One of these two states is a repulsive (dissociative) state. Other excited states can be constructed using linear combinations of other orbitals. Some will be binding and others will be repulsive. Thus for excited states of $\text{H}_2^+$ we obtain the following molecular orbitals:

**Nomenclature**

$$\sigma_{u^*} \ 1s$$

$g$ - gerade
$u$ - ungerade

* - antibonding

<table>
<thead>
<tr>
<th>LCAO Function</th>
<th>MO Nomenclature</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1s_A + 1s_B$</td>
<td>$\sigma_g \ 1s$</td>
</tr>
<tr>
<td>$1s_A - 1s_B$</td>
<td>$\sigma_{u^*} \ 1s$</td>
</tr>
<tr>
<td>$2s_A + 2s_B$</td>
<td>$\sigma_g \ 2s$</td>
</tr>
<tr>
<td>$2s_A - 2s_B$</td>
<td>$\sigma_{u^*} \ 2s$</td>
</tr>
<tr>
<td>$2p_{zA} - 2p_{zB}$</td>
<td>$\sigma_g \ 2p$</td>
</tr>
<tr>
<td>$2p_{xA} + 2p_{xB}$</td>
<td>$\pi_u \ 2p$</td>
</tr>
<tr>
<td>$2p_{xA} - 2p_{xB}$</td>
<td>$\pi_g^* \ 2p$</td>
</tr>
<tr>
<td>$2p_{yA} + 2p_{yB}$</td>
<td>$\pi_u \ 2p$</td>
</tr>
<tr>
<td>$2p_{yA} - 2p_{yB}$</td>
<td>$\pi_g^* \ 2p$</td>
</tr>
<tr>
<td>$2p_{zA} + 2p_{zB}$</td>
<td>$\sigma_{u^*} \ 2p$</td>
</tr>
</tbody>
</table>
Let us look at these various combinations:
First the 1s
Followed by $2p_x$ and $y$

Note the important role of symmetry!
Hydrogen Molecule

The hydrogen molecule plays the same role in molecular electronic structure that the He atom played in the theory of atomic structure. It is a building block and also shows us how to deal with indistinguishability and electron spin. Consider the following diagram for $H_2$.

![Diagram of H2 molecule with labels for $r_{1\alpha}$, $r_{1\beta}$, $r_{1\gamma}$, $r_{2\alpha}$, $r_{2\beta}$, $r_{12}$, $R_{\alpha\beta}$, and $e_1$, $e_2$.]

After making the Born-Oppenheimer approximation, the $H_2$ Hamiltonian becomes

$$\hat{H} = -\frac{\hbar^2}{2m_e} \left[ \nabla_1^2 + \nabla_2^2 \right] - \frac{1}{r_{1\alpha}} - \frac{1}{r_{1\beta}} - \frac{1}{r_{2\alpha}} - \frac{1}{r_{2\beta}} - \frac{1}{r_{12}} + \frac{1}{R_{\alpha\beta}}$$

where I am not paying too much attention to constants.

As in the case of He, we start by dropping the electron-electron repulsion term. Then, following rewriting

$$\hat{H} = -\frac{\hbar^2}{2m_e} \nabla_1^2 - \frac{1}{r_{1\alpha}} - \frac{1}{r_{1\beta}} - \frac{\hbar^2}{2m_e} \nabla_2^2 - \frac{1}{r_{2\alpha}} - \frac{1}{r_{2\beta}} + \frac{1}{R_{\alpha\beta}}$$

we see that the first three terms are a function of the coordinates and momenta of electron 1, while the next three concern only electron 2. The Hamiltonian can be written as

$$\hat{H} = \hat{h}_{H_2^+}(1) + \hat{h}_{H_2^+}(2) + \frac{1}{R_{\alpha\beta}}$$
The wavefunction is the product of two $\text{H}_2^+$ wavefunctions and the energy is the sum of two $\text{H}_2^+$ energies. If we use the LCAO-MO approximate wavefunctions we just developed, then the ground state of $\text{H}_2$ is given by

$$\psi = \sigma_g 1s(1) \sigma_g 1s(2)$$

and after we recognize spin and indistinguishability, we have

$$\psi = \sigma_g 1s(1) \sigma_g 1s(2)[\alpha(1)\beta(2)-\beta(1)\alpha(2)]$$

As before, we can use Slater determinants to produce appropriately antisymmetrized wavefunctions. All the same techniques that we developed for atoms can be utilized to improve the accuracy of the calculations. The following potential energy curves result:
and we can build up diatomic molecular structure:

