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FAST TRACK COMMUNICATION

Renormalized four-point coupling constant in the three-dimensional $O(N)$ model with $N \to 0$

Andrea Pelissetto[1] **and Ettore Vicari**[2]

[1] Dipartimento di Fisica and INFN, Sezione di Roma I, Università degli Studi di Roma La Sapienza, Piazzale Moro 2, I-00185 Roma, Italy
[2] Dipartimento di Fisica and INFN, Sezione di Pisa, Università degli Studi di Pisa, Largo Pontecorvo 2, I-56127 Pisa, Italy

E-mail: Andrea.Pelissetto@roma1.infn.it and Ettore.Vicari@df.unipi.it

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Abstract

We simulate self-avoiding walks on a cubic lattice and determine the second virial coefficient for walks of different lengths. This allows us to determine the critical value of the renormalized four-point coupling constant in the three-dimensional N-vector universality class for $N = 0$. We obtain $\bar{g}^* = 1.4005(5)$, where $\bar{g}$ is normalized so that the three-dimensional field-theoretical β function behaves as $\beta(\bar{g}) = -\bar{g} + \bar{g}^2$ for small $\bar{g}$. As a byproduct, we also obtain precise estimates of the interpenetration ratio Ψ^*, $\Psi^* = 0.246\,85(11)$ and of the exponent ν, $\nu = 0.5876(2)$.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

In the last 30 years, there has been a significant progress in the understanding of critical phenomena. The conceptual setting is now well understood and we are now in a position to check the general framework by comparing the experimental and theoretical results and the different theoretical methods among themselves. The most precise experimental and theoretical results have been obtained for $O(N)$ systems in which the order parameter is an N-component vector and the symmetry breaking pattern corresponds to $O(N) \to O(N-1)$ [1]. With the increase of the precision of the theoretical and experimental estimates, some small discrepancies are beginning to emerge: for instance, there is at present a discrepancy between the experimental [2, 3] and the theoretical [4–6] estimates of the specific-heat exponent α for the three-dimensional XY universality class ($N = 2$); analogously, there are tiny discrepancies between the most precise field-theoretical estimates [7] of γ for the three-dimensional Ising ($N = 1$) and polymer systems ($N = 0$) and those obtained by using high-temperature and Monte Carlo methods [8–12]. These differences should not be taken as an indication of the

failure of the general framework; most likely, they are due to a too optimistic determination of the error bars on the results. For instance, numerical results are affected by scaling corrections which are difficult to take into account, while field-theoretical results may converge slowly due to nonanalyticities of the renormalization-group functions [13–18][3].

The case $N = 0$ is a good testing ground for the different theoretical methods. Indeed, there is a well-known mapping between the $N = 0$ universality class and the statistical model of self-avoiding walks (SAWs) [20]. SAWs can be very efficiently simulated by using several algorithms. In particular, in three dimensions, the pivot algorithm [21–25] allows one to obtain an independent measurement of a global quantity in a time of the order of $\xi^{0.85/\nu} \sim \xi^{1.45}$ (in SAWs the correlation length ξ can be identified with the end-to-end distance) [25], to be compared with conventional algorithms for spin systems in which the autocorrelation time scales as ξ^{3+z}, where z is the dynamic critical exponent (cluster algorithms, which are at present the best ones for N-vector models, have $0 < z \lesssim 0.5$, see [26, 27] for estimates of z and additional references). Thus, for $N = 0$, one is able to probe very carefully the critical limit and get a good control of the scaling corrections that represent the main source of error in high-precision studies. Monte Carlo studies provide therefore accurate estimates of critical quantities that can be used as reference values in other theoretical approaches.

In this paper, we consider the four-point renormalized coupling which is the basic ingredient in any field-theoretical calculation, computing its value at the critical point. We obtain

$$\bar{g}^* = 1.4005(5), \tag{1}$$

where $\bar{g}$ is normalized so that the β function behaves as $\beta(\bar{g}) = -\bar{g} + \bar{g}^2 + O(\bar{g}^3)$ for small values of $\bar{g}$. This result should be compared with the best available estimates. Field theory gives $\bar{g}^* = 1.396(20)$ (ϵ expansion [28]) and $\bar{g}^* = 1.413(6)$ (massive zero-momentum scheme in fixed dimension $d = 3$ [7]). The ϵ-expansion result is perfectly consistent with our final estimate. On the other hand, the fixed-dimension result differs slightly, by approximately two error bars. This is similar to what is observed for the exponent γ: the most precise fixed-dimension calculation gives [7] $\gamma = 1.1596(20)$, which is slightly larger—but fully compatible with the quoted error—than the most precise Monte Carlo estimates, $\gamma = 1.1573(2)$ [12] and $\gamma = 1.1575(6)$ [10]. A similar phenomenon occurs for $N = 1$, where the fixed-dimension estimates [7] of both $\bar{g}^*$ and γ are slightly larger (but note that again the effect is at the level of one error bar) than the Monte Carlo results [8, 9]. The universal constant $\bar{g}^*$ has also been computed by resumming its high-temperature expansion in the lattice N-vector model. It is reported in [29] that $\bar{g}^* = 1.388(5)$ which is not fully compatible with (1). As stressed several times [1, 16], this is probably due to scaling corrections proportional to $(\beta - \beta_c)^\Delta$, where Δ is the leading correction-to-scaling exponent ($\Delta \approx 0.5$ in the present model). Even if in principle standard resummation methods should be able to take them into account, in practice, with the series of moderate length available today, they give rise to systematic deviations that are quite difficult to estimate: as a consequence, error bars are often underestimated. This problem has been overcome by considering improved Hamiltonians characterized by the absence of leading scaling corrections [6, 8, 30], leading to accurate estimates of critical exponents and universal amplitudes for $N = 1, 2, 3$.

