Knots and links in the simple cubic lattice

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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 minimum number of monomers needed to make a knot. Here we address this problem by characterizing, both analytically and numerically, the minimum length needed to form a particular knot in the simple cubic lattice.

Consider the simple cubic lattice $\mathbb{Z}^3$. A step is a line segment of unit length joining two lattice points in $\mathbb{Z}^3$ (namely points with integer coordinates). A lattice polygon K of length n is a polygon embedded in $\mathbb{Z}^3$ with n steps. The minimum step number of a knot type K is the minimum number of steps needed to construct a lattice polygon of knot type K. It is shown that the minimum step number of 3_1 is 24 (See the figure below), 4_1 is 30 and 5_1 is 34. Numerically we determined the upper bound of the minimum step number of knots up to 10 crossing. We also discuss the minimum step numbers and exponential growth rate of knots and links in confined regions