

Energy of the Interacting Self-Avoiding Walk at the θ -point

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We perform a numerical study of a new microcanonical polymer model on the three dimensional cubic lattice, consisting of ideal chains whose range and number of nearest-neighbor contacts are fixed to given values. Our simulations suggest an interesting exact relation concerning the internal energy per monomer of the Interacting Self-Avoiding Walk at the θ -point.

I. INTRODUCTION

It is well known that a polymer chain can collapse from an extended to a compact configuration if the temperature or the solvent quality is lowered below some critical value. This phenomenon, known as Coil-to-Globule transition (CG, [1–3]), arises when the attractive interaction between the monomers overwhelm the excluded volume effect. At the transition temperature (commonly called θ -point) these contributions compensate, resulting in a phase where the chains behave approximately as random walks [1, 4–6].

Let ω_N be an N -steps Simple Random Walk (SRW) on the cubic lattice \mathbb{Z}^d ,

$$\omega_N = \left\{ x_t(\omega_N) \in \mathbb{Z}^d : 0 \leq t \leq N \right\}, \quad (1)$$

by convention we fix the seed monomer at $x_0(\omega_N) = 0$. The chain can be represented through the locations of its monomers $x_t(\omega_N)$ or equivalently by the orientations of its steps

$$x_t(\omega_N) - x_{t-1}(\omega_N) \in \Omega_1, \quad (2)$$

where Ω_1 is the set of possible orientations on \mathbb{Z}^d (for the cubic lattice the number is $|\Omega_1| = 2d$). Then, we indicate with

$$\Omega_N = \Omega_1^N \ni \omega_N \quad (3)$$

the set of all possible chain configurations.

Here we present a micro-canonical model where the number of distinct lattice sites visited by the walk $R(\omega_N)$ (*range*) and the number of nearest-neighbors monomer pairs $L(\omega_N)$ (*links*) are constrained to scale with the number of steps N , formally

$$R(\omega_N) = \lfloor (1-m)N \rfloor, \quad L(\omega_N) = \lfloor \lambda N \rfloor, \quad (4)$$

where we denoted by $\lfloor z \rfloor$ the lower integer truncation of $z \in \mathbb{R}$, (see Figure 1). The model is controlled by the pair of parameters m and λ , and the Interacting Self-Avoiding Walk (ISAW, [7–12, 16, 17]) is recovered by taking $m = 0$.

We numerically investigated the micro-canonical phase diagram on the plane (m, λ) , formulating a conjecture on the location of the transition line $\lambda = \ell_c(m)$ that is expected to separate the SAW like-phase (where the scaling of the average chain displacement is that of the SAW) from the clustered phase (in which the chains configure into compact clusters).

Based on these computer simulations and some additional theoretical arguments, our analysis suggests that at least in the Thermodynamic Limit (TL) $N \rightarrow \infty$ the critical link density is a linear function of m

$$\ell_c(m) = \lambda_c + \delta_c m \quad (5)$$

and the constant λ_c is expected to match the density of contacts per monomer of the ISAW at the θ -point in the TL.

Before going further we introduce the notation and state some basic properties. Without loss of generality, instead of $R(\omega_N)$ we will work with the related quantity

$$M(\omega_N) = N + 1 - R(\omega_N), \quad (6)$$

which represent the number of *intersections* present in the chain ω_N . Our model is then defined by a partition of Ω_N into subsets $\Omega_N(M, L)$ such that each walk has exactly M intersections and L links

$$\Omega_N(M, L) = \{ \omega_N \in \Omega_N : M(\omega_N) = M, L(\omega_N) = L \}, \quad (7)$$

we indicate with the symbol $\langle \cdot \rangle_{M,L}$ the average at fixed N , M and L

$$\langle \cdot \rangle_{M,L} = \frac{1}{|\Omega_N(M, L)|} \sum_{\omega_N \in \Omega_N(M, L)} (\cdot), \quad (8)$$

while the dependence on N is kept implicit. Also, we can define the probability of uniformly extracting a chain with M intersections and L links