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Number of Electrons</th>
<th>Configuration</th>
<th>Term Symbol</th>
<th>Bond Order</th>
<th>R_e, Å</th>
<th>D_e, eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>H_2^+</td>
<td>1</td>
<td>(1σ_g)</td>
<td>2Σ</td>
<td>½</td>
<td>1.06</td>
<td>2.79</td>
</tr>
<tr>
<td>H_2</td>
<td>2</td>
<td>(1σ_g)^2</td>
<td>1Σ</td>
<td>1</td>
<td>0.74</td>
<td>4.75</td>
</tr>
<tr>
<td>He_2^+</td>
<td>3</td>
<td>(1σ_g)^2 (1σ_u)</td>
<td>2Σ</td>
<td>½</td>
<td>1.08</td>
<td>2.5</td>
</tr>
<tr>
<td>He_2</td>
<td>4</td>
<td>(1σ_g)^2(1σ_u)^2</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Li_2</td>
<td>6</td>
<td>[He_2] (2σ_g)^2</td>
<td>1Σ</td>
<td>1</td>
<td>2.67</td>
<td>1.14</td>
</tr>
<tr>
<td>Be_2</td>
<td>8</td>
<td>[He_2] (2σ_g)^2(2σ_u)^2</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>B_2</td>
<td>10</td>
<td>[Be_2] (1π_u)^2</td>
<td>3Σ</td>
<td>1</td>
<td>1.59</td>
<td>3</td>
</tr>
<tr>
<td>C_2</td>
<td>12</td>
<td>[Be_2] (1π_u)^4</td>
<td>1Σ</td>
<td>2</td>
<td>1.24</td>
<td>6.36</td>
</tr>
<tr>
<td>N_2^+</td>
<td>13</td>
<td>[Be_2] (1π_u)^4 (3σ_g)</td>
<td>2Σ</td>
<td>2½</td>
<td>1.11</td>
<td>8.86</td>
</tr>
<tr>
<td>N_2</td>
<td>14</td>
<td>[Be_2] (1π_u)^4 (3σ_g)^2</td>
<td>1Σ</td>
<td>3</td>
<td>1.09</td>
<td>9.90</td>
</tr>
<tr>
<td>O_2^+</td>
<td>15</td>
<td>[N_2] (1π_g)</td>
<td>2Π</td>
<td>2½</td>
<td>1.12</td>
<td>6.77</td>
</tr>
<tr>
<td>O_2</td>
<td>16</td>
<td>[N_2] (1π_g)^2</td>
<td>3Σ</td>
<td>2</td>
<td>1.21</td>
<td>5.21</td>
</tr>
<tr>
<td>F_2</td>
<td>18</td>
<td>[N_2] (1π_g)^4</td>
<td>1Σ</td>
<td>1</td>
<td>1.44</td>
<td>1.34</td>
</tr>
<tr>
<td>Ne_2</td>
<td>20</td>
<td>[N_2] (1π_g)^4 (3σ_u)^2</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
To see all of the levels of the 1st and 2nd row homonuclear diatomics qualitatively, look at the following:

Notice that the ordering of the energy levels is different for different molecules. This will be apparent in calculations, but also is understood from a correlation diagram relating the symmetries of orbitals in the molecular and united atom limits:
Figure 9.15. Contour maps of the various molecular orbitals and the total electron density of the homonuclear diatomic molecules H₂ through F₂. [From A. C. Wahl, Science 197, 961 (1966). Copyright 1966 by the American Association for the Advancement of Science.]
Heteronuclear Diatomic Molecules

The preceding discussion concerned homonuclear diatomic molecules, with the consequence that all of the molecular orbitals were constructed from degenerate components, e.g., \(2p_A\) and \(2p_B\). When we consider heterogeneous molecules, the degeneracy is not present, and we must rethink the results. Thus the terms \(H_{AA}\) and \(H_{BB}\) are no longer equal. The previous LCAO derivation must be modified.

