Convergence of the supercell model for quantum crystals

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In this talk, we consider quantum crystals in the reduced Hartree-Fock (rHF) framework. The nuclei are supposed to be classical particles. We consider two types of crystals. The first ones are perfect crystals, where the nuclei are arraged according to a periodic lattice. The second one are crystals with local defects, where the nuclear distribution is of the form

$$\mu = \mu_{\text{per}} + \nu, \tag{1}$$

where μ_{per} is a periodic nuclear distribution corresponding to a reference perfect crystal and ν represents the defect. We assume that μ decays at infinity (see Figure 1).

Figure 1: Perfect crystals and crystals with local defects.

A good numerical approximation of these materials is obtained using the supercell model. It consists in restricting the system to a box of (large) finite size with periodic boundary conditions. For perfect crystals, we prove in [1] that the supercell model converges to the whole space model exponentially, when the size of the supercell goes to infinity. For crystals with local defects, we prove in [2] that the defect energy admits an expansion of the form

$$\mathcal{F}^{\nu} \simeq \mathcal{F}_L^{\nu} + \frac{a}{L} + O\left(\frac{1}{L^3}\right).$$

when the defect is small. The coefficient a can be computed using the supercell calculation. The convergence is thus accelerated to the order L^{-3} without any additional computational cost.

References

[1] D. Gontier and S. Lahbabi. Convergence rates of supercell calculations in the reduced Hartree-Fock model. *M2AN*, pages 1403–1424, 2015.

[2] D. Gontier and S. Lahbabi. Supercell calculations in the reduced hartree-fock model for crystals with local defects. *Appl. Math. Res. Express*, pages 1–64, 2016.