$$p_0(M, L) = \frac{|\Omega_N(M, L)|}{(2d)^N} \quad (9)$$

that by definition sums to one

$$\sum_{M,L} p_0(M, L) = 1. \quad (10)$$

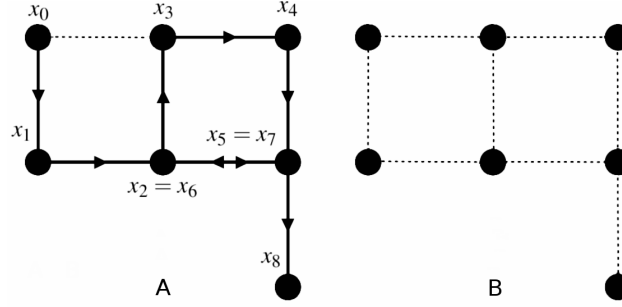


Figure 1. Range and link count for a chain $\omega_8 = \{x_0, x_1, \dots, x_8\}$ of $N = 8$ steps on \mathbb{Z}^2 , shown on top. A shows the actual walk, while B highlights the range points (black circles) and the links (dotted segments) of ω_8 . The total range is $R(\omega_8) = 7$, the number of self-intersections is then $M(\omega_8) = 8 + 1 - R(\omega_8) = 2$, occurring at the 6-th and 7-th steps. The total number of links is $L(\omega_8) = 8$, as it counts also the links imposed by the chain condition (in A the only non-trivial link is that between monomers x_0 and x_3).

We remark that the link counter $L(\omega_N)$ also includes the links between consecutive monomers, hence is always bounded by the range R from below and by dR from above, for $d = 3$

$$1 \leq \frac{L(\omega_N)}{N + 1 - M(\omega_N)} < 3, \quad (11)$$

also, notice that $L(\omega_N)$ can increase only if $M(\omega_N)$ does not (the variables are anti-correlated).

In the simplest case, the CG transition can be modeled by incorporating attractive nearest-neighbors interactions in the Self-Avoiding Walk (SAW) [13–15, 17, 29, 36], the canonical version of our model is described by the Hamiltonian

$$H(\omega_N) = \varepsilon M(\omega_N) + \gamma L(\omega_N). \quad (12)$$

The competition between the repulsive range term $\varepsilon M(\omega_N)$ versus the attractive nearest-neighbor interaction $\gamma L(\omega_N)$ allows for the CG transition.

Given the parameters $\beta_1/\beta = \varepsilon$ and $\beta_2/\beta = \gamma$ the associated Gibbs measure is

$$\mu_\beta(\omega_N) = \frac{e^{-\beta_1 M(\omega_N) - \beta_2 L(\omega_N)}}{Z_\beta} \quad (13)$$

Notice that the partition function can be expressed as a sum over M and L using the formula

$$Z_\beta = \sum_{\omega_N \in \Omega_N} e^{-\beta_1 M(\omega_N) - \beta_2 L(\omega_N)} = \sum_{M, L} |\Omega_N(M, L)| e^{-\beta_1 M - \beta_2 L}, \quad (14)$$

and we can also define a pseudo-Gibbs measure

$$p_\beta(M, L) = \frac{|\Omega_N(M, L)| e^{-\beta_1 M - \beta_2 L}}{Z_\beta} \quad (15)$$

that allows to express the thermal averages

$$\langle \cdot \rangle_\beta = \sum_{\omega_N \in \Omega_N} \mu_\beta(\omega_N) \langle \cdot \rangle = \sum_{M, L} p_\beta(M, L) \langle \cdot \rangle_{M, L} \quad (16)$$

in terms of the microcanonical averages $\langle \cdot \rangle_{M, L}$.

Based on the existing literature on the IDJ model [17–19], the limit $N \rightarrow \infty$ of our model should exist for any choice of the parameters, and then we expect that for any β and any ratio β_1/β_2 the probability measure $p_\beta(\lfloor mN \rfloor, \lfloor \lambda N \rfloor)$ concentrates on some point of the (m, λ) plane.

