Geometrical properties of two-dimensional interacting self-avoiding walks at the $\theta$-point

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Abstract
We perform a Monte Carlo simulation of two-dimensional $N$-step interacting self-avoiding walks at the $\theta$-point, with lengths up to $N = 3200$. We compute the critical exponents, verifying the Coulomb-gas predictions, the $\theta$-point temperature $T_\theta = 1.4986(11)$, and several invariant size ratios. Then, we focus on the geometrical features of the walks, computing the instantaneous shape ratios, the average asphericity, and the end-to-end distribution function. For the latter quantity, we verify in detail the theoretical predictions for its small- and large-distance behaviour.

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

1. Introduction

Self-avoiding walks (SAWs) have been extensively studied over the years. They have a rich mathematical structure and represent one of the simplest models of critical behaviour. Moreover, they are also relevant for the understanding of the universal features of large-molecular-weight macromolecules in solution [1–8]. Indeed, the study of the asymptotic behaviour of long SAWs (and also of walks with different architecture, like self-avoiding rings or stars) allows one to obtain predictions for several structural and thermodynamical properties—for instance, critical exponents, structure factors, osmotic pressure, etc—of polymers both in dilute and semidilute good-solvent solutions in the limit of infinite degree
of polymerization. These predictions are in good agreement with the (usually much less precise) experimental results. By adding an attractive interaction, SAWs also allow us to study the critical transition (θ-point) between good-solvent and poor-solvent behaviour [5–8]. The phase diagram of interacting SAWs is well known. Above the θ-temperature $T_\theta$, the large-\(N\) behaviour is temperature independent and in the same universality class as that observed for athermal SAWs, which correspond to the case $T = \infty$. On the other hand, for $T < T_\theta$ typical walks are compact: this is the so-called collapsed or poor-solvent regime. At the θ temperature, interacting SAWs show a quite interesting tricritical behaviour. The two-dimensional case has been extensively studied by Coulomb-gas techniques and conformal field theory (CFT). They have provided exact predictions for the critical exponents [9], which have been confirmed by several high-precision numerical studies [10–22]. Also the collapsed phase has been discussed in detail [23–27], including the crossover behaviour close to the θ-point [28].

In this paper we perform a Monte Carlo (MC) simulation of two-dimensional interacting SAWs close to the θ-point, with the purpose of determining some geometrical features of the walks. In particular, we focus on the instantaneous shape of the walks and on the end-to-end distribution function (EEDF). As is well known, walks are not instantaneously spherical. Their shape is usually characterized by considering combinations of the eigenvalues of the gyration tensor. One of them, the mean asphericity, is an essential ingredient in theoretical studies of the hydrodynamic behaviour of dilute polymer solutions [29–31]. The EEDF has been extensively studied in three dimensions, because of its theoretical interest [32–44]. Under the mapping of SAWs onto the $n \to 0 \sigma$ model (or $\lambda \phi^4$ theory), it corresponds to the spin–spin correlation function, which is the basic object of field-theoretical calculations. Moreover, it can also be accessed experimentally, by performing neutron-scattering experiments on solutions of end-marked polymers [7].

In this paper, we obtain a high-precision determination of the EEDF, which will be compared with several predictions obtained by using the standard mapping onto the $n = 0$ spin model and with phenomenological expressions that have been shown to be quite accurate in three dimensions. As for the shape of the walks, we will determine the average asphericity, comparing it with results obtained in the good-solvent regime [45, 46] and for non-interacting random walks [47].

The paper is organized as follows. In section 2, we define the interacting SAWs and some basic quantities. In section 3, we use our MC results to determine the θ temperature and verify the theoretical predictions for the critical exponents. In section 4, we study the walk shape and in section 5, the EEDF. In section 6, we summarize our conclusions.

2. Model and definitions

In this paper, we consider SAWs on a two-dimensional square lattice. An $N$-step SAW $\omega$ is a set of $N+1$ lattice sites $\omega_0 = 0$, $\omega_1$, $\ldots$, $\omega_N$, such that $\omega_i$ and $\omega_{i+1}$ are lattice nearest neighbours. For each walk, we define the energy $E$ as the number of nearest-neighbour contacts between non-bonded monomers:

$$E \equiv -\sum_{i=0}^{N-3} \sum_{j=i+3}^{N} c_{ij},$$

where

$$c_{ij} \equiv \begin{cases} 1 & \text{if } |\omega_i - \omega_j| = 1, \\ 0 & \text{otherwise}. \end{cases}$$

\[ \text{(2.1)} \]

\[ \text{(2.2)} \]
Table 1. Estimates of $\beta_\theta$ on the square lattice. EE stands for exact enumeration, MC for Monte Carlo.

| Reference | Year | Method | $\beta_\theta$ |
|-----------|------|--------|--------------|
| [10]      | 1987 | EE     | 0.75         |
| [11]      | 1988 | MC     | 0.65(3)      |
| [12]      | 1990 | EE     | 0.67(4)      |
| [13]      | 1990 | MC     | 0.658(4)     |
| [14]      | 1992 | EE     | 0.657(16)    |
| [15]      | 1993 | MC     | 0.658(4)     |
| [16]      | 1994 | EE     | 0.660(5)     |
| [17]      | 1995 | MC     | 0.665(2)     |
| [18]      | 1996 | MC     | 0.664, 0.666 |
| [48]      | 1997 | MC     | 0.667(1)     |
| [49]      | 2009 | MC     | 0.664(8)     |
| This work | 2011 | MC     | 0.6673(5)    |

We consider the ensemble of $N$-step walks with partition function $Z_N = \sum_{\{\omega\}} e^{-\beta E}$, where $\beta \equiv 1/T$ is the inverse temperature and the sum is extended over all $N$-step walks. We will study the behaviour close to the $\theta$ temperature $\beta_\theta$. For the model we consider, the best present-day estimates of $\beta_\theta$ on the square lattice are reported in table 1.