In table 1, we summarize the best available estimates of $\bar{g}^*$ for the three-dimensional N-vector systems with $0 \leqslant N \leqslant 3$. Monte Carlo or high-temperature expansions computed in

[3] Nonanalyticity effects are expected to be small in three dimensions. For instance, the leading nonanalytic terms appearing in the β function have the form $(g^* - g)^{1+1/\Delta}$ and $(g^* - g)^{\Delta_2/\Delta}$ [14, 16]. In three dimensions, $1 + 1/\Delta \approx \Delta_2/\Delta \approx 2$, so that nonanalyticities are weak [1, 17]. This is not the case in two dimensions [18]. In the two-dimensional Ising model, a correction of the form $(g^* - g)^{8/7}$ is expected. This term is probably the reason why field-theory results [19] differ significantly from the exact ones [17, 18].

Table 1. Estimates of the critical value of the four-point renormalized coupling $\bar{g}^*$ in the three-dimensional N-vector model with $0 \leqslant N \leqslant 3$. We normalize $\bar{g}$ so that the three-dimensional β function behaves as $\beta(\bar{g}) = -\bar{g} + \bar{g}^2 + O(\bar{g}^3)$. In [6, 8, 30], a different normalization is used and $g^* = 48\pi\bar{g}^*/(N+8)$ is reported. In the second column, we indicate the method used in the determination of the coupling constant. FD refers to the field-theoretical fixed-dimension zero-momentum scheme, ϵ-exp to the ϵ expansion, MC stands for Monte Carlo and IHT for the analysis of high-temperature expansions specialized to improved models (i.e. models without leading scaling corrections).

Reference	Method	$N=0$	$N=1$	$N=2$	$N=3$
[7]	FD	1.413(6)	1.411(4)	1.403(3)	1.390(4)
[28]	ϵ-exp	1.396(20)	1.408(13)	1.425(24)	1.426(9)
[6, 8, 30]	IHT		1.406(1)	1.4032(7)	1.395(7)
Present work	MC	1.4005(5)			

improved models provide the most accurate results. Field theory is in substantial agreement, although small differences appear for $N = 0$ (fixed-dimension expansion) and $N = 3$ (ϵ expansion). Other results are reported in [1].

The paper is organized as follows. In section 2, we define the basic quantities that are computed in the present work. In section 3, we present our numerical results. First, we derive the correction-to-scaling function associated with the second virial coefficient, then we determine $\bar{g}^*$. Finally, in section 3.3, we use our numerical data to obtain a new estimate of the exponent ν.

2. Definitions

We consider a simple cubic lattice and N-step SAWs. A SAW is a lattice walk $\{\mathbf{r}_0, \ldots, \mathbf{r}_N\}$ such that $\mathbf{r}_i$ and $\mathbf{r}_{i+1}$ are nearest neighbours and each lattice site is visited at most once. We also introduce an effective attraction $-\mathcal{E}$ ($\mathcal{E} > 0$) between nonconnected nearest-neighbour walk sites. If $\beta \equiv -\mathcal{E}/k_B T$ is the dimensionless inverse temperature in the scaling limit, the statistical properties are independent of β as long as the system is in the good-solvent (swollen) regime. Scaling corrections instead depend on β and thus, by properly fixing β, one can reduce them significantly. Following [31], we fixed $\beta = 0.054$. The extensive Monte Carlo work of [32] indicates that for this value of β the leading scaling corrections are at least a factor of 10 smaller than those occurring in the athermal model with $\beta = 0$.[4] For the simulation, we used the pivot algorithm [21–25], which is very efficient for the determination of SAW global properties. In order to estimate the zero-momentum renormalized coupling g^*, we computed the second virial coefficient for SAWs of different lengths [33]. For this purpose, we used the hit-or-miss algorithm discussed in [34].

We performed a large-scale simulation, considering walks of length N varying between 100 and 64 000, determining the radius of gyration and the end-to-end distance for 67 different values of N and the second virial coefficient for 369 pairs of walks of different length. Some results (those corresponding to pairs with $N_2 > N_1 \geqslant 8000$) are reported in table 2. The statistics vary between 8×10^7 and 24×10^7 pivot trials for each value of N. Our runs were performed on a cluster of Intel Xeon (3.20 GHz) processors and lasted approximately eight CPU years of a single processor.

