Energy of the interacting self-avoiding walk at the θ point

Simone Franchini and Riccardo Balzan
Dipartimento di Fisica, Sapienza Universitá di Roma, Piazzale Aldo Moro 1, 00185 Roma, Italy

(Received 19 June 2020; revised 10 September 2020; accepted 14 September 2020; published 29 September 2020)

We perform a numerical study of a new microcanonical polymer model on a 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.

DOI: 10.1103/PhysRevE.102.032143

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 (CG) transition [1–3], arises when the attractive interaction between the monomers overwhelms the excluded volume effect. At the transition temperature (commonly called the 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-step simple random walk (SRW) on the cubic lattice $\mathbb{Z}^d$:

$$\omega_N = \{x_t(\omega_N) \in \mathbb{Z}^d : 0 \leqslant t \leqslant N\}. \tag{1}$$

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

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

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

$$\Omega_N = \Omega_1^N \ni \omega_N \tag{3}$$

the set of all possible chain configurations.

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

$$R(\omega_N) = \lfloor (1-m)N \rfloor, \qquad L(\omega_N) = \lfloor \lambda N \rfloor, \tag{4}$$

where we denoted by $\lfloor z \rfloor$ the lower integer truncation of $z \in \mathbb{R}$ (see Fig. 1). The model is controlled by the pair of parameters m and λ, and the interacting self-avoiding walk (ISAW, [7–15]) is recovered by taking $m = 0$.

We numerically investigated the microcanonical 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) $N \to \infty$ the critical link density is a linear function of m,

$$\ell_c(m) = \lambda_c + \delta_c m, \tag{5}$$

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

$$M(\omega_N) = N + 1 - R(\omega_N), \tag{6}$$

which represents 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:

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

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

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

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,

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

that by definition sums to 1:

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

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 $d = 3$:

$$1 \leqslant \frac{L(\omega_N)}{N + 1 - M(\omega_N)} < 3. \tag{11}$$

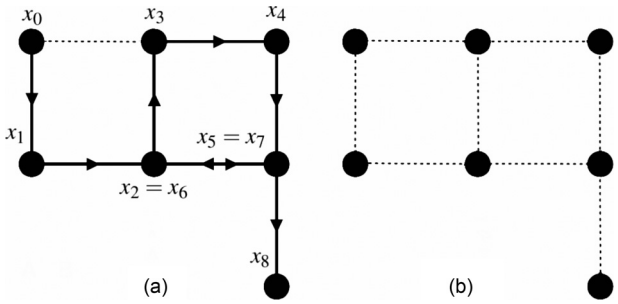

FIG. 1. Range and link count for a chain $\omega_8 = \{x_0, x_1, \ldots, x_8\}$ of $N = 8$ steps on $\mathbb{Z}^2$, shown on top. (a) shows the actual walk, while (b) highlights the range points (black circles) and the links (dotted segments) of ω_8. The total range is $R(\omega_8) = 7$, the number of self-intersections is then $M(\omega_8) = 8 + 1 - R(\omega_8) = 2$, occurring at the sixth and seventh 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 nontrivial link is that between monomers x_0 and x_3].

Also, notice that $L(\omega_N)$ can increase only if $M(\omega_N)$ does not (the variables are anticorrelated).

In the simplest case, the CG transition can be modeled by incorporating attractive nearest-neighbor interactions in the self-avoiding walk (SAW) [14–22]. The canonical version of our model is described by the Hamiltonian

$$H(\omega_N) = \epsilon M(\omega_N) + \gamma L(\omega_N). \tag{12}$$

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

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

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

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

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

and we can also define a pseudo-Gibbs measure

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

that allows us to express the thermal averages

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

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

Based on the existing literature on the IDJ model [13–15], the limit $N \to \infty$ 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,

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

while L_N is the average number of links,

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

By standard SRW theory [13,18,22,23], the average densities of intersections and links are given by the formulas

