[2x2] Matrix

$H\psi = E\psi$ $\quad$ ψ to be expanded in terms of φ_1 and φ_2
with $\langle \varphi_i | \varphi_j \rangle = \delta_{ij}$ (orthonormal)

$$\rightarrow \psi = \alpha\varphi_1 + \beta\varphi_2 .$$

$*$ $H\psi = H(\alpha\varphi_1 + \beta\varphi_2) = H\varphi_1 \cdot \alpha + H\varphi_2 \cdot \beta .$

$**$ $E\psi = E(\alpha\varphi_1 + \beta\varphi_2) = E\varphi_1 \cdot \alpha + E\varphi_2 \cdot \beta .$

$*$ $\langle \varphi_1 | H | \psi \rangle = \langle \varphi_1 | H | \varphi_1 \rangle \cdot \alpha + \langle \varphi_1 | H | \varphi_2 \rangle \cdot \beta \equiv H_{11} \cdot \alpha + H_{12} \cdot \beta$

$*$ $\langle \varphi_2 | H | \psi \rangle = \langle \varphi_2 | H | \varphi_1 \rangle \cdot \alpha + \langle \varphi_2 | H | \varphi_2 \rangle \cdot \beta \equiv H_{21} \cdot \alpha + H_{22} \cdot \beta$

$**$ $\langle \varphi_1 | E | \psi \rangle = \langle \varphi_1 | E | \varphi_1 \rangle \cdot \alpha + \langle \varphi_1 | E | \varphi_2 \rangle \cdot \beta = E\alpha + 0 \cdot \beta = E\alpha$

$**$ $\langle \varphi_2 | E | \psi \rangle = \langle \varphi_2 | E | \varphi_1 \rangle \cdot \alpha + \langle \varphi_2 | E | \varphi_2 \rangle \cdot \beta = 0 \cdot \alpha + E\beta = E\beta .$

$$H\psi = E\psi \quad \longleftrightarrow \quad \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

Two solutions: $\psi_1 = \alpha_{11}\varphi_1 + \alpha_{12}\varphi_2$ with energy E_1
$\psi_2 = \alpha_{21}\varphi_1 + \alpha_{22}\varphi_2$ with energy E_2 .

Diagonalization routine:

Input: $\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \equiv \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}$

Output $\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \equiv \begin{bmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \end{bmatrix}$ $\quad$ (note: mirrored!)

$\begin{bmatrix} R_1 & R_2 \end{bmatrix} \equiv \begin{bmatrix} E_1 & E_2 \end{bmatrix}$