

The computation of a large number nev of eigenvalues and eigenvectors of the Hamiltonian is still an outstanding problem.

Preconditioners through Davidson methods helpful only for a few tens of lowest eigenvalues.

Orthogonalization is the limiting factor of classical Davidson methods.

We have developed theory and software based on an unpreconditioned, dynamic inner-outer Jacobi-Davidson. We call it JDQMR.

Pros: No orthogonalization against converged eigenvalues during inner steps.
Scales almost linearly with nev (not nev^2)

Cons: Convergence deteriorates for interior eigenvalues, **but very slowly**

100 lowest evals of ∇^2	Davidson (no precondition)	ARPACK	JDQMR
Matrix-vector products	51673	4612	60462
Time (sec)	1533	826	237