The general secular determinant

\[
\begin{vmatrix}
H_{AA} - E & H_{AB} \\
H_{AB} & H_{BB} - E
\end{vmatrix} = 0
\]

can be expanded out to

\[
H_{AA}H_{BB} - H_{AA}E - EH_{BB} + E^2 - H_{AB}^2 + 2H_{AB}E - E^2S^2 = 0
\]

which has rather complex solutions for \(E\),

\[
\begin{vmatrix}
1 & H_{AA} + H_{BB} - 2H_{AB}S + \frac{1}{2}(H_{BB} - H_{AA})^2 - 4H_{AA}H_{AB}S + 4H_{BB}H_{AB}S + 4H_{AB}^2 + 4S^2H_{AA}H_{BB} \\
H_{AA} + H_{BB} - 2H_{AB}S + \frac{1}{2}(H_{BB} - H_{AA})^2 - 4H_{AA}H_{AB}S + 4H_{BB}H_{AB}S + 4H_{AB}^2 + 4S^2H_{AA}H_{BB}
\end{vmatrix}
\]

IF, however, we can neglect overlap (\(S=0\)), then the secular determinant simplifies to

\[
\begin{vmatrix}
H_{AA} - E & H_{AB} \\
H_{AB} & H_{BB} - E
\end{vmatrix} = 0
\]

Again expanding to

\[
H_{AA}H_{BB} - H_{AA}E - EH_{BB} + E^2 - H_{AB}^2 = 0
\]

which has the following less complex solutions for \(E\)

\[
\begin{vmatrix}
\frac{1}{2}H_{AA} + \frac{1}{2}H_{BB} + \frac{1}{2}(H_{BB} - H_{AA})^2 + 4H_{AB}^2 \\
\frac{1}{2}H_{AA} + \frac{1}{2}H_{BB} - \frac{1}{2}(H_{BB} - H_{AA})^2 + 4H_{AB}^2
\end{vmatrix}
\]

IF, in addition, \(|H_{AA} - H_{BB}| >> H_{AB}\), the two solutions simplify to
This result corresponds essentially to the energies of the parent atomic states being very different, i.e. having very different ionization energies. Namely, the energies of the molecular orbitals are little changed from those of the parent, and there is very little bonding interaction. The two molecular orbitals are essentially the atomic orbitals, \( \Psi_A \) and \( \Psi_B \). This result shows why only those orbitals close to each other in energy make significant contributions to the bonding in heteronuclear molecules.

To be specific, consider now the heteronuclear diatomic molecule HF. We approximate the coulomb integrals \( H_{AA} = \alpha_H = 13.6 \text{ eV} \), and \( H_{BB} = \alpha_F = 19.6 \text{ eV} \). We will let the resonance integral \( H_{AB} = \beta = 2 \text{ eV} \). These values are approximately correct. The general secular determinant now becomes for this HF case

\[
\begin{pmatrix}
13.6 - E & 2 \\
2 & 18.6 - E
\end{pmatrix}
= 0
\]

which expands to

\[
248.96 - 32.2 \cdot E + E^2 = 0
\]

with two solutions for \( E \),

\[
\begin{pmatrix}
19.301562118716424343 \\
12.898437881283575657
\end{pmatrix}
\]

These results are given pictorially below
When each of these values for $E$ are substituted into the secular equations, we obtain two wave functions,

$$
\Psi_{\text{lower}} = 0.33 \psi_H + 0.94 \psi_F $$

and

$$
\Psi_{\text{upper}} = 0.94 \psi_H - 0.33 \psi_F $$

One orbital is bonding and the other is antibonding. The bonding orbital has 94% F character and the antibonding one has 94% H character. There are two electrons to place in these orbitals, and they will go into the lower energy one to form the ground state. It is immediately clear why we refer to the HF ground state as being **ionic**, with structure $\text{H}^+ \text{F}^-$. We also see that the excited state represented here is not ionic.

We have implicitly considered only those orbitals that are close to each other energetically. To get a feeling for the reasonableness of this approximation, let us add a 2s orbital to the HF molecular orbitals above.

