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Small-world phenomena and the statistics of linear polymers

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Abstract

A regular lattice in which the sites can have long-range connections at a distance l with a probability $P(l) \sim l^{-\delta}$, in addition to the short-range nearest neighbour connections, shows small-world behaviour for $0 \leq \delta < \delta_c$. In the most appropriate physical example of such a system, namely, the linear polymer network, the exponent δ is related to the exponents of the corresponding n -vector model in the $n \rightarrow 0$ limit, and its value is less than δ_c . Still, the polymer networks do not show small-world behaviour. Here, we show that this is due to a (small value) constraint on the number, q , of long-range connections per monomer in the network. In the general δ - q space, we obtain a phase boundary separating regions with and without small-world behaviour, and show that the polymer network falls marginally in the regular lattice region.

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A small-world network (SWN) develops out of regular lattices having local connections with additional long-range links or connections with a finite probability. It acquires the intriguing property that while the local connectivity structure remains similar to the original underlying lattice, the shortest path between any two lattice sites becomes similar to that of random graphs [1, 2]. Specifically, if we take a regular d -dimensional lattice, then the neighbourhood of any site of the lattice is given by the structure of the lattice and the shortest path between any two sites of the lattice is of the order of $N^{1/d}$, where N is the total number of sites in the lattice. For a random graph, having random connections at all ranges, a similar shortest path distance between any two points grows as $\ln N$ implying that the effective lattice dimensionality $d \rightarrow \infty$. The local structure of a random graph is completely amorphous. Watts and Strogatz [1] in their model showed that starting from a regular lattice, when some of the nearest neighbour bonds are replaced by long-range connections at random with a finite probability p , the network shows an interesting feature: while the local connectivity remains practically the same as in the regular lattice, the global shortest path distance S_N scales as $\ln N$ for a network of size N for any non-vanishing p .

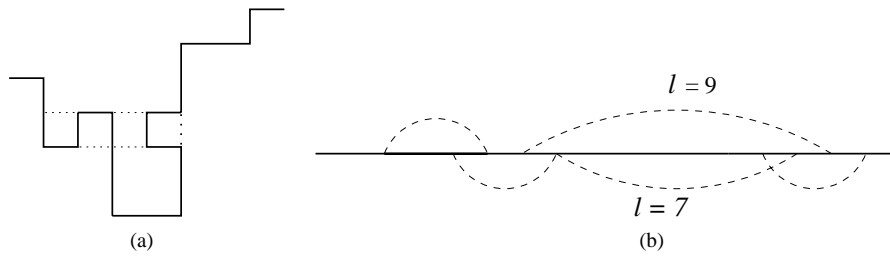


Figure 1. (a) Portion of a SAW network: the solid line represents the polymer or the street and the dashed lines represent the nearest neighbour bridges. (b) A stretched chain equivalent: it contains long-range connections with probability $P(l)$.

This property of the SWN is of importance in various social communication networks, such as internet links, disease spreading, etc. This also explains the amazingly low value of the number of steps connecting any two members of such networks, e.g., the ‘six degrees of separation’ observed in Milgram’s experiment and similar situations [3]. The minimal step number connecting two members of these networks scales as $\ln N$, rather than as N , the total population of the network, while the local coordination structure remains almost the same. Recently, the propagation of thermal correlations in such networks have also been studied; particularly, the effect of such random long-range connections on the nearest neighbour interacting Ising chain [4, 5]. With long-range interactions occurring with probability p , the transition temperature becomes non-zero for $p > p_c$ for the Ising chain; $p_c = 0$ according to Barrat and Weigt [4] and $p_c \neq 0$ according to Gitterman [5]. Estimates of this transition temperature and the nature of the correlations near the transition point have been investigated in the above mentioned studies [4, 5].

In such SWN, the probability p of the long-range connections is simply the fraction of such connections which are added randomly and are independent of the range. Recently, in some extended SWN models, the probability $P(l)$ that two points at a distance l along the chain are connected has been taken to be dependent on l such that $P(l) \sim l^{-\delta}$; $\delta = 0$ corresponds to the original model [1]. These studies indicate that for $\delta \geq \delta_c$ the network effectively reduces to the regular lattice, while for $\delta \leq \delta_c$ it effectively becomes a SWN. There is apparently some disagreement over the value of δ_c : according to [6] $\delta_c = 2$, while in [7] δ_c is found to be equal to d . Our study here is essentially for one-dimensional chains and we find that for the corresponding unrestricted cases (defined later), $\delta_c = 2$.

