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Corrections to scaling in multicomponent polymer solutions

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We calculate the correction-to-scaling exponent ω_T that characterizes the approach to the scaling limit in multicomponent polymer solutions. A direct Monte Carlo determination of ω_T in a system of interacting self-avoiding walks gives $\omega_T = 0.415 \pm 0.020$. A field-theory analysis based on five- and six-loop perturbative series leads to $\omega_T = 0.41 \pm 0.04$. We also verify the renormalization-group predictions for the scaling behavior close to the ideal-mixing point.

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I. INTRODUCTION

The behavior of dilute or semidilute solutions of long polymers have been investigated at length by using the renormalization group [1–3], which has explained the scaling behavior observed in these systems and has provided quantitative predictions that become exact when the degree of polymerization becomes infinite. Most of the work has been devoted to binary systems, i.e., to solutions of one polymer species in a solvent. The method, however, can be extended to multicomponent polymer systems, i.e., to solutions of several chemically different polymers. The general theory has been worked out in detail in Refs. [4–6]. In the good-solvent regime in which polymers are swollen, the scaling limit does not change. For instance, the radius of gyration R_g increases as N^ν, where [7,8] $\nu \approx 0.5876$ and N is the length of the polymer. However, the presence of chemically different polymers gives rise to scaling corrections in quantities that are related to the polymer-polymer interaction. In the dilute regime one may consider, for instance, the second virial coefficient B_2 between two polymers of different species. Its scaling behavior is [4–6]

$$B_2 = A(R_{g,1}R_{g,2})^{3/2}[1 + a(R_{g,1}R_{g,2})^{-\omega_T/2} + \cdots + b(R_{g,1}R_{g,2})^{-\omega/2} + \cdots], \tag{1.1}$$

where $R_{g,1}$ and $R_{g,2}$ are the gyration radii of the two polymers, A, a, b are functions of $R_{g,1}/R_{g,2}$, and ω_T, ω are correction-to-scaling exponents. Equation (1.1) is valid for long polymers in the good-solvent regime; more precisely, for $N_1, N_2 \to \infty$ at fixed N_1/N_2 (or, equivalently, at fixed $R_{g,1}/R_{g,2}$), where N_1 and N_2 are the lengths of the two polymers. The exponent ω is the one that controls the scaling corrections in binary systems. The most accurate estimate of the exponent so far yields [7] $\Delta = \omega\nu = 0.517 \pm 0.007^{+0.010}_{-0.000}$, corresponding to $\omega = 0.880 \pm 0.012^{+0.017}_{-0.000}$. The exponent ω_T is an exponent that characterizes multicomponent systems. Perturbative calculations [9,6] indicate that ω_T is quite small, $\omega_T \approx 0.4$. Thus, scaling corrections decrease very slowly in multicomponent systems and can be quite relevant for the values of N_1 and N_2 that can be attained in practice. Therefore, the determination of the scaling behavior in multicomponent systems may require extrapolations in N_1 and N_2, which, in turn, require a precise knowledge of the scaling exponents.

In this paper we improve the previous determinations [9,6] of ω_T. First, we extend the perturbative three-loop calculations of Ref. [6]. We analyze the five-loop expansion of ω_T in powers of $d = 4 - \epsilon$, d being the space dimension, and the six-loop expansion of ω_T in the fixed-dimension massive zero-momentum (MZM) scheme. Second, we compute ω_T by numerical simulations. For this purpose we consider interacting self-avoiding walks and compute the second virial coefficient. A careful analysis of its scaling behavior provides us with an estimate of ω_T. We also consider the ideal-mixing point where the interaction between the two different chemical species vanishes. A renormalization-group analysis of the behavior close to this point was presented in Ref. [6]. An extensive Monte Carlo simulation allows us to verify the theoretical predictions.

The paper is organized as follows. In Sec. II we present our renormalization-group calculations. In Sec. III we determine the correction-to-scaling exponent by means of a Monte Carlo simulation. In Sec. IV we discuss the ideal-mixing point where the effective interaction between the two chemically different species vanishes. Conclusions are presented in Sec. V.

II. PERTURBATIVE DETERMINATION OF ω_T

The starting point of the calculation is the Landau-Ginzburg-Wilson Hamiltonian [6]

$$\mathcal{H} = \int d^d x \left\{ \tfrac{1}{2}[(\partial_\mu \phi_1)^2 + (\partial_\mu \phi_2)^2 + r_1 \phi_1^2 + r_2 \phi_2^2] + \tfrac{1}{4!}(u_0 \phi_1^4 + 2 w_0 \phi_1^2 \phi_2^2 + v_0 \phi_2^4) \right\}, \tag{2.1}$$

where ϕ_1 and ϕ_2 are n-component fields. As usual, the poly-

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mer theory is obtained in the limit $n \to 0$. In this specific case, the fixed-point structure of the theory is particularly simple and is explained in detail in Ref. [6]. One finds that the β functions satisfy the following properties: $\beta_u(u,v,w) = \bar{\beta}(u)$, $\beta_v(u,v,w) = \bar{\beta}(v)$, $\beta_w(g,g,g) = \bar{\beta}(g)$, where $\bar{\beta}(g)$ is the β function in the vector $O(n=0)\varphi^4$ model and u, v, w are renormalized four-point couplings normalized so that $u \approx Cu_0$, $v \approx Cv_0$, $w \approx Cw_0$ at tree level, C being a constant. The relevant fixed point is the symmetric one $u^* = v^* = w^* = g^*$, where g^* is the zero of $\bar{\beta}(g)$. The exponent ω_T is given by

$$\omega_T = \left. \frac{\partial \beta_w}{\partial w} \right|_{u=v=w=g^*}. \tag{2.2}$$

