Degenerate perturbation theory
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- First order perturbation theory review
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- First order perturbation theory review
- Treating a two-fold degeneracy
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- First order perturbation theory review
- Treating a two-fold degeneracy
- Lifting the degeneracy
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- First order perturbation theory review
- Treating a two-fold degeneracy
- Lifting the degeneracy
- Higher order degeneracies
First order perturbation theory review

Full Hamiltonian includes solvable portion plus a small perturbative component
First order perturbation theory review

\[ H = H^0 + H' \]

Full Hamiltonian includes solvable portion plus a small perturbative component.

There is a BIG problem with these results.

What can we do about degenerate states where the energy denominator vanishes?
First order perturbation theory review

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expand the energy and eigenfunction solutions of the full Hamiltonian

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\[ H = H^0 + H' \]
\[ E_n = E_n^0 + E_n^1 + E_n^2 + \cdots \]
First order perturbation theory review

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First order perturbation theory review

Full Hamiltonian includes solvable portion plus a small perturbative component

expand the energy and eigenfunction solutions of the full Hamiltonian

obtain the first and second order corrections to the energy and the first order correction to the eigenfunctions

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\[ E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle \]

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$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle$$

$$\psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} \psi_m^0$$

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\[ E_n^2 = \sum_{m \neq n} \left| \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \right|^2 \]
Full Hamiltonian includes solvable portion plus a small perturbative component

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First order perturbation theory review

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expand the energy and eigenfunction solutions of the full Hamiltonian

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\[ E_n^2 = \sum_{m \neq n} \frac{|\langle \psi_m^0 | H' | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0} \]

There is a BIG problem with these results

What can we do about degenerate states where the energy denominator vanishes?
Two-fold degeneracy

For the case where two states have the same energy, we can find the linear combinations which properly solve the total Hamiltonian

\[ H_0 \psi_0^a = E_0 \psi_0^a \]

\[ H_0 \psi_0^b = E_0 \psi_0^b \]

As \( \lambda \to 0 \) these two split states devolve back to two good linear combinations of the original degenerate states

\[ \psi^+ = \alpha \psi_0^a + \beta \psi_0^b, \quad \psi^- = \gamma \psi_0^a + \delta \psi_0^b, \]

\[ \langle \psi^+ | \psi^- \rangle = 0 \]
Two-fold degeneracy

For the case where two states have the same energy, we can find the linear combinations which properly solve the total Hamiltonian.

We denote the two degenerate states as $\psi^0_a$ and $\psi^0_b$ with their associated eigenvalue equations.

As $\lambda \to 0$ these two split states devolve back to two “good” linear combinations of the original degenerate states.
Two-fold degeneracy

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$$H^0 \psi_0^a = E^0 \psi_0^a$$
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Suppose that we apply the full potential, $H = H^0 + \lambda H'$ and let $\lambda \to 1$.

$$H^0 \psi_0^a = E^0 \psi_0^a$$
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Two-fold degeneracy

For the case where two states have the same energy, we can find the linear combinations which properly solve the total Hamiltonian

we denote the two degenerate states as \( \psi_0^a \) and \( \psi_0^b \) with their associated eigenvalue equations

suppose that we apply the full potential, \( H = H^0 + \lambda H' \) and let \( \lambda \to 1 \)

the degeneracy is lifted and the two states have different energies.
Two-fold degeneracy

For the case where two states have the same energy, we can find the linear combinations which properly solve the total Hamiltonian

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\[
H^0 \psi_a^0 = E^0 \psi_a^0 \\
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in general, as $\lambda \to 0$ these two split states devolve back to two “good” linear combinations of the original degenerate states.

\[
\begin{align*}
H^0 \psi_a^0 &= E^0 \psi_a^0 \\
H^0 \psi_b^0 &= E^0 \psi_b^0 \\
E_{\pm} &= \gamma \psi_0^a + \delta \psi_0^b \\
\langle \psi_+ | \psi_- \rangle &= 0
\end{align*}
\]
Two-fold degeneracy

For the case where two states have the same energy, we can find the linear combinations which properly solve the total Hamiltonian.

We denote the two degenerate states as $\psi_0^a$ and $\psi_0^b$ with their associated eigenvalue equations.

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In general, as $\lambda \to 0$ these two split states devolve back to two “good” linear combinations of the original degenerate states.

\[
\psi_+ = \alpha \psi_0^a + \beta \psi_0^b, \quad H^0 \psi_\pm = E^0 \psi_\pm \\
\psi_- = \gamma \psi_0^a + \delta \psi_0^b, \quad \langle \psi_+ | \psi_- \rangle = 0
\]
Lifting the degeneracy

The task is to determine the “good” combinations, which are not known \textit{a priori}. 