We indicate with M_N the average number of intersections for a SRW of N steps

$$M_N = \sum_{M, L} p_0(M, L) \cdot M, \quad (17)$$

while L_N is the average number of links

$$L_N = \sum_{M,L} p_0(M,L) \cdot L, \quad (18)$$

By standard SRW theory [16, 28–30], the average densities of intersections and links are given by the formulas

$$M_N = m_0 N + u_0 \sqrt{N} + o(\sqrt{N}), \quad (19)$$

$$L_N = \lambda_0 N + w_0 \sqrt{N} + o(\sqrt{N}), \quad (20)$$

the constants can be exactly computed (for example $m_0 = C_3$ Polya constant [20]). Also, the fluctuations

$$\Delta M(\omega_N) = M(\omega_N) - M_N, \quad (21)$$

$$\Delta L(\omega_N) = L(\omega_N) - L_N, \quad (22)$$

are expected to satisfy a joint Central Limit Theorem (CLT) centered at zero, and $p_0(M, L)$ should concentrate in a $O(\sqrt{N})$ neighborhood of the point $(m_0 N, \lambda_0 N)$ on the (M, L) space. As we shall see in short, this fact is of central importance to locate the critical line in three dimensions. We will discuss its grounds when dealing with the conjectured phase diagram.

II. LOCATING THE TRANSITION LINE

It is easy to verify that the proposed Hamiltonian converges to the ISAW in the limit $\varepsilon \rightarrow \infty$ (if also $\beta_2 = 0$ corresponds to the SAW). Under the assumption that $\log p_0(0, \lfloor \lambda N \rfloor)$ is convex in λ at least in the SAW phase, we can expect that

$$\lim_{N \rightarrow \infty} \lim_{\beta_1 \rightarrow \infty} \lim_{\beta_2 \rightarrow \beta_c} \frac{\langle L(\omega_N) \rangle_\beta}{N} = \lim_{N \rightarrow \infty} \frac{\langle L(\omega_N) \rangle_{0, \lfloor \lambda_c N \rfloor}}{N} = \lambda_c, \quad (23)$$

ie, that in the TL the critical energy densities should be the same in both the canonical and microcanonical versions.

To present the essential features of the phase diagram we will first discuss the quantity

$$\nu(m, \lambda) = \lim_{N \rightarrow \infty} \frac{\log \langle x_N^2(\omega_N) \rangle_{\lfloor mN \rfloor, \lfloor \lambda N \rfloor}}{2 \log N}, \quad (24)$$

which represents the critical exponent of the squared end-to-end distance when M and L are constrained to grow proportionally to N .

For $\gamma \rightarrow 0$ we obtain the so called Stanley model for $\varepsilon > 0$, of Hamiltonian $H_0(\omega_N) = \varepsilon M(\omega_N)$, while for $\varepsilon < 0$ is the Rosenstock Trapping model. The corresponding microcanonical model is

$$\Omega_N(M) = \bigcup_L \Omega_N(M, L) \quad (25)$$

and has been studied in [20, 21] where numerical simulations and additional theoretical arguments support the conjecture that the displacement exponent of the set $\Omega_N(\lfloor mN \rfloor)$

$$\nu(m) = \lim_{N \rightarrow \infty} \frac{\log \langle x_N^2(\omega_N) \rangle_{\lfloor mN \rfloor}}{2 \log N}, \quad (26)$$

has a drop around $m_c = C_3$, with a drop band slowly narrowing as $O(1/N^\alpha)$ and $\alpha = 0.29 \pm 0.1$ ([20], an independent scaling analysis, not shown, gave 0.31 ± 0.1).

Based on these preliminary studies we conjecture that for any value of m there is some critical link density $\ell_c(m)$ such that if $\lambda < \ell_c(m)$ the exponent $\nu(m, \lambda)$ matches the critical exponent ν_3 of the SAW. The conjectured phase diagram is then

$$\nu(m, \lambda) = \begin{cases} \nu_3 & \lambda < \ell_c(m) \\ 1/2 & \lambda = \ell_c(m) \\ 1/3 & \lambda > \ell_c(m) \end{cases} \quad (27)$$

