

Scale-free network hidden in a collapsing polymer

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We show that the collapsed globular phase of a polymer accommodates a scale-free incompatibility graph of its contacts. The degree distribution of this network is found to decay with the exponent $\gamma=1/(2-c)$ up to a cutoff degree $d_c \propto L^{2-c}$, where c is the loop exponent for dense polymers ($c=11/8$ in two dimensions) and L is the length of the polymer. Our results exemplify how a scale-free network can emerge from standard criticality.

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The underlying network structures of the world-wide-web, power grids, social contacts, protein interactions, etc. [1], bear peculiar properties absent in random networks. The graphs associated with them not only share a power law degree distribution commonly referred as “scale-free,” but also an unusually small diameter (a measure of the average shortest distance between two nodes) [2] and typically a high degree of clustering. The advantages/disadvantages of these qualities on the efficiency of the network have been thoroughly discussed in the context of epidemic spreading [3] and resilience against random or malicious attacks [4].

The search for nongrowing scale-free networks (SFNs) originating from equilibrium statistics and/or optimization has been the focus of attention recently [5–7]. And yet, although some statistical models on SFNs have already been studied [8], there is, to our knowledge, no demonstrated link from conventional critical models to the criticality hinted by the network’s scale freeness. As shown here, this link may be established by associating a network with each microstate of the model. Such a network representation is also convenient for studying the system’s complexity and may have wider applicability. For example, a recipe similar to ours was recently adopted for investigating the navigational complexity of cities [9] while earlier connections between graphs and polymers have proven useful to the study of polymer physics [10,11].

We demonstrate here that a SFN is associated with the collapsed phase at low temperature, T , and presumably also with the θ point ($T=T_\theta$) of a polymer. By modeling the collapsed polymer as a self-attracting self-avoiding walk [12] on a square lattice we obtain the degree exponent in terms of a critical index known exactly for two dimensions (2D). Numerical simulations confirm the analytically predicted degree exponent and show that the scale-free character of the network is a direct consequence of the polymer criticality.

The configuration of a polymer chain of L monomers can be represented by an arc diagram [see Figs. 1(a) and 1(b)] which carries the same information as the contact map [10]. It is obtained when one imagines stretching the polymer into a horizontal straight line while pairs of monomers that were

originally in contact are joined by arcs on the upper half plane (the diagram is drawn on a plane even though the polymer may be embedded in arbitrary dimensions). The arc diagram is said to be *planar* if no two arcs cross each other, i.e., if there are no interpenetrating contacts. Otherwise, a nontrivial incompatibility graph (IG) can be associated with the arc diagram [Fig. 1(c)], such that, each arc (contact) represents a node on the IG and two nodes are connected by an edge if the corresponding arcs cross. More precisely, if the monomer units of the polymer are indexed $1, \dots, L$ and the contacts are labeled by indices of the involved monomer pair (i, j) with $i < j$, then the two nodes (i_1, j_1) and (i_2, j_2) of the IG are joined by an edge if and only if there exists an integer n satisfying $i_1 < n < j_1$ and $i_2 < n < j_2$.

The IG provides a representation for the complexity of the contact structure of a folded polymer with particular reference to the arrangement of pseudoknots. This representation is frequently used in RNA folding research [13–15] where pseudoknots are biologically active structural components. An empty IG (no edges, meaning no pseudoknots) is a common simplifying assumption in RNA prediction algorithms [16–18]. Whereas pseudoknots and the IG are not unfamiliar concepts in structural biology and graph theory, the original aspect of the present work is to utilize them as a means to study scaling properties of the polymer.

Alternatively, in case of the traveling salesman problem (TSP) the same complexity refers to the shortest path connecting a given number of cities on a map where repeated visitations of a neighborhood compounds to a contact. In $d=2$, TSP has recently been conjectured to be in the same

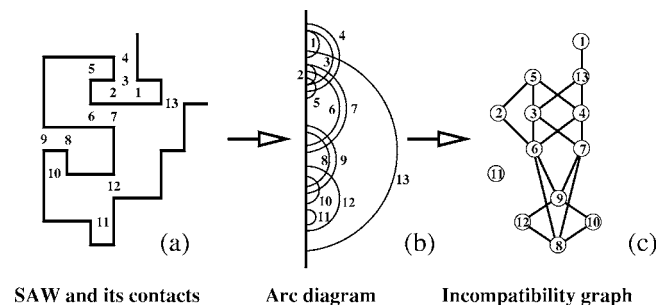


FIG. 1. A polymer on a square lattice and its self-contacts together with the corresponding arc diagram and the incompatibility graph.