Carlo Segre  (Illinois Tech)  
PHYS 406 - Fundamentals of Quantum Theory II  
Degenerate perturbation theory
Lifting the degeneracy

The task is to determine the “good” combinations, which are not known \textit{a priori} instead of working with both $\psi_+$ and $\psi_-$, assume a generic solution

\[ \psi_0 = \alpha \psi_0^a + \beta \psi_0^b \]
Lifting the degeneracy

The task is to determine the “good” combinations, which are not known \textit{a priori}

instead of working with both $\psi_+$ and $\psi_-$, assume a generic solution

$$\psi^0 = \alpha \psi^0_a + \beta \psi^0_b$$
Lifting the degeneracy

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instead of working with both $\psi_+$ and $\psi_-$, assume a
generic solution

as before, we solve the full Schrödinger equation, $H\psi = E\psi$, by expanding the wavefunction
and energy to higher perturbative orders

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Lifting the degeneracy

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$$
H = H^0 + \lambda H' \\
\psi = \psi^0 + \lambda \psi^1 + \lambda^2 \psi^2 + \cdots
$$

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$$\psi = \psi^0 + \lambda \psi^1 + \lambda^2 \psi^2 + \cdots$$
$$E = E^0 + \lambda E^1 + \lambda^2 E^2 + \cdots$$

$$H^0 \psi^0 + \lambda (H' \psi^0 + H^0 \psi^1) + \cdots = E^0 \psi^0 + \lambda (E^1 \psi^0 + E^0 \psi^1) + \cdots$$
Lifting the degeneracy

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$$H^0 \psi^0 + \lambda (H' \psi^0 + H^0 \psi^1) + \cdots = E^0 \psi^0 + \lambda (E^1 \psi^0 + E^0 \psi^1) + \cdots$$

$$H' \psi^0 + H^0 \psi^1 = E^1 \psi^0 + E^0 \psi^1$$
Determining equations

\[ H' \psi^0 + H^0 \psi^1 = E^1 \psi^0 + E^0 \psi^1 \]
Determining equations

\[ H' \psi^0 + H^0 \psi^1 = E^1 \psi^0 + E^0 \psi^1 \]

Apply \( \langle \psi_a^0 \rangle \),
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi_0^a | \) ,

\[ \langle \psi_0^a | H' | \psi^0 \rangle + \langle \psi_0^a | H^0 | \psi^1 \rangle = E^1 \langle \psi_0^a | \psi^0 \rangle + E^0 \langle \psi_0^a | \psi^1 \rangle \]
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi^0_a | \), substitute \( \psi^0 = \alpha\psi^0_a + \beta\psi^0_b \), and integrate through

\[ \langle \psi^0_a | H' | \psi^0 \rangle + \langle \psi^0_a | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_a | \psi^0 \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \]
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\[
\langle \psi_a^0 | H' | \psi^0 \rangle + \langle \psi_a^0 | H^0 | \psi^1 \rangle = E^1 \langle \psi_a^0 | \psi^0 \rangle + E^0 \langle \psi_a^0 | \psi^1 \rangle \\
\langle \psi_a^0 | H' | \alpha\psi_a^0 \rangle + \langle \psi_a^0 | H' | \beta\psi_b^0 \rangle
\]
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi^0_0 | \), substitute \( \psi^0 = \alpha \psi^0_a + \beta \psi^0_b \), and integrate through

\[ \langle \psi^0_a | H' | \psi^0 \rangle + \langle \psi^0_a | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_a | \psi^0 \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \]

\[ \langle \psi^0_a | H' | \alpha \psi^0_a \rangle + \langle \psi^0_a | H' | \beta \psi^0_b \rangle + \langle \psi^0_a | H^0 | \psi^1 \rangle \]
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi^0_a| \), substitute \( \psi^0 = \alpha \psi^0_a + \beta \psi^0_b \), and integrate through

\[ \langle \psi^0_a|H'|\psi^0 \rangle + \langle \psi^0_a|H^0|\psi^1 \rangle = E^1\langle \psi^0_a|\psi^0 \rangle + E^0\langle \psi^0_a|\psi^1 \rangle \]

\[ \langle \psi^0_a|H'|\alpha \psi^0_a \rangle + \langle \psi^0_a|H'|\beta \psi^0_b \rangle + \langle \psi^0_a|H^0|\psi^1 \rangle = E^1\langle \psi^0_a|\alpha \psi^0_a \rangle + E^1\langle \psi^0_a|\beta \psi^0_b \rangle \]
Determining equations

\[ H' \psi^0 + H^0 \psi^1 = E^1 \psi^0 + E^0 \psi^1 \]

