Mathematics > Numerical Analysis

A Bloch decomposition based split-step pseudo spectral method for quantum dynamics with periodic potentials

Zhongyi Huang, Shi Jin, Peter Markowich, Christof Sparber

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We present a new numerical method for accurate computations of solutions to (linear) one dimensional Schr\"odinger equations with periodic potentials. This is a prominent model in solid state physics where we also allow for perturbations by non-periodic potentials describing external electric fields. Our approach is based on the classical Bloch decomposition method which allows to diagonalize the periodic part of the Hamiltonian operator. Hence, the dominant effects from dispersion and periodic lattice potential are computed together, while the non-periodic potential acts only as a perturbation. Because the split-step communicator error between the periodic and non-periodic parts is relatively small, the step size can be chosen substantially larger than for the traditional splitting of the dispersion and potential operators. Indeed it is shown by the given examples, that our method is unconditionally stable and more efficient than the traditional split-step pseudo spectral schemes. To this end a particular focus is on the semiclassical regime, where the new algorithm naturally incorporates the adiabatic splitting of slow and fast degrees of freedom.

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