Low-energy structures

Lanczos method + conjugate gradient (CG) method
[Conventional exact diagonalization (ex. TITPACK)]

Lanczos[eigenvalues,2 vectors] → Lanczos[eigenvectors,3 vectors] → Inverted iteration [5 vectors]

[merit] Only two vectors are necessary
[demerit] Redundant, *Failure* of orthogonality, degeneracy, etc…

Locally Optimal (Preconditioning) Block Conjugate [LO(P)BCG]

A. V. Knyazev, SIAM J. Sci. Compute. 23, 517 (2001)

Eigenvectors $\{|\Phi_0\rangle, |\Phi_1\rangle, \cdots, |\Phi_{M-1}\rangle\}$
residual vectors $\{|r_i\rangle = H|\Phi_i\rangle - \epsilon_i|\Phi_i\rangle\}$
conjugate gradient vectors $\{|p_0\rangle, |p_1\rangle, \cdots, |p_{M-1}\rangle\}$

Diagonalize & Optimize with 3M vectors

[merit]
- Obtaining many low-energy states at once
- Degeneracy & orthogonality can be well reproduced
[demerit] Required memory is slightly larger (~3M-6M vectors)