}$$

we take the continuous chain limit ($l \to 0$ with $\beta_\mathrm{e} l^{-\epsilon}, nl^2$ fixed) to find the dimensionally regularized theory, which exists in $2 < d < 4$. Note that this regularization scheme is equivalent to a cut-off regularization in the sense that both regularization schemes yield the same renormalized theory (up to finite renormalization) [27]. The continuous chain limit therefore can be used to calculate the renormalized partition functions, which is the only use of that limit made in this paper. Renormalization proceeds by λ-independent renormalization factors, which have to absorb poles found for $\epsilon \to 0$. In accord with [18] we have the following one loop results:

$$Z_u(u) = \frac{1}{2}\left\{ 1 + \frac{4}{\epsilon}u + \mathcal{O}(u^2) \right\} \tag{A.3}$$

$$Z_n(u) = 1 - \frac{1}{\epsilon}u + \mathcal{O}(u^2) \tag{A.4}$$

$$Z(u) = 1 + \mathcal{O}(u^2). \tag{A.5}$$

The renormalized expression for the partition function is given as

$$\mathcal{Z}_\mathrm{R} = \frac{(4\pi l^2)^{d/2}}{\Omega}\, \mathrm{e}^{-\mu_\mathrm{s}^*(\beta_\mathrm{e})\, n}\, \frac{Z_n}{Z}\, \mathcal{Z} \tag{A.6}$$

$$= 1 + u\left[\frac{n_\mathrm{R}^{\epsilon/2}}{2-\epsilon} + \frac{n_\mathrm{R}^{\epsilon/2} - 1}{\epsilon} \right] + \mathcal{O}(u^2). \tag{A.7}$$

As required the renormalized result exists in $2 < d \leq 4$.

By differentiating both sides of equation (A.6) with respect to λ (keeping all bare parameters fixed) we obtain the RG equation for the partition function

$$\left\{ 2 - \frac{1}{\nu(u)} - \eta(u) - W(u)\frac{\partial}{\partial u} - \frac{1}{\nu(u)} n_\mathrm{R} \frac{\partial}{\partial n_\mathrm{R}} \right\} \mathcal{Z}_\mathrm{R} = 0. \tag{A.8}$$

The derivation makes use of the fact that $\mathcal{Z}_\mathrm{R}$ by the theorem of renormalizability depends on λ only implicitly *via* u, n_R. RG equations like equation (A.8) form a differential formulation of the scale invariance of the renormalized theory.

Evaluating equation (A.6) directly in three dimensions one finally has to fix the renormalized chain length $n_\mathrm{R} \approx \mathcal{O}(1)$. From the appendix of [28] we adopt the value $n_\mathrm{R} = 0.53$ (note that we set the parameter b_u introduced there as $b_u \equiv 1$ from the outset). Our final result for the renormalized partition function in one loop approximation therefore reads:

$$\mathcal{Z}_\mathrm{R} = 1 + 0.456u + \mathcal{O}(u^2) \qquad (d = 3). \tag{A.9}$$

We should stress that the results we found in Section 3 are not very sensitive to the precise numerical value in equation (A.9). The main functional dependence of the scaling function $H(u)$ (*cf.* Eq. (3.17)) is governed by the functions $\nu(u)$, $\eta(u)$, and $W(u)$ (*cf.* Eqs. (2.12–2.14)), which have been calculated by resummation of perturbative results up to five and six loop order respectively [8].

Appendix B: One loop perturbation theory for the partition function of two mutually repelling chains

B.1 The copolymer

Bare one loop perturbation theory yields

$$\mathcal{Z}_\mathrm{co} = \left(\frac{\Omega}{(4\pi l^2)^{d/2}} \right)^2 \left\{ 1 - \beta_{12} \sum_{\substack{0<j_1<n_1 \\ 0<j_2<n_2}} (j_2 + j_1)^{-d/2} - \beta_{11} \sum_{0<i<j<n_1} (j-i)^{-d/2} - \beta_{22} \sum_{0<i<j<n_2} (j-i)^{-d/2} + \mathcal{O}({\beta_{ab}}^2) \right\}. \tag{B.1}$$

As pointed out in Section 4, equation (4.11), this expression needs a new renormalization factor $Z_2^{(12)}$. The general form of the renormalized result reads (*cf.* Eq. (A.6))

$$\begin{aligned}\mathcal{Z}_{\mathrm{co,R}} = \left(\frac{(4\pi l^2)^{d/2}}{\Omega}\right)^2 \exp[-\mu_{\mathrm{s}}^*(\beta_{11})n_1 - \mu_{\mathrm{s}}^*(\beta_{22})n_2] \\ \times \frac{Z_n(u_{11})Z_n(u_{22})}{Z(u_{11})Z(u_{22})} Z_2^{(12)}(u_{12},u_{11},u_{22})\mathcal{Z}_{\mathrm{co}}. \qquad \text{(B.2)}\end{aligned}$$