[4] According to [32], scaling corrections vanish for $\beta = 0.048(7)$. Our simulations started before [32] was completed. For this reason we used the older estimate of [31].

Table 2. Estimates of $V_2(N_1, N_2; \beta)$ for $\beta = 0.054$. We report the Monte Carlo results such that $N_2 > N_1 \geqslant 8000$.

λ	N_1	N_2	$V_2(N_1, N_2; \beta)$
0.1250	8000	64 000	0.389 72(20)
0.1406	9000	64 000	0.385 64(20)
0.1563	10 000	64 000	0.382 49(20)
0.2135	10 250	48 000	0.373 62(20)
0.2240	10 750	48 000	0.372 36(18)
0.2292	11 000	48 000	0.371 54(19)
0.2656	8500	32 000	0.367 87(19)
0.2969	9500	32 000	0.365 61(17)
0.4063	9750	24 000	0.359 63(14)
0.4432	9750	22 000	0.358 21(13)
0.4625	9250	20 000	0.357 57(8)
0.5000	12 000	24 000	0.356 70(15)
0.5455	12 000	22 000	0.355 36(13)
0.5469	8750	16 000	0.355 23(17)
0.7188	11 500	16 000	0.353 20(15)
0.7609	8750	11 500	0.352 86(15)
0.8000	8000	10 000	0.352 78(15)
0.8125	9750	12 000	0.352 68(15)
0.8889	8000	9000	0.352 35(14)
0.8947	8500	9500	0.352 17(15)
0.9000	9000	10 000	0.352 48(14)
0.9167	22 000	24 000	0.352 10(13)
0.9318	10 250	11 000	0.352 43(12)
0.9535	10 250	10 750	0.352 41(15)
0.9697	8000	8250	0.352 14(13)
0.9773	10 750	11 000	0.352 41(15)

We measured the following quantities:

(1) The radius of gyration of a SAW of length N,

$$R_g^2(N; \beta) \equiv \frac{1}{2(N+1)^2} \sum_{i,j} \langle (\mathbf{r}_i - \mathbf{r}_j)^2 \rangle, \tag{2}$$

where the sums go over the $N + 1$ sites of the chain and $\mathbf{r}_i$ is the corresponding position.

(2) The end-to-end distance of a SAW of length N,

$$R_e^2(N; \beta) \equiv \langle (\mathbf{r}_0 - \mathbf{r}_N)^2 \rangle. \tag{3}$$

(3) The second virial coefficient for two SAWs of lengths N_1 and N_2,

$$B_2(N_1, N_2; \beta) \equiv \frac{1}{2} \sum_{\mathbf{r}} \langle 1 - \mathrm{e}^{-\beta H(1,2)} \rangle_{\mathbf{0},\mathbf{r}}, \tag{4}$$

where the average is over two walks of lengths N_1 and N_2, the first one starting at the origin and the second at $\mathbf{r}$. The sum is over all lattice sites and $H(1, 2)$ is the interaction energy between the two chains: $H(1, 2) = +\infty$ if the two walks intersect each other; otherwise, $H(1, 2) = -\mathcal{E} N_{nnc}$, where N_{nnc} is the number of lattice bonds $\langle \mathbf{r}_a \mathbf{r}_b \rangle$, such that $\mathbf{r}_a$ belongs to the the first walk and $\mathbf{r}_b$ belongs to the second walk (or vice versa).

The second virial coefficient is not universal. A universal quantity is obtained by considering the following dimensionless ratio:

$$V_2(N_1, N_2; \beta) \equiv \frac{B_2(N_1, N_2; \beta)}{R_e(N_1; \beta)^{3/2} R_e(N_2; \beta)^{3/2}}. \tag{5}$$

In the scaling limit, i.e. for $N_1, N_2 \to \infty$, we have

$$R^2(N_1; \beta) = a_R(\beta) N_1^{2\nu} \left(1 + b_R(\beta) N_1^{-\Delta} + \cdots\right) \tag{6}$$

$$V_2(N_1, N_2; \beta) = V^*(\lambda) + b_V(\beta) f(\lambda) (N_1 N_2)^{-\Delta/2} + \cdots \tag{7}$$

where $\lambda \equiv N_1/N_2$, $f(1) = 1$ (normalization condition) and we have neglected additional subleading scaling corrections. The functions $V^*(\lambda)$ and $f(\lambda)$ as well as the exponents ν and Δ are universal. On the other hand, the amplitudes $a_R(\beta)$, $b_R(\beta)$ and $b_V(\beta)$ are model dependent and therefore depend explicitly on β.[5] The exponent ν is known quite precisely. At present, the most accurate estimates are $\nu = 0.587\,58 \pm 0.000\,07$ [36], $\nu = 0.5874 \pm 0.0002$ [37] and $\nu = 0.587\,65 \pm 0.000\,20$ [12] (for an extensive list of results, see [1]). In section 3.3, we confirm these results, obtaining $\nu = 0.5876 \pm 0.0002$. Also the exponent Δ has been determined quite accurately [36]: $\Delta = 0.515 \pm 0.007^{+0.010}_{-0.000}$. In [32], the second virial coefficient for walks of equal length was determined, leading to the estimate $V^*(1)(A^*_{ge})^{-3/2} = 5.500(3)$. Using [35] $A^*_{ge} \equiv \left(a_{R_g}/a_{R_e}\right)^2 = 0.159\,88(4)$, we obtain $V^*(1) = 0.3516(2)$.