Now we have paid attention only to the two states closest in energy, the H 1s and the F 2p states. Were we justified to neglect the other states? We find out by adding in the next closest state, the F 2S state. The ionization energy of the F 2s orbital is approximately 40.2 eV. If we couple this orbital to F 2p with a resonance integral of 1 eV, then we obtain the secular determinant

$$
\begin{vmatrix}
13.6 - E & 2 & 0 \\
2 & 18.6 - E & 1 \\
0 & 1 & 40.2 - E
\end{vmatrix} = 0
$$

![Figure 1](image-url)
which expands to the cubic equation in $E$,

$$9994.592 - 1542.4 \cdot E + 72.4 \cdot E^2 - E^3 = 0$$

with three solutions,

$$
\begin{bmatrix}
40.246519404241607709 \\
12.894404784997342795 - 2 \cdot 10^{-20} \cdot i \\
19.259075810761049496 - 2 \cdot 10^{-20} \cdot i
\end{bmatrix}
$$

Note how the positions of the two original levels are essentially unchanged by the addition of the 2s level, and how the position of the new level is essentially that of the F 2s level. This result is really our justification for considering only those levels that are close to each other in energy.

To give a final example, consider the molecular orbitals of CO, another interesting case. We can construct LCAO-MO’s that are very similar to those of isoelectronic N$_2$. Since the oxygen nuclear charge is greater than that of carbon, all of the bonding LCAO-MO’s will have somewhat larger coefficients for the oxygen orbitals and the antibonding ones will have somewhat larger coefficients for the carbon component than for the oxygen component.

In analogy with N$_2$, the electron configuration of CO is

$$(\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2 (\sigma^* 2s)^2 (\pi 2px)^2 (\pi 2py)^2 (\sigma 2pz)^2$$

I have dropped the u and g designations, since the orbitals no longer have inversion symmetry. I retain the * to indicate antibonding orbitals. The bond order is three, as for N$_2$. The bonding and antibonding aspects of the lowest four orbitals essentially cancel, and we can equally well represent the CO molecule in the alternate basis,

$$(1s C)^2 (1s O)^2 (2s C)^2 (2s O)^2 (\pi 2px)^2 (\pi 2py)^2 (\sigma 2pz)^2$$

Carbon    CO    Oxygen
Semi-Empirical Methods

We can see from this discussion that one might employ semi-empirical wavefunctions using the quantities $\alpha$ and $\beta$ as parameters in calculations. Thus there would be an $\alpha$ for each different orbital, and a $\beta$ for each bonding pair. One could determine these parameters from experiments on one molecule (e.g., the C-H bond in methane) and then use these parameters for C-H bonds in other molecules (maybe \textit{t}-butyl radical!). This empirical method is not as bad as it might seem to guide your reasoning, and it has proven especially useful in cases where one can keep the number of adjustable parameters to a minimum! Especially useful in this context has been the conceptual understanding of the electronic structure of hydrocarbons with extended $\pi$ electron systems.

Consider the ethylene molecule, \textit{C}_2\textit{H}_4. There are 16 electrons: the 4 carbon 1s electrons are localized near a carbon nucleus and are non-bonding, 10 electrons (the 4 H 1s electrons and 4 carbon n=2 electrons) are involved in 4 C-H $\sigma$ bonds and the C - C $\sigma$ bond and the remaining 2 in a C-C $\pi$ bond.

To a good first approximation, we can write the Hamiltonian operator for ethylene as

$$\hat{H}_{\text{ethylene}} = \hat{H}_\sigma + \hat{H}_\pi$$

The $\sigma$ electrons by and large form the molecular frame and do not take part in the distinctive $\pi$ electron chemistry of conjugated hydrocarbons. A large amount of experimental data can be qualitatively rationalized with this model of $\sigma$-$\pi$ separability.

If we make further approximations in the form of the Hückel approximation, then we can parametrize general $\pi$ - conjugated systems:

**Hückel Approximation**

for $\pi$ electrons in planar Hydrocarbons

1. The in plane p orbitals are part of the $\sigma$ bond frame and are separable from the $\pi$ electrons.
2. The resonance integrals between bonded C atoms are given the value $\beta$ (typically about -20 kcal/mol)
3. The resonance integrals between non-bonded C atoms are set to 0.
4. All overlap terms are set to 0.
5. The coulomb integrals are all set to $\alpha$ (typically about -200 kcal/mol). This number is approximately the ionization energy of atomic carbon.

Note that $\alpha$ is exactly the same as $H_{AA}$ and $\beta$ is the same as $H_{AB}$ in our earlier discussion of the LCAO method.

