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Higher order calculations of the renormalization group flow for multicomponent polymer solutions

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Abstract. — We calculate to three-loop order the renormalization group flow of the interaction constants for polymer solutions containing several chemically different polymer species. Close to the fixed points we determine the flow by a Padé-Borel analysis using information on the asymptotic behaviour of the perturbation expansion. We furthermore derive exact relations which connect the correction to scaling exponents to exponents of binary solutions or of star polymers, and in the cross over region we integrate the flow equations numerically to get a global picture. To clarify the relation to previous work based on « direct renormalization » we present a detailed discussion of the interpenetration ratio for two chains of different chemistry or size.

1. Introduction.

Solutions of long macromolecules are among the most extensively studied systems [1] with renormalization group (RG) symmetry. The RG not only explains the universal scaling behaviour observed in the « excluded volume » limit where the two body repulsion dominates, but it also allows for an approximate calculation of the crossover functions which interpolate among the noninteracting and strongly interacting limits. Using RG equations based on a two-loop calculation, combined with theoretically well established values of critical exponents, we in fact can explain many experimental data almost quantitatively [2].

Some time ago this successful theory has been extended [3-5] to describe the physics of two chemically different polymer species in a common solvent (« ternary solutions »). For that system we deal with three different coupling constants $g_{ab} = g_{ba}$; $a, b = 1, 2$; representing the effective interaction of monomers of type (a) and (b). The RG equations define a flow in coupling constant space which governs the crossover phenomena. For ternary solutions this flow is especially rich, possessing eight different fixed points. Furthermore, with increasing concentration the system typically separates into two phases which differ in composition, and this phase transition generically is not governed by a fixed point of the excluded volume problem but takes place in the crossover domain. Thus a good representation of the RG flow in all the accessible parameter region is of great interest.

The present paper is devoted to a detailed discussion of the RG flow for multicomponent polymer solutions. Using field theoretical methods we calculate the flow equations to three-

loop order. For certain fixed points we establish a scaling relation which expresses the important « correction to scaling » exponents ω_{ab} in terms of well known exponents of the binary subsystems. For the other fixed points we relate the ω_{ab} to exponents of « star » polymers, and we furthermore estimate the ω_{ab} by Borel resummation of our three-loop result, including information on the high orders of perturbation theory.

Somewhat surprisingly, part of our results differs from previous work based on « direct renormalization » in the polymer language. Since in that method the coupling constant flow is extracted from an analysis of appropriately normalized virial coefficients of two polymer chains, we reconsider the nonlinear scaling properties of these so-called « interpenetration ratios » to point out the flaw in the argument of reference [3].

The organization of our paper is as follows. In section 2 we derive the RG equations. We calculate fixed points and correction to scaling exponents, and we discuss the flow of the coupling constants. Section 3 is devoted to the analysis of the second virial coefficients and the interpenetration ratios. With regard to the calculations of reference [3] we carry through a careful analysis of the limit where the two interpenetrating chains are of very different size, a limit which has been discussed before in reference [6] using a somewhat different technique. Section 4 summarizes our results. Our work heavily relies on previous field theoretical or polymer work. Some technical details are presented in appendices.

2. Renormalization group flow.

2.1 MAPPING OF POLYMER THEORY ON LANDAU-GINZBURG MODEL. — We consider a system containing (A) chemically different polymer species $a = 1, ..., A$. Using Edwards' continuous chain model we represent the configuration of a chain by a curve $r(s)$, $0 \leqslant s \leqslant S$ in d-dimensional space. The parameter S measures the chain length which is proportional to the molecular weight. To eliminate microscopic length parameters in the Hamiltonian of the model both s and S are taken to have dimensions of a length squared. The partition function of a system containing a single chain of each species $a = 1, .., A$ is written as integral over all configurations $r^{(1)}(s), .., r^{(A)}(s)$:

$$Z(S^{(1)}, .., S^{(A)}) = \int D[r^{(1)}, .., r^{(A)}] \exp\left\{ - \sum_{a=1}^{A} \int_0^{S(a)} ds \left(\frac{dr^{(a)}(s)}{2\, ds} \right)^2 - \right.$$

$$\left. - \frac{1}{2} \sum_{a,b=1}^{A} u_{ab} \int d^d r\, \rho^{(a)}(r)\, \rho^{(b)}(r) \right\} . \quad (2.1)$$

Here

$$\rho^{(a)}(r) = \int_0^{S(a)} ds\, \delta^d(r - r^{(a)}(s)) \quad (2.2)$$

is the fluctuating density of the chain of species (a), and $u_{ab} = u_{ba}$ denotes the matrix of excluded volume interactions. Stability of the model under renormalization requires $u_{ab} \geqslant 0$ for all a, b. (Note that positivity of the *matrix* u_{ab} is not required since the densities are positive semidefinite.) To suppress short distance singularities a cut-off must be imposed. We recall that the expression (2.1) is purely formal and is to be understood as shorthand notation for an appropriate limit of discrete chains. We furthermore note that our choice (2.1) of the partition function differs from the from used for instance in reference [1] by an additional factor 1/2 in the first part of the exponent. This factor is needed to get the equivalent Landau-Ginzburg model in its standard form (2.3).

The model (2.1) can be mapped onto a Landau-Ginzburg theory of (A) n-component spin fields $\sigma_\alpha^{(a)}(r)$; $\alpha = 1, .., n$; $a = 1, .., A$ interacting *via* the Hamiltonian

$$\mathcal{H} = \int \mathrm{d}^d r \left\{ \frac{1}{2} \sum_{a=1}^{A} \sum_{\alpha=1}^{n} \sigma_\alpha^{(a)}(r)(\mu^{(a)} - \Delta)\, \sigma_\alpha^{(a)}(r) + \right.$$
$$\left. + \frac{1}{8} \sum_{a,b=1}^{A} u_{ab} \sum_{\alpha\beta=1}^{n} (\sigma_\alpha^{(a)}(r))^2 (\sigma_\beta^{(b)}(r))^2 \right\} . \quad (2.3)$$

Here $\mu^{(a)}$ is the chemical potential conjugate to $S^{(a)}$. The Laplace transform of the partition function (2.1) can be expressed as a correlation function of the spin model

$$\tilde{Z}(\mu^{(1)}, .., \mu^{(A)}) = \int_0^\infty \prod_a (\mathrm{d}s^{(a)} \mathrm{e}^{-\mu^{(a)} S^{(a)}})\, Z(S^{(1)}, .., S^{(A)}) =$$
$$= \int \prod_{j=1}^{2A} \mathrm{d}^d r_j \left\langle \prod_{a=1}^{A} \sigma_1^{(a)}(r_{2a-1})\, \sigma_1^{(a)}(r_{2a}) \right\rangle \Bigg|_{n=0} \quad (2.4)$$

where at the end of the calculation we for all spin fields have to set the number n of components equal to zero. This procedure is well defined in perturbation theory, and indeed relation (2.4) is proven most directly order by order in the perturbation expansion. For a single chemical species ($A = 1$) a more elegant formal proof uses a Gaussian transformation to linearize the interaction terms. For $A > 1$ this trick works only provided the matrix u_{ab} is positive definite, which is not guaranteed by the positiveness of the matrix elements. It is thus of some interest to sketch a formal proof which holds for general $u_{ab} \geqslant 0$. We present such a proof in appendix A. The argument is easily extended to a grand canonical ensemble or to a canonical ensemble containing any number of chains of the different species.

2.2 RENORMALIZATION. — As mentioned above the model needs a small distance cut-off Λ^{-1} to suppress divergent contributions in perturbation theory. Renormalization is a way to extract the universal scale invariant content of the theory by eliminating the cut-off which reflects the microscopic structure of the system and breaks the scale invariance. The limit $\Lambda \to \infty$ can be taken after an appropriate redefinition of the fields and the parameters occurring in the Hamiltonian (2.3). The field $\sigma^{(a)}(r)$, for instance, is related to its renormalized counterpart $\sigma_{\mathrm{R}}^{(a)}(r)$ by the relation

$$\sigma^{(a)}(r) = Z^{(a)1/2} \sigma_{\mathrm{R}}^{(a)}(r) \quad (2.5)$$

where the renormalization factor $Z^{(a)}$ is determined by imposing a finite « normalization condition » on appropriate expectation values of the renormalized fields. Details of the procedure have been extensively discussed in the literature. (See Refs. [1, 7], for instance.)

For a theory of many fields, renormalization in general mixes the « mass » terms $\mu^{(a)}$ or the couplings u_{ab} among themselves. Fortunately in the limit $n = 0$ the renormalization scheme simplifies to the extent that the field $\sigma^{(a)}$, the mass $\mu^{(a)}$, and the diagonal coupling u_{aa} renormalize as if all other species $\bar{a} \neq a$ were absent : the relevant cut-off dependent contributions of perturbation theory involve only propagators and couplings of type (a). For these quantities we therefore can take over the results of the standard (single species) $O(n)$ model in the limit $n = 0$. Several renormalization schemes are at our disposal, and we use the massless scheme, exploiting results of reference [7], section 9. We in particular need the expression for the field renormalization factor $Z^{(a)}$

$$Z^{(a)} = 1 + K_1 g_{aa}^2 + (8 I_1 K_1 - 4 K_2) g_{aa}^3 + O(g_{aa}^4) . \quad (2.6)$$

The K_ℓ or I_ℓ stand for integrals which are pure numbers depending only on the dimension d of the system. In table I we give K_ℓ, I_ℓ as expansion in powers of $\varepsilon = 4 - d$. (See Ref. [7], Figs. 10, 11.) The renormalized coupling g_{aa} is defined by equations (2.7), (2.9) below for $b = a$. With our convention g_{aa} differs from the coupling defined in reference [7], section 9 by a factor of 3 : (g_{aa}, Ref. [7]) = (3 g_{aa}, here). This explains the difference in numerical prefactors of equation (2.6) as compared to figure 12 of reference [7].

