

Essentially we use the Rayleigh-Ritz method

$$\psi = \sum_{i=1}^2 c_i f_i$$

The variational upper bounds to the energies, E , and the corresponding approximate wave functions (defined by $\{c_i\}$) are found by solving the generalized eigenvalue problem

$$Hc = \epsilon Sc$$

In our case

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 1 & 4 \end{pmatrix}$$

$$S = \begin{pmatrix} S_{11} & S_{21} \\ S_{12} & S_{22} \end{pmatrix} = \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix}$$

The resulting secular equation $\det(H - \epsilon S) = 0$ yields:

$$\begin{vmatrix} 2 - \epsilon & 1 - \frac{1}{2}\epsilon \\ 1 - \frac{1}{2}\epsilon & 4 - \epsilon \end{vmatrix} = (2 - \epsilon)(4 - \epsilon) - (1 - \frac{1}{2}\epsilon)^2 = \frac{3}{4}\epsilon^2 + 5\epsilon + 7 = 0$$
$$\epsilon_{1,2} = \frac{5 \pm \sqrt{25 - 21}}{2 \cdot \frac{3}{4}} = 2, \frac{14}{3}$$

The smaller of the two ϵ 's correspond to the ground state. Hence the upper bound to the ground state energy is

$$\epsilon = 2 \quad (\text{in the same units as matrix elements } \langle f_i | H | f_j \rangle \text{ are given})$$