Consider ethylene as the simplest $\pi$ electron system. There are two electrons, and after we make the Hückel approximations, the secular determinant becomes

$$\begin{vmatrix}
\alpha - E & \beta \\
\beta & \alpha - E
\end{vmatrix} = 0$$

which expands to

$$\alpha^2 - 2\alpha \cdot E + E^2 - \beta^2 = 0$$

with roots

$$\left\{ \begin{array}{l}
\alpha + \beta \\
\alpha - \beta
\end{array} \right.$$  

Since both $\alpha$ and $\beta$ are negative, the lowest energy level is $\alpha + \beta$. The energy level pattern is given by the following diagram:

$$\alpha - \beta \quad \psi_{\text{antibonding}} = 2p_z(1) - 2p_z(2)$$

$$\alpha + \beta \quad \psi_{\text{bonding}} = 2p_z(1) + 2p_z(2)$$

The wave functions indicated in the figure arose from substituting the two energies separately back into the secular equations and solving them for the orbital coefficients. In this case, I assumed that the ethylene molecule was in the x-y plane, so that the $p_z$ orbitals were the ones making up the $\pi$ bond.

The total $\pi$ electron energy here is $2\alpha + 2\beta$. This is our reference isolated $\pi$-bond energy. We will look at other $\pi$ electron bonds and compare against this to see whether there is additional stability or instability in the more complex systems.

As a next step, consider butadiene, $\text{H}_2\text{C}=$\text{CH-CH}=$\text{CH}_2$ . There are 4 $\pi$ electrons to place in $\pi$ orbitals. We make a trial variational function with a $2p_z$ function centered on each carbon atom. In the Hückel approximation, the secular determinant becomes
which expands to
\[
\begin{bmatrix}
\alpha - E & \beta & 0 & 0 \\
\beta & \alpha - E & \beta & 0 \\
0 & \beta & \alpha - E & \beta \\
0 & 0 & \beta & \alpha - E
\end{bmatrix} = 0
\]
which has solutions for E of
\[
\begin{bmatrix}
.618034 \cdot \beta + \alpha \\
-1.61803398 \cdot \beta + \alpha \\
\alpha + 1.61803398 \cdot \beta \\
\alpha - .618034 \cdot \beta
\end{bmatrix}
\]
Both α and β are again negative, and α > β as we saw earlier for HF. In fact, α is essentially the ionization energy out of the initial 2p_z orbital. This gives rise to the following picture:

We calculate the total π electron energy for butadiene. The total π electron energy is \(4\alpha + 4.472 \beta\). There are two π bonds and the energy per π bond is thus \(2\alpha + 2.236 \beta\). The bonds in butadiene stabilize each other by about 0.236 \(\beta\). Since \(\beta\) is typically \(\sim -25\) kcal/mol, this amounts to about 6 kcal/mol, a chemically significant, but modest, stabilization energy.
Now consider cyclobutadiene. We modify our previous determinant by allowing bonding between C\textsubscript{1} and C\textsubscript{4}.

\[
\begin{bmatrix}
\alpha - E & \beta & 0 & \beta \\
\beta & \alpha - E & \beta & 0 \\
0 & \beta & \alpha - E & \beta \\
\beta & 0 & \beta & \alpha - E \\
\end{bmatrix} = 0
\]

The determinant expands to
\[
\alpha^4 - 4\cdot\alpha^3 \cdot E + 6\cdot\alpha^2 \cdot E^2 - 4\cdot\alpha^2 \cdot \beta^2 - 4\cdot\alpha \cdot E^3 + 8\cdot\alpha \cdot E \cdot \beta^2 + E^4 - 4\cdot E^2 \cdot \beta^2 = 0
\]
which has four solutions for \(E\),

\[
\begin{bmatrix}
\alpha \\
\alpha \\
\alpha + 2\cdot\beta \\
\alpha - 2\cdot\beta \\
\end{bmatrix}
\]
and we have a different pattern of energy levels.

\[
\begin{array}{c}
\alpha - 2\beta \\
\alpha \\
\alpha + 2\beta \\
\alpha \\
\end{array}
\]

Compare the total \(\pi\) electron energy in the two cases. We have 4 electrons. For butadiene, the total \(\pi\) electron energy was \(4\alpha + 4.48 \beta\).

For cyclobutadiene, we obtain is \(4\alpha + 4 \beta\).