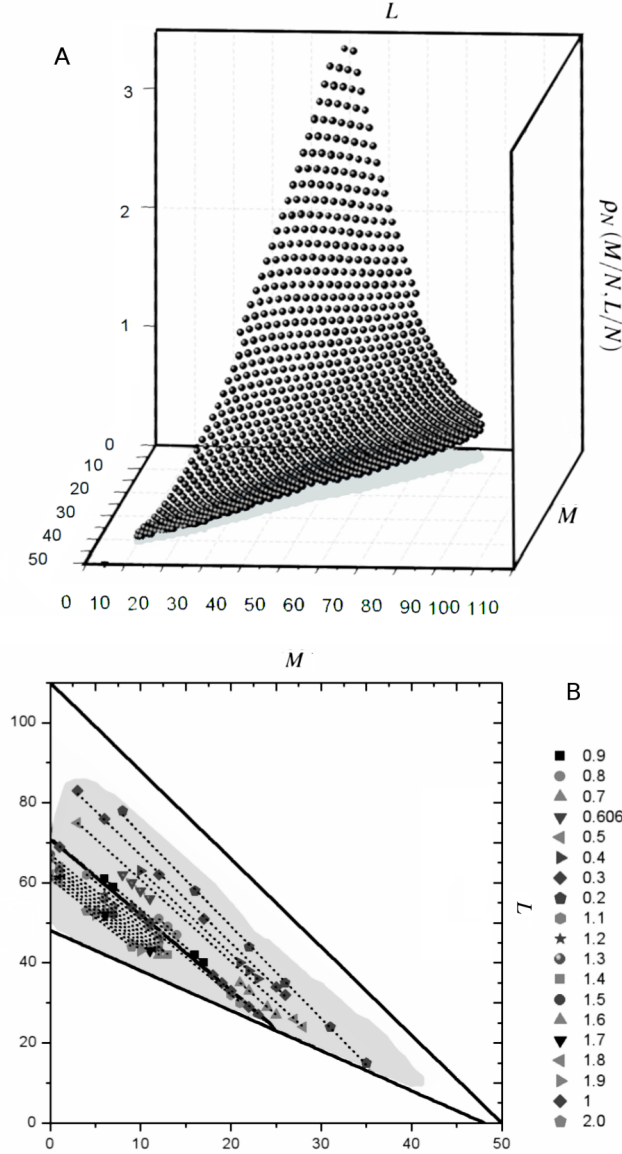


Figure 2. Surface $\rho_N(m, \lambda)$ for a ISAW of $N = 50$. In figure A the surface $\rho_N(m, \lambda)$ is computed for a large part of the parameter space using a PERM algorithm (gray area in B). Figure B shows some level lines $\rho_N(m, \lambda) = r$ as scatter points, the line $\rho_N(m, \lambda) = 1$ and the boundaries of the allowed parameter space are highlighted by solid lines. Although the considered chains are very small, the linear behavior of the level lines in B is still surprising. A simulation of a larger chain of $N = 100$ steps (not shown) gave the same picture.

where ν_3 is the critical exponent of the SAW governing the end-to-end distance [17–19]. If the link density is exactly $\lambda = \ell_c(m)$ the energy contributions from range and links should balance, giving a SRW-like critical behavior with exponent $\nu(m, \ell_c(m)) = 1/2$, while for $\lambda > \ell_c(m)$ we expect to be in the cluster phase, then $\nu(m, \lambda) = 1/3$. Notice that for $m \rightarrow 0$ we must have $\ell_c(0) = \lambda_c$ energy density of the ISAW at the theta point.

Although an investigation of the parameter $\nu(m, \lambda)$ should be carried on to verify the phase exponents (as is done in [20] for the Range Problem), we believe that the existing literature on IDJ-like models [4–9, 11–13, 15–17] already support the existence of a non-trivial transition line, and we decided to locate $\ell_c(m)$ by computing the level lines of the estimator

$$\rho_N(m, \lambda) = \frac{\langle x_N^2(\omega_N) \rangle_{[mN], [\lambda N]}}{N}, \quad (28)$$

that by previous considerations satisfy

$$\rho_N(m, \lambda) = \begin{cases} O(N^{2\nu_3-1}) & \lambda < \ell_c(m) \\ O(1) & \lambda = \ell_c(m) \\ O(N^{-2/3}) & \lambda > \ell_c(m) \end{cases} \quad (29)$$