The exponent ω_T can be computed directly in the $O(n=0)\varphi^4$ model. Indeed, as discussed in Ref. [6], $\omega_T = -y_4$, where y_4 is the renormalization-group dimension of $\phi_1^2 \phi_2^2$ in the symmetric theory with $u_0 = v_0 = w_0$. It corresponds to an $O(2n)$ vector theory and, for $n \to 0$, one is back to the $O(n=0)\varphi^4$ model. Using the results of Ref. [10] one can also show that, for $n \to 0$, $\phi_1^2 \phi_2^2$ is a spin-4 perturbation of the $O(2n)$ model and thus y_4 is the renormalization-group dimension of the cubic-symmetric perturbation $\Sigma_a \varphi_a^4$ of the $O(n=0)\varphi^4$ model. Thus, one can use the perturbative expansions reported in Refs. [11,12]. The ϵ expansion of ω_T is

$$\omega_T = \tfrac{1}{2}\epsilon - \tfrac{19}{64}\epsilon^2 + 0.777\,867\epsilon^3 - 2.652\,11\epsilon^4 + 11.0225\epsilon^5 + O(\epsilon^6). \tag{2.3}$$

At order ϵ^3 it agrees with that given in Ref. [6]. In the fixed-dimension MZM scheme we have at six loops

$$\omega_T = -1 + \tfrac{3}{2}g - \tfrac{185}{216}g^2 + 0.916\,668g^3 - 1.228\,68g^4 + 1.975\,99g^5 - 3.597\,53g^6 + O(g^7), \tag{2.4}$$

where g is the four-point zero-momentum renormalized coupling normalized so that $\bar{\beta}(g) = -g + g^2 + O(g^3)$, as used in, e.g., Ref. [13]; the fixed point corresponds to [14–18] $g^* = 1.40 \pm 0.02$. In order to obtain quantitative predictions, the perturbative series must be properly resummed. We use here the conformal-mapping method [13,19] that takes into account the large-order behavior of the perturbative series.

From the standard ϵ expansion we obtain in three dimensions ($\epsilon = 1$) $\omega_T = 0.42 \pm 0.04$, while in the fixed-dimension MZM scheme we find $\omega_T = 0.37 \pm 0.04$. Using the pseudo-ϵ expansion, Ref. [20] obtained $\omega_T = 0.380 \pm 0.018$ in the MZM scheme. Though compatible, the MZM result is lower than the ϵ-expansion one. This phenomenon also occurs for other exponents and is probably related to the nonanalyticity of the renormalization-group functions at the fixed point [14,21,15,16].

A more precise estimate is obtained by considering $\zeta \equiv \omega_T - \omega/2$. The perturbative expansion of ζ has smaller coefficients than that of ω_T and thus ζ can be determined more precisely. Its ϵ expansion is

$$\zeta = \tfrac{1}{32}\epsilon^2 - 0.133\,936\epsilon^3 + 0.490\,572\epsilon^4 - 2.414\,05\epsilon^5 + O(\epsilon^6). \tag{2.5}$$

The term proportional to ϵ is missing, while the other coefficients are smaller by a factor of 5–10 approximately. Similar cancellations occur in the MZM scheme,

$$\zeta = -\tfrac{1}{2} + \tfrac{1}{2}g - \tfrac{85}{432}g^2 + 0.136\,823g^3 - 0.110\,394g^4 + 0.074\,425g^5 + 0.024\,718g^6 + O(g^7). \tag{2.6}$$

Resumming the perturbative series, we obtain

$$\zeta = -0.006 \pm 0.009 \quad (\text{MZM}),$$

$$\zeta = -0.008 \pm 0.012 \quad (\epsilon\,\text{exp}). \tag{2.7}$$

We can combine these estimates with those for ω. If we use the Monte Carlo result of Ref. [7] reported in the Introduction, we obtain

$$\omega_T = 0.433 \pm 0.016^{+0.008}_{-0.000}. \tag{2.8}$$

If instead we use the field-theory estimates of ω reported in Ref. [17], we obtain

$$\omega_T = 0.399 \pm 0.018 \quad (\text{MZM}),$$

$$\omega_T = 0.407 \pm 0.022 \quad (\epsilon\,\text{exp}). \tag{2.9}$$

Collecting results, we estimate

$$\omega_T = 0.41 \pm 0.04, \tag{2.10}$$

where the error should be quite conservative.

III. MONTE CARLO RESULTS

In order to determine ω_T numerically, we consider lattice self-avoiding walks (SAWs) with an attractive interaction $-\epsilon$ between nonbonded nearest-neighbor pairs. If $\beta \equiv \epsilon/kT$ is the reduced inverse temperature, this model describes a polymer in a good solvent as long as $\beta < \beta_\theta$, where $\beta_\theta \approx 0.269$ corresponds to the collapse θ transition [22,23]. We consider two walks with different interaction energies ϵ_1 and ϵ_2, i.e., with different β_1 and β_2. We assume $\beta_1, \beta_2 < \beta_\theta$, so that both walks are in the good-solvent regime. Then, we consider the second virial coefficient

$$B_2(N_1,N_2;\beta_1,\beta_2,\beta_{12}) \equiv \frac{1}{2}\int d^3\mathbf{r}\langle 1 - e^{-H(1,2)}\rangle_{\mathbf{0},\mathbf{r}}, \tag{3.1}$$