We consider the square end-to-end distance $R^2_e$, the square radius of gyration $R^2_g$ and the square monomer distance from an endpoint $R^2_m$:

$$R^2_e \equiv (\omega_N - \omega_0)^2,$$

$$R^2_g \equiv \frac{1}{N+1} \sum_{i=0}^{N} \left( \omega_i - \frac{1}{N+1} \sum_{k=0}^{N} \omega_k \right)^2 = \frac{1}{2(N+1)^2} \sum_{i,j=0}^{N} (\omega_i - \omega_j)^2,$$

$$R^2_m \equiv \frac{1}{N+1} \sum_{i=0}^{N} (\omega_i - \omega_0)^2.$$

Correspondingly, we define the universal ratios

$$A_N \equiv \frac{\langle R^2_e \rangle_N}{\langle R^2_e \rangle_N}, \quad B_N \equiv \frac{\langle R^2_g \rangle_N}{\langle R^2_e \rangle_N}, \quad C_N \equiv \frac{\langle R^2_m \rangle_N}{\langle R^2_e \rangle_N},$$

and the combination (the exponents $y_\theta$ and $v_\theta$ are defined below)

$$F_N \equiv \left( 2 + \frac{2}{y_\theta + 2v_\theta} \right) A_N - 2B_N + \frac{1}{2} = \frac{23}{8} A_N - 2B_N + \frac{1}{2}.$$

For two-dimensional non-interacting SAWs, it has been proved [50, 51] that the corresponding $F_N$ (with the appropriate exponents $\gamma$ and $\nu$) vanishes in the limit $N \to \infty$. It has been conjectured and verified numerically [16] that $F_\infty = 0$ also at the $\theta$-point.

In a neighbourhood of $\beta_\theta$, the radii have a scaling behaviour of the form

$$\langle R^2 \rangle_N = N^{2v_\theta} f(x), \quad x \equiv N^{\phi}(\beta - \beta_\theta),$$

with $f(0) \neq 0$. More precisely, this scaling form is valid for $\beta \to \beta_\theta$, $N \to \infty$ at fixed $x$. In two dimensions, CFT and Coulomb-gas techniques allow us to compute the universal exponents $\phi$ and $v_\theta$. They are given by [9]

$$v_\theta = \frac{4}{7}, \quad \phi = \frac{3}{7}.$$
The crossover exponent $\phi$ can be measured directly at $\beta = \beta_0$ by considering the specific heat $h_N$, which scales as
\[
h_N \equiv \frac{1}{N} \left( \langle E^2 \rangle_N - \langle E \rangle_N^2 \right) \sim N^{2\phi - 1},
\] (2.10)
or the temperature dependence of the radii,
\[
D_N \equiv -\frac{1}{\langle R^2 \rangle_N} \frac{d\langle R^2 \rangle_N}{d\beta} = \langle E \rangle_N - \frac{\langle R^2 E \rangle_N}{\langle R^2 \rangle_N} \sim N^\phi.
\] (2.11)

In the analysis of the EEDF, we will also consider the exponent $\gamma\theta$, which controls the large-$N$ behaviour of the partition function at the $\theta$ temperature, $Z_N \sim N^{\gamma\theta}$. The exponent $\gamma\theta$ is universal; CFT and Coulomb-gas calculations predict $[9]$ $\gamma\theta = 8/7$.

### 3. Determination of the critical exponents

We performed a MC simulation using the extended reptation algorithm discussed in detail in [52, 53]$^4$. We fixed $\beta = 0.665$, which is the estimate of $\beta_0$ presented in [17], and performed runs for $N = 100, 800, 1600, 3200$. Some results are reported in table 2. Since $\beta_0$ is not exactly known, we also computed several quantities for $\beta = 0.665 - 0.0005n, n = 1, 2, 3, 4$, using the standard reweighting method.

In order to determine $\psi$ we perform fits of the radii to the scaling form (2.8). Since $x$ is small for our data, assuming that the function $f(x)$ is regular at $x = 0$, we can expand it in powers of $x$. At first order, we obtain the scaling form
\[
\langle R^2 \rangle_N = a N^{2\psi} + b N^{2\psi + \phi} (\beta - \beta_0),
\] (3.1)
valid for $x \equiv N^{\psi}(\beta - \beta_0) \ll 1$. We first perform fits taking $a$, $b$, $\psi$, $\phi$, and $\beta_0$ as free parameters. The results are reported in table 3, as a function of $N_{\text{min}}$, the minimum length allowed in the fits. The results obtained in the analysis of the three ratios are reasonably close and indicate
\[
\psi = 0.570(2),
\] (3.2)

$^4$ For non-interacting SAWs, the pivot algorithm [54–56] is extremely efficient. At the $\theta$-point, we do not expect it to be equally good. Still, it might be worthwhile to use it in combination with the extended reptation moves and the multiple Markov chain method [57].
\[ \phi = 0.479(6), \]
\[ \beta_0 = 0.6673(5), \]
\[ T_\nu = 1/\beta_0 = 1.4986(11). \]

These estimates take into account the results of all fits; the reported error is such to include all results and the corresponding errors. The exponent \( \nu_0 \) is in good agreement with the Coulomb-gas prediction \( \nu_0 = 4/7 \approx 0.571 \). On the other hand, the exponent \( \phi \) is significantly larger than \( \phi = 3/7 \approx 0.429 \). This may be due to neglected scaling corrections and/or to the neglected terms in the expansion of the function \( f(x) \), although, we must admit, we have no evidence of corrections in our results, which are stable with respect to \( N_{\text{min}} \) and to the observable considered.

The estimate of \( \beta_0 \) is in good agreement with the most recent one obtained in [48], in which much longer walks were used. The fit in which we assume the theoretical values of the exponents gives estimates of \( \beta_0 \) that have a significantly smaller statistical error. However, note that we neglect here scaling corrections which can—and probably do, given the observed discrepancy for the exponent \( \phi \)—give rise to systematic deviations which are larger than the tiny statistical errors. Hence, we shall keep the conservative estimate (3.4).

In order to obtain independent estimates of the crossover exponent, we also analyse \( D_N \) and \( h_N \). By fitting the MC data we obtain \( \phi = 0.450(4) \) (from \( h_N \)) and \( \phi = 0.436(5) \) (from \( D_N \)). They differ significantly from the estimate (3.3), and thus provide evidence that the apparent stability observed in the fits of the radii and, therefore, the relatively small error should not be trusted. The estimate from the analysis of \( h_N \) and \( D_N \) is in better agreement with the theoretical value than estimate (3.3). The still present tiny discrepancies indicate that corrections to scaling and/or crossover effects are relevant and give rise to systematic deviations, which are larger than the statistical errors. This is consistent with the results of [17] which found \( \phi = 0.435(6) \) with significant scaling corrections. Other recent estimates of \( \phi \) are \( \phi = 0.419(3) \) [20], \( \phi = 0.436(7) \) (in a model with explicit solvent) [21], and \( \phi = 0.422(12) \) from the analysis of the partition-function zeros [22].