We computed the set $\ell_N(m, r)$ that satisfy

$$\rho_N(m, \ell_N(m, r)) = r \quad (30)$$

by numerical simulations using a PERM algorithm [22–25]. For very short chains ($N \leq 100$) we were able to explore a large portion of the space (m, λ) , with r ranging from small values up to the scale of $\rho_N(0, 1)$. We found that for very short chains

$$N\ell_N(m, r) = \lfloor \lambda_N(r)N + \delta_N(r) \cdot mN \rfloor \quad (31)$$

is verified with extremely high accuracy at any observed r . For small chains we observe that the level curves of $\rho_N(m, \lambda)$ appears to be straight lines (see Figure 3).

Given the small size of the chains we cannot conclude much from this observation, but driven by this preliminary experiment we decided to fix $r = 1$, that is the diffusion behavior of the SRW, and perform an intensive investigation of the curve $\ell_N(m, 1)$,

$$\rho_N(m, \ell_N(m, 1)) = 1, \quad (32)$$

that by Eq.(29) is expected to converge to the critical line in the thermodynamic limit [26]

$$\lim_{N \rightarrow \infty} \ell_N(m, 1) = \ell_c(m). \quad (33)$$

The PERM algorithm, which is very efficient in simulating θ -point chains, allowed to evaluate $\ell_N(m, 1)$ up to chains with $N = 500$ in a macroscopic portion of the (M, L) space. We found stronger evidences that at least the curve $\ell_N(m, 1)$ is still a line up to integer truncation,

$$N\ell_N(m, 1) = \lfloor \lambda_N(1)N + \delta_N(1) \cdot mN \rfloor, \quad (34)$$

suggesting the conjecture that the critical line may remain a line in the thermodynamic limit, with critical coefficients eventually satisfying

$$\lim_{N \rightarrow \infty} \lambda_N(1) = \lambda_c, \quad \lim_{N \rightarrow \infty} \delta_N(1) = \delta_c. \quad (35)$$

This property can be explained as follows. As in [21], let us partition the chain ω_N into a number n of sub-chains

$$\omega_N = \{ \omega_T^0, \omega_T^1, \dots, \omega_T^n \} \quad (36)$$

each of size $T = N/n$. The sub-chains are indicated with

$$\omega_T^i = \{ x_0^i, x_1^i, \dots, x_T^i \} \subset \omega_N \quad (37)$$

and satisfy the chain constraint $x_T^i = x_0^{i+1}$. If we neglect the self-intersections between the blocks, as is expected in a SRW-like chain [17], we can approximate the probability measure conditioned on the transition line with a product measure.

Now, as in [21] we assume that each sub-chain can be either a critical ISAW, with local densities $(0, \lambda_0)$, or a SRW, with average local densities (m_0, λ_0) . Then we could write

$$p_0(\lfloor mN \rfloor, \lfloor \ell_c(m)N \rfloor) \simeq \prod_{i=1}^n p_0(0, \lfloor \lambda_c N \rfloor)^{\varphi_i T} p_0(\lfloor m_0 N \rfloor, \lfloor \lambda_0 N \rfloor)^{(1-\varphi_i)T} \quad (38)$$

with $\varphi^i \in \{0, 1\}$ keeping record of the subchain type. One in the end finds that under the above product measure condition the averages of $M(\omega_T)$ and $L(\omega_T)$ satisfy the relation

$$\langle L(\omega_N) \rangle_{\lfloor mN \rfloor, \lfloor \ell_c(m)N \rfloor} \simeq \lambda_c N - \left(\frac{\lambda_c - \lambda_0}{m_0} \right) \langle M(\omega_N) \rangle_{\lfloor mN \rfloor, \lfloor \ell_c(m)N \rfloor}. \quad (39)$$

Notice that three dimensional θ -polymers should include logarithmic corrections to the simple mean-field factorization [4]. Even if these corrections are important in the usual Range Problem [21, 27] here the constraint to stay on the transition line forces the chains to behave like SRWs, and we are persuaded that neglecting these correlations should not affect the shape of the line in the thermodynamic limit.

