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SQUARE SPIRALS, DIMENSIONALITY AND BIOPOLYMERS

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Abstract—This paper illustrates the diversity and esthetic beauty of the spatial patterns produced by a class of heuristic procedures describable by a one-parameter algorithm. While the patterns may provide insight into the structures of biopolymers and other macromolecules, the main focus of this work is the demostration of how two-dimensional order may arise from one-dimensional processes.

We begin this article with a discussion of an organized one-dimensional arrangement of points. These points are so chosen to correspond to a one-dimensional lattice and so we consider only those points that are an integer distance from the origin. It may appear more correct to consider all the points, both a positive and negative distance, than just the positive even if one immediately acknowledges the computational expediency of our simplifying assumption. However counterintuitive be the assumption,† the set of all points corresponding to 0 and the positive integers has the same number of points as the seemingly larger set of the points that correspond to all of the integers. Nothing is thus conceptually lost by our decision to just consider points that are a positive integer from the origin. Our selection of points is equivalent to the elementary mathematical function $f(x) = 0$ for all non-integer x and $f(x) = 1$ for all positive integers x. Our one-dimensional lattice is also equivalent to an infinite string which has been knotted every cm.

This paper presents a simple—perhaps far too simple—picture for the emergence of higher-dimensional order from "merely" the one-dimensional order of a one parameter paradigm. In particular, we consider the transformation of a one- to a two-dimensional lattice, and with this so consider evolution from one- to two-dimensional order. We opt to take our (half-) infinite one-dimensional lattice and "proceed on a [square] spiral starting at the origin" [2]. Proceeding in a rather related way to that of this just cited Ref. [2], one may identify each lattice point of the half-infinite line with a lattice point in the plane.‡ That is, the "1-point" $x = 0$ corresponds to the "2-point" $(x, y) = (0, 0)$, $x = 1$ to $(x, y) = (0, 1)$, $x = 2$ to $(x, y) = (-1, 1)$, $x = 3$ to $(x, y) = (-1, 0)$, $x = 4$ to $(x, y) = (-1, -1)$, etc. We now define an n-spiral by "decorating" the original line every nth lattice point. This decoration can be described in various ways. For example, we may say that our earlier function $f(x)$ is non-zero only when x is an integer multiple on n. We may opt to tie a bow instead of "merely" a knot every n cm.

The one-dimensional lattice is seemingly analogous to an arbitrarily long polymer composed of one type of monomeric subunit. However, many such "real" polymers twist and turn upon themsleves and thus have secondary and tertiary structure that are ordered or organized in all three spatial dimensions. Simple examples include the α-helices that are formed by the "polypeptide that would be a protein" poly-aaaa [3]. Of course, the majority of the distinct chemical species called proteins are ever so more involved, and thereby interesting, because they contain more than one type of amino acid monomeric subunit and the arrangement of the subunits is manifestly

†This assertion, and many others that are even less intuitively reasonable, may be rigorously proven in terms of the analysis given by G. Cantor [1].

‡Strictly speaking, our spiral is left-handed while that in Ref. [2] is right-handed. As such, there is a symmetric relation between our spiral and that earlier given, and the spiral handedness may "merely" subconsciously reflect the fact that the coauthor responsible for programming the spiral (JMR) is left-handed and another author (JFL) has often considered himself to be "ambi-levorous", i.e. equally bad with both hands. The reader should also note that because of the nature of our computer code and printer, our square spirals look rectangular. S/he should also be assured that they are mathematically, if not pictorially, square and, again for computatorial reasons have 66 characters across and 66 lines down.

aperiodic.† Indeed, it has been argued that one reason why catalytically active proteins, more commonly called enzymes, are as large as they are is to allow for the proper three-dimensional arrangement, flexibility, orientation and general organization of active sites. Two quotes from recent reviews are worth citing. From Rebek [5] we cite:

> "It would be most desirable to have access to systems in which the distance between convergent functional groups could be specified in increments of say, even 0.5 Å. It is unlikely that access to such structures will be possible without a tremendous synthetic investment, and we have already suggested [elsewhere, 6] that enzyme structure may be a response to the problems involved with such fine-tuning of small molecules."

Taking a somewhat different tack, Kell [7] suggested: "Enzymes [may be] so big in order . . . to act as channellers of thermal energy to their active sites."

Whether either analysis has validity or not, the design of enzymes constitutes a rather major "engineering feat" because there are some rather tight tolerances for atomic sizes, bond lengths and both bond and torsion angles and because proteins/enzymes are, by definition, all composed of the universal —NHCHRCO— building block. However obvious it is to the biochemist, it should be nonetheless be noted that there are even greater structural restrictions on polypeptides than that just implied. This building block is directional, i.e. they are only joined "head-to-tail" to form the larger "dimeric" units —NHCHRCONHCHR′CO— and seemingly never do either of the alternative "head-to-head" —NHCHRCOCOCHR′NH— or "tail-to-tail" dimers —COCHRNHNHCHR′CO— appear. Furthermore, while except for R = H, all of the building blocks are chiral and so "should" appear equally often in both mirror-image forms. However, real proteins are composed of but one type of handed amino acids, and all of their handedness is the same. Admittedly, we have omitted here any appended coenzymes, i.e. small, non-protein species that contain the catalytically active sites of many enzymes. The presence of coenzymes adds considerable diversity to both structure and activity.

This is all rather complicated. Nonetheless, in a severely simplified form, the protein metaphor may be used if one prefers a polypeptide chain wherein every nth amino acid is a recurring special one that is somehow functionalized and the rest are featureless, say for $n = 5$ corresponding to, say a 1-aspartyltetraglycyl [i.e. {—NHCH(CH_2COOH)CO[$NHCH_2CO]_4$—} or asp-gly-gly-gly-gly] repeat unit. Of course, the analogy is somewhat belied in that our square spiral is imposed on the one-dimensional "species" while the real molecule that is such a copolymer of aspartic acid and glycine would have its own and certainly different secondary structure. As such, our model is rather artificial and so the term "special" rather than "catalytically active" was chosen as to not to alienate any biochemist of confuse anyone else.

With the above caveats, most of the remainder of this article is dedicated to pictures of the special sites generated by n-spirals. In all that follows a * in the center denotes the beginning of the spiral while # is used for all of the other special sites. The 1-spiral is of course every lattice point. The 2-spiral looks like a chessboard or two-dimensional NaCl lattice. This, too, is rather obvious—given a point described by the integer coordinates (x, y). It is a special site when the sum of the coordinates $x + y$ is divisible by 2. This occurs only when both x and y are even or both odd. As such, "alternate" points in the two-dimensional lattice are decorated, and hence the observed pattern. What occurs for the higher n-spirals? Figures 1–14 reproduce our computer generated n-spirals: n was chosen somewhat artificially as the prime numbers 1, 2, 3, 5 and 7 and their lower powers. Numerous two-dimensional patterns seem to arise, although "explanations" for them analogous to that of the chessboard still evade us. Nonetheless, they demonstrate how one-dimensional order can be transformed into two-dimensional order by a simple geometric wrapping and mapping, and so give inferences as to how the one-dimensional primary structures of proteins are transformed through chemical interactions into their much more complicated, though also much more beautiful, three-dimensional secondary and tertiary structures and with this, into the highly efficient and selective species that are usually called enzymes.