where the statistical average is over all pairs of SAWs such that the first one starts at the origin, has N_1 steps, and corresponds to an inverse reduced temperature β_1; the second one starts at $\mathbf{r}$, has N_2 steps, and corresponds to an inverse reduced temperature β_2. Here $H(1,2)$ is the reduced interaction energy: $H(1,2) = +\infty$ if the two walks intersect each other; otherwise, $H(1,2) = -\beta_{12}\mathcal{N}_{nnc}$, where $\mathcal{N}_{nnc}$ is the number of nearest-neighbor contacts between the two walks and $\beta_{12} \equiv \epsilon_{12}/kT$ is the reduced inverse temperature. In order to generate the walks we use the pivot algorithm [24–28] with a Metropolis test, while the second virial coefficient is determined by using the hit-or-miss algorithm discussed in Ref. [29]. We study the invariant ratio

$$A_2(N_1,N_2;\beta_1,\beta_2,\beta_{12}) = \frac{B_2(N_1,N_2;\beta_1,\beta_2,\beta_{12})}{[R_g(N_1;\beta_1)R_g(N_2;\beta_2)]^{3/2}}, \tag{3.2}$$

where $R_g(N;\beta)$ is the radius of gyration. This quantity is directly related to the interpenetration ratio Ψ that is extensively discussed in the polymer literature, $\Psi \equiv 2(4\pi)^{-3/2}A_2$. As we have already discussed, in the limit $N_1,N_2\to\infty$ at $R_g(N_2;\beta_2)/R_g(N_1;\beta_1)$ fixed, A_2 obeys a scaling law of the form [6]

$$A_2(N_1,N_2;\beta_1,\beta_2,\beta_{12}) = f\left(\frac{R_g(N_2;\beta_2)}{R_g(N_1;\beta_1)}\right), \tag{3.3}$$

where $f(x)$ is universal. This applies for β_1, $\beta_2<\beta_\theta$ and, as we shall see, for β_{12} sufficiently small. Note that all the dependence on the inverse temperatures is encoded in a function of a single variable. Moreover, $f(x)$ is also the scaling function associated with a polymer solution made of two different types of polymers that have the same chemical composition (hence $\beta_1=\beta_2=\beta_{12}$) but different lengths. In that case $R_g(N_2;\beta_2)/R_g(N_1;\beta_1)=(N_2/N_1)^\nu$, so that Eq. (3.3) implies that $A_2(N_1,N_2;\beta,\beta,\beta)=g(N_1/N_2)$, with $g(x)=f(x^\nu)$ universal. The function $f(x)$ satisfies the condition $f(x)=f(1/x)$ and de Gennes' relation [30] $f(x)\sim x^p$, $p=3/4-1/(2\nu)$, for $x\to 0$.

We will be interested here in the corrections to Eq. (3.3). In the scaling limit we can write

$$A_2(N_1,N_2;\beta_1,\beta_2,\beta_{12}) = f(\rho) + \sum_{n+m\geq 1}\frac{a_{nm}(\beta_1,\beta_2,\beta_{12})}{x^{n\omega_T+m\omega}} f_{nm}(\rho) + \cdots, \tag{3.4}$$

where

$$\rho \equiv R_g(N_2;\beta_2)/R_g(N_1;\beta_1),$$

$$x \equiv [R_g(N_2;\beta_2)R_g(N_1;\beta_1)]^{1/2},$$

and we have neglected the contributions of the additional correction-to-scaling operators with renormalization-group dimensions $-\omega_i$. They give rise to additional corrections proportional to x^{-p}, $p=n\omega_T+m\omega+\Sigma n_i\omega_i$. Little is known about ω_i, though we expect them to satisfy $\omega_i>\omega_T$, $\omega_i>\omega$. In the following we will assume that all such exponents satisfy $\omega_i \gtrsim 3\omega_T \approx \omega_T+\omega$. The scaling functions $g_{nm}(\rho)$ are universal once a specific normalization has been chosen. Instead, the coefficients a_{nm} depend on the model and, in particular, on the specific values of the parameters β_1, β_2, and β_{12}.

We have simulated two SAWs with $\beta_1=0.05$ and $\beta_2=0.15$, two values that are well within the good-solvent region. Then, we have computed A_2 for $100\leqslant N_1=N_2\leqslant 64\,000$ and several values of β_{12} in the range $0\leqslant\beta_{12}\leqslant 0.30$. The results are plotted in Fig. 1. For $\beta_{12}<0.25$, as $N=N_1=N_2$ increases, the estimates of A_2 tend to become independent of β_{12} although the convergence is very slow. The behavior changes for $\beta_{12}\gtrsim 0.25$ and indeed the data indicate that $A_2=0$ for $N\to\infty$ for some $\beta_{12}=\beta_{12,c}$ slightly larger than 0.25. This value corresponds to the case in which the short-distance repulsion is exactly balanced by the solvent-induced attraction proportional to β_{12}. In field-theoretical terms, this means that the renormalization-group flow is no longer attracted by the symmetric fixed point discussed in Sec. II, but rather by the unstable fixed point with $w^*=0$. Thus, at $\beta_{12}=\beta_{12,c}$ there is effectively no interaction between the chemically different polymers. For $\beta_{12}>\beta_{12,c}$, A_2 becomes negative signaling demixing. The behavior of A_2 does not change significantly if β_1 and β_2 are varied. In Fig. 2 we report results for shorter walks for different pairs of β_1 and β_2, and also for walks with $N_1=4N_2$. Note that $\beta_{12,c}$ depends very little on the parameters β_1 and β_2.