Finally, we consider the invariant ratios \( A_N, B_N, C_N, \) and \( F_N \). MC estimates at \( \beta = 0.665 \) are reported in table 2. If we exclude the data with \( N = 100 \), they are constant within error bars, indicating that scaling corrections and crossover effects are smaller than the statistical errors. Conservatively, we estimate the asymptotic value by averaging the results with \( N \geq 1600 \). We obtain \( A_\infty = 0.18151(10), B_\infty = 0.511063(31), C_\infty = 0.35516(17), \) and \( F_\infty = -0.0003(7) \). The ratios \( A_\infty \) and \( B_\infty \) are in good agreement with the results of [16]: \( A_\infty = 0.180(1), B_\infty = 0.510(2) \). The estimate of \( F_\infty \) is fully compatible with zero, providing further support to the conjecture \( F_\infty = 0 \) of [16].

| \( N_{\text{min}} \) | \( \nu \) | \( \phi \) | \( \beta_0 \) | \( \beta_0 \) (f.exp.) |
|-------------------|--------|--------|----------------|------------------|
| \( R_g \)         | 100    | 0.5720(2) | 0.480(4) | 0.6669(1) | 0.6675(1) |
|                   | 800    | 0.5721(2) | 0.480(5) | 0.6669(1) | 0.6675(1) |
| \( R_\nu \)       | 100    | 0.5678(3) | 0.480(5) | 0.6677(1) | 0.6670(1) |
|                   | 800    | 0.5683(3) | 0.480(5) | 0.6676(1) | 0.6670(1) |
| \( R_m \)         | 100    | 0.5706(3) | 0.478(6) | 0.6672(1) | 0.6671(1) |
|                   | 800    | 0.5711(3) | 0.478(5) | 0.6670(1) | 0.6671(1) |
Figure 1. Rescaled distribution functions $\langle q_\alpha \rangle_N P_{\alpha,N}(q_\alpha)$ for the two eigenvalues $q_\alpha$ of the gyration tensor.

Table 4. MC estimates of the eigenvalues of the gyration tensor, of the shape factor $s_1$, and of the mean asphericity.

| $N$  | $\langle q_1 \rangle_N$ | $\langle q_2 \rangle_N$ | $s_1$    | $\mathcal{A}$   |
|------|-------------------------|-------------------------|----------|-----------------|
| 100  | 35.543(8)               | 7.8954(8)               | 0.8182(2)| 0.37668(8)     |
| 800  | 386.85(30)              | 85.871(34)              | 0.8183(8)| 0.37569(28)    |
| 1600 | 859.93(37)              | 190.262(41)             | 0.8188(5)| 0.37653(16)    |
| 3200 | 1916.6(1.5)             | 422.06(17)              | 0.8195(8)| 0.37805(28)    |

4. Gyration tensor and asphericity

It has been known for many years that polymers are not instantaneously spherical in shape [29]. In order to characterize the shape, we consider the gyration tensor defined by

$$Q_{N,\alpha\beta} \equiv \frac{1}{2(N+1)^2} \sum_{i,j=0}^{N} (\omega_{i,\alpha} - \omega_{j,\alpha})(\omega_{i,\beta} - \omega_{j,\beta}),$$

(4.1)

which is such that $\text{Tr } Q_N = R_g^2$. The tensor $Q_{N,\alpha\beta}$ is symmetric and positive definite; hence, it has two positive eigenvalues $q_1 \geq q_2$. For $N \to \infty$ they are expected to scale as

$$\langle q_\alpha \rangle_N \approx B_\alpha N^{2\alpha},$$

(4.2)

and to obey a scaling law of the form

$$P_{\alpha,N}(q_\alpha) = \frac{1}{\langle q_\alpha \rangle_N} F_\alpha \left( \frac{q_\alpha}{\langle q_\alpha \rangle_N} \right).$$

(4.3)

In figure 1, we report the rescaled eigenvalue distributions. All points fall quite well onto two different universal curves, confirming the validity of the scaling form (4.3). Note that, although the average eigenvalues differ approximately by a factor of 4.5, see table 4, the two distribution functions are similar. They have a sharp peak for $q_\alpha/\langle q_\alpha \rangle_N \approx 0.55$ ($\alpha = 1$) and 0.75 ($\alpha = 2$), a long tail, and go to zero sharply for $q_\alpha/\langle q_\alpha \rangle_N \approx 0.25$. 
To characterize quantitatively the shape of θ walks, we introduce the shape factors
\[ s_1 \equiv \frac{\langle q_1 \rangle_N}{\langle R^2 \rangle_N} = 1 - s_1, \quad s_2 \equiv \frac{\langle q_2 \rangle_N}{\langle R^2 \rangle_N} = \frac{s_1}{1 - s_1}, \quad r_{12} \equiv \frac{\langle q_1 \rangle_N}{\langle q_2 \rangle_N} = \frac{s_1}{1 - s_1}, \tag{4.4} \]
and the mean asphericity
\[ A \equiv \frac{1}{2} \sum_\alpha \left( \frac{(q_\alpha - \bar{q})^2}{\bar{q}^2} \right)_N = \left( \frac{\langle q_1^2 - q_2^2 \rangle}{\langle q_1 + q_2 \rangle^2} \right)_N, \tag{4.5} \]
where \( \bar{q} = \sum_\alpha q_\alpha / 2 = \frac{R^2_g}{2} \). For a disc we have \( s_1 = 1/2, A = 0 \), while a rod gives \( s_1 = 1, A = 1 \).

