

# Ground state energies and configurations of nanoclusters in 2 and 3 dimensions

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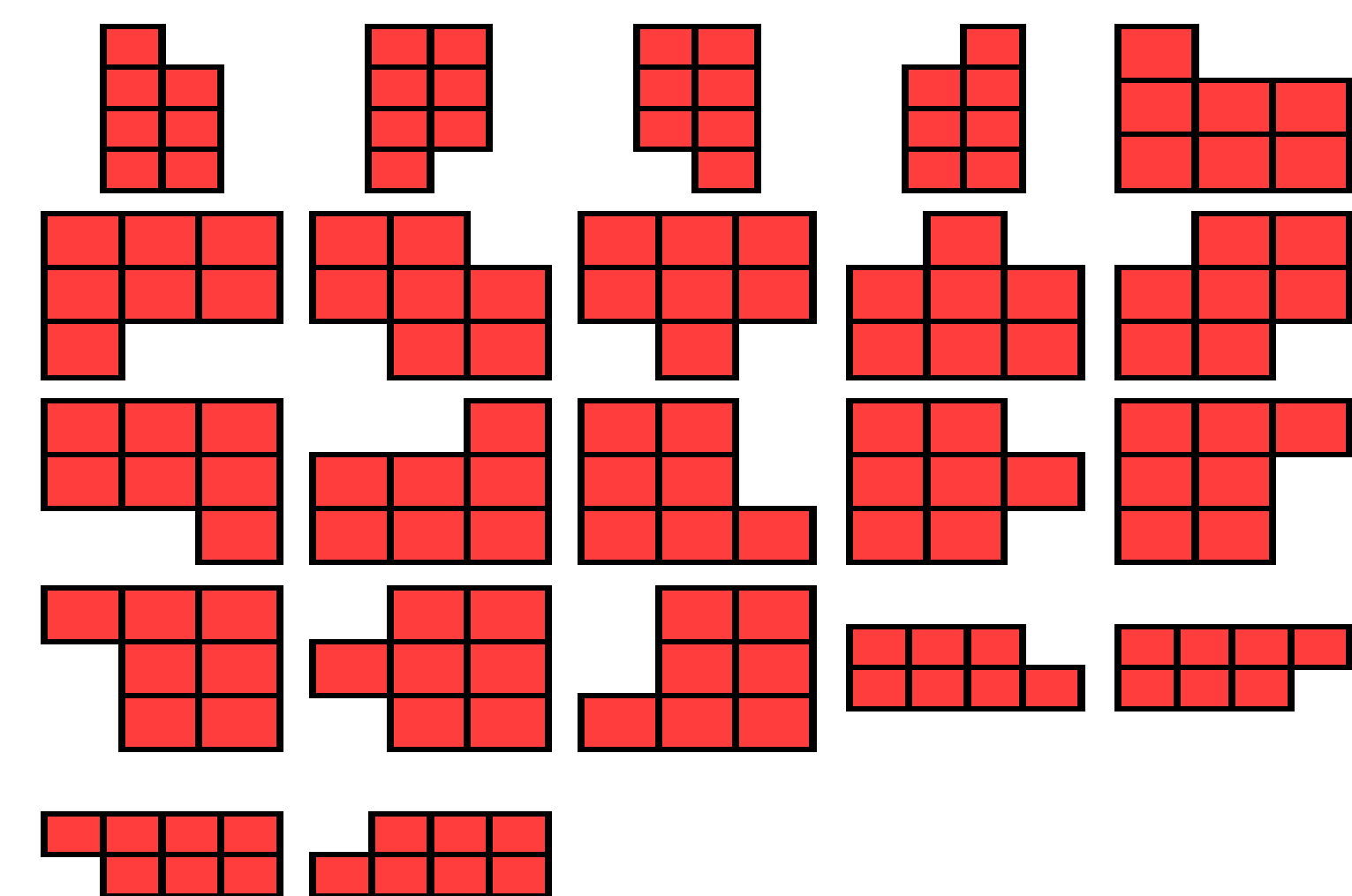
## Introduction

The process of self-assembly of particles into nanoclusters is an open problem in condensed matter physics. The configuration of nanoclusters is determined by thermodynamic consideration. For low temperature, the entropic contribution to the partition function is vanishingly small, and only energetics contributions are at play. Although it is relatively simple to find the ground state energy of such nanoclusters, the number of degenerate states for a given number of particle N had not been understood in a generalized manner.

## Materials and methods

We tackled the problem using a divide and conquer approach. We first investigated the degenerate states in 2 dimensions with particles assembling with 90 degree bonding angles, followed then by a 60 degree bonding angle, and finally 3-dimensional structures in a 90 degree bonding pattern.