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†Aperiodicity is important in biomolecules. Another example of what we are referring to are polynucleotides wherein helical structures arise from chains of just one type of base instead of all four bases normally found in DNA or the even greater number of bases normally found in RNA. Indeed quoting Schrödinger: "We believe a gene—or perhaps the whole chromosome fibre—to be an aperiodic solid." [4]

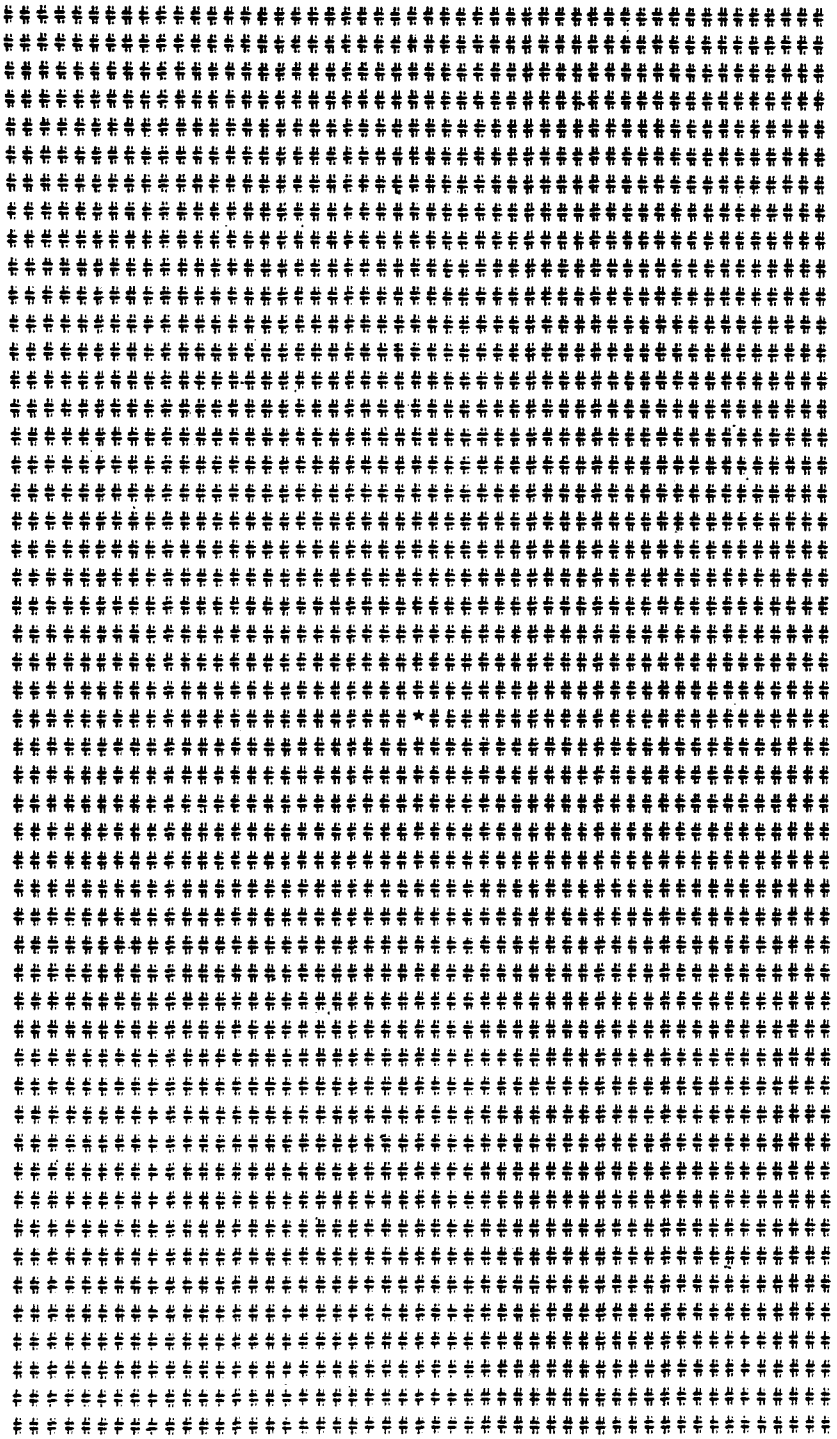

Fig. 1. Performing an interval of 1 spacing; finish printing 1 spiral.