Using the one loop results for $Z_u^{(12)}$ and $Z_2^{(12)}$,

$$\begin{aligned}Z_u^{(12)}(u_{12},u_{11},u_{22}) =& \frac{1}{2}\left\{1+\frac{u_{11}+u_{22}}{\epsilon}+2\frac{u_{12}}{\epsilon}\right\} \qquad \text{(B.3)}\\ Z_2^{(12)}(u_{12},u_{11},u_{22}) =& 1+\frac{1}{\epsilon}u_{12}, \qquad \text{(B.4)}\end{aligned}$$

we find, proceeding as in Appendix A,

$$\begin{aligned}\mathcal{Z}_{\mathrm{co,R}} =& 1+\left(\frac{1}{\epsilon}+\frac{1}{2-\epsilon}\right)\Big\{u_{12}(n_{1\mathrm{R}}+n_{2\mathrm{R}})^{\epsilon/2} \\ &+ (u_{11}-u_{12})\,n_{1\mathrm{R}}^{\epsilon/2} + (u_{22}-u_{12})\,n_{2\mathrm{R}}^{\epsilon/2}\Big\} \\ &- \frac{1}{\epsilon}(u_{11}+u_{22}-u_{12}) + \mathcal{O}(u_{ab}^2). \qquad \text{(B.5)}\end{aligned}$$

This result includes equation (2.7) in the case of identical blocks, $u_{11}=u_{22}=u_{12}=u$, $n_{1\mathrm{R}}+n_{2\mathrm{R}}=n_{\mathrm{R}}$, as well as the case of two independent blocks: $\mathcal{Z}_{\mathrm{co,R}} = \mathcal{Z}_{\mathrm{R}}^{(1)}\mathcal{Z}_{\mathrm{R}}^{(2)}$ if $u_{12}=0$.

B.2 Finite distance between the endpoints of the chains

Defining

$$\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}} = 1 - \int \frac{\mathrm{d}^d p}{(2\pi)^d}\,\mathrm{e}^{i\mathbf{pR}} A_2^{(12)}(p), \qquad \text{(B.6)}$$

we first note that $A_2^{(12)}(0)$ is the second virial coefficient of a ternary solution [29]. The diagrams which contribute to $A_2^{(12)}(p)$ differ from that of the second virial coefficient (see *e.g.* [20]) only by nonzero external momentum $\mathbf{p}$ flowing into one end of one chain resp. $-\mathbf{p}$ flowing into one end of the other. The unrenormalized one loop approximation reads

$$\begin{aligned}A_2^{(12)}(p) = (4\pi l^2)^{d/2}\beta_{12}\Big\{T(p) - \beta_{11}L^{(11)}(p) \\ - \beta_{22}L^{(22)}(p) - \beta_{12}L^{(12)}(p) + \mathcal{O}(\beta_{ab}^2)\Big\}, \qquad \text{(B.7)}\end{aligned}$$

where

$$\begin{aligned}T(p) =& \sum_{0<j_1<n_1}\sum_{0<j_2<n_2} \mathrm{e}^{-p^2l^2(n_1-j_1+j_2)} \\ L^{(11)}(p) =& \sum_{0<j_4<n_2}\mathrm{e}^{-p^2l^2j_4}\sum_{0<j_1<j_2<j_3<n_1}(j_2-j_1)^{-d/2} \\ &\times \mathrm{e}^{-p^2l^2(n_1-j_3)} \\ &+ \sum_{0<j_4<n_2}\mathrm{e}^{-p^2l^2j_4}\sum_{0<j_1<j_3<j_2<n_1}(j_2-j_1)^{-d/2} \\ &\times \mathrm{e}^{-p^2l^2\left(n_1-j_3-\frac{(j_2-j_3)^2}{(j_2-j_1)}\right)} \\ &+ \sum_{0<j_4<n_2}\mathrm{e}^{-p^2l^2j_4}\sum_{0<j_3<j_1<j_2<n_1}(j_2-j_1)^{-d/2} \\ &\times \mathrm{e}^{-p^2l^2(n_1-j_3+j_1-j_2)} \\ &- T(p)\sum_{0<j_1<j_2<n_1}(j_2-j_1)^{-d/2} \\ L^{(22)}(p) =& L^{(11)}(p)\Big|_{n_1\leftrightarrow n_2} \\ L^{(12)}(p) =& \sum_{0<j_1<j_2<n_1}\sum_{0<j_3<j_4<n_2}(j_4-j_3+j_2-j_1)^{-d/2} \\ &\times \mathrm{e}^{-p^2l^2\left(n_1+j_4-j_2-\frac{(j_4-j_3)^2}{(j_4-j_3+j_2-j_1)}\right)} \\ &+ \sum_{0<j_1<j_2<n_1}\sum_{0<j_3<j_4<n_2}(j_4-j_3+j_2-j_1)^{-d/2} \\ &\times \mathrm{e}^{-p^2l^2(n_1+j_3-j_2)}. \qquad \text{(B.8)}\end{aligned}$$