Table I. — *ε-expansion of diagrams.*

$$J_1 = \frac{1}{\varepsilon}\left(1 + \frac{\varepsilon}{2} + \frac{\varepsilon^2}{2}\right)$$

$$J_2 = \frac{1}{2\,\varepsilon^2}\left(1 + \frac{3}{2}\,\varepsilon + \frac{5}{2}\,\varepsilon^2 - \frac{\mathrm{J}}{2}\,\varepsilon^2\right)$$

$$J_3 = \frac{1}{3\,\varepsilon^3}\left(1 + 2\,\varepsilon + \frac{13}{4}\,\varepsilon^2\right)$$

$$J_4 = \frac{1}{3\,\varepsilon^3}\left(1 + \frac{5}{2}\,\varepsilon + \frac{23}{4}\,\varepsilon^2 - \frac{3\,\mathrm{J}}{2}\,\varepsilon^2\right)$$

$$J_5 = \frac{1}{6\,\varepsilon^3}\left(1 + 3\,\varepsilon + \frac{31}{4}\,\varepsilon^2 - \frac{3\,\mathrm{J}}{2}\,\varepsilon^2\right)$$

$$J_6 = \frac{1}{2\,\varepsilon}\,\xi(3)$$

$$J_7 = -\frac{1}{24\,\varepsilon^2}\left(1 + \frac{15}{4}\,\varepsilon\right)$$

$$K_1 = -\frac{1}{8\,\varepsilon}\left(1 + \frac{5}{4}\,\varepsilon\right)$$

$$K_2 = -\frac{1}{6\,\varepsilon^2}(1 + 2\,\varepsilon)$$

The essential new aspect of the present problem is the renormalization of u_{ab}, $b \neq a$. We define g_{ab} as

$$g_{ab} = \kappa^{-\varepsilon} Z^{(a)} Z^{(b)} (Z_4^{(ab)})^{-1} \frac{2(4\pi)^{-d/2}}{\Gamma(d/2)}\, u_{ab}\,, \tag{2.7}$$

where κ is the momentum scale of the renormalized theory. $Z_4^{(ab)}$ and thus g_{ab} is fixed by the renormalization condition

$$\frac{2(4\pi)^{-d/2}}{\Gamma(d/2)}\, \Gamma^{(4)}_{\mathrm{R},ab}\left(\frac{q_1}{\kappa}, .., \frac{q_4}{\kappa}, g_{11}, g_{22}, g_{12}\right)\Big|_{\mathrm{sp}} = g_{ab} \tag{2.8}$$

where $\Gamma^{(4)}_{\mathrm{R},ab}$ is the (dimensionless) renormalized 4-point vertex function with exactly two polymer lines of species a, b, respectively (see Fig. 1). « sp » indicates the symmetry point

$$\frac{q_i\, q_j}{\kappa^2} = \frac{1}{4}\,(4\,\delta_{ij} - 1)\,. \tag{2.9}$$

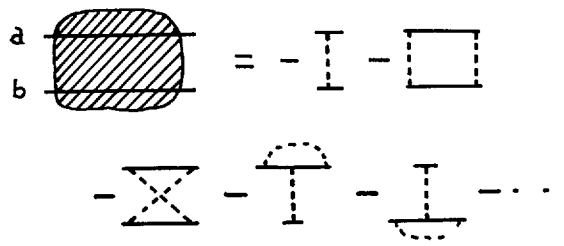

Fig. 1. — Diagrams for $\Gamma^{(4)}_{ab}$ to order of one loop.

Evaluating these equations to three-loop order we find

$$
\begin{aligned}
(Z_4^{(ab)})^{-1} = {} & 1 - I_1(g_{aa} + g_{bb}) - 2\,I_1\,g_{ab} + (4\,I_2 - 2\,I_1^2)\,g_{ab}^2 + \\
& + (6\,I_2 - 2\,I_1^2)\,g_{ab}(g_{aa} + g_{bb}) + I_1^2\,g_{aa}\,g_{bb} + 3(I_2 - I_1^2)(g_{aa}^2 + g_{bb}^2) \\
& + (43\,I_1\,I_2 - 20\,I_1^3 + 2\,I_1\,K_1 - 3\,I_3 - 4\,I_4 - 16\,I_5 - 2\,I_7)(g_{aa}^3 + g_{bb}^3) \\
& + 3(I_1^2 - I_1\,I_2)\,g_{aa}\,g_{bb}(g_{aa} + g_{bb}) \\
& + (34\,I_1\,I_2 - 8\,I_1^3 + 2\,I_1\,K_1 - 12\,I_4 - 16\,I_5 - 6\,I_6 - 2\,I_7)\,g_{ab}(g_{aa}^2 + g_{bb}^2) \\
& + (12\,I_1\,I_2 - 2\,I_1^3 - 2\,I_3 - 8\,I_4 - 8\,I_5)\,g_{ab}\,g_{aa}\,g_{bb} \\
& + (28\,I_1\,I_2 - 8\,I_1^3 - 2\,I_3 - 6\,I_4 - 20\,I_5 - 4\,I_6)\,g_{ab}^2(g_{aa} + g_{bb}) \\
& + (20\,I_1\,I_2 - 6\,J_1^3 - 2\,I_3 - 6\,I_4 - 8\,I_5 - 2\,I_6)\,g_{ab}^3 + O(g^4)\,. \qquad (2.10)
\end{aligned}
$$

For $a = b$ this reduces to the known result.

The flow of the coupling constants under a change of the momentum scale κ of the renormalized theory is governed by the renormalization group equations

$$
\kappa \frac{\mathrm{d}}{\mathrm{d}\kappa}\bigg|_{u_{cd},\,\Lambda\ \text{fixed}} g_{ab} = W_{ab}(g_{11}, g_{22}, g_{12})\,. \qquad (2.11)
$$

The function W_{ab} can be calculated by renormalized perturbation theory. In the application of the theory, κ is taken as a parameter adjusted such that κ^{-1} equals some characteristic macroscopic length scale of the problem. Since this length scale depends on chain lengths and concentrations, the κ dependence of the « running coupling constant » g_{ab} incorporates an important part of the physics of our system. Close to fixed points of the flow it in particular gives rise to the well known power law scaling. A good representation of W_{ab} is therefore of great interest.

An expression of W_{ab} in terms of the renormalization factors can be derived from equation (2.7) :

$$
W_{aa} = -\,\varepsilon g_{aa}\left[1 + g_{aa}\frac{\partial}{\partial g_{aa}} \ln\,(Z_4^{(aa)}/Z^{(a)^2})\right]^{-1} \qquad (2.12)
$$

$$
\begin{aligned}
W_{12} = {} & -\,g_{12}\left[\varepsilon + W_{11}\frac{\partial}{\partial g_{11}} \ln\,(Z_4^{(12)}/Z^{(1)}) + W_{22}\frac{\partial}{\partial g_{22}} \ln\,(Z_4^{(12)}/Z^{(2)})\right] \times \\
& \times \left[1 + g_{12}\frac{\partial}{\partial g_{12}} \ln Z_4^{(12)}\right]^{-1} \qquad (2.13)
\end{aligned}
$$

These expressions can be evaluated with the help of equations (2.6), (2.10).

$$\frac{W_{aa}}{g_{aa}} = -\varepsilon + (4 + 2\varepsilon + 2\varepsilon^2)\, g_{aa} - \left(\frac{21}{2} + \frac{215}{8}\varepsilon - 11 J\varepsilon\right) g_{aa}^2 + \\ + (79 - 22 J + 33\,\zeta(3))\, g_{aa}^3 + O(g_{aa}^4) \quad (2.14)$$

$$\frac{W_{12}}{g_{12}} = -\varepsilon + \left(1 + \frac{\varepsilon}{2} + \frac{\varepsilon^2}{2}\right)(g_{11} + g_{22}) + (2 + \varepsilon + \varepsilon^2)\, g_{12} - \\ - \left(\frac{5}{4} + \frac{55}{16}\varepsilon - \frac{3}{2} J\varepsilon\right)(g_{11}^2 + g_{22}^2) - \left(3 + \frac{15}{2}\varepsilon - 3 J\varepsilon\right) g_{12}(g_{11} + g_{22}) \\ - (2 + 5\varepsilon - 2 J\varepsilon)\, g_{12}^2 + \frac{1}{2}(15 - J)\,(g_{11}^3 + g_{22}^3) + \\ + \left(\frac{27}{2} + 9\,\zeta(3) - 6 J\right) g_{12}(g_{11}^2 + g_{22}^2) + (7 - 3 J)\, g_{12}\, g_{11}\, g_{22} \\ + (12 + 6\,\zeta(3) - 2 J)\, g_{12}^2(g_{11} + g_{22}) + (6 + 3\,\zeta(3) - 2 J)\, g_{12}^3 + O(g^4)\,. \quad (2.15)$$

Here $\zeta(3) \approx 1.202$ is the value of Riemann's ζ-function and $J \approx 0.7494$ represents an integral given in reference [7], equation (9.9). Equation (2.15) is the basic new result exploited in the next subsections. Previously only the therms linear in g_{ab} had been calculated.