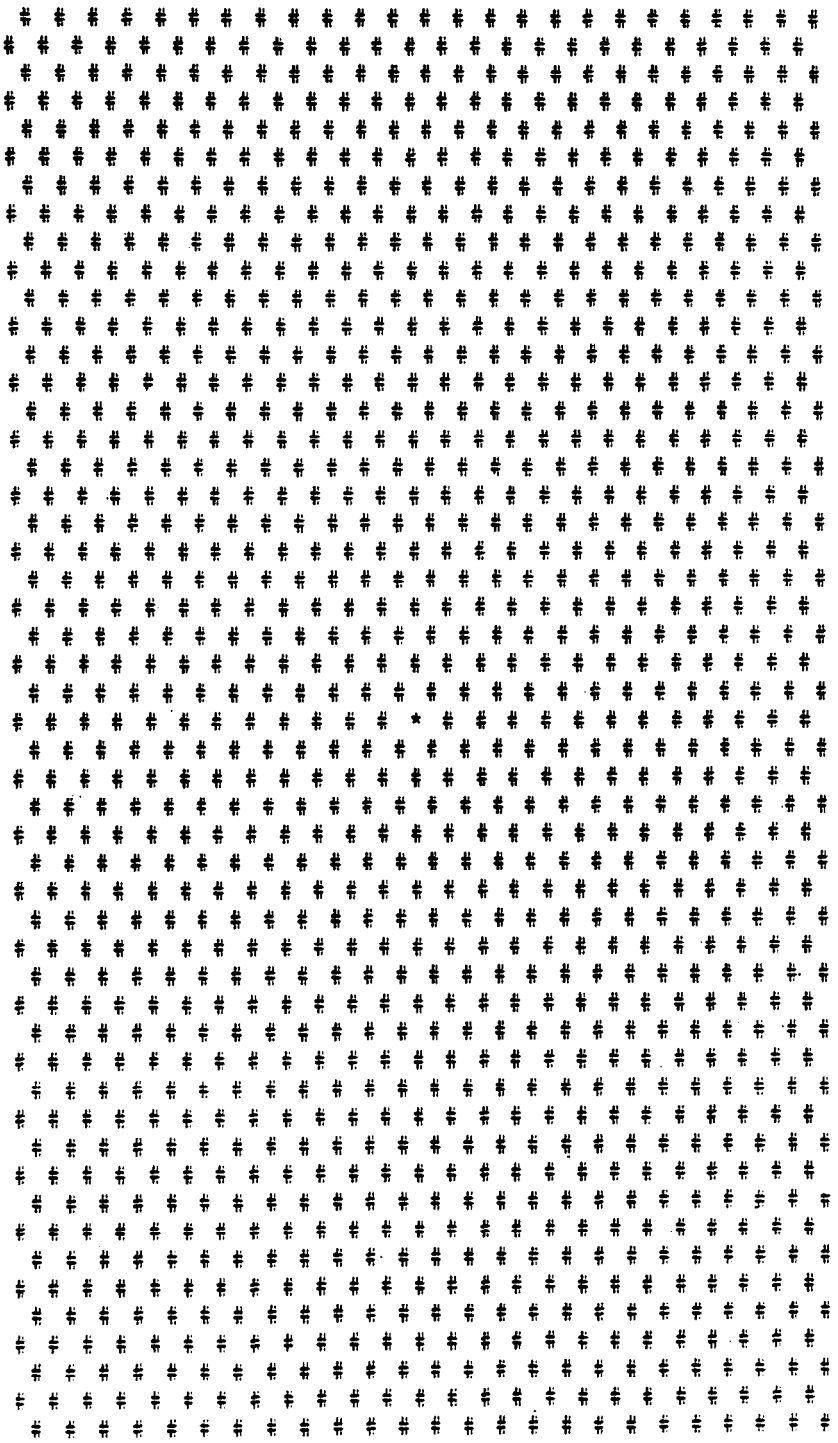

Fig. 2. Performing an interval of 2 spacing; finish printing 2 spiral.

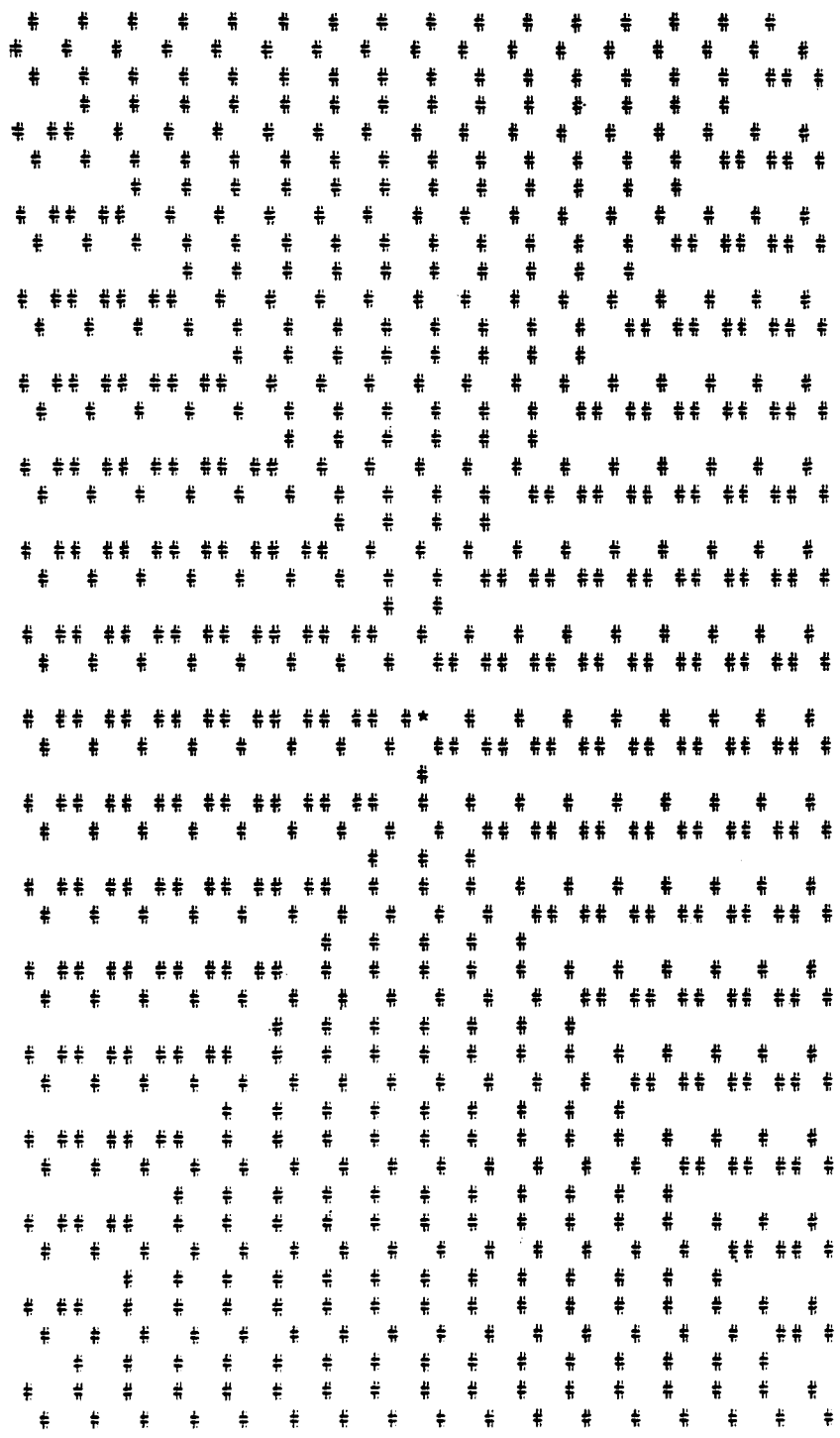

Fig. 3. Performing an interval of 3 spacing; finish printing 3 spiral.