It appears that the most appropriate example of SWN in physics is the example of linear polymers or the self-avoiding walk (SAW) model [8]. Here, the long-range connections over the nearest neighbour monomer–monomer connections (called the ‘streets’) come from the random folding (forming the local loops or the ‘bridges’) of the chain in the embedding dimension d . Figure 1 shows how long-range connections develop out of random folding in a SAW. In fact, the structure of such a network has been studied intensively some time back [9–11]. Here, of course, the probability P of a connection at a (long) range l is given by the SAW statistics: $P(l) = G_l^{\text{SAL}}/G_l^{\text{SAW}}$, where $G_l^{\text{SAW}} = \mu^l l^{\gamma-1}$ is the number of SAWs of length l and $G_l^{\text{SAL}} = \mu^l l^{-2+\alpha}$ is the number of loops of length l [8]. Here μ is the connectivity coefficient of the SAW on the embedding lattice and γ and α are, respectively, the susceptibility and specific heat exponent of the equivalent n -vector model in the limit $n \rightarrow 0$. Hence

$$P(l) \sim l^{-\delta} \quad (1)$$

where $\delta = 1 + \gamma - \alpha$. Using the approximate Flory formula $\nu = 3/(2+d)$ for the correlation length exponent and $\gamma \simeq 1$, we get $\delta \simeq d\nu = 3d/(2+d)$. Hence $\delta < 2$ for $d = 2$ and $\delta = 2$

for $d = 4$. In fact, with the best estimates of α and γ [8], one would also get $\delta < 2$ for $d \leq 3$ and $\delta = 2$ for $d = 4$. The average number, q , of such additional long-range connections per site can also be estimated easily [8]; e.g. $q = (z - 1) - \mu$, where z is the lattice coordination number. This is because out of the $z - 1$ options left for the SAW to grow for the next step, on an average μ options are chosen, the rest being visited earlier due to random folding of the chain. With $\mu \simeq 2.638, 4.151$ and 4.686 , one gets $q \simeq 0.36, 0.85$ and 0.31 in square, triangular and simple cubic lattices, respectively.

The above comparison and the observations [10, 11] on the SAW networks indicate that the requirement $P(l) \sim l^{-\delta}$ with $\delta < 2$ for $d < 4$ for small-world effects is not sufficient as the small-world phenomena is certainly not observed in such SAW networks. In particular, it was found that the shortest path length S_N in a SAW network of N steps grows only linearly in N for any finite-range interactions or bridges [11]. The SAW network therefore always remains a linear one, and no small-world effect ($S_N \sim \ln N$) or, for that matter, no extra dimensional effect ($S_N \sim N^x, x < 1$) can be seen. Of course, the structures of the linear polymer network and the SWN are inherently different, although the effective probability of connections in both cases are given by the same power law (1). In SAW network, there is a structural restriction on the total number of neighbours: at any point along the SAW chain, the total number of connections $q + 2$ (as there are q long-range connections and two short-range connections for each site) cannot exceed the coordination number of the underlying lattice. In SWN, however, no such restriction exists (theoretically, here q can go upto $N - 3$ at each site for $\delta = 0$). In the SAW network, there also exists a correlation between the bridges. Such correlations are absent in SWN (see e.g. in figure 1, two long connections lie very close; such configurations are more likely in a SAW than in a general SWN).

Here we explore the differences that emerge from the constraint on the total number of long-range connections in SAWs to find whether it is responsible for the non-SWN-like behaviour of the SAW networks. Precisely, we investigate the crossover from small-world behaviour to regular lattice behaviour indicated by the crossover in the behaviour of N (from $S_N \sim \ln N$ to $S_N \sim N$).

For a fixed finite average number, q , of long-range connections (per site) in the SWN, we vary δ to obtain $\delta_c(q)$ at which the S_N behaviour changes. We then vary q in the range $0 < q < 2$, which corresponds to the real physical situation of SAWs in a square lattice. Note that for the infinite chain, the probability in (1) is easily normalizable for any δ greater than unity.