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universality class as dense polymers [19]. Rosvall *et al.* use a similar mapping from a city road map to the IG, through which they quantify the information content [9].

Our goal here is to show that the IG of a homopolymer at low temperatures is a scale-free network. To this end, we will approximate the true arc diagram of the polymer with a random arc diagram where the probability of having an arc between two monomers m distance apart along the chain is given by its asymptotic value for an infinite polymer, i.e., $P(m) \sim m^{-c}$. The exponent c is related to the return probability and equals $d/2$ for a random walk [20]. Its counterpart for the self-avoiding polymer is $c = d\nu - \sigma_4$ [21,22]. Note that, apart from the modified radius of gyration exponent ν ($\nu = 1/2$ for the random walk) it additionally involves the four-leg vertex exponent σ_4 which, e.g., plays a key role in DNA physics [23]. The exponents ν and σ_4 are known exactly or to high precision for all integer dimensions, except for $T < T_\theta$ in three-dimensions (3D) [12]. We will find below that the tail of the degree distribution for the IG of such a random arc diagram obeys the power law

$$P(d) \sim d^{-\gamma}, \quad (1)$$

with $\gamma = 1/(2-c)$ in an infinitely long polymer.

Consider an arc diagram of the polymer with the discrete monomer centers labeled by integers $1, \dots, L$. As discussed above, we set the arc-length distribution to be

$$P(m) = m^{-c} / [\zeta(c, 1) - \zeta(c, L + 1)], \quad (2)$$

where the proper normalization is given in terms of the generalized (Hurwitz) zeta function

$$\zeta(c, a) \equiv \sum_{n=0}^{\infty} (n+a)^{-c}. \quad (3)$$

Throughout the paper we will take $c > 1$, as is the case for all systems of interest. We start by considering a single arc in the arc diagram, corresponding to a loop of length m . We label the monomers lying on the loop as $1 < i < m-1$, so that the contacting monomer pair $(0, m)$ which closes the loop is excluded. We want to calculate the probability distribution for the corresponding node in the equivalent incompatibility graph to have degree d .

The probability that the considered arc crosses another one which has one of its legs at monomer i ($1 < i < m-1$) is

$$\pi_{i,m} = \frac{1}{2} \frac{\zeta(c, i+1) + \zeta(c, m-i+1)}{\zeta(c, 1) - \zeta(c, L+1)}. \quad (4)$$

Below, we fix the average density of contacts (which is a function of temperature only) through the arc fugacity, z , so that the arc density satisfies

$$\sigma = z[\partial(1-z)^{-1}/\partial z]/(1-z)^{-1} = z/(1-z). \quad (5)$$

The probability that out of the n arcs originating from the site i , d_i will cross the reference arc $(0, m)$ is

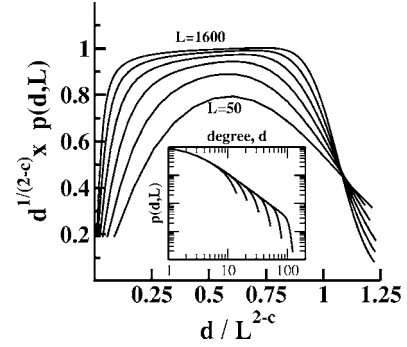


FIG. 2. The plots for increasing L converge to the expected scaling function of Eq. (10). The inset shows the degree distribution for different chain lengths before scaling the axes.

$$\Pi_{i,m}(d_i) = (1-z) \sum_{n=d_i}^{\infty} z^n \binom{n}{d_i} \pi_{i,m}(c)^{d_i} [1 - \pi_{i,m}(c)]^{n-d_i}. \quad (6)$$