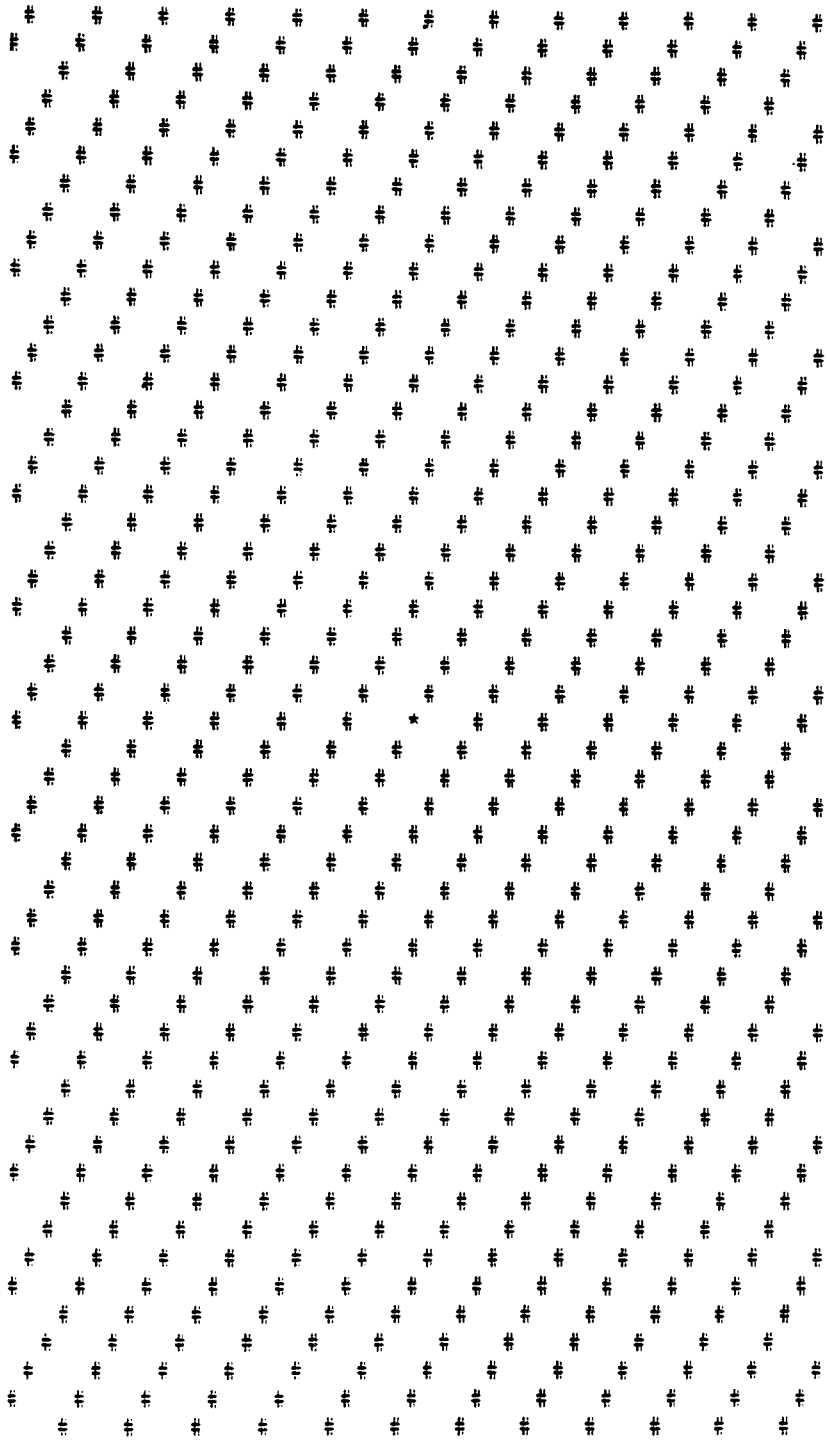

Fig. 4. Performing an interval of 4 spacing; finish printing 4 spiral.

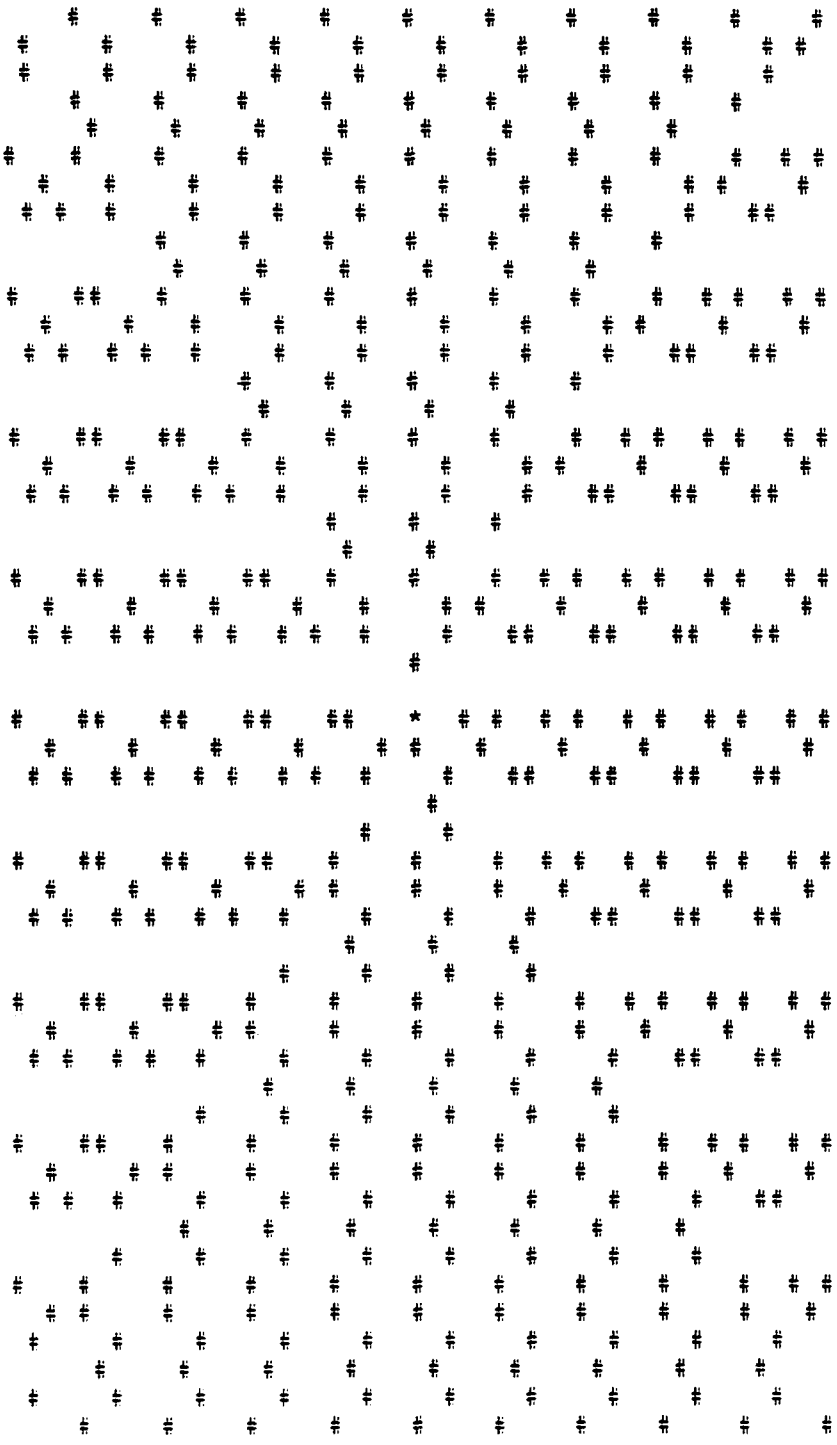

Fig. 5. Performing an interval of 5 spacing; finish printing 5 spiral.