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

$$L_N = \lambda_0 N + w_0 \sqrt{N} + o(\sqrt{N}). \tag{20}$$

The constants can be exactly computed (for example $m_0 = C_3$ Polya constant [24]). Also, the fluctuations

$$\Delta M(\omega_N) = M(\omega_N) - M_N, \tag{21}$$

$$\Delta L(\omega_N) = L(\omega_N) - L_N \tag{22}$$

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 shortly, 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 $\epsilon \to \infty$ (if also $\beta_2 = 0$ corresponds to the SAW). Under the assumption that $\ln p_0(0, \lfloor \lambda N \rfloor)$ is convex in λ at least in the SAW phase, we can expect that

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

i.e., 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

$$\nu(m,\lambda) = \lim_{N\to\infty} \frac{\ln \left\langle x_N^2(\omega_N) \right\rangle_{\lfloor mN \rfloor, \lfloor \lambda N \rfloor}}{2 \ln N}, \tag{24}$$

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

For $\gamma \to 0$ we obtain the so-called Stanley model for $\epsilon > 0$, of Hamiltonian $H_0(\omega_N) = \epsilon M(\omega_N)$, while for $\epsilon < 0$ it is the Rosenstock trapping model. The corresponding microcanonical model is

$$\Omega_N(M) = \bigcup_L \Omega_N(M,L) \tag{25}$$

and has been studied in [24,25], where numerical simulations and additional theoretical arguments support the conjecture

that the displacement exponent of the set $\Omega_N(\lfloor mN \rfloor)$,

$$\nu(m) = \lim_{N\to\infty} \frac{\ln \left\langle x_N^2(\omega_N)\right\rangle_{\lfloor mN\rfloor}}{2\ln N}, \tag{26}$$

has a drop around $m_c = C_3$, with a drop band slowly narrowing as $O(1/N^\alpha)$ and $\alpha = 0.29 \pm 0.1$ ([24]; 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

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

where ν_3 is the critical exponent of the SAW governing the end-to-end distance [14,20,21]. 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 $m \to 0$ we must have $\ell_c(0) = \lambda_c$ energy density of the ISAW at the θ point.

Although an investigation of the parameter $\nu(m,\lambda)$ should be carried out to verify the phase exponents (as is done in [24] for the range problem), we believe that the existing literature on IDJ-like models [4–9,11–15,17] already supports the existence of a nontrivial transition line, and we decided to locate $\ell_c(m)$ by computing the level lines of the estimator,

$$\rho_N(m,\lambda) = \frac{\left\langle x_N^2(\omega_N)\right\rangle_{\lfloor mN\rfloor,\lfloor \lambda N\rfloor}}{N}, \tag{28}$$

that by previous considerations satisfy

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

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

$$\rho_N(m, \ell_N(m,r)) = r \tag{30}$$

by numerical simulations using a pruned-enriched Rosenbluth method (PERM) algorithm [26–29]. For very short chains ($N \leqslant 100$) 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,

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

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 Fig. 2).