2.3 RG FLOW CLOSE TO FIXED POINTS. — The fixed points g_{ab}^* of the RG flow are determined as points in coupling constant space where all W_{ab} vanish. Since W_{aa} depends only on g_{aa}, its zeros determine the possible values of g_{aa}^*.

$$g_{aa}^* = \begin{cases} 0 \\ g^* = \dfrac{\varepsilon}{4}\left[1 + \dfrac{5}{32}\varepsilon + \left[\dfrac{37}{512} - \dfrac{33}{64}\xi(3) - \dfrac{11}{32} J\right]\varepsilon^2 + O(\varepsilon^3)\right]. \end{cases} \quad (2.16)$$

The trivial « Gaussian » fixed point $g_{aa}^* = 0$ describes a polymer chain without self interactions. The nontrivial « excluded volume » fixed point $g_{aa}^* = g^*$ represents fully developed self-repulsion.

The fixed point values $g_{a\bar{a}}^*$, $\bar{a} \neq a$, are determined by the zeros of $W_{a\bar{a}}$. Again we have a trivial solution

$$g_{a\bar{a}}^* = 0 \quad (2.17)$$

representing a system in which species (a) and $(\bar{a})$ do not interact. The nontrivial solution depends on g_{aa}^*, $g_{\bar{a}\bar{a}}^*$, and its expansion to order ε^3 is given in table II, where we explicitly consider a ternary solution : a, $\bar{a} \leqslant 2$. (This amounts to no essential restriction.) We note that at the symmetric fixed point S all coupling constants are identical, with important consequences for the behaviour of ternary solutions [3-5].

Close to a fixed point we can linearize the flow equations. Again restricting ourselves to a ternary solution we introduce the vector

$$|\delta g\rangle = \begin{pmatrix} \delta g_{11} \\ \delta g_{22} \\ \delta g_{12} \end{pmatrix}, \qquad \delta g_{ab} = g_{ab} - g_{ab}^*, \quad (2.18)$$

and we define a dimensionless scale parameter λ by

$$\kappa = \lambda \kappa_0 \quad (2.19)$$

Table II. — *Nontrivial fixed points for a ternary solution.*

Fixed point	g_{11}^*	g_{22}^*	g_{12}^*
—	—	—	—
G	0	0	$\frac{\varepsilon}{2} - \left(J + \frac{3}{2}\zeta(3)\right)\frac{\varepsilon^3}{8}$
U	g^*	0	$\frac{3}{8}\varepsilon + \frac{13}{256}\varepsilon^2 + \left(\frac{89}{4\,096} - \frac{231}{1\,024}\zeta(3) - \frac{63}{512}J\right)\varepsilon^3$
U′	0	g^*	
S	g^*	g^*	g^*

where κ_0^{-1} is some fixed microscopic length. The linearized flow equations take the form

$$\lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} |\delta g\rangle = \Omega |\delta g\rangle \tag{2.20}$$

where the 3×3 matrix Ω has the structure

$$\Omega = \begin{pmatrix} \omega_{11} & 0 & 0 \\ 0 & \omega_{22} & 0 \\ \delta_1 & \delta_2 & \omega_{12} \end{pmatrix} \tag{2.21}$$

$$\omega_{ab} = \left.\frac{\partial W_{ab}}{\partial g_{ab}}\right|_{\{g_{cd}^*\}} \tag{2.22}$$

$$\delta_a = \left.\frac{\partial W_{12}}{\partial g_{aa}}\right|_{\{g_{cd}^*\}} \tag{2.23}$$

The right hand eigenvectors $|\delta g^{(i)}\rangle$, $i = 1, 2, 3$ of Ω obey particularly simple flow equations :

$$|\delta g^{(i)}(\lambda)\rangle = \lambda^{y_i} |\delta g^{(i)}(1)\rangle \,. \tag{2.24}$$

The general form (2.21) yields

$$\left.\begin{aligned} y_a &= \omega_{aa} \\ \delta g_{aa}^{(a)} &\neq 0\,, \quad \delta g_{\bar{a}\bar{a}}^{(a)} = 0 \\ \delta g_{12}^{(a)} &= \frac{\delta_a}{\omega_{aa} - \omega_{12}}\, \delta g_{22}^{(3)} \end{aligned}\right\} \begin{matrix} \bar{a} \neq a \\ a = 1, 2 \end{matrix} \tag{2.25}$$

$$\begin{aligned} y_3 &= \omega_{12} \\ \delta g_{11}^{(3)} &= 0 = \delta g_{22}^{(3)}\,; \quad \delta g_{12}^{(3)} \neq 0\,. \end{aligned} \tag{2.26}$$

The role of these eigenvectors becomes clear if we note that we are interested in the limit where the macroscopic length scale $\sim \kappa^{-1}$ diverges, implying $\lambda \to 0$. In that limit the fixed point considered is stable in direction $|\delta g^{(i)}\rangle$ with $y_i > 0$. In contrast, perturbations $|\delta g^{(i)}\rangle$ with $y_i < 0$ grow for $\lambda \to 0$, implying unstability of the fixed point in that direction.

With the explicit form of W_{ab} given in equations (2.14), (2.15), the matrix elements of Ω are easily calculated. We collect the results in table III. Table IIIa gives the results for fixed

Table IIIa.

Fixed point	g_{11}^*	g_{22}^*	ω_{11}	ω_{22}	ω_{12}
—	—	—	—	—	—
G_0	0	0	$-\varepsilon$	$-\varepsilon$	$-\varepsilon$
U_0	g^*	0	ω	$-\varepsilon$	$-\frac{3}{4}\varepsilon+\frac{11}{128}\varepsilon^2+\left(\frac{83}{2\,048}-\frac{33}{256}\zeta(3)\right)\varepsilon^3$
U_0'	0	g^*	$-\varepsilon$	ω	
S_0	g^*	g^*	ω	ω	$-\frac{1}{2}\varepsilon+\frac{11}{64}\varepsilon^2+\left(\frac{83}{1\,024}-\frac{33}{128}\zeta(3)\right)\varepsilon^3$

Table IIIb.

Fixed point	ω_{11}	ω_{22}	ω_{12}	δ_1	δ_2
—	—	—	—	—	—
G	$-\varepsilon$	$-\varepsilon$	$\varepsilon-\frac{\varepsilon^2}{2}+(1+3\zeta(3))\frac{\varepsilon^3}{4}$	$\frac{\varepsilon}{2}-\frac{\varepsilon^2}{2}+$ $+\left(3J+\frac{9}{2}\zeta(3)-1\right)\frac{\varepsilon^3}{4}$	$\delta_1(G)$
U	ω	$-\varepsilon$	$\frac{3}{4}\varepsilon-\frac{47}{128}\varepsilon^2+$ $+\left(\frac{481}{2\,048}+\frac{21}{32}\zeta(3)\right)\varepsilon^3$	$\frac{3}{8}\varepsilon-\frac{107}{256}\varepsilon^2+$ $+\left(\frac{631}{8}+3J+\frac{247}{2}\zeta(3)\right)\frac{3\varepsilon^3}{512}$	$\delta_1(U')$
U'	$-\varepsilon$	ω		$\frac{3}{8}\varepsilon-\frac{47}{256}\varepsilon^2+$ $+\left(15J+\frac{31}{2}\zeta(3)-\frac{227}{24}\right)\frac{3\varepsilon^3}{512}$	$\delta_1(U)$
S	ω	ω	$\frac{\varepsilon}{2}-\frac{19}{64}\varepsilon^2+$ $+\left(\frac{133}{1\,024}+\frac{69}{128}\zeta(3)\right)\varepsilon^3$	$\frac{1}{4}\varepsilon-\frac{23}{128}\varepsilon^2+$ $+\left(\frac{465}{8}+63\zeta(3)\right)\frac{\varepsilon^3}{256}$	$\delta_1(S)$

points with $g_{12}^*=0$ where $\delta_1=\delta_2=0$ holds. ω is the correction to scaling exponent of the single field $n=0$ model:

$$\omega=\frac{\partial}{\partial g_{aa}}W_{aa}\Big|_{g^*}=\varepsilon-\frac{21}{32}\varepsilon^2+\left(\frac{299}{512}+\frac{33}{32}\zeta(3)\right)\varepsilon^3+O(\varepsilon^4)\,. \tag{2.27}$$

The results for fixed points with $g_{12}^*>0$ are collected in table IIIb. An independent test is possible for $\omega_{12}(S)$. As explained in appendix B this exponent is related to the anomalous

dimension of some composite operator in field theory which is in the class of operators treated in reference [8] to the order of three loops. The result agrees with $\omega_{12}(S)$ as given here.

Our results support the general opinion that the ε-expansion for the correction to scaling matrix Ω is not particularly well behaved. To get estimates which are more reliable in three dimensions ($\varepsilon = 1$) we therefore need additional information. This is the subject of the next subsections.