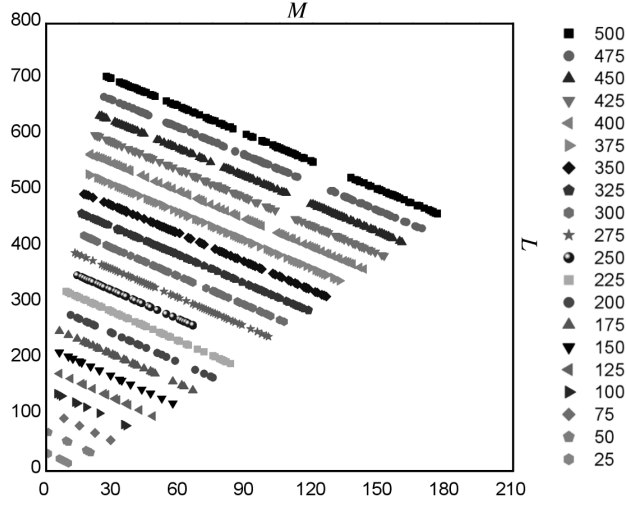


Figure 3. Transition line $\rho_N(m, \lambda) = 1$ for chains up to $N = 500$ for a large portion of the parameter space using a PERM algorithm. The line from different N are shown on the same graph to allow comparison. The length of the chains varies from $N = 25$ to 500 . The linear behavior of the critical level line seems present also for longer chains. The intercepts at $M = 0$, extrapolated from linear fits, are shown as white squares in Figure 4 A.

III. A CONSEQUENCE FROM SRW THEORY

An important consequence of the previous conjecture is that the critical energy density of the ISAW λ_c would be computable in terms of SRW measurable quantities.

In fact, we remark that the $p_0(\lfloor mN \rfloor, \lfloor \lambda N \rfloor)$ is expected to concentrate on (m_0, λ_0) . Since the average squared end-to-end distance in the SRW is exactly N we can conclude that also this point must lie on the transition line

$$\ell_c(m_0) = \lambda_0 \quad (40)$$

Then, by the previous linearity conjecture we should be able to conclude that the ratio

$$\delta_N^* = \frac{\langle L(\omega_N) \rangle_\beta - \langle L(\omega_N) \rangle_0}{\langle M(\omega_N) \rangle_\beta - \langle M(\omega_N) \rangle_0} \quad (41)$$

converges to the actual δ_N (and then to the angular coefficient of the critical line in the TL) under the constraint of constant end-to-end distance

$$\langle x_N^2(\omega_N) \rangle_\beta = \langle x_N^2(\omega_N) \rangle_0. \quad (42)$$

To compute this estimator we expand the Boltzmann factor in the limit of infinite temperature, ie for small β

$$e^{-\beta_1 M - \beta_2 L} = 1 - \beta_1 M - \beta_2 L + O(\beta^2) \quad (43)$$

and then compute the averages. It can be shown after some algebra that in the limit of infinite temperature the differences are approximated by the expressions

$$\langle L(\omega_N) \rangle_\beta - \langle L(\omega_N) \rangle_0 = -\beta_2 \Delta L_N^2 - \beta_1 \Delta Q_N \quad (44)$$

$$\langle M(\omega_N) \rangle_\beta - \langle M(\omega_N) \rangle_0 = -\beta_2 \Delta Q_N - \beta_1 \Delta M_N^2$$

where in order to simplify the formulas we introduced a notation for the variances of links and intersections,

$$\Delta L_N^2 = \langle \Delta L^2(\omega_N) \rangle_0, \Delta M_N^2 = \langle \Delta M^2(\omega_N) \rangle_0, \quad (45)$$

and one for the the correlations between $M(\omega_N)$ and $L(\omega_N)$ under the SRW measure

$$\Delta Q_N = \langle \Delta M(\omega_N) \Delta L(\omega_N) \rangle_0. \quad (46)$$

