Effect of Periodic Arrays of Defects on Lattice Energy Minimizers

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In this talk, I will consider interaction energies $E_f[L]$ between a point $O \in \mathbb{R}^d$, $d \geq 2$, and a lattice L containing O, where the interaction potential f is assumed to be radially symmetric and decaying sufficiently fast at infinity. The idea is to investigate the conservation of optimality results for E_f when integer sublattices kL are removed (periodic arrays of vacancies) or substituted (periodic arrays of substitutional defects). In particular, I will consider separately the non-shifted ($O \in kL$) and shifted ($O \notin kL$) cases and I will present several general conditions ensuring the (non-)optimality of a universal optimizer among lattices for the new energy including defects. Furthermore, in the case of inverse power laws and Lennard-Jones type potentials, I will present necessary and sufficient conditions on non-shifted periodic vacancies or substitutional defects for the conservation of minimality results at fixed density. Different examples of applications will be presented, including optimality results for the Kagome lattice and energy comparisons of certain ionic-like structures. This work can be read more in details in [1].

References

[1] L. Bétermin. Effect of periodic arrays of defects on lattice energy minimizers. *Annales Henri Poincaré*, 22:2995-3023, 2021.