For renormalization along the lines of Appendices A or B.1 we note that due to the normalization of $\mathcal{Z}^{(12)}$ by $\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}$ no explicit renormalization factors occur (this is guaranteed by Eq. (4.8)). By means of equations (A.3, A.4, B.3) we thus write, defining $\bar{p} := pl_{\mathrm{R}}$,

$$\begin{aligned}A_2^{(12)}(p) =& \left(A_2^{(12)}(p)\right)_{\mathrm{R}} \\ =& (4\pi)^{\mathrm{d}/2}\frac{1}{2}n_{1\mathrm{R}}n_{2\mathrm{R}}u_{12}l_{\mathrm{R}}^{\mathrm{d}}\Big\{T_{\mathrm{R}}(\bar{p}) - u_{11}L_{\mathrm{R}}^{(11)}(\bar{p}) \\ &- u_{22}L_{\mathrm{R}}^{(22)}(\bar{p}) - u_{12}L_{\mathrm{R}}^{(12)}(\bar{p}) + \mathcal{O}(u_{ab}^2)\Big\}. \qquad \text{(B.9)}\end{aligned}$$

With the definition

$$P_{a\mathrm{R}} := \bar{p}^2 n_{a\mathrm{R}} = p^2 l_{\mathrm{R}}^2 n_{a\mathrm{R}} \qquad \text{(B.10)}$$

we find for the tree term (note the continuous chain limit)

$$T_{\mathrm{R}}(\bar{p}) = \int_0^1 \mathrm{d}s_1\,\mathrm{e}^{-P_{1\mathrm{R}}s_1}\int_0^1 \mathrm{d}s_2\,\mathrm{e}^{-P_{2\mathrm{R}}s_2}. \qquad \text{(B.11)}$$

The one loop terms clearly are more complicated:

$$
\begin{aligned}
L_{\mathrm{R}}^{(11)}(\bar{p}) = & \int_0^1 \mathrm{d}s_2 \mathrm{e}^{-P_{2\mathrm{R}} s_2} \Big\{ \frac{1}{\epsilon} \int_0^1 \mathrm{d}s \left(1 - n_{1\mathrm{R}}^{\epsilon/2} s^{\epsilon/2}\right) \\
& \times \left(\mathrm{e}^{-P_{1\mathrm{R}}} - \mathrm{e}^{-P_{1\mathrm{R}} s}\right) + \frac{1}{2} \frac{n_{1\mathrm{R}}^{\epsilon/2}}{P_{1\mathrm{R}}} \int_0^1 \mathrm{d}s\, s^{1-d/2} \\
& \times \left(1 - \mathrm{e}^{-P_{1\mathrm{R}}(1-s)}\right) \int_0^1 \mathrm{d}t\, \mathrm{e}^{-P_{1\mathrm{R}} s t} \left(\mathrm{e}^{P_{1\mathrm{R}} s t^2} - 1\right) \\
& + \frac{1}{2} \frac{n_{1\mathrm{R}}^{\epsilon/2}}{P_{1\mathrm{R}}^2} \mathrm{e}^{-P_{1\mathrm{R}}} \int_0^1 \mathrm{d}s\, s^{-d/2} \left(\mathrm{e}^{P_{1\mathrm{R}} s} - P_{1\mathrm{R}} s - 1\right) \\
& \times \left(\mathrm{e}^{P_{1\mathrm{R}}(1-s)} - P_{1\mathrm{R}}(1-s) - 1\right) \Big\} \\
L_{\mathrm{R}}^{(22)}(\bar{p}) = & L_{\mathrm{R}}^{(11)}(\bar{p}) \Big|_{n_{1\mathrm{R}} \leftrightarrow n_{2\mathrm{R}}} \\
L_{\mathrm{R}}^{(12)}(\bar{p}) = & \frac{2}{\epsilon} T_{\mathrm{R}}(\bar{p}) \Big\{ \frac{2}{2-\epsilon} \left[n_{1\mathrm{R}}^{\epsilon/2} + n_{2\mathrm{R}}^{\epsilon/2} - (n_{1\mathrm{R}} + n_{2\mathrm{R}})^{\epsilon/2} \right] - 1 \Big\} \\
& + \frac{1}{2} \frac{n_{1\mathrm{R}} n_{2\mathrm{R}}}{P_{1\mathrm{R}} P_{2\mathrm{R}}} \int_0^1 \mathrm{d}s \int_0^1 \mathrm{d}t (n_{1\mathrm{R}} s + n_{2\mathrm{R}} t)^{-d/2} \\
& \times \Big\{ \left(\mathrm{e}^{-\left(\frac{1}{P_{1\mathrm{R}} s} + \frac{1}{P_{2\mathrm{R}} t}\right)^{-1}} - 1 \right) \left(1 - \mathrm{e}^{-P_{1\mathrm{R}}(1-s)}\right) \\
& \times \left(1 - \mathrm{e}^{-P_{2\mathrm{R}}(1-t)}\right) + 2\mathrm{e}^{-(P_{1\mathrm{R}} + P_{2\mathrm{R}})} \\
& \times \Big[\left(\mathrm{e}^{P_{1\mathrm{R}}} - 1\right) \left(1 - \mathrm{e}^{P_{2\mathrm{R}} t}\right) + \left(\mathrm{e}^{P_{2\mathrm{R}}} - 1\right) \\
& \times \left(1 - \mathrm{e}^{P_{1\mathrm{R}} s}\right) + \left(1 - \mathrm{e}^{P_{1\mathrm{R}} s}\right) \left(1 - \mathrm{e}^{P_{2\mathrm{R}} t}\right) \Big] \Big\}.
\end{aligned}
\tag{B.12}
$$