Given $V^*(\lambda)$, the critical value of the four-point renormalized coupling constant is given by [33]

$$\bar{g}^* = \frac{6^{3/2}}{\pi} \frac{\Gamma(3\nu + 2\gamma)}{\Gamma(\gamma)^{1/2} \Gamma(\gamma + 2\nu)^{3/2}} \int_0^\infty d\lambda\, \lambda^{3\nu/2+\gamma-1} (1+\lambda)^{-3\nu-2\gamma} V^*(\lambda). \tag{8}$$

We use here the standard field-theoretical normalization in which the $O(N)$ β function behaves as $\beta(\bar{g}) = -\bar{g} + \bar{g}^2$ for small $\bar{g}$. In (8) the universal critical exponent γ appears. At present, the most precise estimates are $\gamma = 1.1575(6)$ [10] and $\gamma = 1.1573(2)$ [12].

Let us note that $V_2(N_1, N_2; \beta)$ is symmetric under the interchange of N_1 and N_2. This implies that $V^*(\lambda)$ and $f(\lambda)$ are both symmetric under the transformation $\lambda \to 1/\lambda$. In order to make this symmetry explicit, we introduce a new variable

$$\mu \equiv \frac{2\lambda}{1+\lambda^2}, \tag{9}$$

which varies in the interval $[0, 1]$ and is symmetric under $\lambda \to 1/\lambda$. We take μ as fundamental variable, considering V^* and f to be functions of the variable μ. In terms of μ, integral (8) becomes

$$\bar{g}^* = \frac{6^{3/2}}{\pi} \frac{\Gamma(3\nu + 2\gamma)}{\Gamma(\gamma)^{1/2} \Gamma(\gamma + 2\nu)^{3/2}} \int_0^1 \frac{2\, d\mu}{\mu\sqrt{1-\mu^2}} \left[\frac{2(1+\mu)}{\mu}\right]^{-3\nu/2-\gamma} V^*(\mu). \tag{10}$$

We wish now to compute the small-μ behaviour of the scaling functions. For this purpose, we extend a scaling argument due to de Gennes [38]. For $N_1/N_2 \to 0$, we can compute the second virial coefficient by dividing the longest walk (of length N_2) in N_2/N_1 blobs, which have a size of the order of the size of the shortest walk (of length N_1). The shortest SAW interacts only with a single blob, so that $B(N_1, N_2) \sim (N_2/N_1) B_{\rm bl}(N_1)$, where $B_{\rm bl}(N_1)$ is the second virial coefficient that takes into account the interaction between the blob and the

[5] The amplitude ratio $b_R(\beta)/b_V(\beta)$ is universal and therefore β-independent. Estimates are reported in [35]: $b_{R_g}/b_V = -1.5(3)$, $b_{R_e}/b_V = -1.1(3)$. Also the ratio a_{R_g}/a_{R_e} is universal. It is reported in [35] that $A^*_{ge} \equiv (a_{R_g}/a_{R_e})^2 = 0.159\,88(4)$.

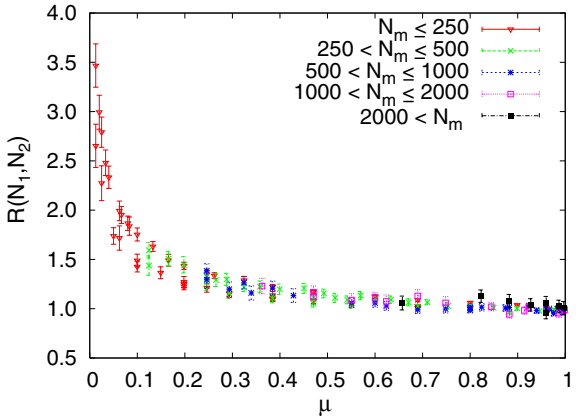

Figure 1. Plot of $R(N_1, N_2)$ as a function of $\mu \equiv 2N_1N_2/(N_1^2 + N_2^2)$, for $\Delta = 0.515$. We use different symbols according to the value of $N_m = \min(N_1, N_2)$.

shortest walk. Since $B_{\rm bl}(N_1)$ depends on a single length scale, the length N_1, by dimensional reasons we have $B_{\rm bl}(N_1) \sim N_1^{3\nu}\left(1 + cN_1^{-\Delta}\right)$. It follows

$$B(N_1, N_2) \sim N_2 N_1^{3\nu-1}\left(1 + cN_1^{-\Delta}\right), \tag{11}$$

and then

$$V_2(N_1, N_2) \sim \frac{N_2 N_1^{3\nu-1}\left(1 + cN_1^{-\Delta}\right)}{N_1^{3\nu/2}\left(1 + d_1 N_1^{-\Delta}\right) N_2^{3\nu/2}\left(1 + d_2 N_2^{-\Delta}\right)} \sim \lambda^{3\nu/2-1}[1 + k\lambda^{-\Delta/2}(N_1N_2)^{-\Delta/2}]. \tag{12}$$

