Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky (Texas), Yousef Saad and Renata Wentzcovitch (Minnesota), Steven Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR- 0551195): Unrestarted Lanczos diagonalization with limited memory

Without preconditioning, the Lanczos algorithm provides optimal eigenvalue and eigenvector approximations from the Krylov space:

$$\{v_0, Av_0, \ldots, A^k v_0\}$$

In practice, the Lanczos method is restarted every *m* steps because:
(a) storing all *k* iteration vectors requires too much memory
(b) implicit orthogonality is lost after many iterations.
Restarts cause loss of optimality and slower convergence. In the past we have developed methods (GD+k and JDQMR) that converge nearly optimal (i.e., similar to unrestarted Lanczos) for one eigenvalue. However, this cost had to be repeated for each eigenvalue sought in the diagonalization of the Kohn-Sham equation. Workers at the Institute have developed a method that during the *unrestarted Lanczos iteration* it keeps track of the lowest *nev* eigenpairs through a recursive, CG-like formula

$$u_{1:nev}^{(i+1)} = \mathrm{RayleighRitz}\left(\{u_{1:nev}^{(i-1)}, u_{1:nev}^{(i)}, g^{(i)}\}\right),\ i > 1,$$

where $g^{(i)}$ are the *m* recent Lanczos vectors, and *i* the update index.

- **For large enough nev convergence of unrestarted Lanczos achieved!**
- **Optimal convergence for all nev eigenvalues**
- **Loss of orthogonalization easily corrected**