The renormalized result is symmetric with respect to interchanging the chains and finite in $2 < d \leq 4$.

In a next step we perform the Fourier transformation in equation (B.6). A closed expression in arbitrary dimension can be obtained for the tree approximation (Eq. (B.11)) only. Defining

$$x := \frac{R}{l_{\mathrm{R}}} \tag{B.13}$$

we find

$$
\begin{aligned}
\tilde{T}_{\mathrm{R}}(x) := & \int \frac{\mathrm{d}^d \bar{p}}{(2\pi)^{\mathrm{d}}} \mathrm{e}^{i \bar{\mathbf{p}} \mathbf{x}} T_{\mathrm{R}}(\bar{p}) \\
= & \frac{(4\pi)^{-d/2}}{n_{1\mathrm{R}} n_{2\mathrm{R}}} \Big\{ (n_{1\mathrm{R}} + n_{2\mathrm{R}})^{\epsilon/2} \mathrm{e}^{-\frac{x^2}{4(n_{1\mathrm{R}} + n_{2\mathrm{R}})}} \\
& \times \left[\Psi(1, 2 - \frac{\epsilon}{2}; \frac{x^2}{4(n_{1\mathrm{R}} + n_{2\mathrm{R}})}) - \Psi(1, 1 - \frac{\epsilon}{2}; \frac{x^2}{4(n_{1\mathrm{R}} + n_{2\mathrm{R}})}) \right] \\
& - n_{1\mathrm{R}}^{\epsilon/2} \mathrm{e}^{-\frac{x^2}{4 n_{1\mathrm{R}}}} \\
& \times \left[\Psi(1, 2 - \frac{\epsilon}{2}; \frac{x^2}{4 n_{1\mathrm{R}}}) - \Psi(1, 1 - \frac{\epsilon}{2}; \frac{x^2}{4 n_{1\mathrm{R}}}) \right] \\
& - n_{2\mathrm{R}}^{\epsilon/2} \mathrm{e}^{-\frac{x^2}{4 n_{2\mathrm{R}}}} \\
& \times \left[\Psi(1, 2 - \frac{\epsilon}{2}; \frac{x^2}{4 n_{2\mathrm{R}}}) - \Psi(1, 1 - \frac{\epsilon}{2}; \frac{x^2}{4 n_{2\mathrm{R}}}) \right] \Big\}.
\end{aligned}
\tag{B.14}
$$

$\Psi(\alpha, \gamma; z)$ denotes the degenerate hypergeometric function [23].

For the complete one loop expression we restrict ourselves to the symmetric case $n_{1\mathrm{R}} = n_{2\mathrm{R}} =: n_{\mathrm{R}}$, $u_{11} = u_{22} =: u$ and we perform an ϵ-expansion. Furthermore we replace l_{R} by the observable R_{g}, the radius of gyration of an isolated chain (*cf. e.g.* [27]),

$$R_{\mathrm{g}}^2 = \frac{\mathrm{d}}{3} n_{\mathrm{R}} l_{\mathrm{R}}^2 \Big\{ 1 + \frac{\epsilon}{8} f \left[\ln n_{\mathrm{R}} - \frac{13}{12} \right] + \mathcal{O}(\epsilon)^2 \Big\}, \tag{B.15}$$