The ratio β_1/β_2 is obtained from the constraint of having a constant average end-to-end distance applied to the first order expansion in β ,

$$\langle x_N^2(\omega_N) \rangle_\beta - \langle x_N^2(\omega_N) \rangle_0 \simeq -\beta_1 \Delta P_N - \beta_2 \Delta T_N = 0 \quad (47)$$

where we again simplified the notation by introducing a symbol for the correlation between $M(\omega_N)$ and $x_N^2(\omega_N)$,

$$\Delta P_N = \langle \Delta M(\omega_N) \Delta x_N^2(\omega_N) \rangle_0 \quad (48)$$

and another symbol for the correlation between $L(\omega_N)$ and $x_N^2(\omega_N)$, which is

$$\Delta T_N = \langle \Delta L(\omega_N) \Delta x_N^2(\omega_N) \rangle_0. \quad (49)$$

Finally, substituting the ratio β_2/β_1 obtained from the last formula into the approximate expression for δ_N^* we obtain the relation

$$\delta_N^* = \frac{\Delta Q_N + \left(\frac{\Delta P_N}{\Delta T_N}\right) \Delta L_N^2}{\Delta M_N^2 + \left(\frac{\Delta P_N}{\Delta T_N}\right) \Delta Q_N} \quad (50)$$

that, assuming true our conjecture, would allow to compute the critical energy density of the ISAW in the TL from the formula

$$\lambda_N^* N = L_N + \delta_N^* M_N. \quad (51)$$

We generated SRW samples with an unbiased algorithm and compared the above estimators with the critical energy from PERM simulations of the ISAW. Our simulations up to $N = 1000$ support the hypothesis that the estimator λ_N^* does eventually converge to λ_c (see Figure 4). We remark that such relation is due to the fact that both the extended phase and the clustered phase scale differently from the SRW. In higher dimensions we cannot rely on this property because for $d > 4$ the SAW is expected to scale like the SRW.

IV. CONCLUSIONS AND OUTLOOKS

Concerning the form of the transition line, it is important to remark that the conjecture in Eq. (51) would open interesting analytic possibilities. In fact, the quantity δ_N^* does not depend on β and all the averages are taken with respect to the SRW measure. We expect that, apart from messy algebra, the asymptotics of the necessary correlation functions can be computed using the very same techniques developed by Jain and Pruitt to compute the variance of the SRW range [29, 31–33, 35]. This would be a nice result, since to the best of our knowledge no exact expression is known or even conjectured for the ISAW critical energy.

Another interesting fact is that the model can be described by a generalized urn model. Since $L(\omega_N)$ can increase only if $M(\omega_N)$ does not, it holds

$$L(\omega_{N+1}) - L(\omega_N) = 2d \cdot \pi(\omega_{N+1}) \{1 - [M(\omega_{N+1}) - M(\omega_N)]\} \quad (52)$$

where we used the symbol

$$\pi(\omega_N) = \langle M(\omega_{N+1}) - M(\omega_N) | \omega_N \rangle_0 \quad (53)$$

to indicate the atmosphere of the chain (see [21]). Given the urn kernels

$$\pi_N^{(k)}(M, L) = \langle I(L(\omega_N) - L(\omega_{N-1}) = k) \rangle_{M, L} \quad (54)$$

for $0 \leq k \leq 2d$ we conjecture that

$$\pi^{(k)}(m, \lambda) = \lim_{N \rightarrow \infty} \pi_N^{(k)}(\lfloor mN \rfloor, \lfloor \lambda N \rfloor) \quad (55)$$

exists for all considered k , and that it would be possible to extend the urn techniques presented in [21, 34] to deal with the urn model controlled by the kernels $\pi^{(k)}(m, \lambda)$. Notice that for $k = 0$ one would have

$$\pi_N^{(0)}(M, L) = \langle I(L(\omega_N) - L(\omega_{N-1}) = 0) \rangle_{M, L} = \langle I(M(\omega_N) - M(\omega_{N-1}) = 1) \rangle_{M, L} \quad (56)$$