To solve the problems we used computer algebra systems as well as programs written in c++ to devise algorithms that enable us to enumerate all possible geometric arrangements for a large set of particles. Our approach is based on the partition and permutation sequence's of the number of particles.



**Figure 1.** Isomers: A cluster of 7 squares can have a maximum 8 contacts. There are 22 isomers with 7 particles.

## Results

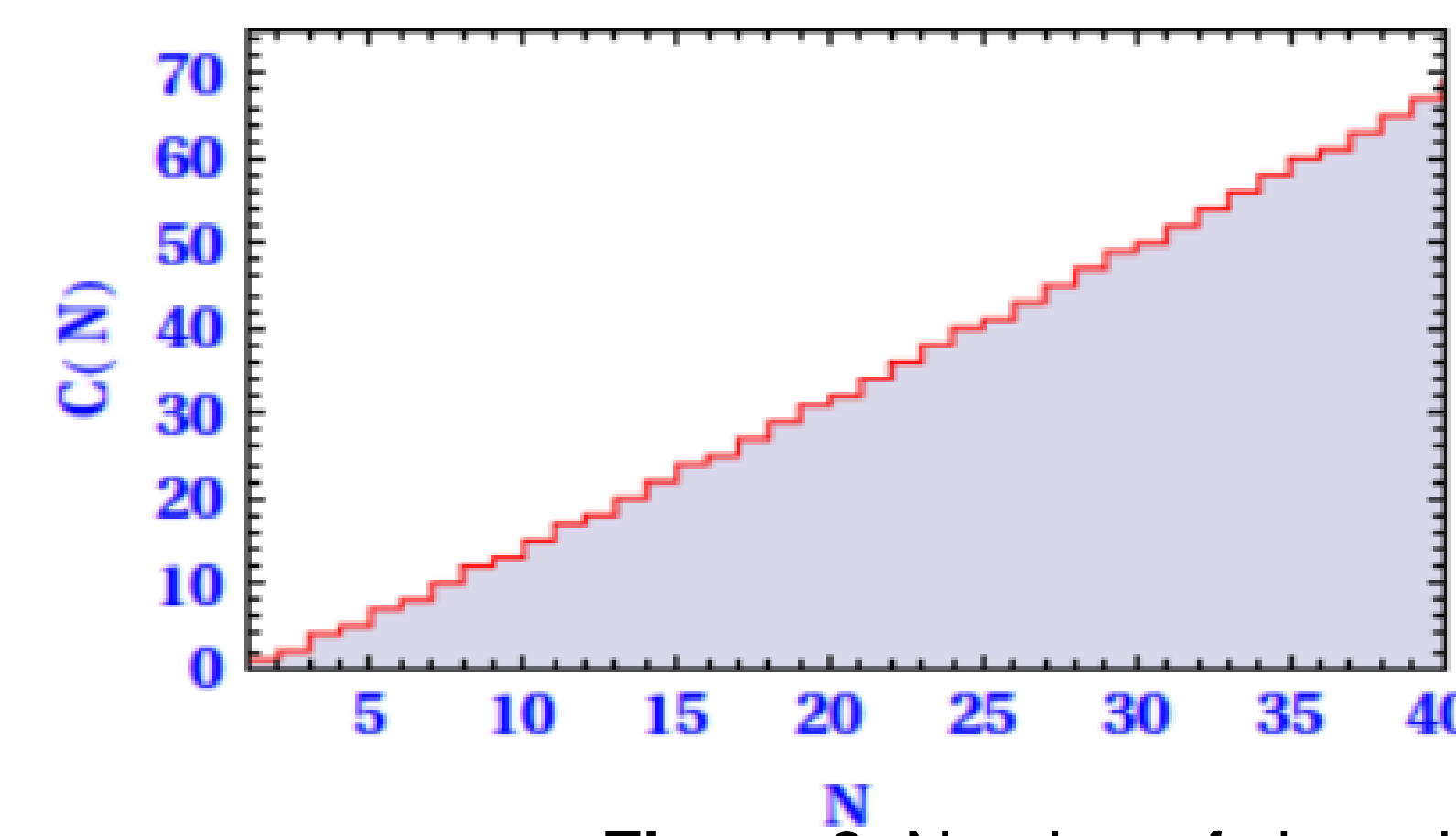
The starting point for our work was to study where square particles were allowed to bond with a 90° angle. Each time there is a shared edge, the overall energy of the nanocluster decreases. With this and defining C as the number of contacts we are able to get the following:

$$C = \frac{1}{2} \sum_i C_i.$$

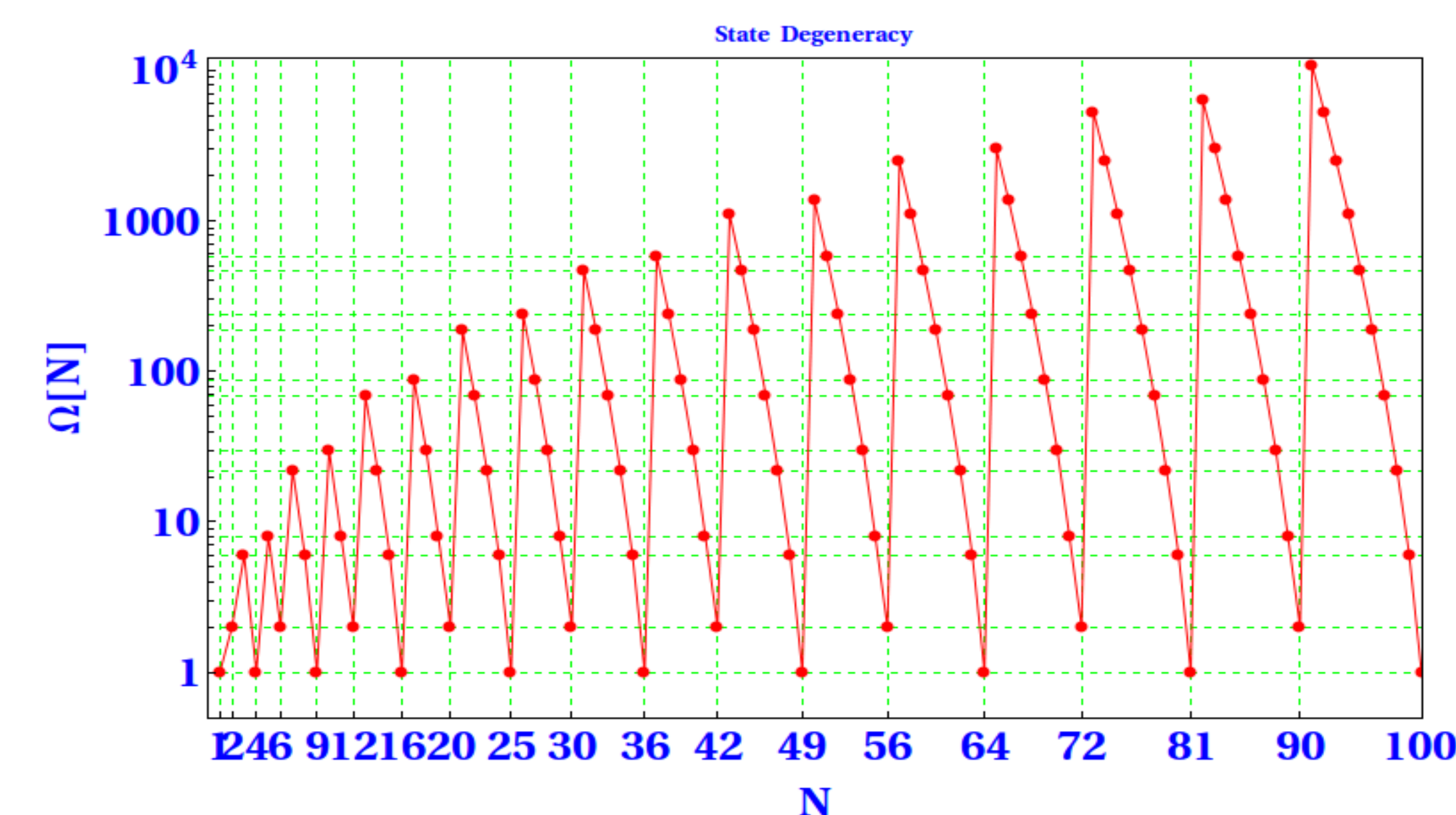
The number of contacts  $C(N)$  for N square particles on a two dimensional lattice is given by the number of shared edges in a spiral of N unit squares as shown in Table I. We would then use the data obtained to figure out ground states that have the same number of contact points as shown in

