Calculation of Selected Eigenvalues using a Jacobi-Davidson Solver[1]

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There are many materials physics problems that require knowledge of only some select eigenvalues and corresponding eigenvectors of the system Hamiltonian. To this end, Wang and Zunger[2] developed a "folded spectrum (FS)" method which scales linearly with system size rather than the usual cubic scaling required by traditional matrix diagonalization techniques. Using Hamiltonians constructed from semi-empirical pseudopotentials, the above authors have successfully applied the technique to a number of interesting problems including the calculation of the dielectric properties of quantum dots[3], variation of the band gap with quantum dot size[2], and the solution of the "inverse band-structure problem"[4]. In all of these cases only a relatively small fraction of the total number of eigensolutions of the Schrödinger equation are determined around a specific energy.

We present an alternative approach using a Jacobi-Davidson[5] technique that does not require "squaring" the Hamiltonian operator as in the FS method but solves the eigenvalue equation directly. The "squaring" of the Hamiltonian operator in the FS method greatly increases the difficulty in solving the original eigenvalue equation. The FS method can, in principle, be extended to generalized eigenvalue problems but at the cost of a significant increase in solving difficulty over the standard FS method. The novel technique we propose does not suffer from either of these problems and can easily be extended to generalized eigenvalue problems as in the projector augmented wave (PAW) method[6].

A few example calculations will be presented using both the PAW method and empirical pseudopotentials.

[1]This work was supported by NSF grants DMR-9403009 and DMR-9706575 and SUR grant from IBM.
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