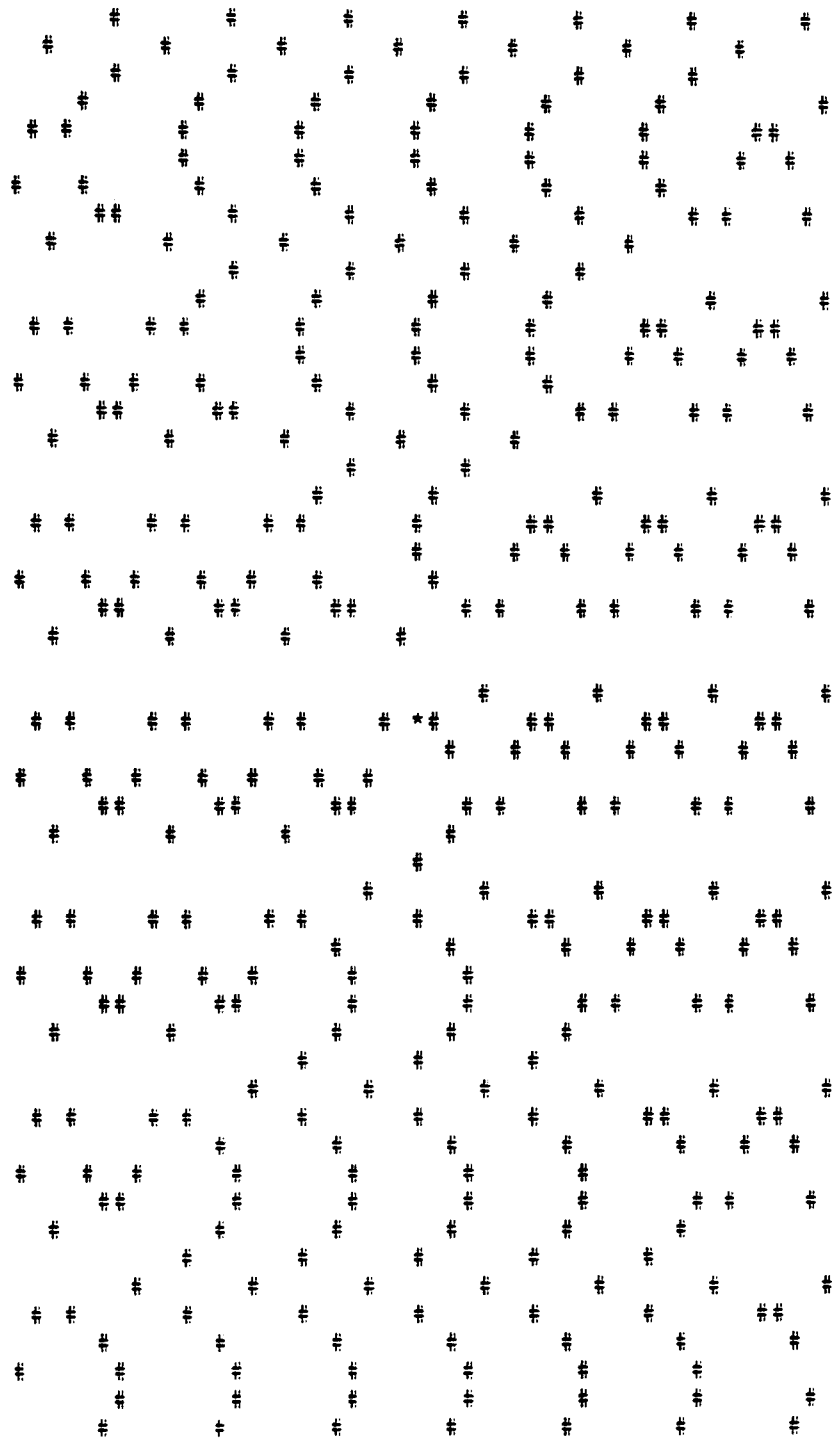

Fig. 6. Performing an interval of 7 spacing; finish printing 7 spiral.

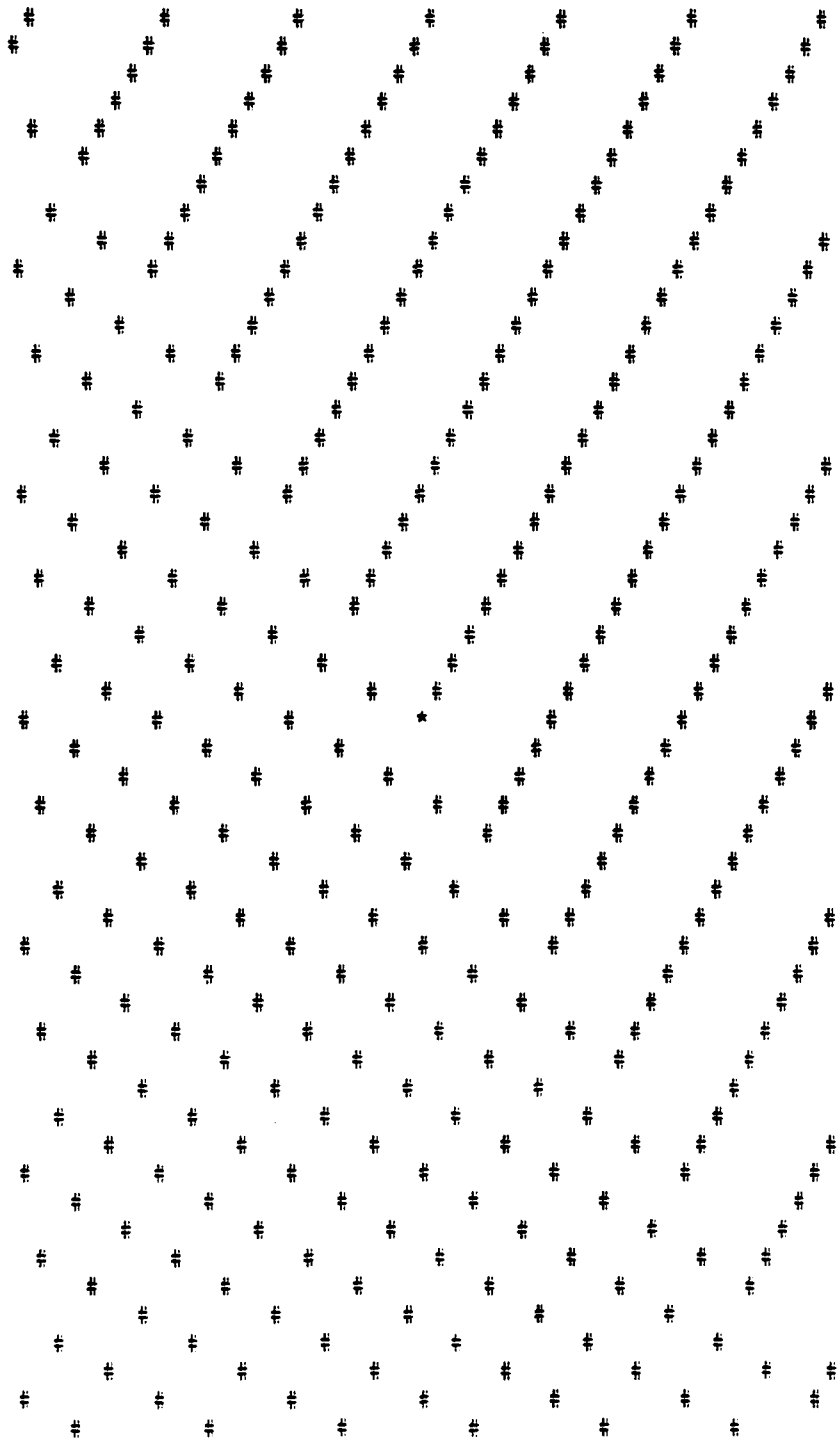

Fig. 7. Performing an interval of 8 spacing; finish printing 8 spiral.