At variance with the ratios \( A_N \), the quantities \( s_1 \) and \( A \) at \( \beta = 0.665 \) show a systematic drift with \( N \), which may be an indication of the crossover towards the asymptotic good-solvent value. To take it into account, we use the expected scaling behaviour close to the θ-point:
\[ s_1, A = f[(\beta - \beta_0)N^\phi]. \tag{4.6} \]
Expanding the function \( f(x) \) to first order, we obtain
\[ s_1, A = a_1 + a_2(\beta - \beta_0)N^\phi. \tag{4.7} \]
This implies that we should fit our data to \( a_1 + b N^\phi \). The parameter \( a_1 \) gives the θ-point estimate of the universal ratio. Using \( \phi = 3/7 \), we obtain \( s_1 = 0.8179(4) \) if we fit all data, and \( s_1 = 0.8169(20) \) if we discard \( N = 100 \). Conservatively, we quote as the final result
\[ s_1 = 0.817(2). \tag{4.8} \]
From \( s_1 \) we can compute the ratio of the average eigenvalues:
\[ r_{12} = 4.46(6). \tag{4.9} \]
Note that the walks are elliptical, with the major axis being approximately a factor of 2 longer than the minor one.

The \( N \) dependence of the average asphericity is not monotonic, and thus the fitting form (4.7) cannot describe the data up to \( N = 100 \). We thus only fit the data satisfying \( N \geq 800 \), obtaining
\[ A = 0.3726(7). \tag{4.10} \]
Note that the error is purely statistical and thus it does not include the systematic uncertainty due to the scaling corrections. It is interesting to compare the results for the asphericity with those obtained under good-solvent conditions [45, 46]:
\[ A_{GS} = 0.503(1). \tag{4.11} \]
Clearly, at the θ-point, walks are more symmetric than in the good-solvent regime. Note that our result is closer to the random-walk value [47]
\[ A_{RW} = \frac{5}{2} - \frac{2}{7} \xi(3) \approx 0.3964. \tag{4.12} \]
Thus, also in two dimensions, θ-point interacting SAWs can be reasonably described by random walks (in three dimensions interacting SAWs are effectively random walks in the limit \( N \to \infty \), although for finite \( N \) there are quite strong logarithmic corrections), as far as the shape is concerned.
5. End-to-end distribution function

5.1. Definitions

If \( c_N(r) \) is the number of SAWs starting at the origin and ending in \( r \), we define the normalized EEDF as

\[
P_N(r) = \frac{c_N(r)}{\sum_r c_N(r)}. \tag{5.1}
\]

The mean squared end-to-end distance is related to \( P_N(r) \) by

\[
\langle R_e^2 \rangle_N = \sum_r |r|^2 P_N(r). \tag{5.2}
\]

In most of the studies of the EEDF, one usually defines a correlation length \( \xi \) which is trivially related to \( R_e^2 \):

\[
\xi^2 = \frac{1}{4} \langle R_e^2 \rangle_N. \tag{5.3}
\]

In the following we shall always use \( \xi \) to characterize the polymer size. In the limit \( N \to \infty \), \( |r| \to \infty \), with \( |r|/N^{1-\nu} \) fixed, the function \( P_N(r) \) has the scaling form \([33, 35, 37]\)

\[
P_N(r) \approx \frac{1}{\xi^2} f(\rho) \left[ 1 + O(N^{-\Delta}) \right], \tag{5.4}
\]

where \( \rho = r/\xi \), \( \rho = |\rho| \), and \( \Delta \) is a correction-to-scaling exponent. By definition

\[
\int_0^\infty 2\pi \rho \, d\rho f(\rho) = 1, \tag{5.5}
\]

\[
\int_0^\infty 2\pi \rho^3 \, d\rho f(\rho) = 4. \tag{5.6}
\]

Several facts are known about \( f(\rho) \). For large values of \( \rho \), it behaves as \([32, 33, 35, 37]\)

\[
f(\rho) \approx f_\infty \rho^\sigma \exp(-D\rho^\delta), \tag{5.7}
\]

where \( \sigma \) and \( \delta \) are given by

\[
\delta = \frac{1}{1 - \nu} = \frac{7}{3} \approx 2.33, \tag{5.8}
\]

\[
\sigma = \frac{4v_0 - 2\gamma_0}{2(1 - v_0)} = 0. \tag{5.9}
\]

For \( \rho \to 0 \), we have \([35, 37]\) instead

\[
f(\rho) \approx f_0 \rho^\theta, \tag{5.10}
\]

where

\[
\theta = \frac{\gamma_0 - 1}{v_0} = \frac{1}{4}. \tag{5.11}
\]

For the purpose of computing \( D \) and \( \delta \) from MC data, it is much easier to consider the ‘wall–wall’ distribution function

\[
P_{w,N}(x) = \sum_y P_N(x, y), \tag{5.12}
\]

which represents the probability that the endpoint of the walk lies on a plane at a distance \( x \) from the origin of the walk. In the large-\( N \) limit, \( P_{w,N}(x) \) has the scaling form

\[
P_{w,N}(x) = \frac{1}{\xi} f_w(\rho) \left[ 1 + O(N^{-\Delta}) \right], \quad \rho = \frac{|x|}{\xi}. \tag{5.13}
\]
Figure 2. The wall–wall EEDF: rescaled combination $\xi P_{w,N}(x)$ versus $\rho$ for different values of $N$.

For large $\rho$, we have

$$f_w(\rho) \approx f_{w,\infty}\rho^{\sigma_w} \exp(-D\rho^d),$$  \hspace{1cm} (5.14)

where $\delta$ is given by equation (5.8), $D$ is the same constant appearing in (5.7), and \[44\]

$$\sigma_w = \delta \left(\nu_\theta - \gamma_\theta + \frac{1}{2}\right) = -\frac{1}{6}. \hspace{1cm} (5.15)$$

5.2. MC study

We studied the EEDF following closely the strategy employed in [44] to analyse the same quantity for three-dimensional non-interacting SAWs. Since our runs were performed at $\beta = 0.665 < \beta_\theta$, in principle, we should reweight the MC data to obtain the EEDF at the $\theta$-point. This correction is apparently negligible compared to the statistical errors, so that we directly analyse the results for $\beta = 0.665$ without additional corrections.

