

Scalable block-tridiagonal eigensolvers in the context of electronic structure calculations

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Abstract. In computer-based numerical simulations, some methods to determine the electronic and optical properties of semiconductor nanostructures, require computing the energies that correspond to the interior eigenvalues of a Hamiltonian matrix. We study the case in which the Schrödinger equation is expanded into a matrix that has a block-tridiagonal structure. Additionally, the matrix can have two extra non zero blocks in the corners due to periodic boundary conditions. Given that not the whole eigenspectrum is required, we choose to use projection methods to compute the necessary set of eigenvalues. The shift-and-invert Lanczos method requires to solve a linear system at each iteration. We have developed a parallel code that improves the scalability of this step by exploiting the block structure. Results show that, to solve these specific cases, this method offers better scalability when compared to a general-purpose solver such as MUMPS.

Keywords. electronic structure calculation, eigenvalue problem, shift-and-invert, cyclic reduction, Schur complement

1. Introduction and motivation

There is an increasing interest in methods that can provide an accurate picture of the electronic structure of large systems. This kind of computations allows the design of new devices that are essential for many emerging technologies.

In order to understand the electronic and optical properties of semiconductor hetero and nanostructures, it is imperative to know the allowed energy levels for electrons and their quantum state, completely determined by their corresponding wavefunctions. These quantities are provided by the Schrödinger equation, a linear partial differential equation (PDE) which, in its single particle (an electron from now on) time-independent version, reads

$$\hat{H}\psi(\mathbf{r}) = \left[-\frac{\hbar^2}{2m_0}\nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}), \quad (1)$$