

The first excited state should be doubly-degenerate

➤ Lanczos only gives one state out of a degenerate multiplet

Go back to the Krylov space

$$H^m |\Psi\rangle = \sum_k C_k E_k^m |\Psi_k\rangle$$

If states k, j are degenerate, we have a term

$$E_j^m (C_j |\Psi_j\rangle + C_k |\Psi_k\rangle)$$

For any m, this vector points in the same direction in the subspace spanned by  $|\Psi_j\rangle, |\Psi_k\rangle$

Acting with H cannot “separate” degenerate states

Since the Lanczos basis spans the same Krylov space, we only get one state out of a degenerate multiplet of states

➤ the particular linear combination depends on the initial state

Numerical round-off errors can lead to apparent degeneracies (multiple copies of the same state). This indicates that the scheme breaks down as the basis becomes non-orthogonal.

Following last Friday's discussion, we went through the program "random" in detail. Please read the commented code and explore what it's doing.