First, we consider the wall–wall distribution $P_{w,N}(x)$. In figure 2, we report the scaling combination $\xi P_{w,N}(x)$ versus the scaling variable $\rho$. The scaling is essentially perfect on the scale of the figure, confirming the correctness of (5.13). Then, we study the large-$\rho$ behaviour with the purpose of verifying the asymptotic behaviour (5.14) and of determining the constants $D$ and $f_{w,\infty}$. Our data are not precise enough to determine $\sigma_w$ and thus we always fix its value in the numerical analysis. We fit the data to

$$\ln \xi P_{w,N} = \ln f_{w,\infty} - D\rho^d, \hspace{1cm} (5.16)$$

$$\ln(\rho^{1/\delta} P_{w,N}) = \ln f_{w,\infty} - D\rho^d. \hspace{1cm} (5.17)$$

The two fits give correct estimates of $D$ and $\delta$, but only the second one provides a correct estimate of $f_{w,\infty}$. We consider only the data belonging to the range $\rho_{\text{min}} \leq \rho \leq \rho_{\text{max}}$. An upper cut-off $\rho_{\text{max}}$ is needed since scaling corrections and numerical errors increase as $\rho$ increases. First, since $P_{w,N}(x) = 0$ for $|x| > N$, the deviations from (5.16) and (5.17) at fixed $N$ become infinitely large as $\rho \rightarrow N/\xi \sim N^{\nu_\theta-1}$. Second, since the EEDF decreases rapidly with $\rho$, for large $\rho$ there is very limited statistics, so that $P_{w,N}(x)$ has a very large
error. But large-$\rho$ data dominate in the fits, providing completely unreliable estimates of the fit parameters.

Results obtained from fits to ansatz (5.16) are reported in table 5, as a function of $N = 100, 800, 1600, 3200$. The results for $\delta$ do not show systematic dependences on the fit parameters $\rho_{\text{min}}$ and $\rho_{\text{max}}$ (at least in the range we consider), while they show a tiny dependence on $N$: apparently, for $N \geq 800$, $\delta$ increases with increasing $N$. The reason is not fully clear but it may be again an effect of the crossover towards the good-solvent value $\delta = 1/(1-\nu) = 4$. In any case, the results are reasonably consistent with the theoretical prediction $\delta = 7/3 \approx 2.333$. The constant $D$ varies roughly between 0.13 and 0.17 for $N \geq 800$, so that we can estimate $D = 0.15(2)$.

In order to estimate $f_{w,\infty}$, we cannot neglect the multiplicative factor $\rho^{a_w}$ and thus only the results of the second fit are relevant. From the data at $N = 1600$, see table 6, we obtain

$$\log f_{w,\infty} = -0.60(5), \quad f_{w,\infty} = 0.55(3), \quad (5.18)$$

where the error takes into account the estimates obtained by using all values of $N$.

Let us consider now the radial distribution $P_N(r)$. Such a quantity is not well suited for a numerical determination of the scaling function $f(\rho)$, because of fluctuations due to the lattice structure. In order to average them out, we will employ a procedure already used in this context in [40, 41, 44].

| $N$  | $\rho_{\text{max}}$ | $\rho_{\text{min}}$ | $\delta$ | $D$   |
|------|---------------------|---------------------|----------|-------|
| 100  | 4 2                 | 2 2                 | 2.517(3) | 0.127(1) |
|      | 3 2                 | 2.50(21)            | 0.131(5) |
| 5    | 2 2                 | 2.466(6)            | 0.142(1) |
|      | 3 2                 | 2.504(13)           | 0.133(3) |
| 6    | 2 2                 | 2.565(14)           | 0.117(3) |
|      | 3 2                 | 2.60(29)            | 0.109(6) |
| 800  | 4 2                 | 2.394(12)           | 0.148(3) |
|      | 3 2                 | 2.410(82)           | 0.144(20)|
| 5    | 2 2                 | 2.318(9)            | 0.173(3) |
|      | 3 2                 | 2.305(29)           | 0.177(9) |
| 6    | 2 2                 | 2.378(20)           | 0.153(6) |
|      | 3 2                 | 2.361(43)           | 0.158(13)|
| 1600 | 4 2                 | 2.426(5)            | 0.141(1) |
|      | 3 2                 | 2.390(30)           | 0.150(8) |
| 5    | 2 2                 | 2.353(7)            | 0.164(2) |
|      | 3 2                 | 2.358(21)           | 0.162(6) |
| 6    | 2 2                 | 2.414(15)           | 0.144(4) |
|      | 3 2                 | 2.430(32)           | 0.139(9) |
| 3200 | 4 2                 | 2.455(11)           | 0.135(2) |
|      | 3 2                 | 2.423(77)           | 0.142(18)|
| 5    | 2 2                 | 2.371(15)           | 0.159(4) |
|      | 3 2                 | 2.375(45)           | 0.158(13)|
| 6    | 2 2                 | 2.469(31)           | 0.132(8) |
|      | 3 2                 | 2.493(67)           | 0.125(16)|
particularly evident for \( /Lambda_1 \), we define \( /Lambda_1 \) with \( /Lambda_1 \). We perform fits of the form (5.6). A point (x, y) is odd (resp. even) if x + y is odd (resp. even).

In figure 3, we report the rescaled EEDF obtained by using the average (5.19), which is in agreement with the estimate obtained by using the wall–wall EEDF.

Results for \( N = 100 \) correspond to fixing the area (hence the number of points). As for \( N = 100 \), this is particularly evident for \( \rho < 1.5 \). This confirms the validity of the scaling relation (5.4).

Let us now again consider the large-\( \rho \) behaviour. In order to determine the parameters, we perform fits of the form

\[
\log[E_{\infty}^{(av)}] = \log f_{\infty} - D\rho^\delta
\]

for each \( N \) and for several \( \rho_{\min} \), \( \rho_{\max} \), and \( \delta \). Note that in this case, theory predicts \( \sigma = 0 \) and thus this fit allows us to determine \( f_{\infty} \), too.

Results for \( N \geq 800 \), \( \Lambda = 1/15 \) and the fixed-width average (5.19) are reported in table 7. The results for \( \delta \) are fully consistent with the theoretical value, while those for \( D \) give roughly \( D = 0.16(2) \), which is in agreement with the estimate obtained by using the wall–wall EEDF. Estimates using \( \Lambda = 1/5 \), or obtained by using the average (5.20), give similar results. As for \( f_{\infty} \) we estimate log \( f_{\infty} = -2.60(15) \) and \( f_{\infty} = 0.082(11) \).