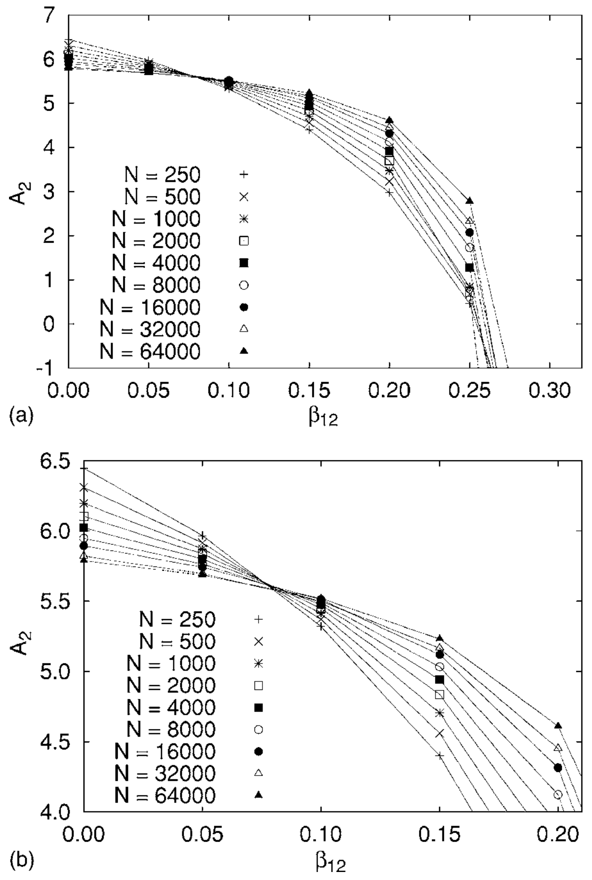

FIG. 1. Invariant ratio A_2 for $\beta_1=0.05$, $\beta_2=0.15$ vs β_{12} for several $N=N_1=N_2$. The two figures differ only by the vertical and horizontal scales. Lines connecting points with different β_{12} are only intended to guide the eye.

In order to determine ω_T, we have considered the data with $\beta_{12}=0$, 0.05, 0.10, 0.15 that are sufficiently far from the critical value $\beta_{12,c}$. We performed a fit that is linear in ω_T,

$$\ln[A_2(N;\beta_{12}=0) - A_2(N;\beta_{12})] = c_1(\beta_{12}) - \omega_T\ln x + \frac{c_2(\beta_{12})}{x^{\omega_a}} + \frac{c_3(\beta_{12})}{x^{\omega_b}}, \tag{3.5}$$

where $\beta_{12}=0.05$, 0.10, 0.15. The exponents ω_a and ω_b should take into account the additional scaling corrections. Since $2\omega_T\approx\omega$, we should have $\omega_a\approx\omega_T\approx\omega-\omega_T$. Using the field-

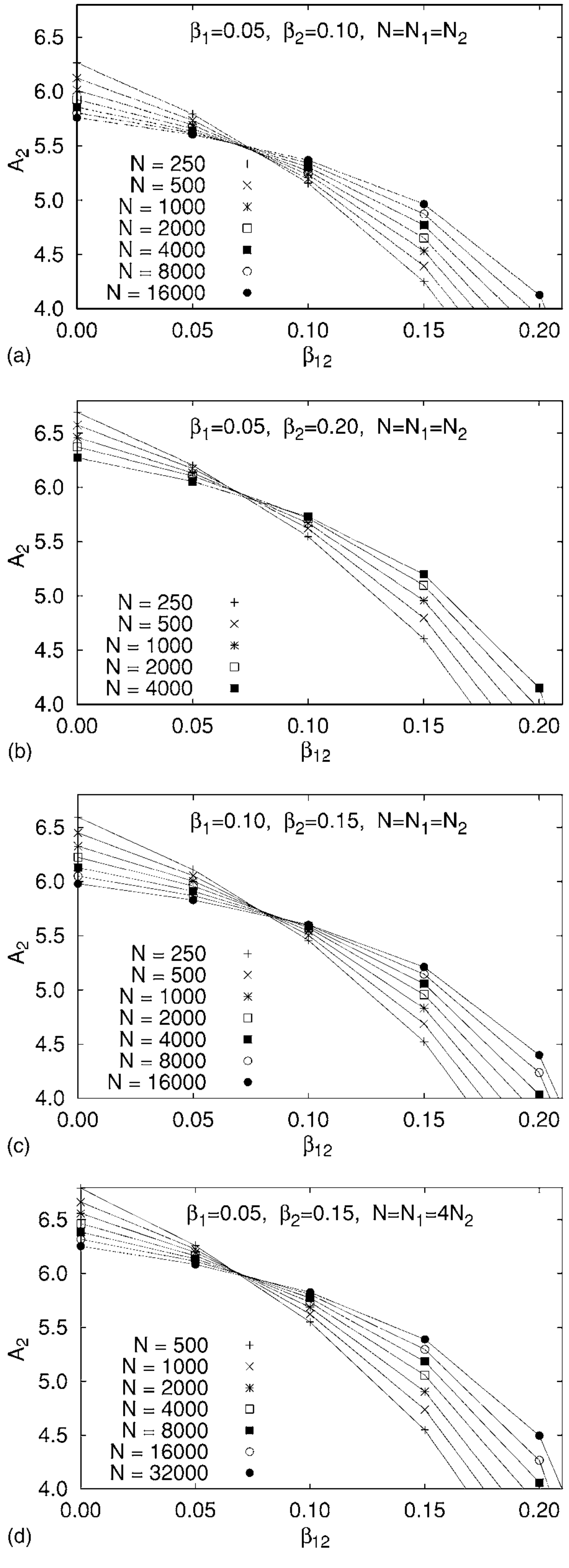

FIG. 2. Invariant ratio A_2 for different choices of β_1 and β_2 vs β_{12}.

