Bounds for the minimum step number of knots confined to slabs in the simple cubic lattice

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Abstract

Volume confinement is a key determinant of the topology and geometry of a polymer. For instance recent experimental studies have shown that the knot distribution observed in bacteriophage P4 cosmids is different from that found in full bacteriophages. In particular it was observed that the complexity of the knots decreases sharply when the length of packed genome decreases. However it is not well understood exactly how the volume confinement affects the topology and geometry of a polymer. This problem is the motivation of this paper. Here a polymer is modeled as a self-avoiding polygon on the simple cubit lattice and the confining condition is such that the polygon is bounded between two parallel planes (i.e., bounded within a slab). We estimate the minimum length required for such a polygon to realize a knot type. Our numerical simulations show that in order to realize a prime knot (with up to 10 crossings) in a 1-slab (i.e. a slab of height one), one needs a polygon with length longer than the minimum length needed to realize the same knot when there is no confining condition. In the case of the trefoil knot, we can in fact establish this result analytically by proving that the minimum length required to tie a trefoil in the 1-slab is 26, which is greater than 24, the known minimum length required to tie a trefoil without a confinement condition. Additionally, we find that in the 1-slab not all geometrical realizations of a given knot type are equivalent to each other, suggesting that the topology of a polymer in confined volume alone is not enough to describe the state of a polymer.

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