Extension of variation principle

- Already solved variational problem with N basis functions:

H_{aa}= NxN hamiltonian matrix

$U\ H_{aa} U^{\dagger} = h_{aa}$= diagonal matrix with eigenvalues h_n, n=1,2…N

- Add one more basis function

⇨

->new (N+1)x(N+1) hamiltonian matrix

- $\mathbf{H_{ab}}$= Nx1 matrix of hamiltonian connecting each old basis function {a} to new one {b}
- $\mathbf{H_{ba}}$= $(\mathbf{H_{ab}})^{\dagger}$=1xN matrix connecting old to new
- $\mathbf{c_a}$= 1st N components of eigenvector
- c_b= N+1st eigenvector component

New eigenvalue problem to be solved:

$$\begin{pmatrix} \mathbf{H}_{\mathbf{aa}} - E\mathbf{1}_{\mathbf{aa}} & \mathbf{H}_{\mathbf{ab}} \\ \mathbf{H}_{\mathbf{ba}} & \mathrm{H}_{\mathrm{bb}} - E \end{pmatrix} \begin{pmatrix} \mathbf{c}_{\mathbf{a}} \\ \mathrm{c}_{\mathrm{b}} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix}$$

Define **W** by $$\mathbf{W} = \begin{pmatrix} \mathbf{U} & \mathbf{0} \\ \mathbf{0}^{\dagger} & 1 \end{pmatrix}$$

Ext-var4

Multiply eq. (1) from the left by **W** and insert $\mathbf{W}^\dagger\mathbf{W} = \mathbf{1}_{(N+1)\times(N+1)}$

$$\mathbf{W}\begin{pmatrix} \mathbf{H_{aa}} - E\mathbf{1_{aa}} & \mathbf{H_{ab}} \\ \mathbf{H_{ba}} & \mathrm{H_{bb}} - E \end{pmatrix}\left(\mathbf{W}^\dagger\mathbf{W}\right)\begin{pmatrix} \mathbf{c_a} \\ \mathrm{c_b} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix}$$

This gives $\begin{pmatrix} \mathbf{h_{aa}} - E\mathbf{1_{aa}} & \mathbf{V_{ab}} \\ \mathbf{V_{ba}} & \mathrm{H_{bb}} - E \end{pmatrix}\begin{pmatrix} \mathbf{d_a} \\ \mathrm{d_b} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix}$

Where $\mathbf{V_{ab}} = \mathbf{U}^\dagger\,\mathbf{H_{ab}}$, $\mathbf{V_{ba}} = \mathbf{H_{ba}}\mathrm{U}$ and $\mathbf{d_a} = \mathbf{U}^\dagger\,\mathbf{c_a}$.

Multiply out the first line of prev. matrix eq.

$$\left(\mathbf{h}_{\mathbf{aa}} - E\,\mathbf{1}_{\mathbf{aa}}\right)\mathbf{d}_{\mathbf{a}} + \mathbf{V}_{\mathbf{a}\mathrm{b}}\,\mathrm{d}_{\mathrm{b}} = \mathbf{0}$$

Solve for $\mathbf{d}_a$

$$\mathbf{d}_{\mathbf{a}} = -\left(\mathbf{h}_{\mathbf{aa}} - E\,\mathbf{1}_{\mathbf{aa}}\right)^{-1}\mathbf{V}_{\mathbf{ab}}\,\mathrm{d}_{\mathrm{b}}$$

Plug this result into 2nd line of matrix eq.

$$\left[-\mathbf{V}_{\mathbf{ab}}\left(\mathbf{h}_{\mathbf{aa}} - E\,\mathbf{1}_{\mathbf{aa}}\right)^{-1}\mathbf{V}_{\mathbf{ab}} + \mathrm{H}_{\mathrm{bb}} - E\right]\mathrm{d}_{\mathrm{b}} = 0$$

This gives a new function f whose roots are the new eigenvalues:

$$f(E) = \mathrm{H}_{\mathrm{bb}} - E - \sum_{\alpha=1}^{N} \frac{\left|\mathrm{V}_{\alpha \mathrm{b}}\right|^2}{\mathrm{h}_\alpha - E} = 0$$

What does this function look like?