theory estimate of ω_T and $\omega \approx 0.88 \pm 0.03$ (Ref. [7]), it should be safe to take [31] $\omega_a = 0.43 \pm 0.06$. As for ω_b we should have $\omega_b \approx 2\omega_T \approx \omega$. Moreover, there is also the possibility that there exists an additional correction exponent ω_1 not very much different from $3\omega_T$, which would contribute a correction with exponent $\omega_1 - \omega_T$. For this reason we have taken $\omega_b = 0.85 \pm 0.20$. The error should be large enough to include all possibilities. The results are reported in Table I. The systematic error reported there gives the variation of the estimate as ω_a and ω_b vary within the reported errors. The results with $N_{\min} = 250$ and 500 are compatible within errors and thus we can take the estimate that corresponds to $N_{\min} = 500$ as our final result. To be conservative, however, the error bar takes also into account the possibility that the observed small trend is a real one. If the neglected corrections are of order $x^{-3\omega_T}$ we expect the results to depend on $N_{\min}$ as $N_{\min}^{-3\nu\omega_T} \approx N_{\min}^{-0.7}$. This implies that the estimate of ω_T can decrease at most by 0.005 when $N_{\min}$ is further increased. This leads to the result

$$\omega_T = 0.415 \pm 0.020. \tag{3.6}$$

As a check we perform a nonlinear fit of the form (fit 2)

$$A_2(N;\beta_{12}) = A_2^* + \frac{a_1(\beta_{12})}{x^{\omega_T}} + \frac{a_2(\beta_{12})}{x^{2\omega_T}} + \frac{a_3(\beta_{12})}{x^{3\omega_T}}; \tag{3.7}$$

since, $x \sim N^\nu$, we can also fit the data to (fit 3)

$$A_2(N;\beta_{12}) = A_2^* + \frac{a_1(\beta_{12})}{N^{\Delta_T}} + \frac{a_2(\beta_{12})}{N^{2\Delta_T}} + \frac{a_3(\beta_{12})}{N^{3\Delta_T}}, \tag{3.8}$$

where $\Delta_T = \omega_T \nu$. The results are reported in Table I. They agree with those obtained before and allow us to estimate the universal constant A_2^* [$A_2^* = f(\rho)$ for $\rho \approx 1.24$; $f(\rho)$ is defined in Eq. (3.3)]: $A_2^* = 5.495 \pm 0.020$ (the corresponding interpenetration ratio is $\Psi^* = 0.2467 \pm 0.0009$).

IV. IDEAL-MIXING POINT

In this section we consider the behavior close to the ideal-mixing point (IMP) $\beta_{12,c}$ where the effective interaction between the two chemically different species vanishes. The renormalization-group analysis is presented in Ref. [6]. The behavior is controlled by an unstable fixed point characterized by an unstable direction with renormalization-group dimension $y_I = 2/\nu - 3$ and by a stable direction with exponent $-\omega$, where $\omega \approx 0.88$ is the usual correction-to-scaling exponent. These results imply that close to the IMP a renormalization-group invariant quantity $\mathcal{R}$ (for instance, the invariant ratio A_2 introduced above) scales as

$$\begin{aligned}\mathcal{R}(\beta_{12}) &= f_{\mathcal{R}}[(\beta_{12} - \beta_{12,c})(R_{g,1}R_{g,2})^{y_I/2}, R_{g,1}/R_{g,2}] \\ &\quad + \frac{1}{(R_{g,1}R_{g,2})^{\omega/2}} g_{\mathcal{R}}[(\beta_{12} - \beta_{12,c})(R_{g,1}R_{g,2})^{y_I/2}, R_{g,1}/R_{g,2}].\end{aligned} \tag{4.1}$$

In this section we wish to verify this scaling behavior for the second virial coefficient. For this purpose we have made simulations for six different pairs of β_1 and β_2 with $N_1 = N_2$ and $0.25 \leqslant \beta_{12} \leqslant 0.28$. Since $N_1 = N_2 = N$ and $R_g(N;\beta) \approx a(\beta)N^\nu$, we can rewrite the previous equation as

TABLE I. Results of the fits. When two errors are quoted, the first one is the statistical error, while the second one is the systematic error. DOF is the number of degrees of freedom of the fit. Fit 3 provides an estimate of $\Delta_T=\nu\omega_T$. We compute $\omega_T=\Delta_T/\nu$ by using $\nu=0.5876\pm0.0001$.

Type	$N_{\min}$	ω_T	A_2^*	χ^2	DOF
fit 1	100	$0.424\pm0.002\pm0.004$		15.2	20
fit 1	250	$0.418\pm0.004\pm0.006$		12.4	17
fit 1	500	$0.415\pm0.007\pm0.008$		11.8	14
fit 2	100	0.426 ± 0.015	5.498 ± 0.011	32.2	26
fit 2	250	0.421 ± 0.030	5.495 ± 0.018	32.1	22
fit 3	100	0.426 ± 0.015	5.499 ± 0.011	32.1	26
fit 3	250	0.423 ± 0.029	5.496 ± 0.017	32.0	22

$$\mathcal{R}(N;\beta_1,\beta_2,\beta_{12}) = \hat{f}_{\mathcal{R}}(b,\rho) + \frac{1}{N^{\Delta}}\hat{g}_{\mathcal{R}}(b,\rho),$$

$$b \equiv (\beta_{12}-\beta_{12,c})N^{\phi},$$

$$\rho \equiv R_g(N;\beta_1)/R_g(N;\beta_2), \tag{4.2}$$

where $\beta_{12,c}$ also depends on β_1 and β_2, and

$$\phi \equiv \nu y_I = 2-3\nu = 0.2372 \pm 0.0003. \tag{4.3}$$

The critical value $\beta_{12,c}$ can be characterized by requiring $A_2(N\to\infty;\beta_1,\beta_2,\beta_{12,c})=0$. We can also define a finite-N IMP as the value of β_{12} where $A_2(N;\beta_1,\beta_2,\beta_{12})$ vanishes (this is the analogous of the Boyle point in θ solutions): we define $\beta_{12,c}^{\mathrm{eff}}(N)$ such that

$$A_2[N;\beta_1,\beta_2,\beta_{12,c}^{\mathrm{eff}}(N)] = 0. \tag{4.4}$$

Inserting in Eq. (4.2) we obtain for $N\to\infty$ the behavior

$$\beta_{12,c}^{\mathrm{eff}}(N) = \beta_{12,c} + \frac{a}{N^{\omega+\phi}}. \tag{4.5}$$