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 $\ell_N(m,1)$,

$$\rho_N(m, \ell_N(m,1)) = 1, \tag{32}$$

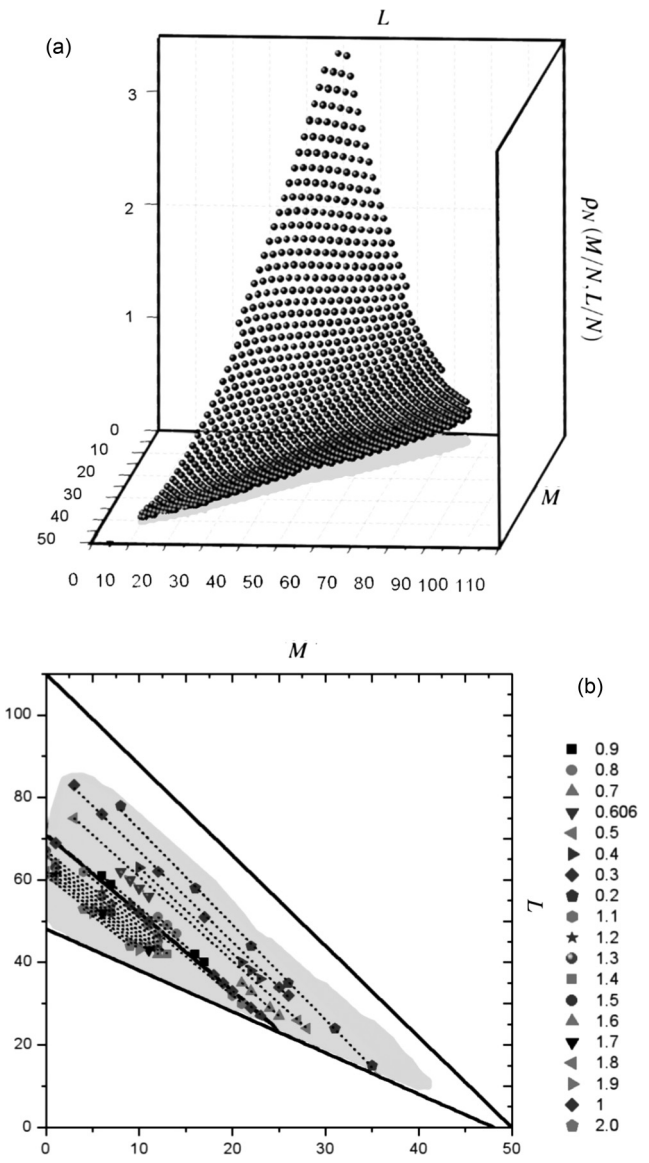

FIG. 2. Surface $\rho_N(m,\lambda)$ for an ISAW of $N = 50$. In (a) the surface $\rho_N(m,\lambda)$ is computed for a large part of the parameter space using a PERM algorithm [gray area in (b)]. (b) shows some level lines $\rho_N(m,\lambda) = r$ as scatter points, the line $\rho_N(m,\lambda) = 1$, and 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.

that by Eq. (29) is expected to converge to the critical line in the thermodynamic limit [30]:

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

The PERM algorithm, which is very efficient in simulating θ-point chains, allowed us to evaluate $\ell_N(m,1)$ up to chains with $N = 500$ in a macroscopic portion of the (M,L) space, see Fig. 3. We found stronger evidence that at least the curve $\ell_N(m,1)$ is still a line up to integer truncation,

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

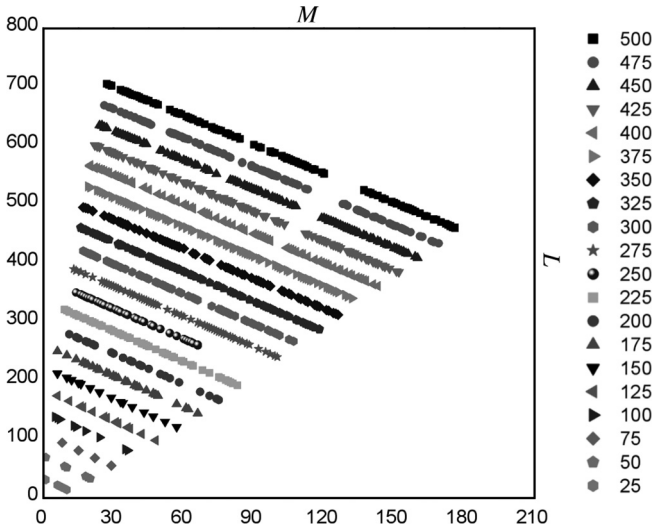

FIG. 3. Transition line $\rho_N(m,\lambda)=1$ for chains up to $N=500$ for a large portion of the parameter space using a PERM algorithm. The lines from different N are shown on the same graph to allow comparison. The lengths of the chains vary from $N=25$ to 500. The linear behavior of the critical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

