

BOUNDS FOR MINIMAL STEP NUMBER OF
KNOTS IN THE SIMPLE CUBIC LATTICE

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Abstract

Knots are found in DNA as well as in proteins, and they have been shown to be good tools for structural analysis of these molecules. An important parameter to consider in the artificial construction of these molecules is the minimal number of monomers needed to make a knot. Here we address this problem by characterizing, both analytically and numerically, the minimum length (also called minimum step number) needed to form a particular knot in the simple cubic lattice. Our analytical work is based on an improvement of a method introduced by Diao to enumerate conformations of a given knot type for a fixed length. This method allows to extend the previously known result on the minimum step number of the trefoil knot 3_1 (which is 24) to the knots 4_1 and 5_1 and show that the minimum step numbers for the 4_1 and 5_1 knots are 30 and 34 respectively. We report on numerical results resulting from a computer implementation of this method. We provide a complete list of estimates of the minimum step numbers for prime knots up to 10 crossings, which are improvements over current published numerical results. We enumerate all minimal lattice knots of a given type and partition them into classes defined by BFACF type 0 moves.