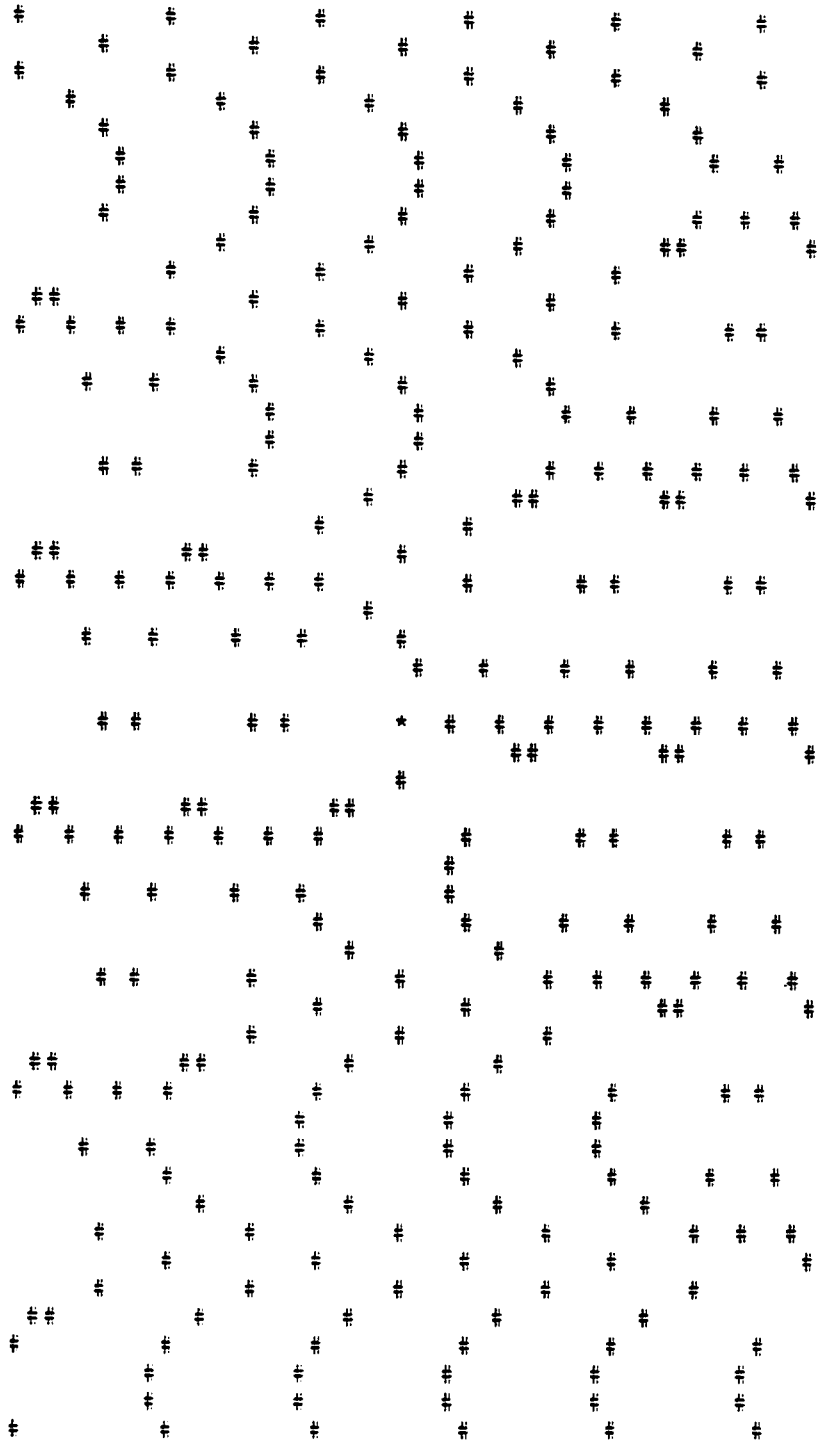

Fig. 8. Performing an interval of 9 spacing; finish printing 9 spiral.