N	C(N)
1	0
2	1
3	2
4	4
5	5
6	7
7	8
8	10
9	12
10	13
11	15

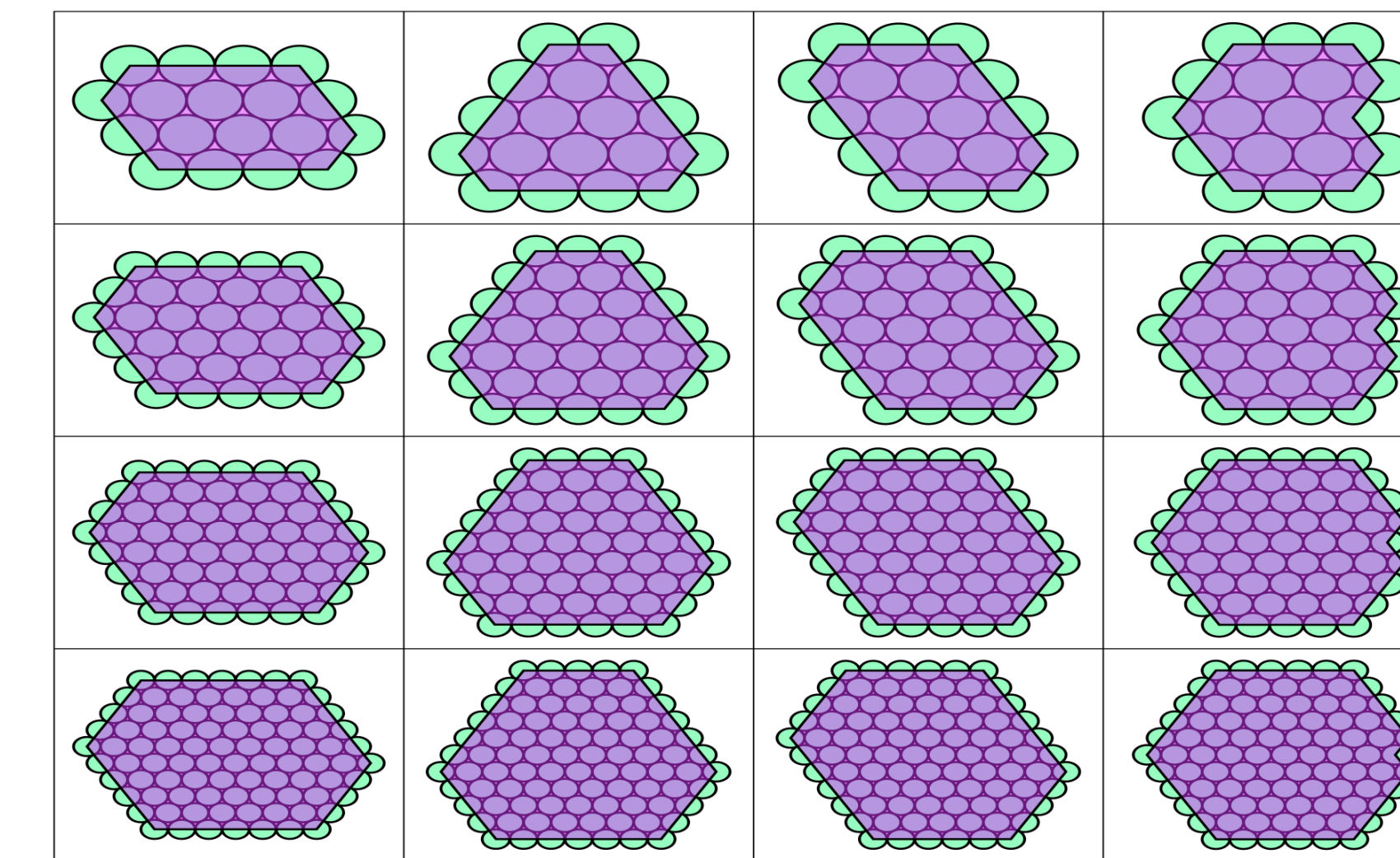
**Table 1.** Maximum number of shared edges  $C(N)$  for square particles ranging for  $N = 1$  to 11