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

$$\lim_{N\to\infty}\lambda_N(1)=\lambda_c,\qquad \lim_{N\to\infty}\delta_N(1)=\delta_c. \tag{35}$$

This property can be explained as follows. As in [25], let us partition the chain ω_N into a number n of subchains,

$$\omega_N=\{\omega_T^0,\omega_T^1,\ldots,\omega_T^n\}, \tag{36}$$

each of size $T=N/n$. The subchains are indicated with

$$\omega_T^i=\{x_0^i,x_1^i,\ldots,x_T^i\}\subset\omega_N \tag{37}$$

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 [14], we can approximate the probability measure conditioned on the transition line with a product measure.

Now, as in [25] we assume that each subchain 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

$$p_0(\lfloor mN\rfloor,\lfloor\ell_c(m)N\rfloor)\simeq\prod_{i=1}^{n}p_0(0,\lfloor\lambda_cN\rfloor)^{\varphi_iT}p_0(\lfloor m_0N\rfloor,\lfloor\lambda_0N\rfloor)^{(1-\varphi_i)T} \tag{38}$$

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

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

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 [25,31], 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.

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

$$\ell_c(m_0)=\lambda_0. \tag{40}$$

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

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

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,

$$\left\langle x_N^2(\omega_N)\right\rangle_\beta=\left\langle x_N^2(\omega_N)\right\rangle_0. \tag{42}$$

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

$$e^{-\beta_1M-\beta_2L}=1-\beta_1M-\beta_2L+O(\beta^2) \tag{43}$$

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

$$\begin{aligned}\langle L(\omega_N)\rangle_\beta-\langle L(\omega_N)\rangle_0&=-\beta_2\Delta L_N^2-\beta_1\Delta Q_N,\\ \langle M(\omega_N)\rangle_\beta-\langle M(\omega_N)\rangle_0&=-\beta_2\Delta Q_N-\beta_1\Delta M_N^2,\end{aligned} \tag{44}$$

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

$$\Delta L_N^2=\langle\Delta L^2(\omega_N)\rangle_0,\qquad \Delta M_N^2=\langle\Delta M^2(\omega_N)\rangle_0, \tag{45}$$

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

$$\Delta Q_N=\langle\Delta M(\omega_N)\Delta L(\omega_N)\rangle_0. \tag{46}$$

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,

$$\left\langle x_N^2(\omega_N)\right\rangle_\beta-\left\langle x_N^2(\omega_N)\right\rangle_0\simeq-\beta_1\Delta P_N-\beta_2\Delta T_N=0, \tag{47}$$

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

$$\Delta P_N=\left\langle\Delta M(\omega_N)\Delta x_N^2(\omega_N)\right\rangle_0, \tag{48}$$

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

$$\Delta T_N=\left\langle\Delta L(\omega_N)\Delta x_N^2(\omega_N)\right\rangle_0. \tag{49}$$

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

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

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

$$\lambda_N^* N = L_N + \delta_N^* M_N. \tag{51}$$

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 Fig. 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 OUTLOOK

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 [18,32–35]. 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 that

$$\begin{aligned} &L(\omega_{N+1}) - L(\omega_N) = \\ &\quad 2d\,\pi(\omega_{N+1})\{1 - [M(\omega_{N+1}) - M(\omega_N)]\} \end{aligned} \tag{52}$$

where we used the symbol

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

to indicate the atmosphere of the chain (see [25]). Given the urn kernels

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

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

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

exists for all considered k, and that it would be possible to extend the urn techniques presented in [25,36] to deal with the urn model controlled by the kernels $\pi^{(k)}(m, \lambda)$. Notice that for $k = 0$ one would have

$$\begin{aligned} \pi_N^{(0)}(M, L) &= \langle I(L(\omega_N) - L(\omega_{N-1}) = 0) \rangle_{M,L} \\ &= \langle I(M(\omega_N) - M(\omega_{N-1}) = 1) \rangle_{M,L} \end{aligned} \tag{56}$$