and we define (*cf.* Eq. (4.25))

$$x_{\mathrm{g}} := \sqrt{\frac{d}{12}} \frac{R}{R_{\mathrm{g}}}. \tag{B.16}$$

After some elementary but lengthy calculation we obtain

$$
\begin{aligned}
\frac{\mathcal{Z}^{(12)}(R)}{\mathcal{Z}^{(1)} \mathcal{Z}^{(2)}} = & 1 - \frac{\epsilon}{4} f_{12} \Big\{ \hat{T}(x_{\mathrm{g}}) \\
& + \epsilon \Big[\hat{L}_0(x_{\mathrm{g}}) + \frac{21}{32} \hat{T}(x_{\mathrm{g}}) + f \hat{L}_1(x_{\mathrm{g}}) + f_{12} \hat{L}_2(x_{\mathrm{g}}) \\
& + \frac{1}{2} \ln n_{\mathrm{R}} \left(1 - \frac{1}{2} f - \frac{1}{2} f_{12}\right) \hat{T}(x_{\mathrm{g}}) \Big] + \mathcal{O}(\epsilon^2) \Big\},
\end{aligned}
\tag{B.17}
$$

where $f := f_{11} = f_{22}$ and $f_{aa} := u_{aa}/u^*$ as in equation (4.5). Note that since

$$2 - \frac{1}{2} (f_{11}^* + f_{22}^*) - f_{12}^*(P) = 0 + \mathcal{O}(\epsilon) \tag{B.18}$$

according to Table 2, equation (B.17) confirms that $\mathcal{Z}^{(12)}(R)/\mathcal{Z}^{(1)}\mathcal{Z}^{(2)}$ also in one loop at all fixed points is a function of R/R_{g} only (universal function). The tree contribution reads (*cf.* Eqs. (4.26, 4.27))

$$\hat{T}(x_{\mathrm{g}}) = \frac{1 - \mathrm{e}^{-\frac{1}{2} x_{\mathrm{g}}^2}}{x_{\mathrm{g}}^2} \mathrm{e}^{-\frac{1}{2} x_{\mathrm{g}}^2} - Ei\left(-x_{\mathrm{g}}^2\right) + \frac{1}{2} Ei\left(-x_{\mathrm{g}}^2/2\right) \tag{B.19}$$

$$\overset{x_{\mathrm{g}} \ll 1}{\sim} \frac{1}{2} \left(1 - \gamma_{\mathrm{Eu}} - \ln 2\right) - \ln x_{\mathrm{g}}, \tag{B.20}$$

while the one loop terms can be written as

$$
\begin{aligned}
\hat{L}_0(x_{\mathrm{g}}) =& \frac{1}{8}\int_{x_{\mathrm{g}}^2/2}^{\infty} \ln^2 t\, \mathrm{e}^{-t}\, \mathrm{d}t - \frac{1}{4}\int_{x_{\mathrm{g}}^2}^{\infty} \ln^2 t\, \mathrm{e}^{-t}\, \mathrm{d}t \\
& - \frac{1}{2} x_{\mathrm{g}}^{-2}\left(\int_{x_{\mathrm{g}}^2/2}^{\infty} \ln t\, \mathrm{e}^{-t}\, \mathrm{d}t - \int_{x_{\mathrm{g}}^2}^{\infty} \ln t\, \mathrm{e}^{-t}\, \mathrm{d}t\right) \\
& - \frac{1}{2}\ln x_{\mathrm{g}}^2 \Bigg[x_{\mathrm{g}}^{-2}\left(\mathrm{e}^{-x_{\mathrm{g}}^2} - \mathrm{e}^{-x_{\mathrm{g}}^2/2}\right) \\
& + \frac{1}{2}\int_{x_{\mathrm{g}}^2/2}^{\infty} \ln t\, \mathrm{e}^{-t}\, \mathrm{d}t - \int_{x_{\mathrm{g}}^2}^{\infty} \ln t\, \mathrm{e}^{-t}\, \mathrm{d}t \Bigg] \\
& - \frac{1}{4}\ln^2 x_{\mathrm{g}}^2\, \mathrm{e}^{-x_{\mathrm{g}}^2} + \frac{1}{8}\ln^2 x_{\mathrm{g}}^2\, \mathrm{e}^{-x_{\mathrm{g}}^2/2} - \frac{1}{8}\ln^2 2\, \mathrm{e}^{-x_{\mathrm{g}}^2/2}
\end{aligned} \tag{B.21}
$$