In the SAW, the values of δ and q are independent. While treating both δ and q as independent quantities in the model where the probability of a long-range connection of length l varies as $l^{-\delta}$, it should be mentioned that strictly speaking the total number of long-range connections qN depends on the value of δ . For example, for $q \sim N$, one does not have a choice for the value of δ as large values of δ will not be allowed in this case. Therefore, when q is taken to be independent of δ , the range of both parameters get restricted. We find that taking $0 < q < 2$ is safe for values of $\delta \leq 2.5$ in the sense that the desired scaling of the bond distributions is intact.

We first generate a linear chain of length N . We then put additional long-range interactions (bridges) following the probability distribution (1), with the restriction that the total number of such connections is qN . We then use a greedy algorithm (see e.g. [12]) to find out the shortest path through the streets and bridges and count the number of steps S_N connecting the endpoints of the SAW network.

In the unrestricted case (large q), we find that the (phase) transition from logarithmic to linear scaling is recovered at $\delta \geq 2$. This agrees with the result of [6]. For the finite N values considered here ($N \leq 10000$), at low values of δ (< 1.4), the logarithmic scaling is clearly observed (figure 2). However, for the intermediate values of δ ($1.4 < \delta < 2$), the variation is apparently power law like. We believe that this is only an effective behaviour and the

logarithmic behaviour will follow as $N \rightarrow \infty$. The justification is *a posteriori*, which can be seen from the results for the constrained cases to be discussed later.

The constraint that the total number of long-range bonds for the whole chain is qN is a global one. It may also be demanded that these bonds are distributed such that each site is not allowed to have more than a fixed number of long-range bonds; this is a local constraint. In a SAW embedded in a square lattice, there is a local constraint as individual sites cannot have more than two long-range neighbours. We have studied both the locally and the globally conserved cases; in the former the number of maximum long-range bonds at every site is