Comparing with the expansion (7) and taking into account that, for small λ, $\lambda \approx \mu/2$, we obtain

$$V^*(\mu) \sim \mu^{3\nu/2-1}, \qquad f(\mu) \sim \mu^{3\nu/2-1-\Delta/2}. \tag{13}$$

As a consequence of this result, for $\mu \to 0$ the integrand that appears in (10) behaves as $\mu^{3\nu+\gamma-2} \sim \mu^{0.92}$. Thus, the small-$\mu$ region is not crucial for a precise determination of $\bar{g}^*$. This is most welcome, since it is quite difficult to determine $V^*(\mu)$ precisely for μ small.

3. Numerical results

3.1. Determination of the correction-to-scaling function $f(\mu)$

In order to determine the correction-to-scaling function $f(\mu)$ (see (7)), we use the numerical data of [31, 39]. The function $V_2(N_1, N_2; \beta)$ was determined for several values of N_1, N_2 in the range $50 \leqslant N_1, N_2 \leqslant 16\,000$ for $\beta = 0$ and $\beta = 0.1$, though not so precisely as in the present work. Following [31] we consider

$$R(N_1, N_2) \equiv \left(\frac{N_1}{N_2}\right)^{-\Delta/2} \frac{V_2(N_1, N_2; \beta = 0) - V_2(N_1, N_2; \beta = 0.1)}{V_2(N_1, N_1; \beta = 0) - V_2(N_1, N_1; \beta = 0.1)}, \tag{14}$$

which converges to $f(\mu)$ as $N_1, N_2 \to \infty$. In figure 1, we show $R(N_1, N_2)$ versus μ. The data approximately fall onto a single curve. However, at a closer look, one observes that, especially for small values of μ, the data fall on two different, though close, lines. This fact can be easily understood. The function $R(N_1, N_2)$ defined in (14) is not symmetric under the

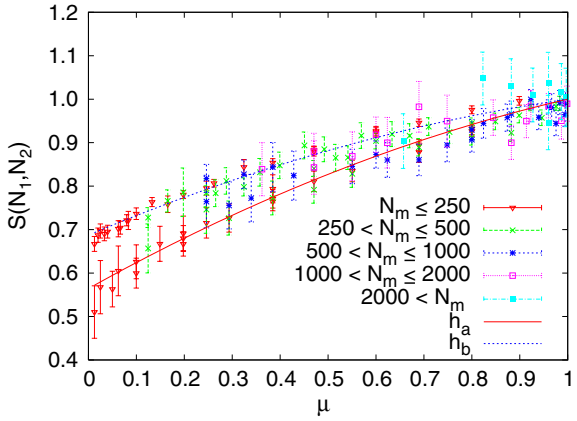

Figure 2. Plot of $S(N_1, N_2)$ as a function of $\mu \equiv 2N_1N_2/(N_1^2 + N_2^2)$, for $\Delta = 0.515$ and $\nu = 0.587\,58$. We use different symbols according to the value of $N_m = \min(N_1, N_2)$. We also report the functions $h_a(\mu)$ and $h_b(\mu)$ discussed in the text, see (19).

interchange of N_1 and N_2 and thus, for finite values of N_1 and N_2, there is no symmetry under $\lambda \to 1/\lambda$. This symmetry is recovered only in the scaling limit. Thus, given a value of μ, the data cluster around two different values: one corresponds to a value of λ such that $\lambda > 1$, while the second one corresponds to a value of λ such that $\lambda < 1$. These differences disappear in the scaling limit and thus they provide us an estimate of the next-to-leading scaling corrections.

It is possible to define a quantity which is symmetric under the interchange of N_1 and N_2 and converges to $f(\mu)$ in the scaling limit. We could have defined

$$R'(N_1, N_2) \equiv \frac{V_2(N_1, N_2; \beta = 0) - V_2(N_1, N_2; \beta = 0.1)}{[\Delta V_2(N_1)\Delta V_2(N_2)]^{1/2}}, \tag{15}$$

where $\Delta V_2(N) \equiv V_2(N, N; \beta = 0) - V_2(N, N; \beta = 0.1)$. We could not use this definition since estimates of $\Delta V_2(N)$ are available only for a few values of N (those computed in [31]), and thus $R'(N_1, N_2)$ can be determined only for 16 pairs of walks.