$$
\begin{aligned}
\hat{L}_1(x_{\mathrm{g}}) =& \frac{13}{96} x_{\mathrm{g}}^{-2}\left(\mathrm{e}^{-x_{\mathrm{g}}^2/2} - \mathrm{e}^{-x_{\mathrm{g}}^2}\right) \\
& + \frac{1}{8}\int_0^1 \mathrm{d}s\, \ln s \int_0^1 \mathrm{d}t \Big[(1+t)^{-2}\mathrm{e}^{-x_{\mathrm{g}}^2/(1+t)} \\
& - (s+t)^{-2}\mathrm{e}^{-x_{\mathrm{g}}^2/(s+t)}\Big] + \frac{1}{8}\int_0^1 \mathrm{d}s\, \ln s \int_0^1 \mathrm{d}t\, x_{\mathrm{g}}^{-2} \\
& \times \Bigg\{ (t-t^2-1)\Big[\mathrm{e}^{-x_{\mathrm{g}}^2/\left(2+s\left(t-t^2-1\right)\right)} \\
& - \mathrm{e}^{-x_{\mathrm{g}}^2/\left(1+s\left(t-t^2-1\right)\right)}\Big] + (t^2-t)\Big[\mathrm{e}^{-x_{\mathrm{g}}^2/\left(1+s\left(t-t^2\right)\right)} \\
& - \mathrm{e}^{-x_{\mathrm{g}}^2/\left(s\left(t-t^2\right)\right)}\Big] + (1-t)\Big[\mathrm{e}^{-x_{\mathrm{g}}^2/(2+s(t-1))} \\
& - \mathrm{e}^{-x_{\mathrm{g}}^2/(1+s(t-1))}\Big] + t\Big[\mathrm{e}^{-x_{\mathrm{g}}^2/(1+st)} - \mathrm{e}^{-x_{\mathrm{g}}^2/(st)}\Big]\Bigg\} \\
& - \frac{1}{8}\int_0^1 \mathrm{d}s\, x_{\mathrm{g}}^{-2}\Bigg\{ s^{-1}\left(\mathrm{e}^{-x_{\mathrm{g}}^2/2} - \mathrm{e}^{-x_{\mathrm{g}}^2/(2-s)}\right) \\
& - 2\left(\mathrm{e}^{-x_{\mathrm{g}}^2/2} - \mathrm{e}^{-x_{\mathrm{g}}^2/(1+s)}\right) + \frac{2s-1}{1-s}\left(\mathrm{e}^{-x_{\mathrm{g}}^2/s} - \mathrm{e}^{-x_{\mathrm{g}}^2}\right)\Bigg\}
\end{aligned} \tag{B.22}
$$

$$
\begin{aligned}
\hat{L}_2(x_{\mathrm{g}}) =& \frac{1}{4}(\ln 2 - 1)\hat{T}(x_{\mathrm{g}}) \\
& + \frac{1}{8} x_{\mathrm{g}}^{-2}\int_0^1 \mathrm{d}s \int_0^1 \mathrm{d}t\, \left[\frac{1}{1+s-t} - \frac{1}{s}\right] \\
& \times \left[\mathrm{e}^{-x_{\mathrm{g}}^2/(1-s+t)} - \mathrm{e}^{-x_{\mathrm{g}}^2/(1+t)}\right] \\
& - \frac{1}{16}\int_0^1 \mathrm{d}s \int_0^1 \mathrm{d}t (s+t)^{-2} \int_0^{1-s} \mathrm{d}s_1 \int_0^{1-t} \mathrm{d}t_1 \\
& \times \Bigg\{ \left(\frac{st}{s+t} + s_1 + t_1\right)^{-2} \mathrm{e}^{-x_{\mathrm{g}}^2/\left(\frac{st}{s+t}+s_1+t_1\right)} \\
& - (s_1+t_1)^{-2}\mathrm{e}^{-x_{\mathrm{g}}^2/(s_1+t_1)} \Bigg\} \\
& + \frac{1}{8}\int_0^1 \mathrm{d}s \int_0^1 \mathrm{d}t (s+t)^{-2} \int_0^1 \mathrm{d}s_1 \int_{1-t}^1 \\
& \times \mathrm{d}t_1\, (s_1+t_1)^{-2}\mathrm{e}^{-x_{\mathrm{g}}^2/(s_1+t_1)}.
\end{aligned} \tag{B.23}
$$

Analyzing the leading logarithmic divergence of the one loop terms we find

$$
\hat{L}_0(x_{\mathrm{g}}) \overset{x_{\mathrm{g}}\to 0}{\sim} -\frac{1}{2}\ln^2 x_{\mathrm{g}} \tag{B.24}
$$

$$
\hat{L}_1(x_{\mathrm{g}}) \overset{x_{\mathrm{g}}\to 0}{\sim} \frac{1}{4}\ln^2 x_{\mathrm{g}} \tag{B.25}
$$

$$
\hat{L}_2(x_{\mathrm{g}}) \overset{x_{\mathrm{g}}\to 0}{\sim} \frac{1}{8}\ln^2 x_{\mathrm{g}}. \tag{B.26}
$$

The coefficients of the logarithms confirm the predicted scaling behaviour of the normalized partition function for $R \ll R_{\mathrm{g}}$, equation (4.33), allowing for an exponentiation of equation (B.17) with the correct exponent $-\eta_2^{(12)}(P)$. In the same spirit equations (B.24–B.26) are found to be necessary to yield the universal short distance scaling function for the number of contacts, equation (4.59), as was mentioned at the end of Section 4.2.2.