2.4 Rigorous relations among exponents.

2.4.1 $g_{12}^* = 0$. — For fixed points with vanishing interchain interaction g_{12} we can relate ω_{12} to the correlation length exponents of subsystems 1 and 2. We exploit the connection of the (unrenormalized) 4-point vertex function $\Gamma_{12}^{(4)}$ to vertex functions $\Gamma_a^{(1,2)}$ having two legs corresponding to field $\sigma^{(a)}$ and one insertion of $(\sigma^{(a)})^2$. Figure 2 yields

$$\Gamma_{12}^{(4)}(q_1, q_2, q_3, q_4; \{u_{ab}\}) = u_{12}\,\Gamma_1^{(1,2)}(-q_1 - q_2, q_1, q_2; u_{11}) \times \times \Gamma^{(1,2)}(-q_3 - q_4, q_3, q_4; u_{22}) + O(u_{12}^2)\,. \quad (2.28)$$

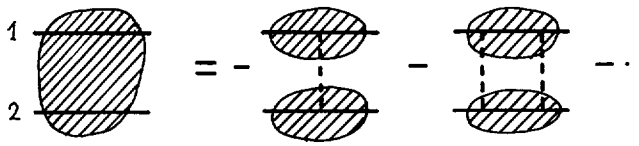

Fig. 2. — Relation of $\Gamma_{ab}^{(4)}$ to $\Gamma_a^{(1,2)}$ $\Gamma_b^{(1,2)}$

Renormalizing this equation according to the standard relations

$$\Gamma_{R,a}^{(1,2)} = Z_2^{(a)}\,\Gamma_a^{(1,2)} \quad (2.29i)$$

$$\kappa^{\varepsilon}\,\Gamma_{R,12}^{(4)} = Z^{(1)}\,Z^{(2)}\,\Gamma_{12}^{(4)} \quad (2.29ii)$$

and using equation (2.17) together with the renormalization condition (2.8) and the standard condition $\Gamma_{R,a}^{(1,2)}(-q_1 - q_2; q_1, q_2)\big|_{sp} = 1$ we immediately find

$$Z_4^{(1,2)} = Z_2^{(1)}\,Z_2^{(2)} + O(g_{12})\,. \quad (2.30)$$

This can be substituted into equation (2.13) to yield

$$W_{12} = -g_{12}\left[\varepsilon + \sum_{a=1}^{2}\left(\frac{1}{\nu(g_{aa})} - 2\right) + O(g_{12})\right] \quad (2.31)$$

where

$$\frac{1}{\nu(g_{aa})} - 2 = W_{aa}\frac{\partial}{\partial g_{aa}}\ln\frac{Z_2^{(a)}}{Z^{(a)}}\,. \quad (2.32)$$

The fixed point values of the correlation length exponent ν are well known [7]:

$$\frac{1}{\nu(g)} - 2 = \begin{cases} 0 & \text{if } g = 0 \\ -\dfrac{\varepsilon}{4}\left[1 + \dfrac{11}{32}\varepsilon + \left(\dfrac{83}{512} - \dfrac{33}{64}\xi(3)\right)\varepsilon^2 + O(\varepsilon^3)\right] & \text{if } g = g^* \end{cases} \quad (2.33)$$

Differentiating equation (2.31) with respect to g_{12} at $g_{12}^* = 0$ we find

$$\omega_{12} = 4 - \varepsilon - \frac{1}{\nu(g_{11}^*)} - \frac{1}{\nu(g_{22}^*)} \tag{2.34}$$

It is easily checked that equations (2.34), (2.33) give back the results of table IIIa.

The exact relation (2.34) can be used to get reliable estimates for ω_{12} in three dimensions, since the nontrivial fixed point value $\nu = \nu(g^*)$ has been calculated to high precision [9] : $\nu = 0.588$ for $d = 3$. (Of course the value $\nu(0) = 1/2$ is exact.) The results are collected in table IVa. Adding the well known [9] value of ω (Eq. (2.27) : $\omega = 0.80$ for $d = 3$, we thus have accurate expressions for the full matrix Ω at all fixed points with $g_{12}^* = 0$.

Relation (2.34) has a simple interpretation in terms of the Hausdorff dimension $d_H^{(a)} = 1/\nu(g_{aa}^*)$ of the polymer coils. It clearly can be written as

$$-\omega_{12} = d_H^{(1)} + d_H^{(2)} - d \tag{2.35}$$

thus identifying $-\omega_{12}$ as Hausdorff dimension of the intersection of the two coils.

Table IVa.

	G_0	U_0, U_0'	S_0
ω_{12}	-1	-0.70	-0.40

Table IVb.

	G	U	U'	S
ω_{12}	0.82	0.68	0.68	0.40
δ_1	0.36	0.25	0.27	0.20
δ_2	0.36	0.27	0.25	0.20
f_{12}^*	1.83	1.48	1.48	1

2.4.2 $g_{12}^* > 0$. — For those fixed points with nonvanishing interaction g_{12}^* the exponent ω_{12} is related to exponents governing the partition function of appropriate four-arm star polymers, which are constructed by tying together endpoints of four chains (see Fig. 3). Consider the partition function $\mathfrak{Z}_*(S_1, ..., S_4)$ of such a star, the arms of lengths S_1, $S_2(S_3, S_4)$ being composed out of monomers of species 1 (2), respectively. In appendix B we prove the following scaling law, being valid at fixed point $P = (g_{11}^*, g_{22}^*, g_{12}^*)$:

$$\exp\{-\mu_c^{(1)}(P)(S_1 + S_2) - \mu_c^{(2)}(P)(S_3 + S_4)\}\ \mathfrak{Z}_*(S_1, .., S_4) = \\ = \lambda^{\hat{\gamma}(P)}\mathfrak{Z}_{*R}\left(\lambda\frac{R_1}{\ell}, \lambda\frac{R_2}{\ell}, \lambda\frac{R_3}{\ell}, \lambda\frac{R_4}{\ell}\right). \tag{2.36}$$

Here $\mu_c^{(a)}$ is the chemical potential per segment of an infinitely long chain of species (a), and R_j is the radius of an isolated chain of length S_j of the corresponding species. The microscopic parameter $\ell \sim \Lambda^{-1}$ is put in for dimensional reasons. The exponent $\hat{\gamma}(P)$ can be related to $\omega_{12}(P)$:

$$\hat{\gamma}(P) = \frac{2}{\nu(g_{11}^*)} + \frac{2}{\nu(g_{22}^*)} + \eta(g_{11}^*) + \eta(g_{22}^*) + \varepsilon - 8 + \omega_{12}(P) \tag{2.37}$$

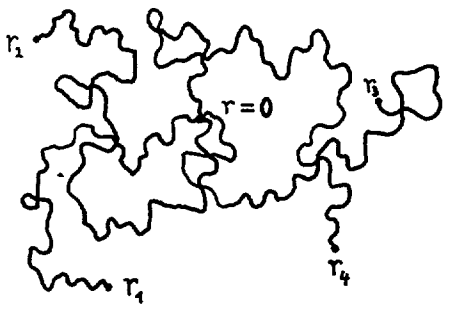

Fig. 3. — Structure of a four arm star polymer.

where [7, 9]

$$\begin{aligned} \eta(0) &= 0 \\ \eta(g^*) \equiv \eta &= \left(\frac{\varepsilon}{8}\right)^2 \left(1 + \frac{17}{16}\varepsilon + O(\varepsilon^2)\right) \\ &\approx 0.027 \quad \text{for} \quad d = 3 . \end{aligned} \tag{2.38}$$

Taking all R_j equal : $R_j \equiv R$ and choosing $\lambda = \ell/R$, we find

$$\mathfrak{Z}_*(S_1,..., S_4) \sim \left(\frac{R}{\ell}\right)^{-\hat{\gamma}(\mathrm{P})} \exp\left\{-\mu_c^{(1)}(\mathrm{P})(S_1 + S_2) - \mu_c^{(2)}(\mathrm{P})(S_3 + S_4)\right\} . \tag{2.39}$$

This relation can be used to measure $\hat{\gamma}(\mathrm{P})$ in Monte Carlo simulations. Such simulations have been carried through [10] at the symmetric fixed point S where we can simplify (2.39) using the well known relation $R/\ell \sim (\bar{S}/\ell^2)^{\nu}$, $S_j = \bar{S}$ for all j.

$$\mathfrak{Z}_*(\bar{S}, .. , \bar{S}) \sim \left(\frac{\bar{S}}{\ell^2}\right)^{\gamma_4 - 1} \exp\left\{-4\,\mu_c\,\bar{S}\right\} \tag{2.40}$$

$$\gamma_4 - 1 = -\nu\,\hat{\gamma}(\mathrm{S}) . \tag{2.41}$$

Thus the determined value of $\gamma_4 = 0.88$ for $d = 3$ with the help of equations (2.41), (2.37) yields $\omega_{12}(\mathrm{S}) = 0.35$, where we used the standard values of ν and η. This result compares favourably with the higher order estimates $\nu\omega_{12}(\mathrm{S}) \approx 0.22$ (or $\omega_{12} \approx 0.37$) of reference [11] or $\omega_{12}(\mathrm{S}) \approx 0.40$ established in the next section. (Note that relation (2.37) is extremely sensitive to the value of ν.) Clearly simulations for appropriate star polymers would make for a useful test of $\omega_{12}(\mathrm{P})$ also for the other fixed points.

2.5 PADÉ-BOREL RESUMMATION. — At fixed points with non-vanishing interchain interaction we use the asymptotic behaviour of the expansions to improve our results. The expansion of the partition function

$$Z(g) = \sum_k Z_k\, g^k \tag{2.42}$$

in the limit of high orders behaves like [12, 13]

$$Z_k = k!\,(-a)^k\, k^{b_0}\, c\left(1 + O\left(\frac{1}{k}\right)\right) . \tag{2.43}$$

This behaviour together with some plausible analyticity assumptions allows for a Padé-Borel resummation. In order to elucidate the basic ideas, we first recall the standard case [13, 14] involving a single coupling constant.

Consider

$$Z(g) = \int \mathrm{D}[\sigma] \exp\{-\mathcal{H}\} \tag{2.44}$$

where $\mathcal{H}$ is given by equation (2.3) with

$$u_{ab} \equiv g\Gamma\left(\frac{d}{2}\right)(4\pi)^{d/2} \tag{2.45}$$

Assuming analyticity of $Z(g)$ in the cut g-plane we may write down the dispersion relation

$$Z(g) = \frac{1}{\pi}\int_{-\infty}^{0} \mathrm{d}g' \frac{\mathrm{Im}\, Z(g')}{g' - g} \tag{2.46}$$

Expansion in powers of g yields

$$Z_k = \frac{1}{\pi}\int_{-\infty}^{0} \mathrm{d}g'\, g'^{-k-1}\, \mathrm{Im}\, Z(g')\,. \tag{2.47}$$

We evaluate $\mathrm{Im}\, Z(g')$ by a saddle point approximation for the σ-integral (2.44). It can be easily shown [14] that the saddle point σ_{sp} dominating $\mathrm{Im}\, Z(g')$ also dominates the higher order terms of the perturbation expansion and leads to the form (2.43) with

$$a = g'\,\mathcal{H}[\sigma_{\mathrm{sp}}] = \text{const.} \tag{2.48}$$

We note a necessary condition for a saddle point which dominates $\mathrm{Im}\, Z$: the matrix of Gaussian fluctuations $\delta\sigma$ around σ_{sp} must show a single negative eigenvalue. In the process of analytic continuation from $\mathrm{Re}\, g' > 0$ to $\mathrm{Re}\, g' < 0$ the amplitude of this mode has to be rotated into the imaginary axis, thus yielding the necessary factor of i.