Since the function $f(\mu)$ behaves as $\mu^{3\nu/2-1-\Delta/2}$ as $\mu \to 0$ (equation (13)), we write

$$f(\mu) = \mu^{3\nu/2-1-\Delta/2} h(\mu), \tag{16}$$

where $h(\mu)$ satisfies $h(0) \neq 0$ and the normalization condition $h(1) = 1$. In order to estimate $h(\mu)$ we consider

$$S(N_1, N_2) \equiv R(N_1, N_2) \left(\frac{2N_1N_2}{N_1^2 + N_2^2} \right)^{-3\nu/2+1+\Delta/2}, \tag{17}$$

which converges to $h(\mu)$ in the scaling limit. The function $S(N_1, N_2)$ is reported in figure 2. As before, note that the data do not fall onto a single curve: two branches, corresponding respectively to $\lambda > 1$ and $\lambda < 1$ are clearly visible. Their difference gives us a rough estimate of the next-to-leading corrections. The two branches of the function $S(N_1, N_2)$ are quite smooth in μ and thus good fits are obtained by taking polynomial interpolations. Therefore, we fit the numerical data to

$$S(N_1, N_2) = 1 + \sum_{k=1}^{n} a_k (\mu - 1)^k, \tag{18}$$

which automatically guarantees $S(N, N) = 1$. In order to take into account the scaling corrections that show up in the presence of two different branches, we perform two fits: in the

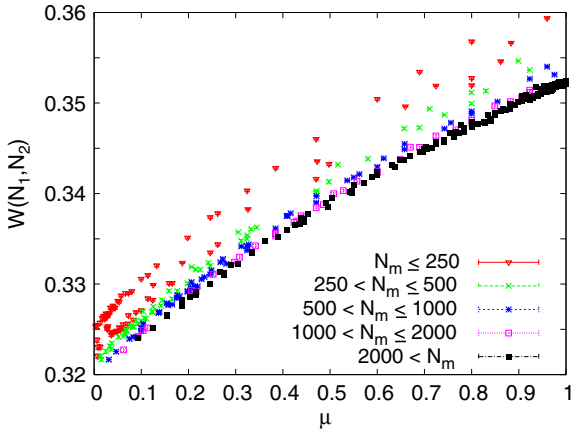

Figure 3. Plot of $W(N_1, N_2; \beta)$ for $\beta = 0.054$ as a function of $\mu \equiv 2N_1N_2/(N_1^2 + N_2^2)$ for $\nu = 0.587\,58$. We use different symbols according to the value of $N_m = \min(N_1, N_2)$.

first one (fit (a)), we use all data for $\mu \geqslant 0.7$ and the data with $N_1 > N_2$ for $\mu < 0.7$; in the second one (fit (b)), we use all data for $\mu \geqslant 0.7$ and the data with $N_1 < N_2$ for $\mu < 0.7$. In case (a) we interpolate the data that belong to the lower branch, while in case (b) we interpolate the upper-branch results. The order n of the polynomial does not play much role and we always use $n = 2$. The results of the two fits are

$$\begin{aligned} h_a(\mu) &= 1 + 0.255\,9953(\mu - 1) - 0.179\,692(\mu - 1)^2, \\ h_b(\mu) &= 1 + 0.160\,4295(\mu - 1) - 0.152\,394(\mu - 1)^2. \end{aligned} \tag{19}$$

The corresponding curves are reported in figure 2. In the following section we use

$$h(\mu) = \tfrac{1}{2}[h_a(\mu) + h_b(\mu)] = 1 + 0.208\,212(\mu - 1) - 0.166\,043(\mu - 1)^2 \tag{20}$$

as our estimate of $h(\mu)$ and take $|h - h_a|$ and $|h - h_b|$ as estimates of the error on $h(\mu)$.

3.2. Estimate of g^*

We now estimate the universal function $V^*(\mu)$. Taking into account the asymptotic behaviour (13), we define a new function

$$W(\mu) \equiv \mu^{1-3\nu/2} V^*(\mu), \tag{21}$$

which is such that $W(0) \neq 0$. In order to estimate $W(\mu)$ we consider

$$W(N_1, N_2; \beta) = V_2(N_1, N_2; \beta) \left(\frac{2N_1N_2}{N_1^2 + N_2^2} \right)^{-3\nu/2+1}. \tag{22}$$

For $N_1, N_2 \to \infty$, it behaves as (see (7))

$$W(\mu) + b_V(\beta) h(\mu) \mu^{-\Delta/2} (N_1N_2)^{-\Delta/2}. \tag{23}$$

The function $W(N_1, N_2; \beta)$ is reported in figure 3. It shows a small dependence on μ, but significant scaling corrections. As before we use a polynomial parameterization for $W(\mu)$ and fit the data to

$$W(N_1, N_2; \beta) = \sum_{k=0}^{n} a_k (\mu - 1)^k + a_{n+1} h(\mu) \mu^{-\Delta/2} (N_1N_2)^{-\Delta/2}, \tag{24}$$

Table 3. Estimates of $\bar{g}^*$ and of $V^*(1)$ for different values of $N_{\min}$. A third-order interpolation ($n = 3$) is used in (24).