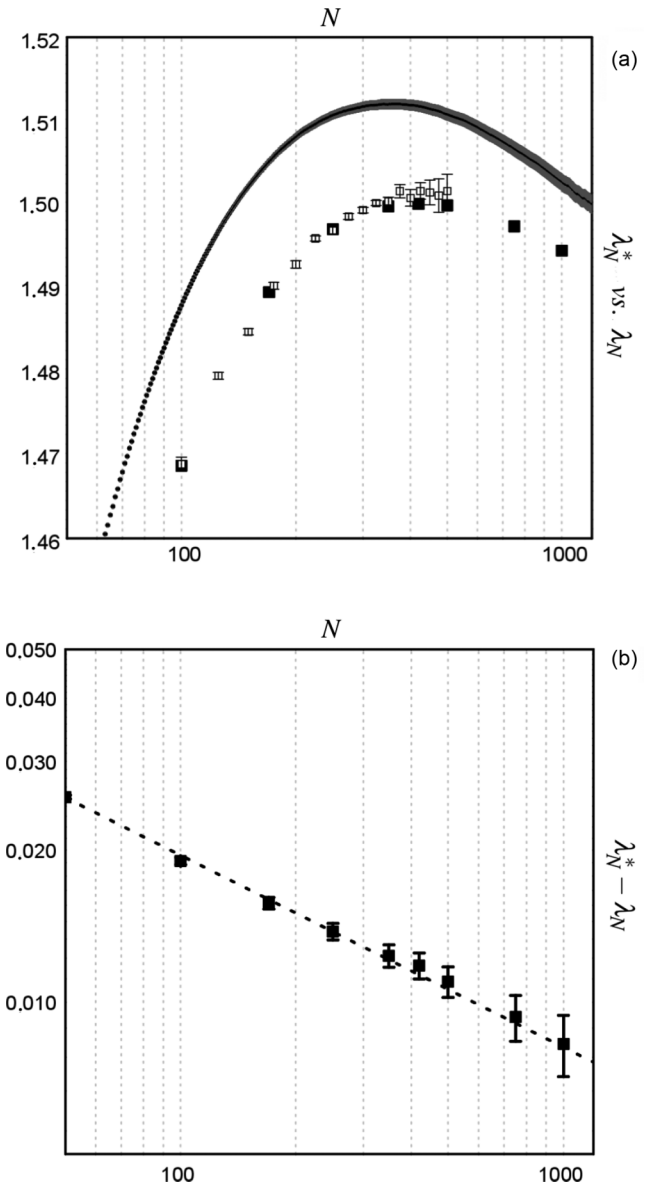

FIG. 4. Comparison between the critical ISAW energy from independent PERM simulations with the estimator of Eq. (51) up to $N = 1000$ computed with an unbiased algorithm. In (a), semilogarithmic scale, the black line is the estimator λ_N^* with its error (standard deviation), obtained from an unbiased 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 Fig. 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 it must hold that

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

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 where 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 $\lambda_0 = 6C_3/(1 + C_3) \simeq 1.005$ and $m_0 = C_3 \simeq 0.3405$ [13]), 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, i.e., $m^* = C_3(\lambda_c - 3)/(\lambda_c - \lambda_0 - 3C_3)$, 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 example, the conjecture would imply that no CG transition can occur for $m < 1$ in the $\Omega_N(\lfloor mN \rfloor, \lfloor (1 - m)N \rfloor)$ model, where the 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.

ACKNOWLEDGMENTS

We would like to thank Giorgio Parisi (Sapienza Univeristá di Roma) and Valerio Paladino (Amadeus IT) for interesting discussions and suggestions. This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Grant Agreement No. 694925).

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