The asymptotic behaviour of the ε-expansion for ω_{12} or δ_a can be derived [12] from the behaviour of the g-expansion. It has the same form (2.43) but with « a » replaced by

$$\hat{a} = \frac{a}{W_1} \tag{2.49}$$

where W_1 is the first nontrivial coefficient of the R.G. flow function $W = \lambda \dfrac{\partial}{\partial\lambda} g$:

$$\frac{W(g, \varepsilon)}{g} = -\varepsilon + W_1 g + O(g^2)\,. \tag{2.50}$$

We now apply this method to our problem involving three *a priori* different coupling constants and two fields. For fixed points G or S the problem essentially reduces to the case discussed above.

Specifically at fixed point S all coupling constants become identical and we immediately can take over the standard results yielding

$$\hat{a}(\mathrm{S}) = \frac{3}{8}\,. \tag{2.51}$$

At fixed point G the two diagonal couplings vanish, leaving us again with a problem of a single nontrivial coupling constant g_{12}. Repeating the calculation sketched above we find the same result as above:

$$\hat{a}(\mathrm{G}) = \frac{3}{8}\,. \tag{2.52}$$

To treat fixed point U : $g_{22}^* = 0$, $g_{11}^* \neq 0 \neq g_{12}^*$ (or fixed point U', equivalently) we write

$$g_{22} = \hat{g} g_{12} \tag{2.53}$$

and we consider the expansion in powers of g_{12}, keeping $\hat{g}$ fixed. To defend this trick we note that at the fixed point $\hat{g}$ takes the form

$$\hat{g} = \frac{2}{3} + O(\varepsilon) \tag{2.54}$$

where the $O(\varepsilon)$ corrections should not influence to leading behaviour $(-\hat{a})^k$. We have checked this with a toy model in which the fields $\sigma_j(r)$ are replaced by complex variables.

We thus write the Hamiltonian as

$$\mathcal{H}[\sigma_1, \sigma_2] = \int \mathrm{d}^d r \left\{ \frac{1}{2} (\nabla \sigma_1)^2 + \frac{1}{2} (\nabla \sigma_2)^2 + \frac{u_{12}}{4} \left(\sigma_1^2 \sigma_2^2 + \frac{\hat{g}}{2} (\sigma_1^2)^2 \right) \right\} \tag{2.55}$$

$$u_{12} = g_{12} \Gamma \left(\frac{d}{2} \right) (4\pi)^{d/2} \tag{2.56}$$

Following the procedure described above we look for saddle points of the σ_1, σ_2 integrations. The saddle point equations

$$\begin{aligned} -\Delta \sigma_2 + \frac{1}{2} u_{12} \sigma_2 \sigma_1^2 &= 0 \\ -\Delta \sigma_1 + \frac{1}{2} u_{12} (\sigma_2^2 \sigma_1 + \hat{g} \sigma_1^3) &= 0 \end{aligned} \tag{2.57}$$

yield the solutions

$$\sigma_{1c} = \sigma_{2c} = 0 \qquad \text{(i)}$$

$$\sigma_{2c} = 0 \, ; \, \sigma_{1c} = \left(\frac{-2}{u_{12} \hat{g}} \right)^{1/2} \psi_c \qquad \text{(ii)} \tag{2.58}$$

$$\sigma_{2c} = \left(\frac{-2}{u_{12} \hat{g}} \right)^{1/2} \psi_c \, ; \; \sigma_{1c} = \left((\hat{g} - 1) \frac{2}{u_{12}} \right)^{1/2} \psi_c \qquad \text{(iii)}$$

Here ψ_c denotes the well known [12] solution of the instanton equation :

$$\Delta \psi_c + \psi_c^3 = 0 \, . \tag{2.59}$$

As explained above we are looking for a saddle point possessing a single unstable mode.

(i) The solution $\sigma_{1c} = 0 = \sigma_{2c}$ is trivially stable and yields no contribution to Im Z.

(ii) With $\sigma_1 = \sigma_{1c} + \delta\sigma_1$, $\sigma_2 = \delta\sigma_2$ we find to order $(\delta\sigma)^2$

$$\delta \mathcal{H} = \int \mathrm{d}^d r \left\{ \frac{1}{2} \sum_\alpha \delta\sigma_{1,\alpha} (-\Delta - (1 + 2\delta_{\alpha 1}) \psi_c^2) \delta\sigma_{1,\alpha} + \right.$$
$$\left. + \frac{1}{2} \sum_\alpha \delta\sigma_{2,\alpha} \left(-\Delta - \frac{1}{\hat{g}} \right) \psi_c^2 \sigma_{2,\alpha} \right\} \tag{2.60}$$

where we assumed that σ_{1c} points into direction $\alpha = 1$ in the n-dimensional space of the spin components. The first quadratic form in (2.60) is known [12] to have one negative eigenvalue. The second quadratic form has a negative eigenvalue provided $1/\hat{g} > 1$, since in that case the potential $-1/\hat{g}\psi_c^2$ is more attractive than the potential $-\psi_c^2$ which by virtue of equation

(2.59) possesses a normalizable eigenstate at zero eigenvalue. In the case of interest here, $\hat{g}$ is smaller than 1 (compare Eq. (2.54)) and thus saddle point (ii) does not contribute to Im Z.

(iii) The corresponding analysis for saddle point (iii) shows that for $\hat{g} < 1$ only one negative eigenvalue exists. This therefore is the relevant saddle point. It yields

$$a = g'_{12}\, \mathcal{R}(\sigma_{1c}, \sigma_{2c}) = \frac{3}{4}\frac{1}{1 - \hat{g}/2} \tag{2.61}$$

To derive $\hat{a}$ according to equations (2.49), (2.50) we write W_{12} (Eq. (2.15)) as

$$\frac{W_{12}}{g_{12}} = -\varepsilon + (2 + \hat{g})\, g_{12} + O(\varepsilon^2) \tag{2.62}$$

to find

$$a = \frac{3}{2}(4 - \hat{g}^2)^{-1} = \frac{27}{64}. \tag{2.63}$$

Having found the asymptotic behaviour of the coefficients $\omega_{12}^{(k)}$ of the formal power series $\omega_{12}(\varepsilon) = \sum_k \omega_{12}^{(k)} \varepsilon^k$ and the corresponding series for δ_a in the form of equation (2.43) we use the standard Borel resummation method in the form discussed in reference [15]. Some details of the procedure are summarized in appendix C. The results are collected in table IVb, where we also give the values of $f_{12}^* = g_{12}^*/g^*$

2.6 GLOBAL CROSS-OVER DIAGRAM. — The global flow of the couplings follows from the solution of the flow equations (2.11) in the whole allowed range of the couplings g_{ab}. First of all we notice the symmetry of the whole flow under exchange of the couplings g_{11} and g_{22}. Furthermore the ternary system contains the binary one as a special case. Thus

$$g_{11}(\lambda) = g_{22}(\lambda) = g_{12}(\lambda), \quad \text{all } \lambda$$

is a special solution of (2.11). Figure 4 gives a schematic plot of the 3-dimensional flow diagram.

To see the main nontrivial features of the flow, it may suffice to evaluate the flow equations in a two-loop approximation. Furthermore it is useful to rescale all couplings with a factor g^*,

$$g_{ab}(\lambda) = g^* f_{ab}(\lambda), \tag{2.64}$$

to arrive at a non loop order dependent frame of the flow. The resulting differential equations to be evaluated are

$$\lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} f_{aa}(\lambda) = -\varepsilon f_{aa}\left[1 - \left(1 + \frac{21}{32}\varepsilon\right) f_{aa} + \frac{21}{32}\varepsilon f_{aa}^2\right] + O(\varepsilon^3) \tag{2.65i}$$

$$\lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} f_{12}(\lambda) = -\varepsilon f_{12}\left[1 - \frac{1}{4}\left(1 + \frac{21}{32}\varepsilon\right)(2f_{12} + f_{11} + f_{22}) + \frac{5}{64}\varepsilon(f_{11}^2 + f_{22}^2) + \right.$$
$$\left. + \frac{\varepsilon}{16} f_{12}(2f_{12} + 3f_{11} + 3f_{22})\right] + O(\varepsilon^3). \tag{2.65ii}$$

As the flow of f_{11} and f_{22} is independent of f_{12}, the three-dimensional flow is structured by planes perpendicular to the flow lines in the $f_{12} = 0$-plane. This flow is pictured in figure 5.

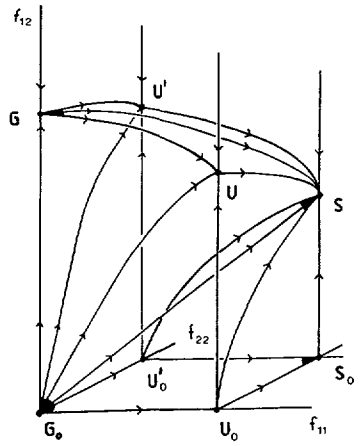

Fig. 4.