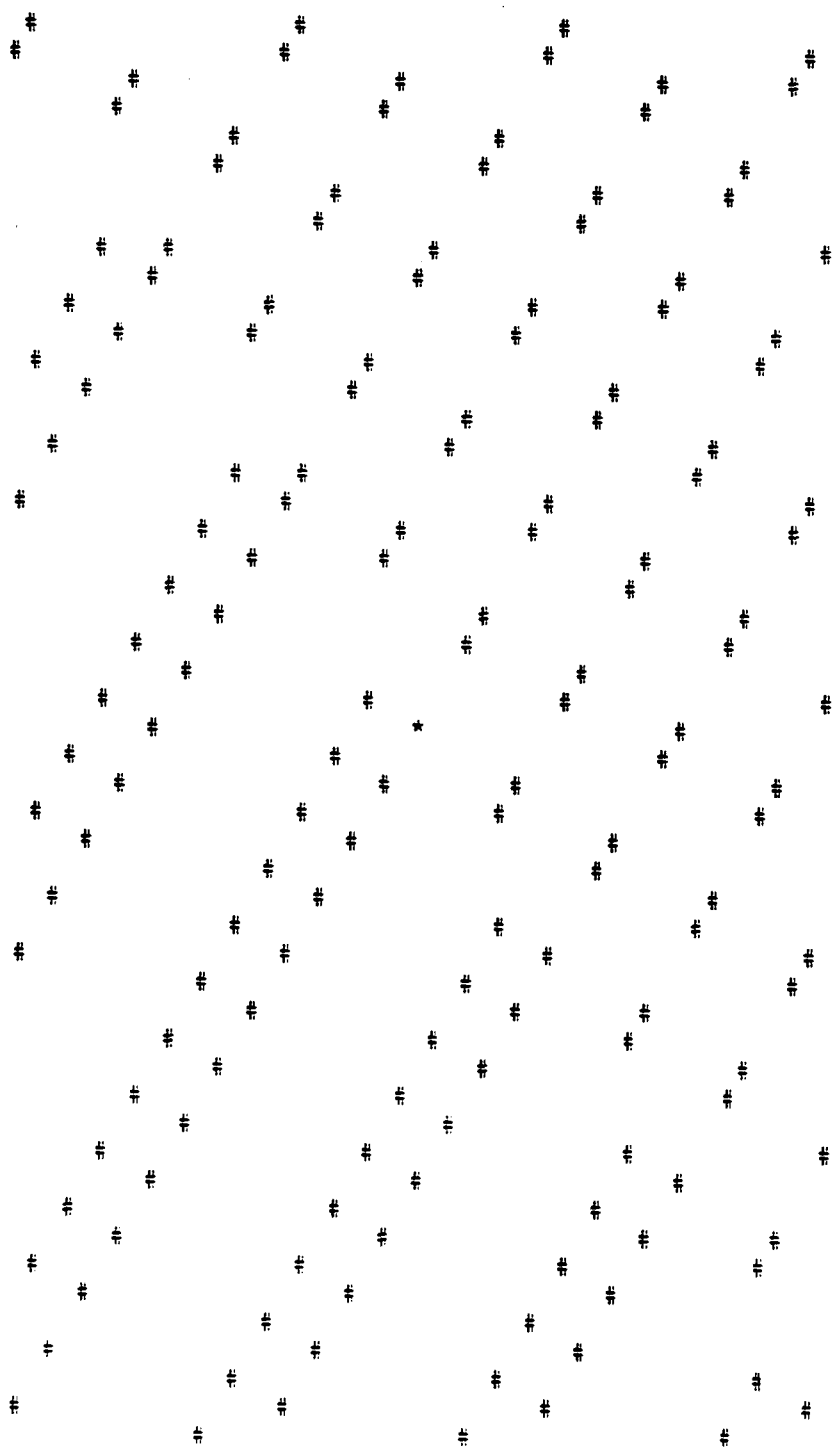

Fig. 9. Performing an interval of 16 spacing; finish printing 16 spiral.

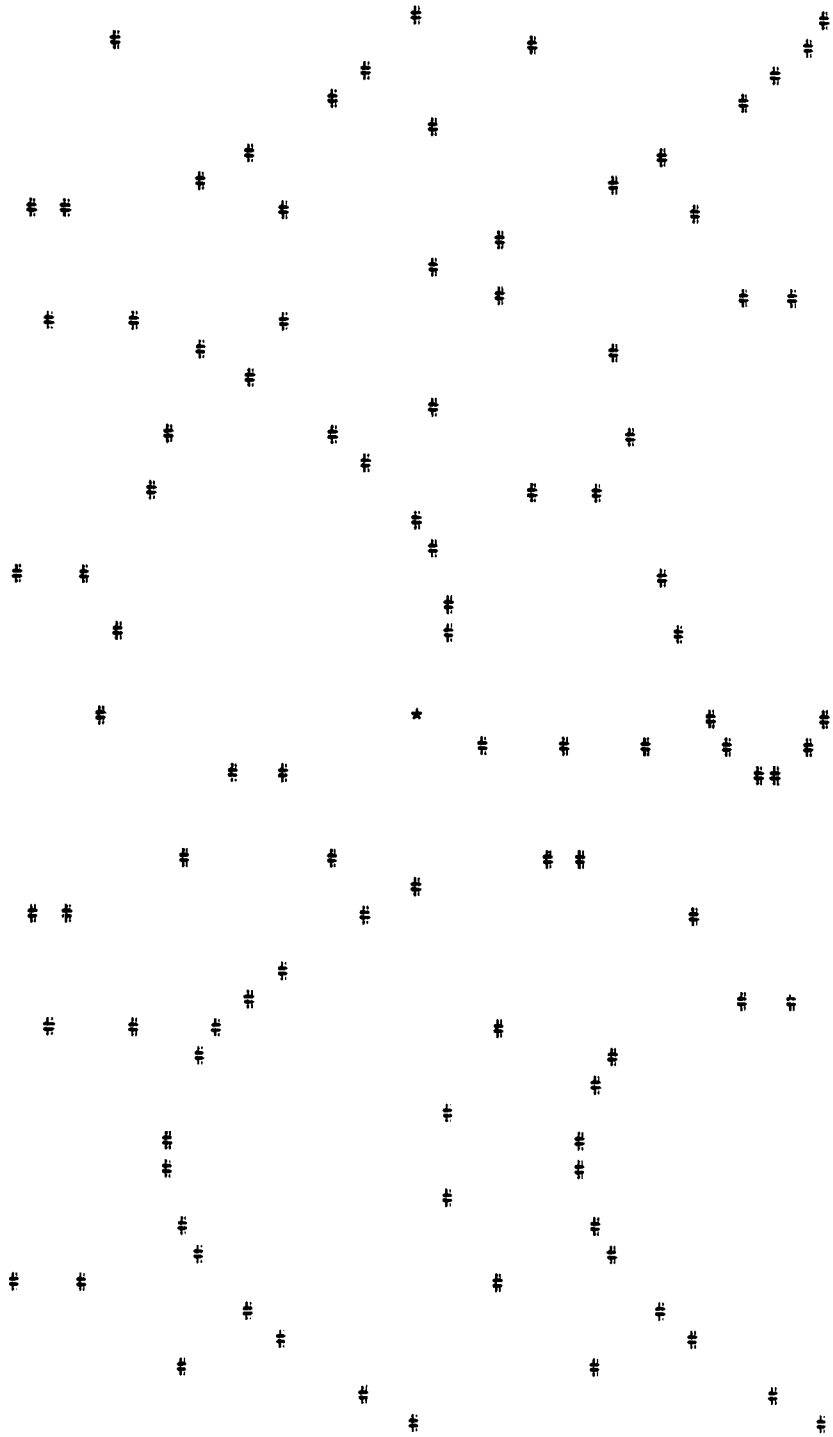

Fig. 10. Performing an interval of 25 spacing; finish printing 25 spiral.