Now we can write down the probability that the reference arc crosses a total of d arcs as

$$P_m(d) = \sum_{\{d_i\}}^{\sum_i d_i = d} \prod_{i=1}^{m-1} \Pi_{i,m}(d_i). \quad (7)$$

The difficulty due to the restricted sum is overcome by shifting to the grand-canonical formulation with an arc-crossing fugacity, μ . If we define $\tilde{P}_m(\mu)$ to be the Laplace transform of Eq. (7), then a further summation over all loop lengths m gives the Laplace transform $\tilde{P}(\mu, L)$ of the degree distribution we are after. Using Eqs. (6) and (7) we obtain

$$\tilde{P}(\mu, L) = \sum_{d=0}^{\infty} P(d, L) \mu^d = \sum_{m=1}^L m^{-c} \prod_{i=1}^{m-1} [1 + \sigma(1-\mu)\pi_{i,m}]^{-1}. \quad (8)$$

We solved for $P(d, L)$ numerically using MATHEMATICA. The probability distribution for the node degrees obtained exhibits a clear power law with a sharp finite size cutoff (Fig. 2, inset). The analysis of the data for a range of lengths L and several values of c gives the finite size scaling form

$$P(d, L) = d^{-1/(2-c)} f(d/L^{2-c}), \quad (9)$$

where $f(x)$ is a scaling function determining the window of validity for the power law

$$f(x) = \begin{cases} \text{const}, & x \lesssim O(1) \\ 0, & \text{otherwise.} \end{cases} \quad (10)$$

When the two axes are normalized in accordance with Eq. (9), we obtain a convincing asymptotic collapse for $P(d, L)$ for increasing L (Fig. 2), hence, assuring the validity of the assumed scaling form.

It is clear from Eqs. (9) and (10) that the power law disappears when $c \geq 2$. This, in fact, is the case for a freely fluctuating self-avoiding coil in two and three dimensions. For convenience, we list below (see Table I) the value of the loop exponent, c , for various cases. For the low T phase in three dimensions no estimate of σ_4 is available yet. In this

TABLE I. Known values of the loop exponent c for a self-attracting self-avoiding walk at various temperature regimes in two and three dimensions.

Temperature	2D	3D
$T < T_\theta$	1.375	
$T = T_\theta$	1.571	1.5
$T > T_\theta$	2.688	2.22 ^a

^aSee Ref. [24].

case, simulations suffer from severe surface effects which add to the difficulties of sampling compact configurations.

The random-graph approximation we employed above omits correlations among contacts in the IG graph. For example, we ignored the fact that the IG is bipartite in two dimensions [13]. Thus, the conclusions of the random-graph scenario are not guaranteed a priori to hold for true polymers and it is necessary to confirm them through numerical simulations. For this purpose, we generated self-avoiding walks on a square lattice up to length $L=3200$ by using the pruned-enriched rosenbluth method (PERM) [25], a particularly efficient Monte-Carlo technique for interacting polymers. A nearest neighbor attractive interaction ϵ was introduced in order to induce collapse [12]. For each sample we obtained the normalized degree distribution of its incompatibility graph and averaged them with their associated Boltzmann weight (Fig. 3).

According to the Table above and Eq. (9), high T polymers do not have scale-free IGs. We first checked through computer simulations at $T > T_\theta$ that this indeed is true. In fact, the IG in this case is composed of many disconnected subgraphs with an exponentially decaying distribution of number of nodes. Our preliminary results show that the c exponent controls the power-law distribution for the span along the polymer backbone of each isolated subgraph comprising the IG.

According to Eqs. (9) and (10) SFN should emerge when c gets smaller than 2, i.e., when we cross the θ point. We confirm this by considering next the case where the scale-free nature of the IG is expected to be most easy to demonstrate, namely the $T < T_\theta$ regime in two dimensions. The small loop exponent c in this regime renders a wider scaling

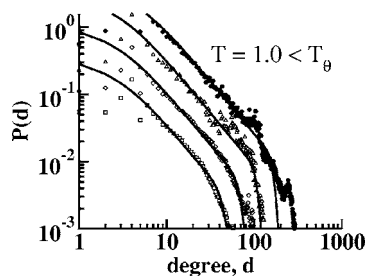


FIG. 3. Averaged degree distribution for the IG of a self-attracting self-avoiding walk of 400 (\square), 800 (\diamond), 1600 (\triangle), 3200 (\bullet) steps on square lattice at $T/\epsilon=1.0 < T_\theta/\epsilon$. The solid curves are the model's predictions with $c=d\nu-\sigma_4=1.375$.

region on the basis of Eq. (9). The temperature was fixed to $T/\epsilon=1.0 < T_\theta/\epsilon \approx 1.54$ [12], deep in the low T phase.