**Figure 2.** Number of shared edges,  $C(N)$  for N square particles bonding at 90°



**Figure 3.** Number of ground states isomers in an N particle cluster using a square lattice.



**Figure 4.** Pattern of some degenerate states formed by building on the outer side of the polygon.

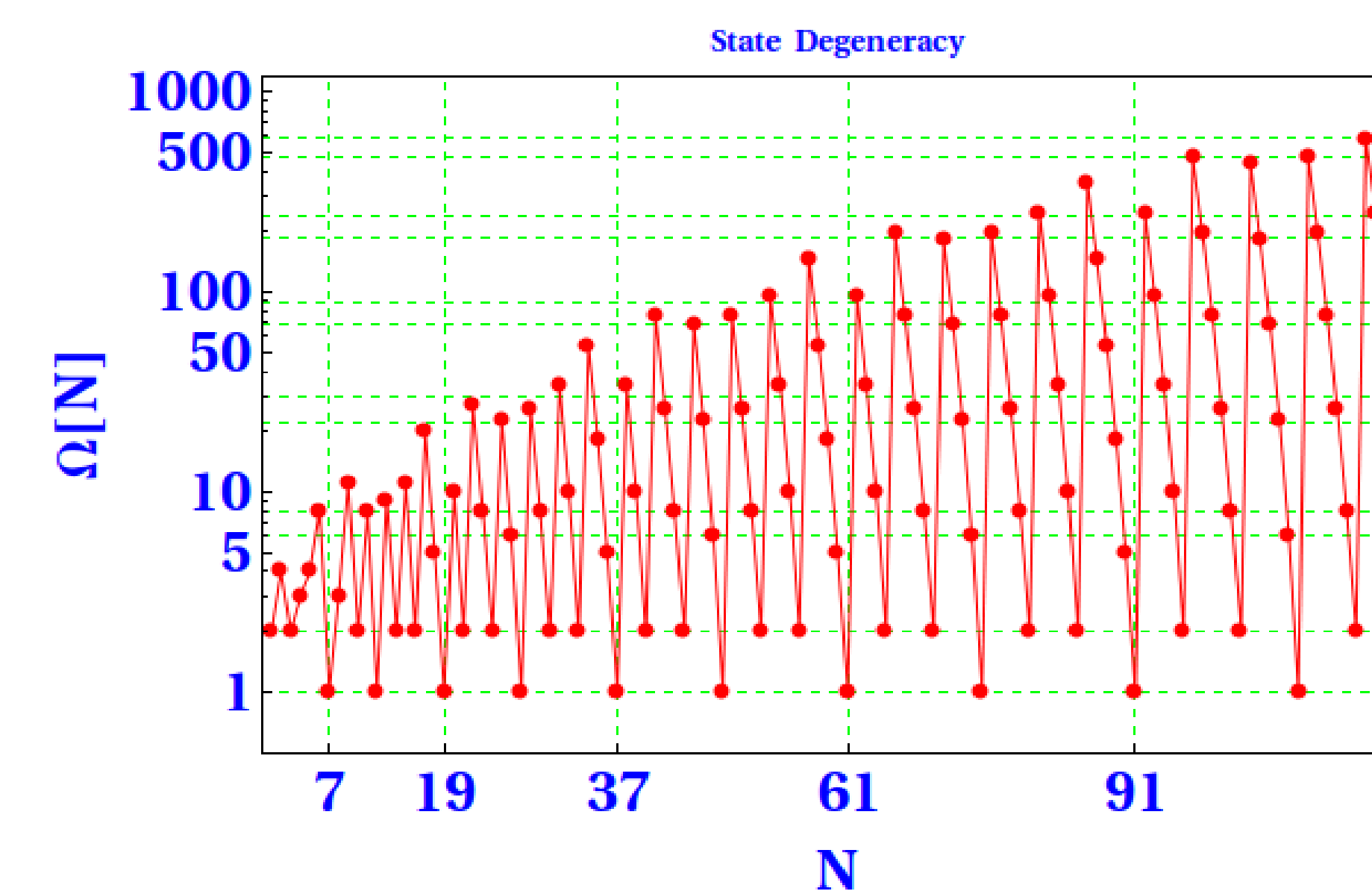
A specific geometric structure, which has the maximum number of bonds for N particles, repeats itself by adding one more layer of circles. But as N gets large the number of these geometric structures gets much higher. Figure 4 shows some of the structures that repeat as N gets larger down the column.

We found the number of contact points to be the following:

$$C(N) = 3N - P(N) - 6 * (1/2)$$

This can also be found from the OEIS sequence A047932.

The number of configurations that share a maximum number of bonds for a given number of disk particles is generally larger than one. There are two ways that we can count configurations: (a) count as similar all configurations that can be obtained by uniform vector translation. (b) count all configurations as similar if they can be obtained through a rotation operation. The number of configuration under the first scheme is given in table V. The Figure 5 shows the degeneracy up to  $N = 120$ , taking into account the translation and rotation operations.



**Figure 5.** Number of ground state isomers in a N particle cluster using a hexagonal lattice.

## Conclusions

In conclusion, we have been able to enumerate isomers for square particles and disk particles for  $N < 120$ . In the case of square particles, we have been able to determine the analytic formula for the degeneracy for all N. For disk particles, there still needs to be further development for an analytic formula to be derived. For future work, we would like to apply a similar analysis to spherical particles with contact interaction as well as find the formula for disk particles. The next step for this research will be to develop our analysis and tactics to move into the third dimension and how these nanoclusters form in nature.

## Literature cited

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## For further information

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