$N_{\min}$	$\bar{g}^*$	$V^*(1)$
100	1.3983(5)	0.351 08(16)
200	1.3990(5)	0.351 20(14)
400	1.3997(4)	0.351 34(11)
800	1.4003(4)	0.351 47(10)
1000	1.4004(4)	0.351 51(10)
1500	1.4005(4)	0.351 53(10)
2000	1.4004(5)	0.351 50(10)
3000	1.4005(5)	0.351 49(12)
5000	1.4007(7)	0.351 54(19)

where we use the function $h(\mu)$ reported in (20), and $a_0, \ldots, a_{n+1}$ are the fit parameters. Once $W(\mu) = \sum_{k=0}^{n} a_k(\mu - 1)^k$ has been determined, we can compute $V^*(\mu)$ and finally $\bar{g}^*$ using (10). There are several sources of the error on the result:

(i) *Statistical errors due to the uncertainty on* $V_2(N_1, N_2; \beta)$. They are computed by means of an auxiliary Monte Carlo procedure. The input data are varied randomly within error bars (at each Monte Carlo step all estimates $V_2(N_1, N_2)$ are replaced by $V_2(N_1, N_2) + r(N_1, N_2)\sigma_V(N_1, N_2)$, where $\sigma_V(N_1, N_2)$ is the error on $V_2(N_1, N_2)$ and $r(N_1, N_2)$ is a random number extracted from a Gaussian distribution with zero mean and unit variance) and $\bar{g}^*$ is recomputed each time. The standard deviation of these estimates provides the statistical error on $\bar{g}^*$.

(ii) *Error due to the uncertainty on* $h(\mu)$. We repeat the analysis with the two functions reported in (19). The difference with the result obtained by using $h(\mu)$ gives the error.

(iii) *Error due to the uncertainty of the exponents*. We consider the best estimates $\nu = 0.587\,58(7)$, $\Delta = 0.515(17)$ and $\gamma = 1.1573(2)$, and determine how $\bar{g}^*$ varies as the exponents change by one error bar.

(iv) *Error due to the additional scaling corrections*. In (7) we have only written the leading scaling correction. There are however other correction terms that vanish faster and that may be relevant at the values of N we are considering. For this purpose, we have repeated the analysis several times, each time considering only data satisfying $N_1, N_2 \geqslant N_{\min}$, for several values of $N_{\min}$.

In table 3, we give estimates of $\bar{g}^*$ for different values of $N_{\min}$. We use a third-order interpolation, i.e. we set $n = 3$ in (24). Similar results are obtained for $n = 2$: for $N_{\min} \lesssim 2000$ the estimates obtained by taking $n = 2$ and $n = 3$ differ by less than $\frac{1}{3}$ of the error bar; for $N_{\min} \gtrsim 2000$ differences are larger bur never exceed one error bar. The error we report is the sum of the errors of types (i), (ii) and (iii). Errors of type (ii) are always small and account for less than 5% of the total error: the somewhat large uncertainty on the function $h(\mu)$ does not have much influence on the final result. For $N_{\min} \lesssim 1000$ most of the error is due to the error on the exponent Δ, while in the opposite case the statistical error (i) dominates. As a check of our results we also report $V^*(1)$. With the parameterization (24) we have simply $V^*(1) = a_0$. The results are perfectly consistent with the estimate $V^*(1) = 0.3516(2)$ reported in section 2, obtained by using the numerical results of [32, 35].

The results reported in table 3 show a tiny dependence on $N_{\min}$. For $N_{\min} \geqslant 800$, the results are approximately constant within error bars. We take our final estimates at $N_{\min} = 3000$:

$$\bar{g}^* = 1.4005(5), \tag{25}$$

$$V^*(1) = 0.351\,49(12). \tag{26}$$

Estimate (25) should be compared with the previous results: $\bar{g}^* = 1.396(20)$ is obtained by using the ϵ expansion [28]; $\bar{g}^* = 1.413(6)$ is obtained by using the massive zero-momentum scheme in three dimensions [7]; $\bar{g}^* = 1.388(5)$ is obtained by resumming its high-temperature expansion [29]. Note that both the fixed-dimension estimate and the high-temperature result are not fully consistent with our results. In the case of the field-theoretical results, this is probably due to the slow convergence of the perturbative expansions, a phenomenon that may be related to the nonanalyticities of the renormalization-group functions at the fixed point. In the case of the high-temperature result, this is probably due to the scaling corrections: resummations are not fully able to cope with the nonanalyticities present at the critical point.

Our precise estimate of $\bar{g}^*$ can also be used as an input in the field-theory determinations of the critical exponents γ and ν. We consider the massive zero-momentum scheme [7] in fixed dimension, in which critical quantities are obtained by evaluating the corresponding renormalization-group functions at $\bar{g}^*$. Instead of using the six-loop estimate $\bar{g}^* = 1.413(6)$, we evaluate the seven-loop resummed renormalization-group functions associated with γ and ν [7, 40, 41] at the Monte Carlo estimate $\bar{g}^* = 1.4005(5)$. This can be easily achieved by using some intermediate results reported in [7]. We obtain

$$\gamma = 1.1583(15), \qquad \nu = 0.5873(7), \tag{27}$$

which are slightly lower than the estimates of [7], $\gamma = 1.1596(20)$ and $\nu = 0.5882(11)$, and in better agreement with the best Monte Carlo estimates $\gamma = 1.1573(2)$ and $\nu = 0.587\,58(7)$ mentioned above[6]. This is a nice consistency check between the lattice Monte Carlo techniques and field-theory methods.