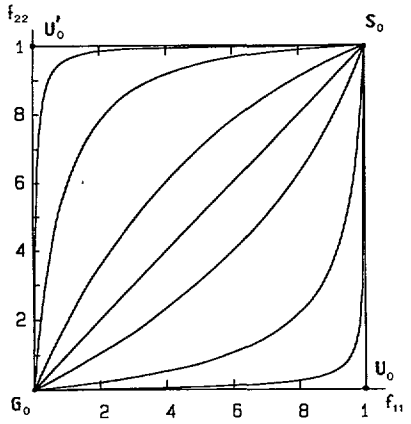

Fig. 5.

Fig. 4. — Position and stability of fixed points. All special lines starting in the direction of eigenvectors are shown. The arrows give the direction of flow under $\lambda \to 0$, the darkened areas indicate directions in which two (G, S_0, S) or three (G_0) eigenvectors are degenerate.

Fig. 5. — Flow of the binary couplings f_{11} and f_{22}. This picture holds for all values of f_{12}.

Typical flow lines in four representative planes are given in figures 6a-d. These planes are lateral planes characterized by $f_{22} = 0$ and $f_{11} = 1$, the symmetry-plane $f_{11} = f_{12}$ and a typical inner plane. A consideration of higher orders in ε would not change the picture qualitatively, since the main qualitative features result from the flow in the neighbourhood of the fixed points, in particular from the stability properties. An interesting special case is given for the two binary couplings $f_{aa}(\lambda)$ taking fixed point values 0 or 1, independent of λ. In that case the flow equation (2.65ii) can be integrated analytically to yield

$$\lambda = \left(\frac{f_{12}(\lambda)}{f_{12}(1)} \right)^{1/\omega_{12}(P_0)} \left(\frac{f^*_{12}(P) - f_{12}(\lambda)}{f^*_{12}(P) - f_{12}(1)} \right)^{1/\omega_{12}(P)} \tag{2.66}$$

This equation describes the flow of $f_{12}(\lambda)$ on the axis connecting fixed points $P_0 = (g^*_{11}, g^*_{22}, 0)$ and $P = (g^*_{11}, g^*_{22}, g^*_{12})$. It is valid to order ε^2 in the sense that taking the logarithmic derivative of equation (2.66) and using values of ω_{12}, f^*_{12} calculated to $O(\varepsilon^2)$ we recover (2.65ii) to order ε^2. In the form (2.66), we however can use the higher order estimates of table IV. This result is the analogue of the representation of the binary flow $f_{aa}(\lambda)$

$$\lambda = \left(\frac{f_{aa}(\lambda)}{f_{aa}(1)} \right)^{-1/\varepsilon} \left(\frac{1 - f_{aa}(\lambda)}{1 - f_{aa}(1)} \right)^{1/\omega} \tag{2.67}$$

which was used in the analysis of experimental data presented in reference [2].

3. Analysis of the interpenetration ratio.

Some time ago Joanny *et al.* [3] calculated fixed points and correction to scaling exponents for ternary solutions using Des Cloizeaux's direct renormalization approach [1]. For the

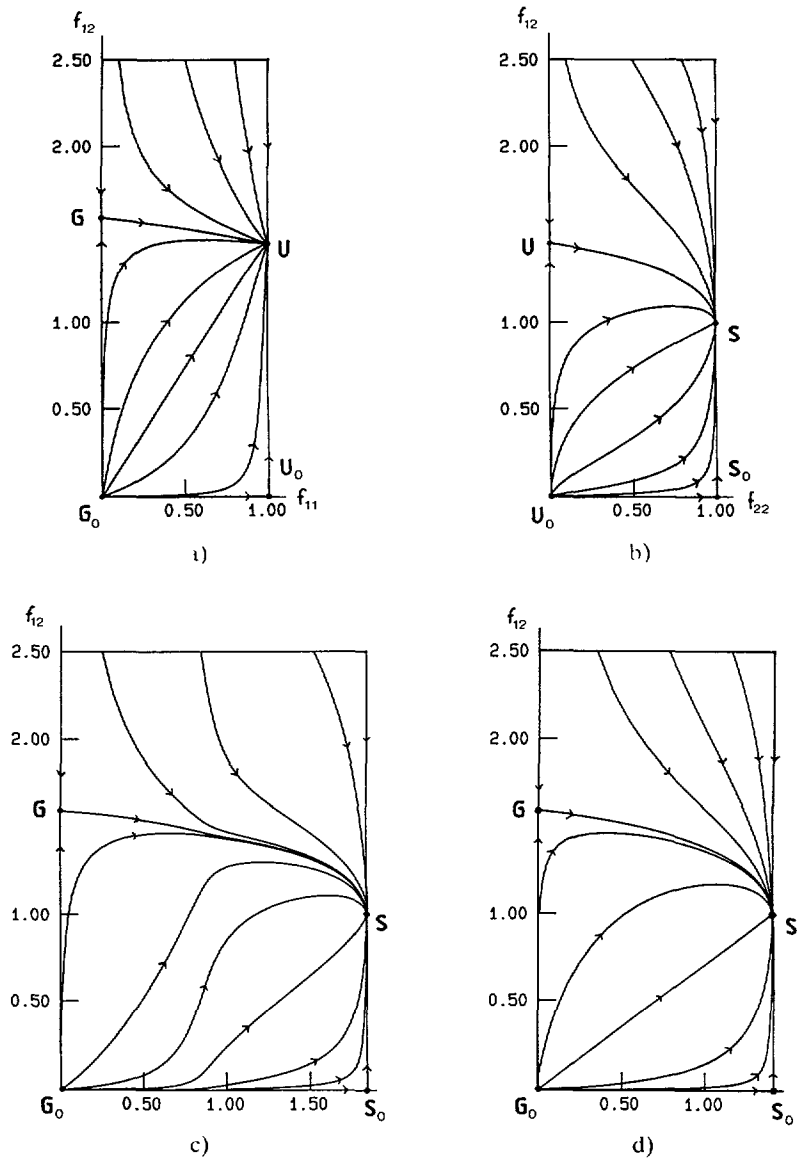

Fig. 6. — a) Flow in the plane $f_{22} = 0$. The singular behaviour at fixed point U is not resolved since the values of ω and ω_{12} at U are close to one another. b) Flow in the plane $f_{11} = 1$. c) Flow in the plane perpendicular to the lowest curve in figure 5. d) Flow in the symmetric plane $f_{11} = f_{22}$. In figures 6c and 6d the abscissa give the curve lengths of the basic lines.

symmetric fixed points of type S, S_0 or G, G_0 their results are consistent with ours, outside the symmetric situation the results differ. To show this we here evaluate the interpenetration ratio which plays the role of the coupling constant in the direct renormalization scheme.

The interpenetration ratio $\psi^{(ab)}$ is defined as

$$\psi^{(ab)} = (4\pi)^{-d/2} A_2^{(ab)} (R_g^{(a)} R_g^{(b)})^{-d/2} \tag{3.1}$$

where $A_2^{(ab)}$ is the osmotic second virial coefficient for two chains of type (a) or (b), respectively, and $R_g^{(a)}$ is the radius of gyration of chain (a). $\psi^{(ab)}$ obeys the nonlinear scaling law [5]

$$\psi^{(ab)} = \psi^{(ab)}\left(\frac{R_g^{(a)^2}}{R_g^{(b)^2}},\ \{g_{cd}(\lambda)\}\right) \tag{3.2}$$

which implies that at fixed points $g_{cd} = g_{cd}^*$ it reduces to a universal function of the scaling variable

$$x = R_g^{(a)^2}/R_g^{(b)^2} \tag{3.3}$$

Note that this quantity is invariant under the renormalization group.

With our renormalization scheme, first-order results for $A_2^{(ab)}$ and $R_g^{(a)^2}$ have been given in reference [4]. We introduce the ratio x defined above as well as the reduced form of the coupling constants :

$$f_{cd} = \frac{g_{cd}}{g^*};\quad c, d = 1, 2\,. \tag{3.4}$$

Some straightforward algebra yields

$$\begin{aligned}\left(\frac{d}{3}\right)^{d/2}\psi^{(ab)} = \frac{\varepsilon}{8}f_{ab}\Big\{1 - \frac{11}{32}\varepsilon + \frac{3}{8}\varepsilon f_{ab} + \frac{37}{96}\varepsilon(f_{aa}+f_{bb}) + \frac{\varepsilon}{4}\left(1-\frac{f_{aa}}{2}\right)\ln(1+x) + \\ + \frac{\varepsilon}{4}\left(1-\frac{f_{bb}}{2}\right)\ln\left(1+\frac{1}{x}\right) + \frac{\varepsilon}{8}f_{ab}\left(x\ln\left(1+\frac{1}{x}\right)+\frac{1}{x}\ln(1+x)\right) \\ + \frac{\varepsilon}{4}\left(f_{ab}+\frac{1}{2}(f_{aa}+f_{bb})-2\right)\ln\left(\frac{d}{3}\frac{\mathrm{e}^{-\gamma_{\mathrm{Eu}}}}{\lambda^2\kappa_0^2}(R_g^{(a)^{-2}}+R_g^{(b)^{-2}})\right)+O(\varepsilon^2)\Big\}\,.\end{aligned} \tag{3.5}$$

Here γ_{Eu} denotes Euler's constant. For $a = b (x \equiv 1)$ this reduces to a well known result. Furthermore at all fixed points with $f_{ab}^* \neq 0$ the relation

$$f_{ab}^* = 2 - \frac{1}{2}(f_{aa}^* + f_{bb}^*) + O(\varepsilon) \tag{3.6}$$

holds. Thus the λ-dependence drops out and $\psi^{(ab)}$ becomes a universal function of x, in keeping with the general scaling law.

