

On linear stability of crystals in the Schrödinger-Poisson model

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Abstract. Crystals are modeled by the Schrödinger–Poisson–Newton equations. The ground state for crystals in \mathbb{R}^3 with 1D, 2D and 3D lattices [1] and N ions per cell is shown to exist. Crystals with 1D lattice is a model of the carbon tube, while the case of 2D lattice corresponds to the graphene.

Second, we consider the Schrödinger–Poisson–Newton equations for crystals with a cubic lattice and one ion per cell, linearized at the ground state [4]. Our key result is the *energy positivity* for the Bloch generators of the linearized equations with small elementary charge $e > 0$ under a novel Wiener-type condition on the ion charge density. The proof relies i) on a suitable factorization of the Hamilton functional, ii) on the asymptotics of the ground state as $e \rightarrow 0$, and iii) on calculation of the energy bifurcation at small quasimomenta. Using these arguments, we show that the minimal zero energy of the Bloch generators, corresponding to $e = 0$, bifurcates into positive eigenvalues $\sim e^2$ for all nonzero quasimomenta except for a Lebesgue nullset.

These Bloch generators are nonselfadjoint (and even nonsymmetric) Hamilton operators. We diagonalize these generators applying our theory of spectral resolution of the Hamilton operators *with positive definite energy* [2, 3], which is an infinite-dimensional version of some Gohberg and Krein ideas from the theory of parametric resonance. Using this spectral resolution, we establish the stability of the linearized dynamics for crystals in the case of small $e > 0$.

References

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