This last result is exactly the same as what one would obtain for 4 electrons in two isolated \(\pi\) bonds (two ethylene molecules). There is no \textbf{delocalization energy} when we form cyclobutadiene. For benzene, we shall see that the result is quite different.
Consider the secular determinant for benzene. We have

\[
\begin{pmatrix}
\alpha - E & \beta & 0 & 0 & 0 & \beta \\
\beta & \alpha - E & \beta & 0 & 0 & 0 \\
0 & \beta & \alpha - E & \beta & 0 & 0 \\
0 & 0 & \beta & \alpha - E & \beta & 0 \\
0 & 0 & 0 & \beta & \alpha - E & \beta \\
\beta & 0 & 0 & 0 & \beta & \alpha - E \\
\end{pmatrix} = 0
\]

Solving for \( E \) gives six energies as below,

\[
\begin{pmatrix}
-2\beta + \alpha \\
2\beta + \alpha \\
\beta + \alpha \\
\beta + \alpha \\
-\beta + \alpha \\
-\beta + \alpha
\end{pmatrix}
\]

with a now familiar energy level pattern,

\[
\begin{array}{cccc}
\alpha & -2\beta & \alpha - 2\beta \\
\alpha - \beta & \alpha - \beta & \alpha - \beta & \alpha - \beta & \alpha - \beta \\
\alpha + \beta & \alpha + \beta & \alpha + \beta & \alpha + \beta & \alpha + \beta \\
\alpha + 2\beta & \alpha + 2\beta & \alpha + 2\beta & \alpha + 2\beta & \alpha + 2\beta
\end{array}
\]

Antibonding

\[
\begin{array}{cccc}
\alpha & \alpha & \alpha & \alpha & \alpha
\end{array}
\]

Bonding

The total \( \pi \) electron energy is now seen to be \( 2(\alpha + 2\beta) + 4(\alpha+\beta) = 6\alpha + 8\beta \). There is an additional stabilization energy of \( 2\beta \) compared to three ethylene
molecules. Typically, $\beta$ is about $-25$ kcal/mol, so this additional stabilization energy is quite significant.

To help us get a feel for what is happening, we will look at a few more $\pi$ electron systems. Consider cyclopentadiene, $\text{C}_5\text{H}_5$, with its 5 $\pi$ electrons. The cation will have 4 and the anion 6. First the secular determinant,

$$
\begin{vmatrix}
\alpha - E & \beta & 0 & 0 & \beta \\
\beta & \alpha - E & \beta & 0 & 0 \\
0 & \beta & \alpha - E & \beta & 0 \\
0 & 0 & \beta & \alpha - E & \beta \\
\beta & 0 & 0 & \beta & \alpha - E \\
\end{vmatrix} = 0
$$

With roots given by

$$
\begin{bmatrix}
2\cdot\beta + \alpha \\
.61803398874989482\cdot\beta + \alpha \\
-1.61803398874989482\cdot\beta + \alpha \\
.61803398874989482\cdot\beta + \alpha \\
-1.61803398874989482\cdot\beta + \alpha \\
\end{bmatrix}
$$

and energy level pattern

$$
\begin{align*}
\alpha - 1.618\beta & \quad \text{Antibonding} \\
\alpha + 0.618 \beta & \quad \text{Bonding} \\
\alpha + 2\beta & \\
\end{align*}
$$

Finally, consider planar cyclooctatetraene, $\text{C}_8\text{H}_8$. 
\[
\begin{bmatrix}
\alpha - E & \beta & 0 & 0 & 0 & 0 & 0 & \beta \\
\beta & \alpha - E & \beta & 0 & 0 & 0 & 0 & 0 \\
0 & \beta & \alpha - E & \beta & 0 & 0 & 0 & 0 \\
0 & 0 & \beta & \alpha - E & \beta & 0 & 0 & 0 \\
0 & 0 & 0 & \beta & \alpha - E & \beta & 0 & 0 \\
0 & 0 & 0 & 0 & \beta & \alpha - E & \beta & 0 \\
\beta & 0 & 0 & 0 & 0 & 0 & \beta & \alpha - E \\
\end{bmatrix} = 0
\]

with solutions
\[
\begin{bmatrix}
\alpha \\
\alpha \\
-2 \cdot \beta + \alpha \\
2 \cdot \beta + \alpha \\
\alpha + \sqrt{2 \cdot \beta} \\
\alpha - \sqrt{2 \cdot \beta} \\
\alpha + \sqrt{2 \cdot \beta} \\
\alpha - \sqrt{2 \cdot \beta} \\
\end{bmatrix}
\]