Blog Entry © Wednesday, September 3, 2025, by James Pate Williams, Jr. Solution of Exercise 1.11 in ***Quantum Chemistry an Introduction to Advanced Electronic Structure Theory*** © 1996 by Attila Szabo and Neil S. Ostlund

Exercise 1.11 Find the eigenvalues and eigenvectors of the following two matrices by the secular determinant method and the unitary diagonalization method.

$$A = \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix} \; and \; B = \begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix}$$

$$|A - \omega I| = \begin{vmatrix} 3-\omega & 1 \\ 1 & 3-\omega \end{vmatrix} = (3-\omega)^2 - 1 = 9 - 6\omega + \omega^2 - 1 = \omega^2 - 6\omega + 8 = 0$$

By the quadratic formula we have:

$$\omega = \frac{6 \pm \sqrt{36 - 32}}{2} = \frac{6 \pm \sqrt{4}}{2} = \frac{6 \pm 2}{2} = 3 \pm 1$$

$$\omega_1 = 3 - 1 = 2$$

$$\omega_2 = 3 + 1 = 4$$

The second eigenvector is as follows:

$$3a + b = 4a$$

$$b = a$$

$$a^2 + a^2 = 1$$

$$2a^2 = 1$$

$$a = b = \frac{1}{\sqrt{2}}$$

The first eigenvector is found to be:

$$3a + b = 2a$$

$$a = -b$$

$$a^2 + a^2 = 1$$

$$a = \frac{1}{\sqrt{2}}$$

$$b = -a = -\frac{1}{\sqrt{2}}$$

$$|B - \omega I| = \begin{vmatrix} 3-\omega & 1 \\ 1 & 2-\omega \end{vmatrix} = (3-\omega)(2-\omega) - 1 = \omega^2 - 5\omega + 6 - 1 = \omega^2 - 5\omega + 5$$

$$\omega = \frac{-5 \pm \sqrt{25 - 20}}{2} = \frac{-5 \pm \sqrt{5}}{2}$$