Finally, we can replace $\beta_{12,c}$ with $\beta_{12,c}^{\mathrm{eff}}(N)$ in Eq. (4.2) obtaining the equivalent form

$$\mathcal{R}(N;\beta_1,\beta_2,\beta_{12}) = \hat{f}_{\mathcal{R}}[(\beta_{12}-\beta_{12,c}^{\mathrm{eff}})N^{\phi},\rho] + \frac{1}{N^{\Delta}}\bar{g}_{\mathcal{R}}[(\beta_{12}-\beta_{12,c}^{\mathrm{eff}})N^{\phi},\rho], \tag{4.6}$$

where $\bar{g}_{\mathcal{R}}(b,\rho)$ vanishes at the IMP $b=0$. Equation (4.6) is more suitable for a numerical check close to the IMP than Eq. (4.2), since scaling corrections vanish at the IMP and are therefore small close to it. In the following we verify numerically predictions (4.5) and (4.6).

In Fig. 3 we show $\beta_{12,c}^{\mathrm{eff}}(N)$ vs $N^{-\omega-\phi}$ for three different pairs of β_1 and β_2. The data show a quite good linear behavior: only the two points corresponding to $N=2000$ and 4000 are in some cases off the linear fit, probably because our sampling is not yet adequate for these large values of N. These results allow us to obtain $\beta_{12,c}$,

$$\beta_{12,c} = 0.2574 \pm 0.0006, \quad \beta_1 = 0.05, \quad \beta_2 = 0.10,$$

$$\beta_{12,c} = 0.2588 \pm 0.0007, \quad \beta_1 = 0.05, \quad \beta_2 = 0.15,$$

$$\beta_{12,c} = 0.2609 \pm 0.0003, \quad \beta_1 = 0.05, \quad \beta_2 = 0.20,$$

$$\beta_{12,c} = 0.2596 \pm 0.0004, \quad \beta_1 = 0.10, \quad \beta_2 = 0.15,$$

$$\beta_{12,c} = 0.2609 \pm 0.0009, \quad \beta_1 = 0.10, \quad \beta_2 = 0.20,$$

$$\beta_{12,c} = 0.2626 \pm 0.0009, \quad \beta_1 = 0.15, \quad \beta_2 = 0.20.$$

Note that the dependence on β_1 and β_2 is tiny.

Then, we verify Eq. (4.6). In Fig. 4 we report A_2 vs the scaling variable $(\beta_{12}-\beta_{12,c}^{\mathrm{eff}})N^{\phi}$ for different β_1,β_2. All points with $100\leq N\leq 1000$ fall on top of each other confirming the scaling behavior predicted by the renormalization group. The scaling functions depend on β_1 and β_2 through the ratio ρ. Moreover, one should also take into account that the scaling variable is only defined up to an arbitrary prefactor. We now show that the dependence on ρ is tiny for the range of values of ρ we have considered, since all data with different values of N, β_1, and β_2 fall on a single curve once one takes as scaling variable $R(\beta_1,\beta_2)(\beta_{12}-\beta_{12,c}^{\mathrm{eff}})N^{\phi}$, where $R(\beta_1,\beta_2)$ is a properly chosen constant that depends on β_1 and β_2. This is evident in Fig. 5, where we report data with different β_1 and β_2. We only consider $N=500$ for clarity, since we have already verified that data with different values of N show the predicted scaling. The scaling is very good, indicating that the ρ dependence is negligible. If we choose $R(0.05,0.10)=1$ the scaling curve can be parametrized as $A_2=-19.773x-46.457x^2$, with $x=R(\beta_1,\beta_2)(\beta_{12}-\beta_{12,c}^{\mathrm{eff}})N^{\phi}$. Finally, note that $R(\beta_1,\beta_2)$ does not depend very much on β_1 and β_2. For instance, $R(0.15,0.20)/R(0.05,0.10)\approx 0.88$.

V. CONCLUSIONS

In this paper we have considered the corrections to scaling expected in multicomponent polymer solutions. A high-precision Monte Carlo simulation with very long walks, up to $N=64\,000$, gives $\omega_T=0.415\pm0.020$. This estimate is consistent with the estimate $\omega_T=0.41\pm0.04$ obtained by using