We now turn to the results of reference [3]. The ratio defined there differs from ours by the use of the end-to-end distance R_e in place of R_g, but with the well known result [16]

$$\frac{R_g^{(a)^2}}{R_e^{(a)^2}} = \frac{1}{6}\left(1 - \frac{\varepsilon}{96}f_{aa} + O(\varepsilon^2)\right) \tag{3.7}$$

we easily can transform it into an expression for $\psi^{(ab)}$ At fixed points G or S, as well as at fixed point U, U′ in the special case $a = b$, the results are identical to ours provided we put $x = 1$. Also the correction to scaling exponents agree, if we take into account that the exponents of reference [3] equal $\nu(g_{aa}^*)\,\omega_{12}$ in our notation. At the unsymmetric fixed points U, U′ and for $a \neq b$, $x = 1$ we find

$$\left(\frac{d}{3}\right)^{d/2}\psi^{(12)*} = \frac{3}{16}\varepsilon\left[1 + \frac{7}{12}\varepsilon + \frac{3}{4}\varepsilon\ln 2 + O(\varepsilon^2)\right]. \tag{3.8i}$$

This is to be compared to the result derived from reference [3]:

$$\left(\frac{d}{3}\right)^{d/2} \psi^{(12)*} = \frac{3}{16}\,\varepsilon\left[1 + \frac{9}{16}\,\varepsilon + \frac{3}{4}\,\varepsilon \ln 2 + O(\varepsilon^2)\right]. \tag{3.8ii}$$

The correction to scaling exponents also turn out to differ. To identify the source of this discrepancy we first note that in reference [3] the unrenormalized chain lengths are taken to be equal: $S_1 = S_2 = S$. In the symmetric situation this is consistent with $x = 1$, but at fixed points U, U′ and for $a \neq b$ the ratio x takes the form

$$x = (\text{const.}\ S)^{2\nu - 1} = 1 + O(\varepsilon). \tag{3.9}$$

From equation (3.5) this effect gives rise to a difference $O(\varepsilon^2)$ and cannot explain the difference in order ε. We therefore believe the source of the discrepancy to be somewhat more fundamental: in reference [3] the RG flow equations are constructed from the variation of $\psi^{(ab)}$ with $S \equiv S_1 \equiv S_2$. In the unsymmetric situation $g_{11} \neq g_{22}$ the different species however scale differently with S and thus a change of S is not uniquely related to a change of the length scale κ^{-1} Therefore the resulting equations are no valid representation of spatial dilatations underlying the renormalization group.

To pursue the matter somewhat further we analyze the limits $x \to 0$ or $x \to \infty$. According to an argument of De Gennes [17] the second virial coefficient $A_2^{(ab)}$ in the limit $R_g^{(a)} \gg R_g^{(b)}$ and at a fixed point g_{cd}^* should behave as

$$A_2^{(ab)} \sim (R_{ga})^{\frac{1}{\nu(g_{aa}^*)}} (R_{gb})^{d - \frac{1}{\nu(g_{aa}^*)}}$$

giving rise to

$$\psi^{(12)*} \sim \begin{cases} \left(\dfrac{1}{x}\right)^{\frac{d}{4} - \frac{1}{2\nu(g_{11}^*)}} & x \to \infty \\ x^{\frac{d}{4} - \frac{1}{2\nu(g_{22}^*)}} & x \to 0\,. \end{cases} \tag{3.10}$$

(For definiteness we take $a = 1$, $b = 2$.) Equation (3.5) indeed can be written in a form which exhibits this behaviour:

$$\begin{aligned} \left(\frac{d}{3}\right)^{d/2} \psi^{(12)} = {} & \frac{\varepsilon}{8} f_{12} (1+x)^{\varepsilon/4 - \varepsilon f_{11}/8} \left(1 + \frac{1}{x}\right)^{\varepsilon/4 - \varepsilon f_{22}/8} \times \\ & \times \left\{1 - \frac{11}{32}\,\varepsilon + \frac{3}{8}\,\varepsilon f_{12} + \frac{37}{96}\,\varepsilon (f_{11} + f_{22}) + \frac{\varepsilon}{8} f_{12}\left[x \ln\left(1 + \frac{1}{x}\right) + \frac{1}{x} \ln (1+x)\right] + \right. \\ & \left. + \frac{\varepsilon}{4}\left[f_{12} + \frac{1}{2}(f_{11} + f_{22}) - 1\right] \ln\left(\frac{d}{3} \frac{\mathrm{e}^{-\gamma_{\mathrm{Eu}}}}{\lambda^2 \kappa_0^2} (R_g^{(1)^{-2}} + R_g^{(2)^{-2}})\right) + O(\varepsilon^2)\right\}. \end{aligned} \tag{3.11}$$

For $x \to 0$ or $x \to \infty$ the part in curly brackets tends to some finite limit. It is easily checked that at all fixed points the powers of $(1 + x)$ or $\left(1 + \dfrac{1}{x}\right)$ are consistent with the hypothesis (3.10). This shows that in all cases $\psi^{(12)}$ diverges for $x \to 0$ or $x \to \infty$. Turning to fixed point U: $f_{11} = 1$, $f_{22} = 0$ and taking $S_1 = S_2 \to \infty$ we find $x \to \infty$. Thus in this limit $\psi^{(12)*}$ diverges, in contrast to the assumption of reference [3], section II-C. (We should note, however, that we agree with the discussion of large ratios of chain size given in reference [3], Sect. III.)

4. Summary.

We have presented a detailed discussion of the renormalization group flow for ternary polymer solutions. Special attention was paid to the vicinity of the fixed points, where the flow equations can be linearized. Our three-loop results together with a determination of the asymptotics of the ε-expansion allow for a Padé-Borel resummation which is expected to give good results for the linearized flow. Furthermore we were able to relate the correction to scaling exponents at the various fixed points to intersection properties of two different polymer molecules or to properties of four arm star polymers. The latter relation allows for a test of these exponents in Monte Carlo simulations. Up to now such computer experiments have been carried through only in the symmetric situation, where the interaction among all pairs of chains becomes equal to a common fixed point value g^*. It would be of interest to carry through similar calculations for a system in which one or both polymer species are in Θ-conditions, the different species still repelling each other.

In the cross-over region away from fixed points the flow equations for g_{ab} in general have to be integrated numerically. This situation is not completely satisfying since we have found no way to build into the numerical procedure the values of the exponents as known from the Padé-Borel resummation. Thus our numerical solution of the flow equations given to L-Loop order employs the exponents also only to L-Loop approximation, which may be far from the Padé-Borel result. If, in contrast, an analytical solution of the flow equations is possible, then the exponents can be explicitly identified in the result and therefore be replaced by their best known values. This program can be carried through in two special cases :

i) the flow of the binary couplings alone is given to a good approximation by equation (2.67) ;

ii) if both binary couplings take on fixed point values, the flow of g_{12} is represented by equation (2.66).

Generally speaking, only if the flow is restricted to the axes, the exact exponents can be built into the flow equations easily.

Choosing an appropriate chemical composition of the ternary system we can reach any point in the flow diagram. Thus the RG flow in principle can be measured. Unfortunately systematic experiments outside the domain of the symmetric fixed point are not yet available. Close to the symmetric fixed point our theory nicely fits the experiments [5, 18].

To clarify a discrepancy with previous calculations we analyzed in detail the interpenetration ratio of two chains of different species. As a result of this analysis we extended and verified a simple scaling argument giving the form of the interpenetration ratio for two chains of very different size. An experimental verification of this result would be very interesting, but presumably is difficult to achieve.

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Note added in proof :

We meanwhile have constructed a form of ω_{12}, correct to $O(\varepsilon^2)$, which allows us to introduce the exact values of ω_{ab} and g^*_{ab}. The expression is of the same structure as the logarithmic derivative of equations (2.66) or (2.67).

Appendix A.

Formal relation of the multicomponent polymer theory to $n = 0$ field theory.

For each species (a) we introduce a continuous product of δ-functions

$$1 = \int D[\varphi^{(a)}] \prod_r \delta(\varphi^{(a)}(r) - \rho^{(a)}(r)) =$$

$$= \int D[\varphi^{(a)}, \tilde{\varphi}^{(a)}] \exp\left\{ i \int \mathrm{d}^d r \, \tilde{\varphi}^{(a)}(r) \, (\varphi^{(a)}(r) - \rho^{(a)}(r)) \right\} . \quad \text{(A1)}$$

It is important to note that by virtue of $\rho^{(a)}(r) \geq 0$ we may restrict the $\varphi^{(a)}$ integration to $\varphi^{(a)}(r) \geq -\delta$, $\delta \to +0$. Substituting equation (A1) into the expression (2.4) for $\tilde{Z}$ we for $u_{ab} \geq 0$ can interchange the $r^{(a)}$ and $(\varphi^{(a)}, \tilde{\varphi}^{(a)})$ integrations to find

$$\tilde{Z}(\mu^{(1)}, .., \mu^{(A)}) = \int \prod_a D[\varphi^{(a)}, \tilde{\varphi}^{(a)}] \times$$

$$\times \exp\left\{ i \sum_a \int \tilde{\varphi}^{(a)} \varphi^{(a)} - \frac{1}{2} \sum_{a,b} u_{ab} \int \varphi^{(a)} \varphi^{(b)} \right\} \prod_a \int \mathrm{d}^d r \, \mathrm{d}^d r \, , \; G(r, r', \mu^{(a)}, [\tilde{\varphi}^{(a)}]) \quad \text{(A2)}$$

where

$$G(r, r', \mu^{(a)}, [\tilde{\varphi}^{(a)}]) = \int_0^\infty \mathrm{d}s \, \mathrm{e}^{-\mu S} \int_{r(0)=r}^{r(S)=r'} D[r] \exp\left\{ - \int_0^S \mathrm{d}s \left[\left(\frac{\mathrm{d}r(s)}{2 \, \mathrm{d}s} \right)^2 \right] + i \tilde{\varphi}(r(s)) \right\}$$

$$= \langle r | (\mu - \Delta + i \tilde{\varphi})^{-1} | r' \rangle . \quad \text{(A3)}$$