Appendix C: Two flow equations

We here derive equations (4.37, 4.42). The derivative $\lambda\, \mathrm{d}/\mathrm{d}\lambda$ in these equations is as always understood with keeping all bare parameters fixed. Applied to functions like the renormalization factors which explicitly depend on the renormalized couplings and on λ we have

$$
\begin{aligned}
\lambda\frac{\mathrm{d}}{\mathrm{d}\lambda} =& \lambda\frac{\partial}{\partial\lambda} + W(u_{11})\frac{\partial}{\partial u_{11}} + W(u_{22})\frac{\partial}{\partial u_{22}} \\
& + W_{12}(u_{12}, u_{11}, u_{22})\frac{\partial}{\partial u_{12}}\cdot
\end{aligned} \tag{C.1}
$$

For the flow of (*cf.* Eq. (4.3))

$$
\frac{\partial\beta_{12}}{\partial u_{12}} = \frac{\beta_{12}}{u_{12}}\left(1 + u_{12}\frac{\partial}{\partial u_{12}}\ln Z_u^{(12)}(u_{12}, u_{11}, u_{22}, \lambda)\right) \tag{C.2}
$$

we thus find

$$
\begin{aligned}
& \lambda\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln\left[\frac{\partial\beta_{12}}{\partial u_{12}}\right]^{-1} = \\
& \frac{W_{12}}{u_{12}} - W_{12}\frac{\partial}{\partial u_{12}}\ln\left(1 + u_{12}\frac{\partial}{\partial u_{12}}\ln Z_u^{(12)}(u_{12}, u_{11}, u_{22}, \lambda)\right) \\
& - \frac{u_{12}\left[\lambda\frac{\partial}{\partial\lambda} + W(u_{11})\frac{\partial}{\partial u_{11}} + W(u_{22})\frac{\partial}{\partial u_{22}}\right]}{1 + u_{12}\frac{\partial}{\partial u_{12}}\ln Z_u^{(12)}(u_{12}, u_{11}, u_{22}, \lambda)} \\
& \times \frac{\partial}{\partial u_{12}}\ln Z_u^{(12)}(u_{12}, u_{11}, u_{22}, \lambda).
\end{aligned} \tag{C.3}
$$

On the other hand, applying equation (C.1) on both sides of equation (4.3) yields *(see Eq. (C.4) next page).*

$$W_{12}(u_{12},u_{11},u_{22}) = \lambda\frac{\mathrm{d}}{\mathrm{d}\lambda}u_{12} = -u_{12}\frac{\epsilon + \left(\lambda\frac{\partial}{\partial\lambda} + W(u_{11})\frac{\partial}{\partial u_{11}} + W(u_{22})\frac{\partial}{\partial u_{22}}\right)\ln\, Z_u^{(12)}(u_{12},u_{11},u_{22},\lambda)}{1 + u_{12}\frac{\partial}{\partial u_{12}}\ln\, Z_u^{(12)}(u_{12},u_{11},u_{22},\lambda)}\cdot \tag{C.4}$$

Inserting equation (C.4) into the last line of equation (C.3) we finally obtain

$$\begin{aligned}
&\lambda\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln\left[\frac{\partial\beta_{12}}{\partial u_{12}}\right]^{-1} = \\
&\frac{W_{12}}{u_{12}} - W_{12}\frac{\partial}{\partial u_{12}}\ln\left(1+u_{12}\frac{\partial}{\partial u_{12}}\ln\, Z_u^{(12)}\right) \\
&+ \frac{u_{12}}{1+u_{12}\frac{\partial}{\partial u_{12}}\ln\, Z_u^{(12)}}\frac{\partial}{\partial u_{12}}\left[\epsilon+\frac{W_{12}}{u_{12}}\left(1+u_{12}\frac{\partial}{\partial u_{12}}\ln\, Z_u^{(12)}\right)\right] \\
&= \frac{\partial}{\partial u_{12}}W_{12}(u_{12},u_{11},u_{22}),
\end{aligned} \tag{C.5}$$

proving equation (4.37).