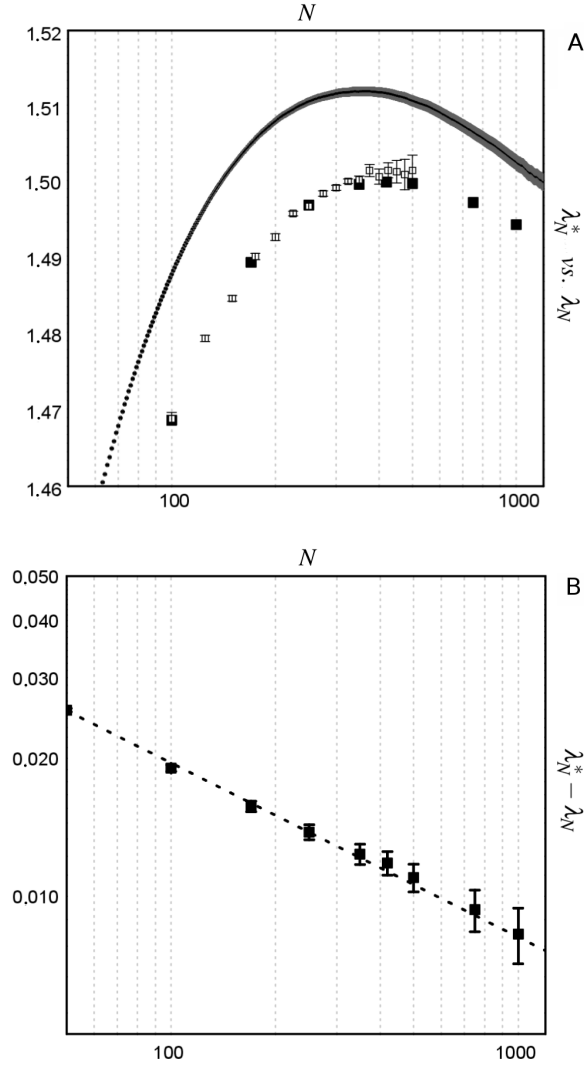


Figure 4. Comparison between the critical ISAW energy from independent PERM simulations with the estimator of Eq. (51) up to $N = 1000$ computed with an unbiased algorithm. In figure A, semi-log scale, the black line is the estimator λ_N^* with its error (standard deviation), obtained from an unbiased simulation, while the black dots are values obtained with an independent PERM simulation. Finally, the white squares are the intercepts at $M = 0$ from linear fits of Figure 3. B shows the difference $\lambda_N^* - \lambda_N$ between ISAW critical energy and Eq. (51) in log-log scale. The difference is fitted with a power law $K_0 x^{-c}$, with $K_0 = 0.1124 \pm 0.0005$ and exponent $c = -0.38 \pm 0.01$.

and that by definition must hold

$$1 - \pi_N^{(0)}(M, L) = \sum_{k=1}^{2d} \pi_N^{(k)}(M, L). \quad (57)$$

We conclude with one last remark. Due to difficulties in simulating long chains when m is close to 1 we were unable to directly check the behavior in this region. At first we were tempted to further push the conjecture and guess that in the TL the critical line hits the value $\lambda = 0$ at $m = 1$, but our PERM estimates seem to exclude this simple ansatz because the observed $\lambda_N(1)$ is always below the value $\lambda_c = \lambda_0 / (1 - C_3) \simeq 1.5238$ for which a “linear” critical line can pass through the point (m_0, λ_0) , that must lie on the critical line in any case (from SRW theory $\lambda_0 = 6 \cdot C_3 / (1 + C_3) \simeq 1.005$ and $m_0 = C_3 \simeq 0.3405$ [16]), and then hit the boundary $3(1 - m)$ of the allowed parameter space at $m = 1$ exactly.

Then, if the linear behavior of $\ell_N(m)$ can be really extended in the whole m range and $\lambda_c < \lambda_0 / (1 - C_3)$ this would imply the existence of a second critical value for the intersection density, ie the $m^* = C_3 \cdot (\lambda_c - 3) / (\lambda_c - \lambda_0 - 3 \cdot C_3)$ at which the crossing between the critical line $\ell_c(m)$ and the boundary $3(1 - m)$ actually happens, and after this value the clustered phase would not be possible anymore except for values of λ concentrating on the boundary of the parameter range. For or example, the

conjecture would imply that no CG transition can occur for $m < 1$ in the $\Omega_N([mN], [(1-m)N])$ model, where the exceeding nearest neighbor pairs are forbidden. This is likely because in a clustered phase we necessarily have a partial saturation of the nearest neighbor sites of each monomer, and such phase would be extremely unfavored by a small link density.

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