More precise estimates of \( D \), \( f_{\infty} \), and \( f_{w,\infty} \) are obtained by fixing \( \delta \) to its theoretical value \( \delta = 7/3 \). From the analysis of the wall–wall EEDF, using the fit function (5.17), we obtain

\[
D = 0.1668(3), \quad f_{w,\infty} = 0.625(4), \quad f_{\infty} = 0.607(9) \quad (5.22)
\]

while from the radial distribution function, we have

\[
D = 0.1656(3), \quad f_{\infty} = 0.607(9) \quad (5.23)
\]

We shall consider two different averages,

\[
\hat{P}_{1,n}^{(aw)}(r_1, n) = \frac{1}{2N_1,n(r_1,n)} \sum_{r_1 \leq r_1, n} P_N(r),
\]

\[
\hat{P}_{2,n}^{(av)}(r_2, n) = \frac{1}{2N_2,n(r_2,n)} \sum_{r_2 \leq r_2, n} P_N(r).
\]

Here \( r_1, n = r_0 + n \Delta \) and \( r_2^2, n = r_0^2 + n \Delta \), where \( r_0 \) and \( \Delta \) are fixed parameters, and \( N_1,n(r_1,n) \) and \( N_2,n(r_2,n) \) are the number of lattice points with the same parity of \( \rho \) that lie in the considered shell. For practical purposes, we measure \( \Delta \) in units of the correlation length: we define \( \Lambda = \Delta / \xi \) and keep it fixed for all values of \( N \). For \( \Delta \) fixed, \( P_N(r), \hat{P}_{1,n}^{(av)}(r), \) and \( \hat{P}_{2,n}^{(av)}(r) \) have the same scaling behaviour as \( N \to \infty \). The same holds for fixed \( \Lambda \), as long as \( \Lambda \ll 1 \). In figure 3, we report the rescaled EEDF obtained by using the average (5.19) with \( \Lambda = 1/15 \). All points fall on top of each other, except for those with \( N = 100 \) (this is particularly evident for \( \rho < 1.5 \)). This confirms the validity of the scaling relation (5.4).

| \( N \) | \( \rho_{\min} \) | \( \delta \) | \( D \) | \( \log f_{w,\infty} \) |
|---|---|---|---|---|
| 100 | 2 | 2.527(4) | 0.125(1) | -0.640(5) |
| | 3 | 2.545(13) | 0.121(3) | -0.670(2) |
| 800 | 2 | 2.377(10) | 0.153(3) | -0.577(13) |
| | 3 | 2.345(30) | 0.162(9) | -0.520(53) |
| 1600 | 2 | 2.412(7) | 0.145(2) | -0.607(9) |
| | 3 | 2.397(22) | 0.149(6) | -0.581(37) |
| 3200 | 2 | 2.431(15) | 0.140(4) | -0.620(18) |
| | 3 | 2.417(46) | 0.144(12) | -0.598(78) |

We consider two different averages, \( \hat{P}_{1,n}^{(av)}(r_1, n) \) and \( \hat{P}_{2,n}^{(av)}(r_2, n) \), which are fixed parameters, and \( N_1,n(r_1,n) \) and \( N_2,n(r_2,n) \) are the number of lattice points with the same parity of \( \rho \) that lie in the considered shell. For practical purposes, we measure \( \Delta \) in units of the correlation length: we define \( \Lambda = \Delta / \xi \) and keep it fixed for all values of \( N \). For \( \Delta \) fixed, \( P_N(r), \hat{P}_{1,n}^{(av)}(r), \) and \( \hat{P}_{2,n}^{(av)}(r) \) have the same scaling behaviour as \( N \to \infty \). The same holds for fixed \( \Lambda \), as long as \( \Lambda \ll 1 \). In figure 3, we report the rescaled EEDF obtained by using the average (5.19) with \( \Lambda = 1/15 \). All points fall on top of each other, except for those with \( N = 100 \) (this is particularly evident for \( \rho < 1.5 \)). This confirms the validity of the scaling relation (5.4).

Let us now again consider the large-\( \rho \) behaviour. In order to determine the parameters, we perform fits of the form

\[
\log[E_{\infty}^{(av)}] = \log f_{\infty} - D\rho^\delta
\]

for each \( N \) and for several \( \rho_{\min} \), \( \rho_{\max} \), and \( \delta \). Note that in this case, theory predicts \( \sigma = 0 \) and thus this fit allows us to determine \( f_{\infty} \), too.

Results for \( N \geq 800 \), \( \Lambda = 1/15 \) and the fixed-width average (5.19) are reported in table 7. The results for \( \delta \) are fully consistent with the theoretical value, while those for \( D \) give roughly \( D = 0.16(2) \), which is in agreement with the estimate obtained by using the wall–wall EEDF. Estimates using \( \Lambda = 1/5 \), or obtained by using the average (5.20), give similar results. As for \( f_{\infty} \) we estimate log \( f_{\infty} = -2.60(15) \) and \( f_{\infty} = 0.082(11) \).

More precise estimates of \( D \), \( f_{\infty} \), and \( f_{w,\infty} \) are obtained by fixing \( \delta \) to its theoretical value \( \delta = 7/3 \). From the analysis of the wall–wall EEDF, using the fit function (5.17), we obtain

\[
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\]

while from the radial distribution function, we have

\[
D = 0.1656(3), \quad f_{\infty} = 0.607(9) \quad (5.23)
\]
The estimates of $D$ obtained in the two cases differ by two combined error bars, indicating that the errors are underestimated by a factor of at least 2. Multiplying all errors by 2, we end up with the final estimates

$$D = 0.1662(6), \quad f_{w.\infty} = 0.625(8), \quad f_{\infty} = 0.088(4).$$

We finally consider the behaviour for $\rho \to 0$, performing fits of the form

$$\log f(\rho) = \log f_0 + \theta \log \rho,$$

see (5.10). Since (5.25) is valid only for $\rho \to 0$ and for $r \to \infty$ (scaling limit), data must be analysed in a window $\rho_{\text{min}} \leq \rho \leq \rho_{\text{max}}$. We find stable results only for $N = 3200$. For lower values of $N$, lattice effects are very strong and equation (5.25) does not describe the low-$r$ data.
Table 8. The non-trivial even moments $M_{2k,N}$, $k \leq 6$, and the corresponding asymptotic values.