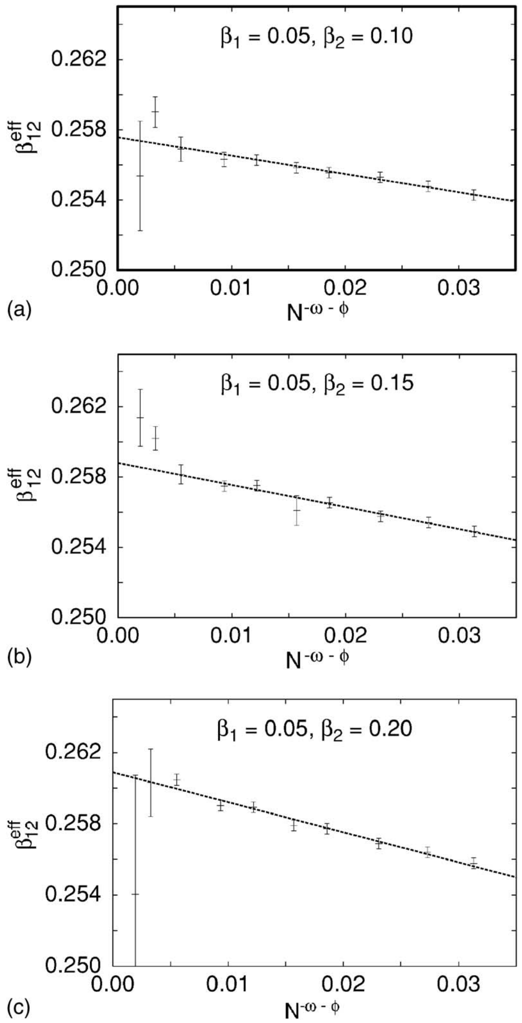

FIG. 3. Finite-N ideal-mixing point $\beta_{12,c}^{\mathrm{eff}}$ vs $1/N^{\omega+\phi}$ for three different pairs of β_1 and β_2. The line corresponds to the fit $\beta_{12,c}^{\mathrm{eff}} = \beta_{12,c} + a/N^{\omega+\phi}$.

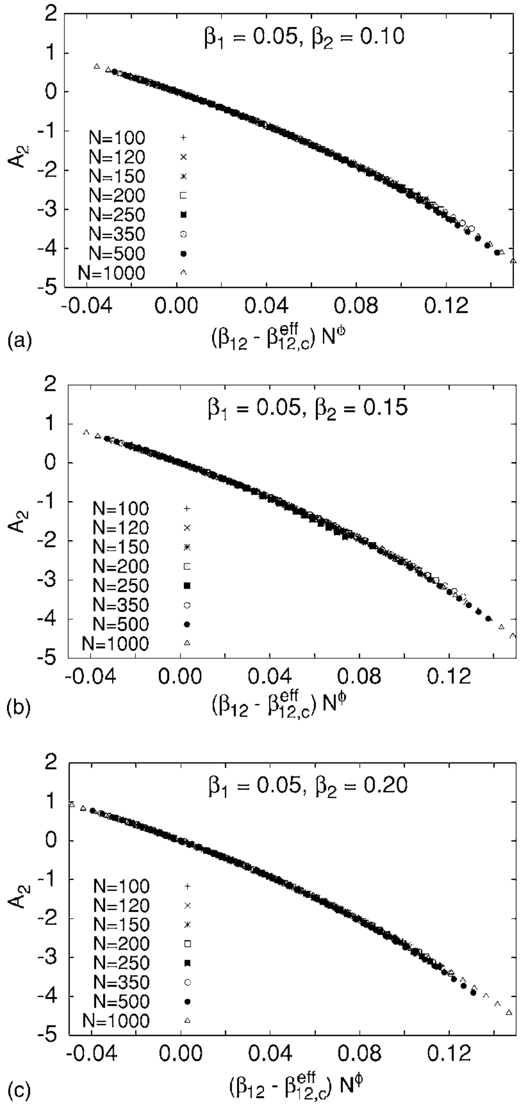

FIG. 4. Invariant ratio A_2 vs $(\beta_{12} - \beta_{12,c}^{\mathrm{eff}})N^{\phi}$ for three different pairs of β_1 and β_2.

the perturbative renormalization group. Previous perturbative renormalization-group calculations gave $\omega_T \approx 0.37$ (Ref. [9]) and $\omega_T \approx 0.40$ (Ref. [6]): they substantially agree with our estimate. On the other hand, the numerical result [6] $\omega_T \approx 0.35$ obtained by exploiting the relation between ω_T and the growth exponent for four-arm star polymers seems slightly too small.

One should note that ω_T is quite small and thus convergence may be quite slow. For instance, in the case we have considered numerically, $A_2^* = 5.495 \pm 0.020$ for $N \to \infty$. On the other hand, for $\beta_{12} = 0$ (respectively, $\beta_{12} = 0.15$) we find $A_2 = 5.790 \pm 0.005$ (respectively, $A_2 = 5.232 \pm 0.005$) for $N = N_1 = N_2 = 64\,000$. Even if the walks are very long, there is still a 5% discrepancy. For $N = 1000$, differences are larger, approximately of 15%.

In order to obtain a better qualitative understanding of the corrections we have also performed additional simulations. The results are reported in Fig. 2. The qualitative behavior is very similar in all cases and almost independent of β_1 and β_2. In particular, corrections appear to vanish in all cases for $0.05 \lesssim \beta_{12} \lesssim 0.10$ and to increase strongly for $\beta_{12} \gtrsim 0.20$. Morever, $\beta_{12,c}$ is always close to β_θ, and shows a tiny dependence on β_1 and β_2.

The discussion presented here addressed the behavior of multicomponent solutions, but it should be noted that the

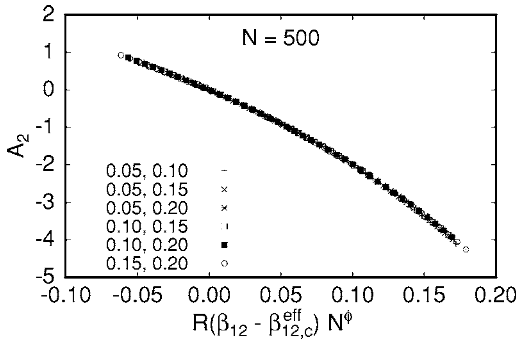

FIG. 5. Invariant ratio A_2 vs $R(\beta_{12} - \beta_{12,c}^{\mathrm{eff}})N^{\phi}$ for $N = 500$. We report results corresponding to six different pairs of β_1 and β_2.

results are also relevant for copolymers in which chemically different polymers are linked together [32]. Also in this case scaling corrections with exponent ω_T are present.

