Optional homework #1

(1) Study and summarize Davidson's algorithm of determining the few lowest eigenvalues of a large matrix. Why is it essential for the matrix to be diagonally dominant for this algorithm to work well?

E. R. Davidson, J. Comput. Phys. **17**, 87 (1975).

(2) Study and summarize the DMRG algorithm of determining the lowest eigenvalue of an even larger matrix than (1)? What is the structure of the Hamiltonian matrix in a "one-dimensional" system treatable by it? How does its sweep algorithm take advantage of that structure? How will the Hamiltonian matrices look in two- and three-dimensional systems?

Y. Kurashige and T. Yanai, J. Chem. Phys. **130**, 234114 (2009).