| $N$  | $M_{4,N}$ | $M_{6,N}$ | $M_{8,N}$ | $M_{10,N}$ | $M_{12,N}$ |
|------|-----------|-----------|-----------|------------|------------|
| 100  | 1.778(1)  | 4.422(4)  | 13.89(2)  | 52.2(1)    | 226.8(6)   |
| 800  | 1.815(4)  | 4.661(1)  | 15.317(7) | 60.84(4)   | 281.3(3)   |
| 1600 | 1.8192(1) | 4.691(1)  | 15.494(4) | 61.82(2)   | 288.2(2)   |
| 3200 | 1.8184(4) | 4.682(2)  | 15.404(7) | 61.24(4)   | 283.2(3)   |

If we write $\rho_{\min} = n_{\min} / \Lambda \xi$, we find stable results for $n_{\min} \gtrsim 1$, $0.15 \lesssim \rho_{\max} \lesssim 0.30$, and $\Lambda$ quite small, $\Lambda \approx 10^{-2}$. If the parameters are in this range, we obtain

$$\theta = 0.255(10),$$

$$f_0 = 0.081(2).$$

The result for $\theta$ is in perfect agreement with the theoretical prediction $\theta = 1/4$. An improved estimate of $f_0$ can be obtained by fixing $\theta$ to its theoretical value. We obtain

$$f_0 = 0.0810(5).$$

Finally, we computed the moments

$$M_{2k,N} = \frac{\sum r^{2k} P_N(r)}{\sum r^2 P_N(r)},$$

see table 8. We extrapolated the results by performing a fit of the form

$$M_{2k,N} = M_{2k,\infty} + a N^{-\Delta},$$

where $M_{2k,\infty}$, $a$, and $\Delta$ are free parameters. The results are reported in table 8.

5.3. Phenomenological expressions

A phenomenological representation for the function $f(\rho)$ has been proposed by McKenzie and Moore [35] and des Cloizeaux [7]:

$$f(\rho) \approx f_{ph}(\rho) = f_{ph} \rho^{\theta_{ph}} \exp(-D_{ph} \rho^{\delta_{ph}}).$$

Here $\delta_{ph}$ and $\theta_{ph}$ are free parameters, while $f_{ph}$ and $D_{ph}$ are fixed by the normalization conditions (5.5) and (5.6):

$$D_{ph} = \left\{ \frac{\Gamma[(4 + \theta_{ph})/\delta_{ph}]}{4\Gamma[(2 + \theta_{ph})/\delta_{ph}]} \right\}^{\delta_{ph}/2},$$

$$f_{ph} = \frac{\delta_{ph} D_{ph}^{(2+\theta_{ph})/\delta_{ph}}}{2\pi \Gamma[(2 + \theta_{ph})/\delta_{ph}]}.$$

In three dimensions, in the good-solvent regime this expression describes the EEDF quite accurately, even taking $\delta$ and $\theta$ equal to their theoretical value [44].

In our case, if we use $\theta_{ph} = \theta = 1/4$ and $\delta_{ph} = \delta = 7/3$ we obtain for the two constants

$$D_{ph} = 0.1794, \quad f_{ph} = 0.06931,$$

which are quite close to the exact results. The resulting curve, curve (a) in figure 4, reasonably describes the EEDF in the large- and small-distance region, but underestimates it in the intermediate region $0.2 \lesssim \rho \lesssim 1.4$. As an additional check we can compute the invariant ratios.
Figure 4. The EEDF against several phenomenological approximations: (a) we set $\delta_{ph} = 7/3$ and $\theta_{ph} = 1/4$ and use (5.32) to fix the constants; (b) $\delta_{ph}$ and $\theta_{ph}$ are determined by fitting the data, while the constants are fixed by (5.32); (c) $\delta_{ph}$, $\theta_{ph}$, $D_{ph}$, and $f_{ph}$ are obtained by fitting the data.

Using the phenomenological expression, we obtain $M_{2k,ph} = 1.77, 4.39, 13.9, 53.1, 237$ for $k = 2, 3, 4, 5, 6$. They are not very different from the exact results reported in table 8, the differences varying between 3% for $k = 2$ and 18% for $k = 6$. Note that discrepancies increase as $k$ increases. This is due to the fact that these ratios are increasingly sensitive to the large-$\rho$ behaviour, and the phenomenological expression underestimates the EEDF for large $\rho$ since $D_{ph} > D = 0.1662(6)$.

In order to obtain a better approximation, we take $\theta_{ph}$ and $\delta_{ph}$ as free parameters, fixing always $D_{ph}$ and $f_{ph}$ by using the normalization conditions (5.32). We obtain

$\quad \theta_{ph} \approx 0.282, \quad \delta_{ph} \approx 2.04.$ \hspace{1cm} (5.34)

Correspondingly $D_{ph} = 0.270, f_{ph} = 0.0795$. The resulting phenomenological expression describes better the EEDF in the relevant region $\rho \lesssim 5$, see figure 4, but clearly overestimates the EEDF in the large-$\rho$ region, given that $\delta_{ph}$ is smaller than $\delta = 7/3 = 2.333$. As a check we again computed the ratios $M_{2k}$. For $k = 2$ we obtain $M_{4,ph} = 1.825$ which agrees with the correct value $M_4 = 1.821(4)$ and confirms the validity of the approximation for $\rho$ is not too large. However, for $k \geq 3$ the obtained estimates $M_{2k,ph}$ are larger than those reported in table 8. For instance, we obtain $M_{6,ph} = 4.96$ and $M_{8,ph} = 17.65$, which overestimate the correct results by 5% and 14%, respectively.