The estimate (26) of $V^*(1)$ allows us to obtain a new estimate of the interpenetration ratio:

$$\Psi^* \equiv 2(4\pi)^{-3/2}(A^*_{ge})^{-3/2}V^*(1) = 0.246\,85(11), \tag{28}$$

where we used $A^*_{ge} = 0.159\,88(4)$ [35]. It is consistent with the result reported in [32]: $\Psi^* = 0.246\,93(13)$.

3.3. Estimate of the exponent ν

As a byproduct of our simulations we obtained the estimates of R^2_g and R^2_e up to $N = 64\,000$. They allow us to obtain a new estimate of the exponent ν. It is crucial to take into account the scaling corrections and thus we have performed fits of the form

$$\ln R^2 = a + 2\nu \ln N + bN^{-\Delta} + cN^{-\Delta_2}, \tag{29}$$

as we did in [32, 35] for the virial coefficients, taking $\Delta = 0.515(17)$ [36] and $\Delta_2 = 1.0(1)$. The last term in (29) is an effective correction that takes into account several terms: nonanalytic corrections proportional to $N^{-2\Delta}$ and $N^{-\Delta_2}$ (Δ_2 is the next-to-leading correction-to-scaling exponent, $\Delta_2 = 0.98(6)$ [42]) and analytic terms behaving as $1/N$. As before, we repeat the fit several times, each time including data corresponding to walks such that $N \geqslant N_{\min}$. The results are reported in table 4. The estimates obtained from the fits of R^2_g are very stable—they essentially do not change for $100 \leqslant L_{\min} \leqslant 500$. Those obtained from the fits of R^2_e show a slight downward trend but are perfectly compatible. As a final estimate we take

$$\nu = 0.5876(2), \tag{30}$$

[6] One may repeat this calculation for other values of N. For example, in the Ising case ($N = 1$), using the most precise estimate $\bar{g}^* = 1.406(1)$, see table 1, one obtains $\gamma = 1.2387(8)$ and $\nu = 0.6299(10)$, which should be compared with the field-theoretical estimates [7] $\gamma = 1.2396(13)$ and $\nu = 0.6304(13)$ (obtained by using the six-loop result $\bar{g}^* = 1.411(4)$), and the lattice results [30, 9] $\gamma = 1.2373(2)$ and $\nu = 0.630\,12(16)$.

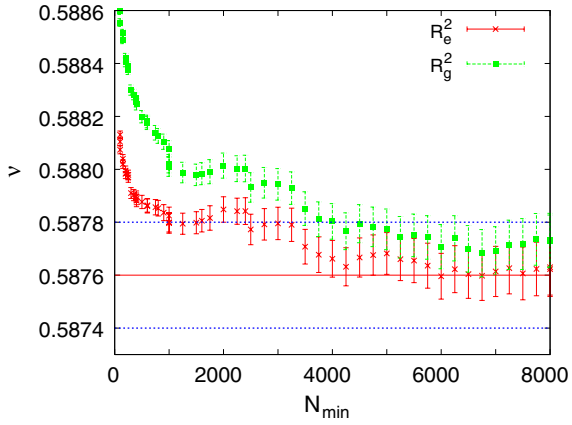

Figure 4. Estimates of ν obtained by fitting R_g^2 and R_e^2 to $\ln R^2 = a + 2\nu \ln N$, as a function of $N_{\min}$, the length of the shortest walk considered in the fit. The thick horizontal line corresponds to our central estimate (30), while the thin dotted lines give the error.

Table 4. Estimates of ν obtained from the analysis of R_e^2 and R_g^2 as a function of $N_{\min}$, the length of the shortest walk considered in the fit.

$N_{\min}$	$\nu\,(R_e^2)$	$\nu\,(R_g^2)$
100	0.587 68(9)	0.587 54(10)
200	0.587 73(14)	0.587 55(14)
300	0.587 61(18)	0.587 54(17)
400	0.587 56(19)	0.587 51(19)
500	0.587 61(23)	0.587 53(23)
600	0.587 50(25)	0.587 43(24)
800	0.587 64(33)	0.587 68(31)
1000	0.587 40(36)	0.587 41(34)

which is compatible with all results reported in table 4. The estimate (30) is in good agreement with the previous ones reported in the literature [12, 36, 37] and mentioned in section 2.

Note that the inclusion of the scaling corrections in the fit is crucial. In figure 4, we report the estimates of ν obtained by using a fit without the scaling corrections, $\ln R^2 = a + 2\nu \ln N$. The results show a clear downward trend, depend on the quantity at hand, and are apparently constant within error bars only for $N_{\min} \gtrsim 6000$. In this range they are in perfect agreement with the estimate (30).

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