To prove equation (4.42) we first derive a flow equation for $\partial/\partial u_{12}\ln Z_2^{(12)}$. With equation (C.1) and the definitions (Eqs. (4.15, 4.36)) we obtain

$$\begin{aligned}
&\lambda\frac{\mathrm{d}}{\mathrm{d}\lambda}\left[\frac{\partial}{\partial u_{12}}\ln Z_2^{(12)}\right] = \\
&\frac{\partial}{\partial u_{12}}\left[\left(\lambda\frac{\partial}{\partial\lambda}+W(u_{11})\frac{\partial}{\partial u_{11}}+W(u_{22})\frac{\partial}{\partial u_{22}}+W_{12}\frac{\partial}{\partial u_{12}}\right)\ln Z_2^{(12)}\right] \\
&- \frac{\partial}{\partial u_{12}}\left[W_{12}\frac{\partial}{\partial u_{12}}\ln Z_2^{(12)}\right] + W_{12}\frac{\partial^2}{\partial u_{12}^2}\ln Z_2^{(12)} \\
&= \frac{\partial}{\partial u_{12}}\eta_2^{(12)} - \omega_{12}\left[\frac{\partial}{\partial u_{12}}\ln Z_2^{(12)}\right].
\end{aligned} \tag{C.6}$$

Restricting to fixed point behaviour we now set $u_{aa} \equiv u_{aa}^* \in \{0,u^*\}$. In this case the general solution of the differential equation (C.6) can be written as

$$\begin{aligned}
\frac{\partial}{\partial u_{12}}\ln Z_2^{(12)} = \exp&\left\{-\int_{u_{12}(1)}^{u_{12}}\mathrm{d}v\,\frac{\omega_{12}(v,u_{11}^*,u_{22}^*)}{W_{12}(v,u_{11}^*,u_{22}^*)}\right\} \\
&\times\left[\hat{c}^{(12)}+\int_{u_{12}(1)}^{u_{12}}\mathrm{d}w\,\frac{\frac{\partial}{\partial u_{12}}\eta_2^{(12)}(w,u_{11}^*,u_{22}^*)}{W_{12}(w,u_{11}^*,u_{22}^*)}\right. \\
&\left.\times\exp\left\{\int_{u_{12}(1)}^{w}\mathrm{d}v\,\frac{\omega_{12}(v,u_{11}^*,u_{22}^*)}{W_{12}(v,u_{11}^*,u_{22}^*)}\right\}\right].
\end{aligned} \tag{C.7}$$

$\hat{c}^{(12)}$ is the integration constant. To evaluate the behaviour of equation (C.7) for $u_{12}\to u_{12}^*(P)$ we expand the integrands

$$\frac{\partial}{\partial u_{12}}\eta_2^{(12)}(u_{12},u_{11}^*,u_{22}^*)=\left(\frac{\partial}{\partial u_{12}}\eta_2^{(12)}\right)_P+\mathcal{O}(u_{12}-u_{12}^*(P)) \tag{C.8}$$

$$\begin{aligned}
W_{12}(u_{12},u_{11}^*,u_{22}^*) = {}&\omega_{12}(P)\,(u_{12}-u_{12}^*(P)) \\
&+\frac{1}{2}\left(\frac{\partial}{\partial u_{12}}\omega_{12}\right)_P(u_{12}-u_{12}^*(P))^2 \\
&+\mathcal{O}(u_{12}-u_{12}^*(P))^3,
\end{aligned} \tag{C.9}$$

$$\begin{aligned}
\omega_{12}(u_{12},u_{11}^*,u_{22}^*) = {}&\omega_{12}(P)+\left(\frac{\partial}{\partial u_{12}}\omega_{12}\right)_P(u_{12}-u_{12}^*(P)) \\
&+\mathcal{O}(u_{12}-u_{12}^*(P))^2.
\end{aligned} \tag{C.10}$$

A consistent expansion of equation (C.7) up to $\mathcal{O}(u_{12}-u_{12}^*(P))$ then finally yields

$$\begin{aligned}
\frac{\partial}{\partial u_{12}}\ln Z_2^{(12)} = {}&\frac{\tilde{c}^{(12)}}{u_{12}-u_{12}^*(P)}-\frac{\tilde{c}^{(12)}}{2\omega_{12}(P)}\left(\frac{\partial}{\partial u_{12}}\omega_{12}\right)_P \\
&+\frac{1}{\omega_{12}(P)}\left(\frac{\partial}{\partial u_{12}}\eta_2^{(12)}\right)_P+\mathcal{O}(u_{12}-u_{12}^*(P)).
\end{aligned} \tag{C.11}$$

The nonuniversal constant $\tilde{c}^{(12)}$ absorbs the dependence on the starting value $u_{12}(1)$. Inserting equation (C.9) we obtain equation (4.42).

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