An isoperimetric approach to the Heitmann-Radin crystallization

We discuss a simple model for finite crystallization in the case of zero temperature, short range pairwise interactions and two dimensions.

For any fixed $N \in \mathbb{N}$, we aim at characterizing the ground states of the Heitmann-Radin energy defined by

$$\mathcal{E}(\{p_1, \dots, p_N\}) := \sum_{i<j} J(|p_i - p_j|) \quad (\{p_1, \dots, p_N\} \subset \mathbb{R}^2),$$

where $J(1) = -1$, $J(t) = 0$ for $t > 1$ and $J(t) = +\infty$ for $t < 1$.

We will see that for any configuration $V_N = \{p_1, \dots, p_N\}$, the energy decomposes as

$$\mathcal{E}(V_N) = \text{bulk} + \text{surface}(V_N) + \text{defect}(V_N),$$

where the bulk is proportional to N (and independent of V_N), the surface term is the *outer perimeter* of the nearest neighbour graph generated by V_N, and the defect term is an *inner perimeter*, measuring how much this graph differs from a subset of the triangular lattice. In virtue of the decomposition above, in order to find the minimizers of $\mathcal{E}$, it is enough to minimize the sum between the inner and the outer perimeter. Following this strategy, we will prove that the minimizers of $\mathcal{E}$ are all the subsets of the triangular lattice minimizing the outer perimeter. We will give a characterization of such minimizers, providing all the uniqueness cases.

This is a joint work with Gero Friesecke (TU München).