(We should note that for $\delta > 0$ and $u_{aa} = 0$ the $\varphi^{(a)}$ integral in equation (A2) still is ill-defined. This is easily cured by adding an appropriate regularizing factor.) The resolvent (A3) in the standard way can be expressed as two spin expectation value of a zero component spin field to yield

$$\tilde{Z}(\mu^{(1)}, .., \mu^{(a)}) = \int \prod_a D[\varphi^{(a)}, \tilde{\varphi}^{(a)}] \exp\left[i \sum_a \int \tilde{\varphi}^{(a)} \varphi^{(a)} - \right.$$

$$\left. - \frac{1}{2} \sum_{a,b} u_{ab} \int \varphi^{(a)} \varphi^{(b)} \right] \prod_a \left\{ \int D[\sigma^{(a)}] \int \mathrm{d}^d r \, \mathrm{d}^d r' \, \sigma_1^{(a)}(r) \, \sigma_1^{(a)}(r') \right.$$

$$\left. \times \exp\left[- \frac{1}{2} \sum_{\alpha=1}^{n} \int \sigma_\alpha^{(a)} (\mu^{(a)} - \Delta + i \tilde{\varphi}^{(a)}) \, \sigma_\alpha^{(a)} \right] \right\} \Bigg|_{n=0} \quad \text{(A4)}$$

Now the $\tilde{\varphi}^{(a)}$ integral yields a continuous product of δ-functions which guarantees that $\varphi^{(a)}(r) \equiv \frac{1}{2} (\sigma^{(a)}(r))^2$. Equation (2.4) results.

Appendix B.

Relation to star polymers.

We consider a four-arm star, with arms S_1, $S_2(S_3, S_4)$ built out of monomers of species 1 or 2, respectively. The Laplace transform of the star partition function $\mathfrak{Z}_*(S_1, .., S_4)$ can be mapped on an expectation value involving four $n = 0$ spin fields :

$$\int_0^\infty \prod_{j=1}^{4} (\mathrm{d}S_j \, \mathrm{e}^{-\mu_j S_j}) \, \mathfrak{Z}_*(S_1, .., S_4) = \int \prod_{j=1}^{4} \mathrm{d}^d r_j \left\langle \prod_{j=1}^{4} \sigma_1^{(j)}(0) \, \sigma_1^{(j)}(r_j) \right\rangle^{\mathcal{H}'} \tag{B1}$$

(We arbitrarily fix the core of the star at $r = 0$.) The Hamiltonian $\mathcal{H}'$ is of the form (2.3), but with two $n = 0$ fields for each chemical species ($\sigma^{(1)}$, $\sigma^{(2)}$ · species 1, $\sigma^{(3)}$, $\sigma^{(4)}$ · species 2). Each field has its own mass μ_j.

It is easily checked that the expectation value in (A1) is multiplicatively renormalizable, the basic relation reading on the level of vertex functions

$$\Gamma_*(q_1, .., q_4) = Z_* \, \Gamma_{*\mathrm{R}}\left(\frac{q_1}{\kappa}, .., \frac{q_4}{\kappa}; g_{11}, g_{22}, g_{12} \right) . \tag{B2}$$

Here q_j is conjugate to r_j. In the exceptional situation $\sum q_j = 0$, $\mu_1 \equiv \mu_2$, $\mu_3 \equiv \mu_4$ the unrenormalized function Γ_* can be expressed as derivative of $\Gamma_{12}^{(4)}$ as calculated from the ternary model

$$\Gamma_* = \frac{\partial}{\partial u_{12}} \Gamma_{12}^{(4)} . \tag{B3}$$

Renormalizing this equation with the help of equation (2.29ii) and using the fact that $\Gamma_{\mathrm{R},12}^{(4)}$ depends on u_{12} only *via* g_{12} we find an expression for Z_*

$$Z_* = Z^{(1)} Z^{(2)} \kappa^{-\varepsilon} \left(\frac{\partial g_{12}}{\partial u_{12}} \bigg|_{\Lambda, \kappa, u_{11}, u_{22} \text{ fixed}} \right)^{-1} \tag{B4}$$

Taking the logarithmic derivative with respect to λ we find

$$\eta_*(g_{11}, g_{22}, g_{12}) \equiv \lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} \bigg|_{u_{cd}, \Lambda \text{ fixed}} \ln Z_* = \eta(g_{11}) + \eta(g_{22}) - \varepsilon - \frac{\partial}{\partial g_{12}} W_{12}(g_{11}, g_{22}, g_{12}) \tag{B5}$$

where

$$\eta(g_{aa}) = \lambda \frac{\mathrm{d}}{\mathrm{d}\lambda} \bigg| \ln Z^{(a)} \tag{B6}$$

with fixed point values given in equation (2.38). At the fixed points equation (B5) yields

$$\eta_*(\mathrm{P}) = \eta(g_{11}^*) + \eta(g_{22}^*) - \varepsilon - \omega_{12}(\mathrm{P}) \tag{B7}$$

where $\mathrm{P} = (g_{11}^*, g_{22}^*, g_{12}^*)$ stands for fixed points G, U, U′ or S.

We note that at the symmetric fixed point S we can calculate $\eta_*(\mathrm{S})$ also within the framework of the normal $O(n)$ model, just interpreting the $\sigma_1^{(j)}$, $j = 1, .., 4$ as different components of a single spin field and taking all masses $\mu^{(j)}$ equal. The composite operator

$\prod_j \sigma_1^{(j)}(r)$ then is in the class of operators discussed in reference [8] to three-loop order ([1]), and a comparison with our formulation yields

$$\eta_*(S) = -(2-\eta)\,\alpha_4 \tag{B8}$$

where α_4 to $O(\varepsilon^3)$ can be taken from reference [8], equation (5) with $k=4$, $n=0$. This allows for an independent check of our result for $\omega_{12}(S)$.

η_* can also be determined in Monte Carlo simulations of four arm stars. To show this we invert the Laplace transformation (B1) to derive the relation of $\mathcal{Z}_*(S_1, .., S_4)$ to its renormalized counterpart

$$\mathcal{Z}_*(S_1, .., S_4) = \exp\{\mu_c^{(1)}(S_1+S_2) + \mu_c^{(2)}(S_3+S_4)\} \times \\ \times (Z_2^{(1)} Z_2^{(2)})^2 Z_*^{-1} \mathcal{Z}_{*R}(S_{R1}^{(1)}, S_{R2}^{(1)}, S_{R3}^{(2)} S_{R4}^{(2)}) \tag{B9}$$

$$S_{R_j}^{(a)} = \kappa^2 \frac{Z_2^{(a)}}{Z^{(a)}} S_j\,. \tag{B10}$$

Here $\mu_c^{(a)}$ is the segment chemical potential of an infinitely long chain of species (a). The variables $S_{R_j}^{(a)}$ can be replaced [5] by $\lambda R_j/\ell$, where R_j is a measure of the size of a polymer coil of contour length $\sim S_j$ of the appropriate species. It, for instance, could be identified with the radius of gyration. ℓ is some microscopic length parameter. Close to a fixed point equations (B5), (B6), (2.32) yield

$$Z_2^{(a)} \sim \lambda^{1/\nu(g_{aa}^*) - 2 + \eta(g_{aa}^*)} \\ Z_* \sim \lambda^{\eta_*(g_{11}^*, g_{22}^*, g_{12}^*)} \tag{B11}$$

Equations (2.36), (2.37) result, which form the basis of our discussion in the main text.

Appendix C.

Borel resummation [13].

Given a formal power series

$$A(x) = \sum_k A_k x^k \tag{C1}$$

with the asymptotic behaviour of A_k being of the form (2.43) we consider the Borel transform

$$B_b(t) = \sum_{k=0}^{\infty} \frac{A_k}{\Gamma(k+b+1)} t^k \tag{C2}$$

where b is used as adjustable parameter to be discussed below. The series (C2) converges for $|t| < 1/a$, and inverting the transformation we find

$$A(x) = \int_0^\infty \mathrm{d}t\, t^b \mathrm{e}^{-t} B_b(xt)\,, \tag{C3}$$

([1]) This has been pointed out to us by B. Duplantier.

Assuming that all singularities of $A(x)$ are located on the negative real axis we use the conformal mapping

$$U = \frac{(1 + axt)^{1/2} - 1}{(1 + axt)^{1/2} + 1} \tag{C4}$$

to map the domain of integration in equation (C3) into the region of convergence of the Borel transform. This yields

$$B_b(xt) = \sum_k U_k (U(xt))^k \tag{C5}$$

where the U_k can be calculated from the A_k. Following reference [9] we furthermore extract a possible power type singularity at $U = 1$ in the form

$$B_{b,\alpha}(xt) = (1 - U(xt))^\alpha B_b(xt) \tag{C6}$$

thus introducing the second fit parameter α. The fit parameters α, b are determined by minimizing the difference between successive approximations constructed by restricting the series of $B_{b,\alpha}$ in powers of U to the first few terms. It turns out that the results are fairly insensitive to b. Having at hand the $x \equiv \varepsilon$-expansion to $O(\varepsilon^3)$ we in the U-expansion are restricted to third order. As with other applications of that method to ε-expansion of exponents it turns out that our final result for $\varepsilon = 1$ is fairly insensitive to the order to which the U-expansion is restricted and in fact is close to a simple (2, 2)-Padé approximant to the original series.

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