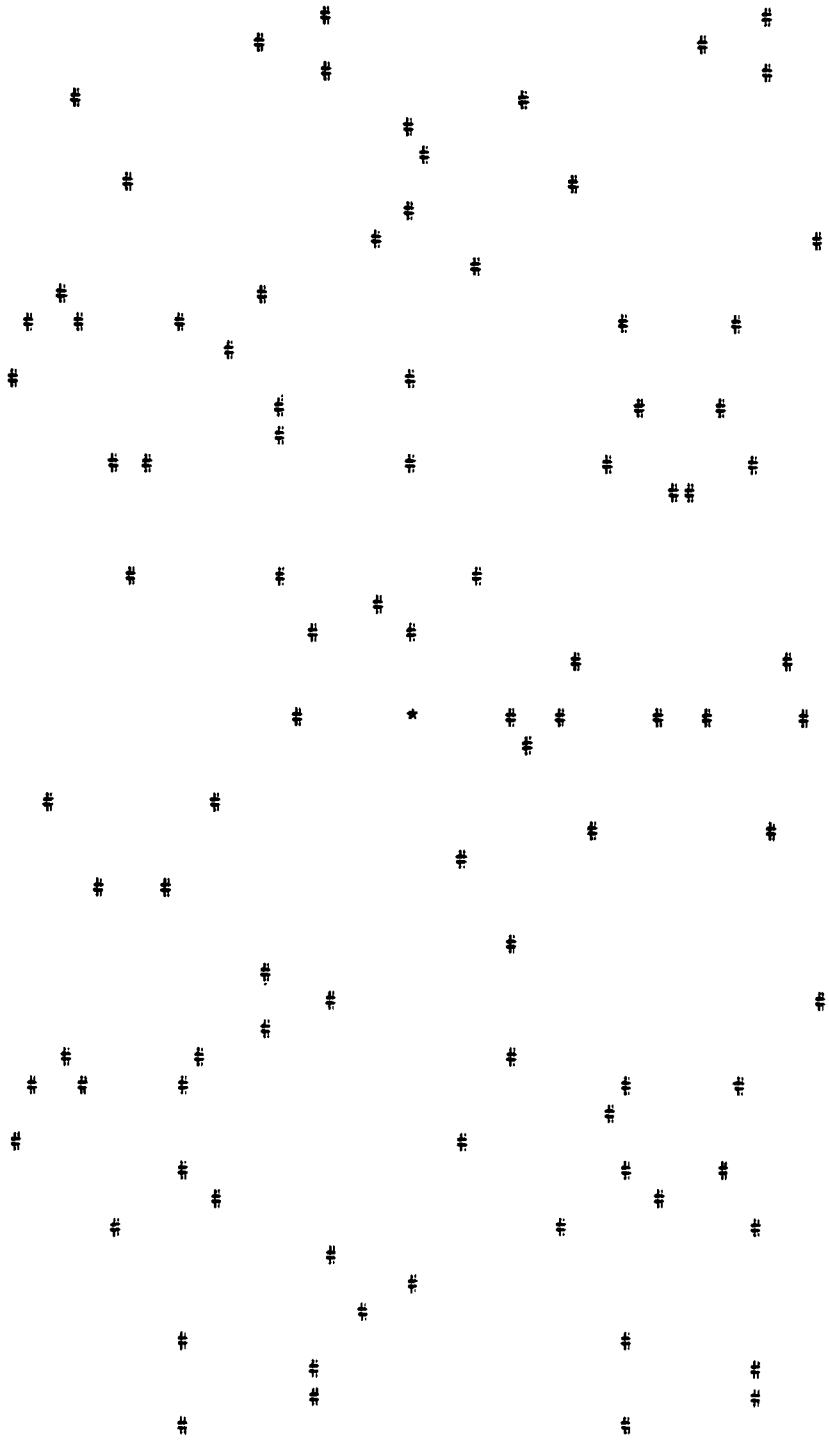

Fig. 11. Performing an interval of 27 spacing; finish printing 27 spiral.

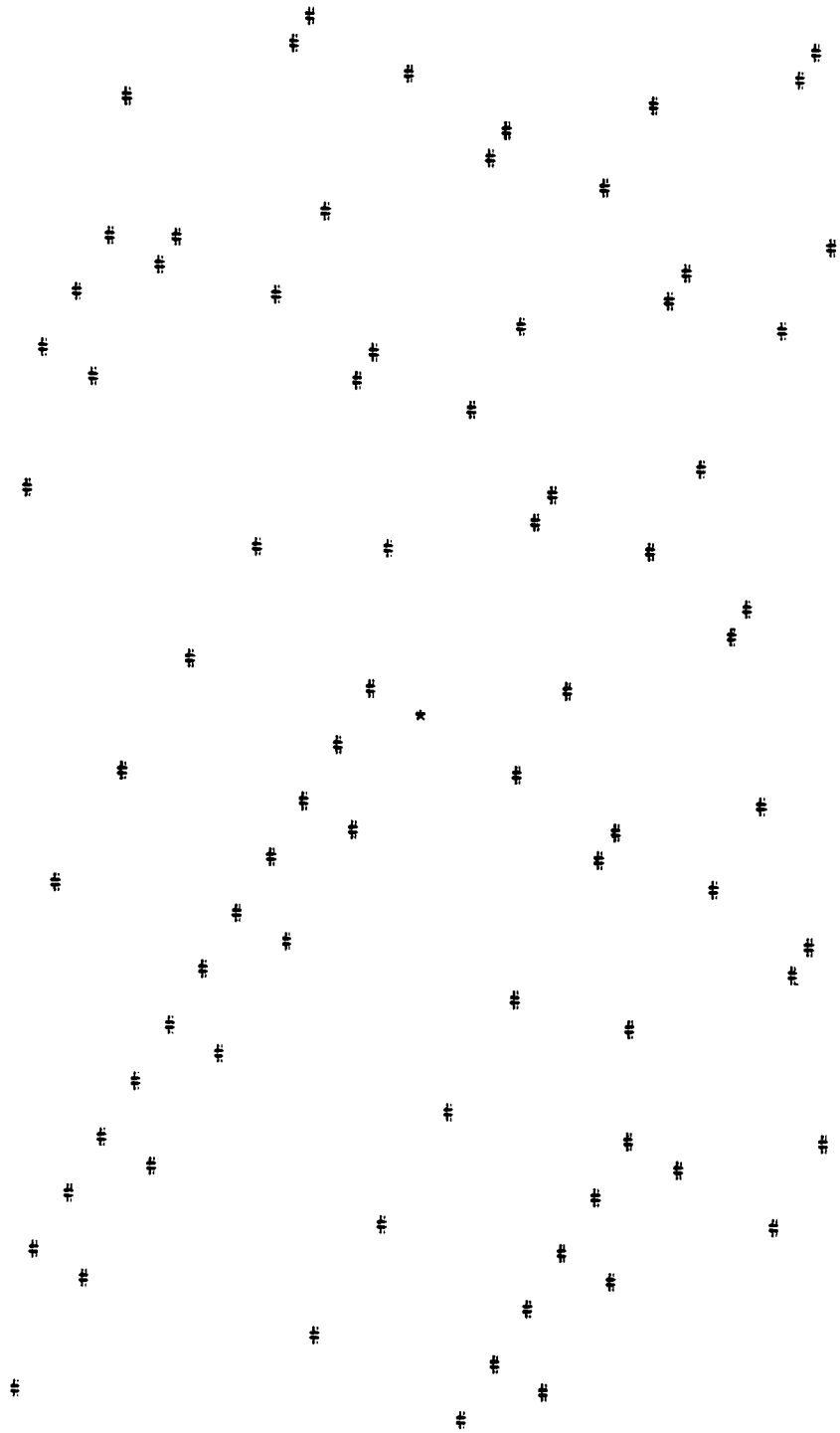

Fig. 12. Performing an interval of 32 spacing; finish printing 32 spiral.

Fig. 13. Performing an interval of 49 spacing; finish printing 49 spiral.

Fig. 14. Performing an interval of 64 spacing; finish printing 64 spiral.

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