# Supercell calculations for the simulation of crystals without/with defects

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**Abstract**: A crystal is mathematically modeled by a periodic Hamiltonian acting on the whole space. In order to compute numerically the properties of such a system, an approximation must be done. One of the most natural approximation consists into studying the Hamiltonian on a supercell, i.e. a box containing $L$ times the periodicity of the crystal, with periodic boundary conditions.

The purpose of this talk is to prove that the error made with this approximation is exponentially small with respect to $L$ if the crystal is perfect. We then consider the case when a local defect is present in the crystal. In this case, the error is of order $L^{-1}$. However, it is possible to identify and correct the main contribution of the error to improve the speed of convergence to the order $L^{-3}$.