For $E \to -\infty$, $f \to \infty$

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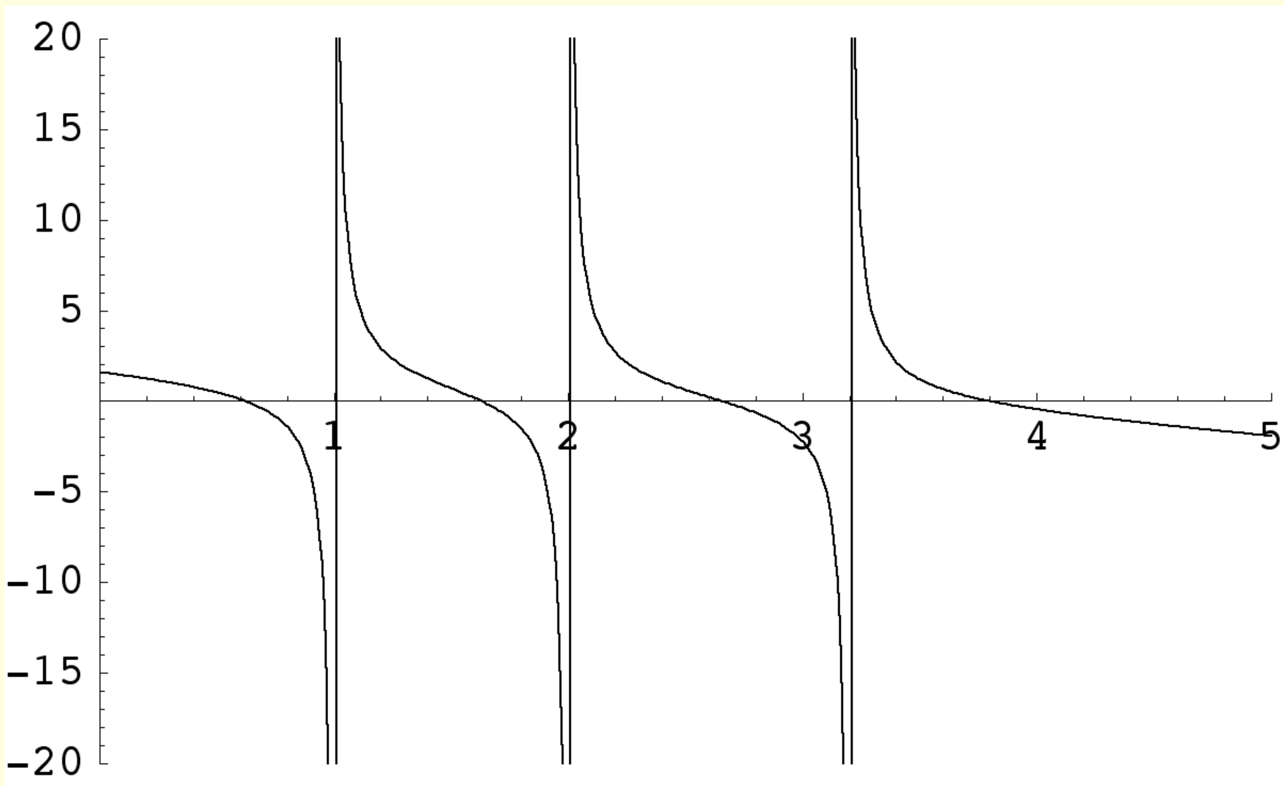
Poles whenever $E = \mathrm{h}_\alpha$

Schematic graph of *f(E)*:



Eigenvalues of the NxN problem interleave those of the (N+1)x(N+1) problem

In the limit N ->∞, the approximate eigenvalues become exact.

Conclusion: Not only is the lowest e'value an upper bound on the true lowest energy, but the 2nd e'value is a bound on the 2nd lowes energy, etc.