The degree distribution for not too high IG node degrees appears to be self-averaging, since we were able to identify the power law behavior even in a single sample. The data presented in Fig. 3 are averaged over at least 1000 independent samples, mainly to determine the cutoff behavior. For comparison, the corresponding random-graph prediction obtained from Eq. (8) is also shown in the same figure with a solid curve. The curve and the data points are overlapped by a suitable *vertical* shift to compensate for the discrepancy between the two at very small degree numbers ($d < 5$): The window $0 \leq d < 5$ is irrelevant for scaling purposes, yet it accounts for a finite fraction of the probability integral. An incorrect prediction in this region [due to deviations from the asymptotic form in Eq. (2)] consequently results in a finite vertical shift on the right-hand side of the distribution.

Figure 3 shows the degree distributions obtained from simulations of chains of various lengths. The agreement with the random-graph estimate calculated above is also shown (solid line). Not only the degree exponent, $\gamma=1/(2-c)=1.6$, which is given by the slope in the log-log plot, but also the L dependence of the finite size cut-off is well predicted by Eqs. (9) and (10).

Although the θ point, too, appears as a good candidate with a predicted network exponent of $\gamma=2.33(2.0)$ for 2D(3D), relatively longer polymers required in order to obtain a convincing power law scaling make simulations harder due to either self-trapping or strong logarithmic corrections, respectively.

Most known examples of SFNs also exhibit a high degree of clustering. Our graphs being ideally bipartite, the standard clustering coefficient based on counting triangles vanishes (except for a small contribution from buried polymer ends). Instead, we considered the probability that two nodes have a common nearest neighbor given that they already share another one and checked how it differs from its expected value for two uncorrelated nodes with the same degree. The latter probability is given by

$$P_{rand}(d_1, d_2) = 1 - \frac{(N-d_1-1) \cdots (N-d_1-d_2)}{(N-1)(N-2) \cdots (N-d_2)}, \quad (11)$$

where N is the number of nodes in the subgraph excluding the two nodes with degrees d_1, d_2 . Note that the Eq. (11) is symmetric under the exchange of degrees. We found that $\langle P(d_1, d_2) - P(d_1, d_2)_{rand} \rangle \approx 0.16$, indicating a high degree of clustering. A feature possibly due to the spatial proximity of the loops corresponding to the two nodes that share a common nearest neighbor.

In conclusion, we showed that a collapsed polymer globule in two dimensions accommodates a scale-free network. By means of a model based on the critical properties of the polymer, we conjecture exact exponents for the scaling of the degree distribution. The model predicts similar behavior also at the θ point, but with different degree exponents. Resulting networks are scale-free upto a degree number obtained by finite size scaling. The cutoff is determined by a power of L which is the inverse of the degree exponent γ , such that the

power law scaling is less prominent (cutoff is more severe) at higher values of γ . It is conceivable that a similar mechanism applying to other known examples of SFNs may serve as a sieve selecting low degree exponents.

The above results show how pseudotopological features of compact polymer conformations concile with the overall scale invariance by displaying universal power law behaviors. The discovery of these scalings can be regarded as a step forward in the more general program of elucidating the interplay between topology and scale invariance in polymer statistics (see, e.g., Refs. [26,27]). The connection between polymers and networks studied here could reveal important

also in other related problems. One possible connection is to the TSP [20], where the topology of the related IG could serve as a checkpoint for the conjectured correspondence with dense polymers. One is also tempted to attribute to the IG of a globular biopolymer, such as a folded protein, a signature of the folding kinetics. For example, since the IG gives a measure of how “interpenetrating” the contacts are, a correlation between high-degree nodes and the earlier formed contacts or the folding nucleus [28] is plausible.

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