We obtain a slightly better approximation if we keep all constants as free parameters, relaxing the normalization conditions (5.32). We obtain

$\quad \theta_{ph} \approx 0.277, \quad \delta_{ph} = 1.95, \quad D_{ph} = 0.285, \quad f_{ph} = 0.0805.$ \hspace{1cm} (5.35)

The corresponding curve is reported in figure 4, as graph (c). It cannot be distinguished on the scale of the figure from graph (b), obtained by using parameters (5.34). This is not unexpected, since the parameters are quite close to each other. For the choice (5.35) of the constants, we have

$\quad \int_0^\infty 2\pi \rho \ d\rho f(\rho) = 1.042.$ \hspace{1cm} (5.36)
\[ \int_0^{\infty} 2\pi \rho^3 \, d\rho f(\rho) = 4.469. \]  
(5.37)

The violations of the normalization conditions are therefore reasonably small (4% and 10% in the two cases).

5.4. Internal-point distribution function

As a byproduct of our simulations, we also determined an exponent which is related to the internal-point distribution function. We consider the probability \( P_{N,M}(r) \) that \( \omega_M - \omega_0 = r \), where \( \omega_M \) is an internal point, i.e. \( M < N \). In the limit \( N, M \to \infty, r \to \infty \) with \( r N^{-\nu} \) and \( M/N \) fixed, we obtain the scaling expression

\[ P_{N,M}(r) \approx \frac{1}{\xi^2} f_{\text{int}}(r/\xi, M/N), \]  
(5.38)

where \( \xi^2 = \langle R^2 \rangle_N / 4 \) as before. The function \( f_{\text{int}}(\rho, M/N) \) is nonanalytic for \( \rho \to 0 \):

\[ f_{\text{int}}(\rho, M/N) \sim \rho^{\theta_{\text{int}}}, \]  
(5.39)

where the exponent \( \theta_{\text{int}} \) is independent of \( M/N \). In two dimensions, \( \theta_{\text{int}} \) has been computed exactly, obtaining \( \theta_{\text{int}} = 5/6 \) for non-interacting SAWs and \( \theta_{\text{int}} = 5/12 \) at the \( \theta \)-point [9].

The exponent \( \theta_{\text{int}} \) can be determined by measuring the probability \( P_{\text{ENN}} \) that the endpoint is a nearest neighbour of the walk. Keeping into account that there are \( N \) internal points, we obtain

\[ P_{\text{ENN}} \sim N \xi^{-\theta_{\text{int}}} \sim N^{2-\nu-\nu\theta_{\text{int}}}. \]  
(5.40)

It should be noted that this expression only takes into account 'distant' contacts, since the scaling form (5.38) is valid only in the limit \( r \to \infty \). To this nonanalytic term we should therefore add the contribution of 'local' contacts, which is expected to be an analytic function of \( N \). Thus, we obtain the prediction

\[ P_{\text{ENN}} \approx a + b/N + c/N^{\nu(2+\nu\theta_{\text{int}})-1} + \cdots, \]  
(5.41)

At the \( \theta \)-point, this gives

\[ P_{\text{ENN}} \approx a + b/N + c/N^{8/21}, \]  
(5.42)

while for non-interacting SAWs, we have

\[ P_{\text{ENN}} \approx a + b/N + c/N^{9/8}. \]  
(5.43)

We have computed \( P_{\text{ENN}} \) at the \( \theta \)-point\(^7 \) and fitted the results with \( a + b/N^\Delta \) (see table 9). The estimates of \( \Delta \) allow us to obtain an estimate of \( \theta_{\text{int}} \):

\[ \theta_{\text{int}} = 0.407(11). \]  
(5.44)

This result is in good agreement with the theoretical value \( 5/12 = 0.4166 \ldots \). Moreover, we obtain

\[ P_{\text{ENN}}^{\infty} = 0.7854(14). \]  
(5.45)

\(^7\) We have also studied \( P_{\text{ENN}} \) for non-interacting SAWs in two and three dimensions. In both cases the data are well fitted by \( a + b/N \), which allows us to conclude that \( \theta_{\text{int}} > 2(1 - \nu) / \nu \). In two dimensions, this is consistent with the theoretical prediction, while in three dimensions it implies \( \theta_{\text{int}} \gtrsim 1.40 \).
Table 9. Probability that the endpoint is a nearest neighbour of the walk.

| $N$  | $p^\text{ENN}_N$  |
|------|------------------|
| 100  | 0.63307(4)      |
| 800  | 0.71579(10)     |
| 1600 | 0.73159(6)      |
| 3200 | 0.74407(10)     |

6. Conclusions

In this paper, we present a detailed study of some geometrical properties of two-dimensional interacting SAWs at the $\theta$-point. For this purpose we have generated walks of length up to $N = 3200$ at $\beta = 0.665$, which is close to the $\theta$-point value $\beta_\theta = 0.6673(5)$.

The main results of this investigation are as follows.

(i) We compute the critical exponents $\nu_\theta$ and $\phi$. Our estimate of $\nu_\theta$, $\nu_\theta = 0.570(2)$, is in perfect agreement with the Coulomb-gas prediction [9] $\nu_\theta = 4/7 \approx 0.571$. For the exponent $\phi$, we find $\phi = 0.479(6)$ from the analysis of the radii, $\phi = 0.436(5)$ from the analysis of their temperature dependence, and $\phi = 0.450(4)$ from the specific heat (errors are purely statistical). The somewhat large differences among these estimates indicate that the neglected scaling corrections are important. A reasonable final estimate would be $\phi = 0.46(3)$, which takes into account all results with their errors. Thus, we also confirm, although with limited precision, the theoretical prediction [9] $\phi = 3/7 \approx 0.429$.

(ii) We compute several invariant ratios involving the radii $R^2_g$, $R^2_m$, and $R^2_e$ and, in particular, we verify a conjecture of [16]. For $N \to \infty$, the combination $F_N$ defined in (2.7) vanishes, as it does for non-interacting SAWs [50, 51].

(iii) We discuss the shape of the walks, determining, in particular, the average asphericity $A$. We obtain

$$A = 0.3726(7),$$

where the error is purely statistical. Walks are typically elliptic, the ratio of the two axes being $2.11(2)$. For comparison, note that for random walks [47], $A = 0.3964$, while under good-solvent conditions [45, 46], $A = 0.503(1)$.

(iv) We compute the EEDF. We verify the theoretical predictions for its small- and large-distance behaviour and provide effective approximations valid in the whole relevant range $r/\xi \lesssim 5$, that is, for $r/(R_e)_N \lesssim 2.5$ (for $r \gtrsim 5\xi$, the EEDF is very small).

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