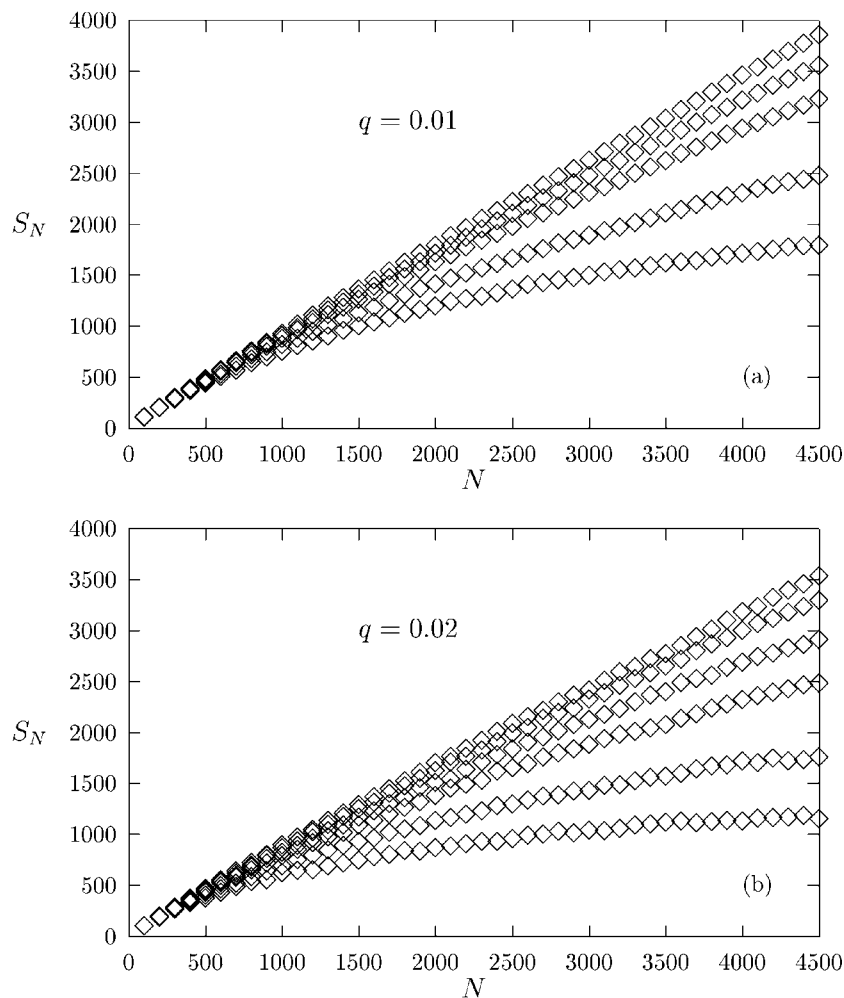


Figure 2. The behaviour of the shortest path length S_N over N steps along the chain. The curves are drawn for higher to lower values of δ from top to bottom: (a) $q = 0.01$; $\delta = 1.6, 1.5, 1.4, 1.2$ and 1.0 . The curves become linear for $\delta = 1.5$ and above. (b) $q = 0.02$; $\delta = 1.7, 1.6, 1.5, 1.4, 1.2$ and 1.0 . The curves are linear above $\delta = 1.6$. (c) $q = 0.2$; $\delta = 2.0, 1.95, 1.9, 1.8, 1.7$ and 1.6 . Linearity is observed above $\delta = 1.90$. (d) $q = 0.5$; $\delta = 1.8, 1.9, 1.95, 2.0$ and 2.1 . Linearity appears above $\delta = 2.0$. In (c) and (d) where larger chains ($N = 10000$) have been considered, the change from the apparent power law to the actual logarithmic behaviour below δ_c is clearly observed. The logarithmic behaviour at $\delta < \delta_c$ can be observed at smaller values of N as q increases.

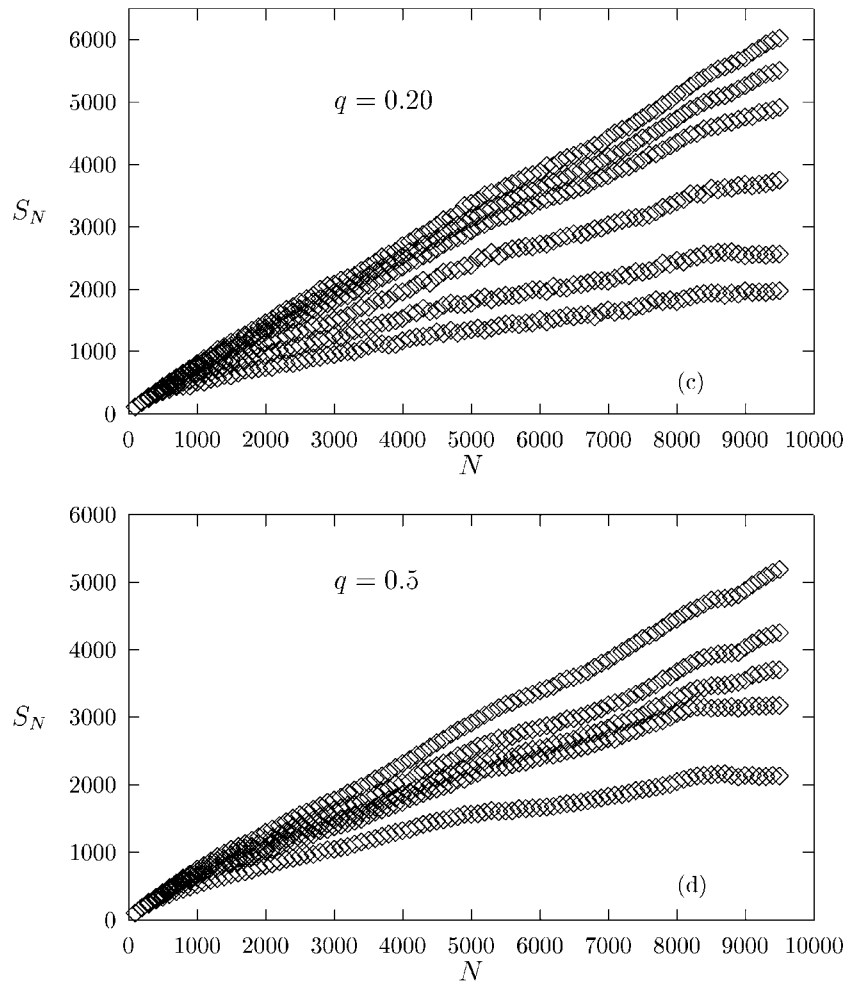


Figure 2. (Continued)

kept equal to 2 in analogy with the SAW (on a square lattice), keeping the total number of long-range connection equal to qN at the same time. However, the results with local and non-local conservation are observed to be the same as far as the scaling of the shortest path is concerned. The total path length in the locally restricted case is smaller because connections which are redundant in the globally restricted case are to some extent lesser in number.

