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 energetic 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 than 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.

Results
The starting point for our work was to study where square particles were allowed to bond with a 90-degree 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:

\[ C = \frac{1}{2} \sum \frac{N}{N} \]

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 than use the data obtained to figure out ground states that have the same number of contact points as shown in a generalized manner.

![Figure 1. Isomers: A cluster of 7 squares can have a maximum 8 contacts. There are 22 isomers with 7 particles.](image1)

![Figure 2. Number of shared edges, C(N) for N square particles bonding at 90°.](image2)

![Figure 3. Number of ground state isomers in an N particle cluster using a square lattice.](image3)

![Figure 4. Pattern of some degenerate states formed by building on the outer side of the polygon.](image4)

![Figure 5. Number of ground state isomers in a N particle cluster using a hexagonal lattice.](image5)

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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![Table 1. Maximum number of shared edges C(N) for square particles ranging for N = 1 to 11](image6)