

Paths and helices in diamond lattice

Alexandru T. Balaban, Kiran B. Chilakamarri, Douglas J. Klein

In 2001, Balaban and Rcker described the overlap operation of two 3-paths (paths with three edges) to produce longer paths in diamond lattice and cubic lattice. These special 3-paths they called protochirons. Labeling these protochirons and recording the labels as one moves through a path in a lattice provides a coding mechanism for the paths in lattices. There are six protochirons in cubic lattice and three in the diamond lattice, such as is the focus of this talk. The three protochirons in diamond lattice are denoted by the letters R, S, and Z. Any path has a unique code in terms of these protochirons. Given a code such as RRSRRZ. and the position of the first protochiron (i.e., the coordinates of the first four points) all the points of the path can be evaluated. We provide a simple algorithm to this effect. Periodic paths have periodic codes. A mild application of the pigeonhole principle yields the converse: A periodic code and the position of the first protochiron determines a periodic path. Since helices are periodic, when searching for helices it is enough to restrict our attention to periodic codes. We provide an algorithm to test if a given code corresponds to a helix. The algorithm involves evaluating the points of a periodic block and projecting them on to an appropriate plane to see if they form a cycle.