The variation of the shortest path with the path length for a given q and various δ values shows that when extrapolated for large N , there are only two kinds of behaviour: logarithmic and linear. The linear behaviour is obtained for $\delta > \delta_c(q)$. The logarithmic behaviour is quite apparent for small δ . For intermediate values of $\delta < \delta_c(q)$, apparently there is an effective power law behaviour $S_N \sim N^x$; but we find that with increasing N , x decreases and one finally obtains the logarithmic behaviour. On the other hand, for $\delta \geq \delta_c$, x is observed to remain practically near unity. This observation may require really large values of N (e.g. $N < 10\,000$ for $q < 0.1$). The transition boundary is difficult to estimate accurately—a problem encountered in many SWNs [6]. At small values of q , we find that the shortest path becomes

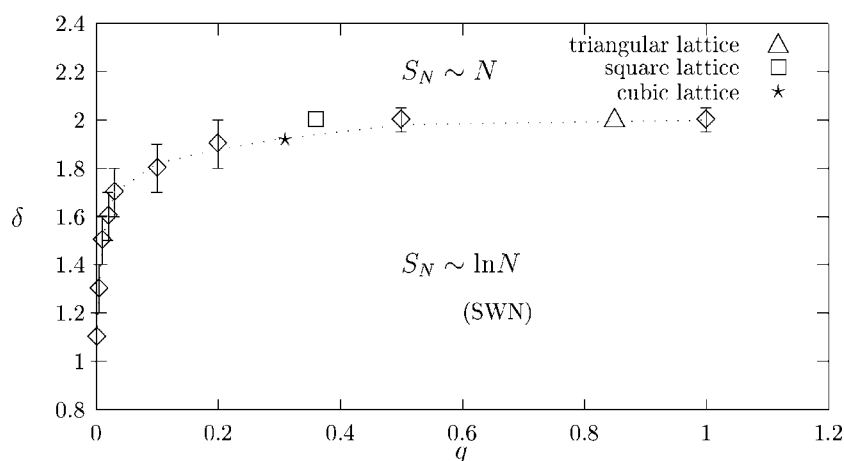


Figure 3. The regions corresponding to the different behaviour of S_N in the δ - q plane. The dashed line is a guide to the eye separating the small-world region from the linear region. At low values of q , there is no small-world-like phenomena even though δ is less than 2.0. The values of q and δ for linear polymers on the square, triangular and cubic lattices are shown by different symbols.

linear at a value $\delta_c(q) < 2$. As q is increased, $\delta_c(q)$ increases, and finally $\delta_c(q)$ approaches a value 2.0 as q becomes large (see figure 3).

In summary, our generalized model in which both δ and q are treated independently shows that the transition from small-world to the regular lattice behaviour occurs across a phase boundary $\delta_c(q)$. Extensive earlier investigations on SAW networks had established [10, 11] that they do not show any small-world behaviour. In view of the recent studies [6, 7] on models having long-range connections with probability distribution (1), and the observation that they show small-world behaviour for $\delta < 2$, together with the fact that δ is indeed less than 2 for SAWs, an apparent contradiction arises. We resolve this here by studying the phase diagram of a generalized model having long-range connection probability distribution (1) and a restricted average number, q (per site), of such additional long-range connections. We show that a crossover from small-world to regular lattice behaviour occurs as one crosses the phase boundary given by $\delta_c(q)$ ($\delta_c \rightarrow 2$ for large q). The points (q, δ) corresponding to the square, triangular and cubic lattices in figure 3 show that linear polymers on these lattices lie marginally in the regular lattice region. We claim that the small value of q (< 1) for linear polymers makes it fall in the regular lattice region in the phase diagram, and excludes the possibility of its small-world behaviour. As mentioned earlier, we have not taken into account the various correlations developing in the SAW, and thus the q values in SAW, and the network studied in the present paper may not be quantitatively identical. Second, the values of q and δ shown in figure 3 for the different lattices are theoretical estimates only and therefore these points may actually lie deeper in the regular lattice region. Hence we believe that the important result $\delta_c(q) < 2$ for small values of q is responsible for the non-SWN-like behaviour in SAW.

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