Finally, we have also considered the behavior close to the ideal-mixing point, where there is no effective interaction between the two chemically different polymer species. Our numerical results are in very good agreement with the renormalization-group predictions of Ref. [6].

[1] P. G. de Gennes, *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaca, NY, 1979).

[2] K. F. Freed, *Renormalization Group Theory of Macromolecules* (Wiley, New York, 1987).

[3] L. Schäfer, *Excluded Volume Effects in Polymer Solutions* (Springer-Verlag, Berlin, 1999).

[4] J.-F. Joanny, L. Leibler, and R. Ball, J. Chem. Phys. **81**, 4640 (1984).

[5] L. Schäfer and C. Kappeler, J. Phys. (France) **46**, 1853 (1985).

[6] L. Schäfer, U. Lehr, and C. Kappeler, J. Phys. I **1**, 211 (1991).

[7] P. Belohorec and B. G. Nickel, Guelph University report (unpublished).

[8] At present the most accurate estimates of ν are $\nu=0.587\,58\pm0.000\,07$ (Ref. [7]), $\nu=0.5874\pm0.0002$ [T. Prellberg, J. Phys. A **34**, L599 (2001)], $\nu=0.587\,65\pm0.000\,20$ [H.-P. Hsu, W. Nadler, and P. Grassberger, Macromolecules **37**, 4658 (2004)]. For an extensive list of results, see A. Pelissetto and E. Vicari, Phys. Rep. **368**, 549 (2002).

[9] D. Broseta, L. Leibler, and J.-F. Joanny, Macromolecules **20**, 1935 (1987).

[10] P. Calabrese, A. Pelissetto, and E. Vicari, Phys. Rev. B **67**, 054505 (2003).

[11] H. Kleinert and V. Schulte-Frohlinde, Phys. Lett. B **342**, 284 (1995).

[12] J. M. Carmona, A. Pelissetto, and E. Vicari, Phys. Rev. B **61**, 15136 (2000).

[13] J. C. Le Guillou and J. Zinn-Justin, Phys. Rev. Lett. **39**, 95 (1977); Phys. Rev. B **21**, 3976 (1980).

[14] B. G. Nickel, Physica A **177**, 189 (1991).

[15] S. Caracciolo, M. S. Causo, and A. Pelissetto, Phys. Rev. E **57**, R1215 (1998).

[16] A. Pelissetto and E. Vicari, Nucl. Phys. B **519**, 626 (1998).

[17] R. Guida and J. Zinn-Justin, J. Phys. A **31**, 8103 (1998).

[18] A. Pelissetto and E. Vicari, Nucl. Phys. B **575**, 579 (2000).

[19] J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena*, 3rd ed. (Clarendon, Oxford, 1996).

[20] P. Calabrese and P. Parruccini, Phys. Rev. B **71**, 064416 (2005).

[21] A. D. Sokal, Europhys. Lett. **27**, 661 (1994); **30**, 123(E) (1995).

[22] P. Grassberger and R. Hegger, J. Chem. Phys. **102**, 6881 (1995); P. Grassberger, Phys. Rev. E **56**, 3682 (1997).

[23] We quote here some additional, less precise estimates of β_θ: $\beta_\theta=0.274\pm0.006$ [H. Meirovitch and H. A. Lim, J. Chem. Phys. **91**, 2544 (1989)] and $\beta_\theta=0.276\pm0.006$ [M. C. Tesi, E. J. J. van Rensburg, E. Orlandini, and S. G. Whittington, J. Stat. Phys. **82**, 155 (1996)].

[24] M. Lal, Mol. Phys. **17**, 57 (1969).

[25] B. MacDonald, N. Jan, D. L. Hunter, and M. O. Steinitz, J. Phys. A **18**, 2627 (1985).

[26] N. Madras and A. D. Sokal, J. Stat. Phys. **50**, 109 (1988).

[27] A. D. Sokal, in *Monte Carlo and Molecular Dynamics Simulations in Polymer Science*, edited by K. Binder (Oxford University Press, Oxford, 1995).

[28] T. Kennedy, J. Stat. Phys. **106**, 407 (2002).

[29] B. Li, N. Madras, and A. D. Sokal, J. Stat. Phys. **80**, 661 (1995).

[30] P. G. de Gennes, talk given at the Yeshiva meeting on statistical mechanics, Fall 1980; cited in Ref. [6].

[31] A precise estimate of $\omega-\omega_T$ can be obtained by writing it as $\omega/2-\zeta$. Using the estimate of Ref. [7] for ω and the estimate of ζ reported in Sec. II we find $\omega-\omega_T=0.447\pm0.025$.

[32] These considerations do not apply to the Widom-Rowlinson model of diblock copolymers considered in C. I. Addison, J. P. Hansen, V. Krakoviack, and A. A. Louis, Mol. Phys. **103**, 3045 (2005), since the two polymers are ideal. In this case scaling corrections are controlled by exponent ω_S, whose ϵ expansion is $\omega_S=\epsilon-\frac{1}{2}\epsilon^2+1.151\,54\epsilon^3-4.204\,39\epsilon^4+16.9338\epsilon^5+O(\epsilon^6)$. A Padé-Borel resummation gives $\omega_S=0.77\pm0.02$. A three-loop analysis gives $\omega_S\approx0.82$ (Ref. [6]).