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AMG eigenbasis solver for the Schrödinger eigenvalue problem

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In this talk the AMG algorithm for solving the Scrödinger eigenvalue problem is discussed. Its goal is to approximate the eigenbasis, i.e., all eigenfunctions, of the Schrödinger operator as it appears in the Kohn-Sham equation.

The algorithm employs multilevel eigenvalues/eigenfunction representations that allows approximation of most of the eigenfunctions on the inexpensive coarse grids and leads to a reduction of both computational and storage costs. In addition this structure is beneficial for performance of a variety of applications essential to the Kohn-Sham equations. Also addressed is the issue of quality of the obtained sets of eigenfunctions, such as their accuracy and independence. Numerical results and discussion of the further extension of the approach will conclude the talk.