Apply \( \langle \psi^0_a | \) substitute \( \psi^0 = \alpha \psi^0_a + \beta \psi^0_b \), and integrate through

\[ \langle \psi^0_a | H' | \psi^0 \rangle + \langle \psi^0_a | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_a | \psi^0 \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \]
\[ \langle \psi^0_a | H' | \alpha \psi^0_a \rangle + \langle \psi^0_a | H' | \beta \psi^0_b \rangle + \langle \psi^0_a | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_a | \alpha \psi^0_a \rangle + E^1 \langle \psi^0_a | \beta \psi^0_b \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \]
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi^0_a | \), substitute \( \psi^0 = \alpha \psi^0_a + \beta \psi^0_b \), and integrate through

\[ \langle \psi^0_a | H' | \psi^0 \rangle + \langle \psi^0_a | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_a | \psi^0 \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \]
\[ \langle \psi^0_a | H' | \alpha \psi^0_a \rangle + \langle \psi^0_a | H' | \beta \psi^0_b \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle = E^1 \langle \psi^0_a | \alpha \psi^0_a \rangle + E^1 \beta \langle \psi^0_a | \psi^0_b \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \]
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi^0_a \rangle \), substitute \( \psi^0 = \alpha\psi^0_a + \beta\psi^0_b \), and integrate through

\[
\langle \psi^0_a | H' | \psi^0 \rangle + \langle \psi^0_a | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_a | \psi^0 \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle
\]

\[
\langle \psi^0_a | H' | \alpha\psi^0_a \rangle + \langle \psi^0_a | H' | \beta\psi^0_b \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle = E^1 \langle \psi^0_a | \alpha\psi^0_a \rangle + E^1 \beta \langle \psi^0_a | \psi^0_b \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle
\]
Determining equations

\[ H' \psi^0 + H^0 \psi^1 = E^1 \psi^0 + E^0 \psi^1 \]

Apply \( \langle \psi_a^0 | \), substitute \( \psi^0 = \alpha \psi_a^0 + \beta \psi_b^0 \), and integrate through

\[ \langle \psi_a^0 | H' | \psi_a^0 \rangle + \langle \psi_a^0 | H^0 | \psi^1 \rangle = E^1 \langle \psi_a^0 | \psi^0 \rangle + E^0 \langle \psi_a^0 | \psi^1 \rangle \]

\[ \langle \psi_a^0 | H' | \alpha \psi_a^0 \rangle + \langle \psi_a^0 | H' | \beta \psi_b^0 \rangle + E^0 \langle \psi_a^0 | \psi^1 \rangle = E^1 \langle \psi_a^0 | \alpha \psi_a^0 \rangle + E^1 \beta \langle \psi_a^0 | \psi_b^0 \rangle + E^0 \langle \psi_a^0 | \psi^1 \rangle \]

\[ \alpha \langle \psi_a^0 | H' | \psi_a^0 \rangle + \beta \langle \psi_a^0 | H' | \psi_b^0 \rangle = \alpha E^1 \langle \psi_a^0 | \psi_a^0 \rangle \]
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi_0^0 | \), substitute \( \psi^0 = \alpha\psi_0^0 + \beta\psi_0^0 \), and integrate through

\[ \langle \psi_0^0 | H' | \psi_0^0 \rangle + \langle \psi_0^0 | H^0 | \psi^1 \rangle = E^1 \langle \psi_0^0 | \psi^0 \rangle + E^0 \langle \psi_0^0 | \psi^1 \rangle \]

\[ \langle \psi_0^0 | H' | \alpha\psi_0^0 \rangle + \langle \psi_0^0 | H' | \beta\psi_0^0 \rangle + E^0 \langle \psi_0^0 | \psi^1 \rangle = E^1 \langle \psi_0^0 | \alpha\psi_0^0 \rangle + E^1 \beta \langle \psi_0^0 | \psi_0^0 \rangle + E^0 \langle \psi_0^0 | \psi^1 \rangle \]

\[ \alpha \langle \psi_0^0 | H' | \psi_0^0 \rangle + \beta \langle \psi_0^0 | H' | \psi_0^0 \rangle = \alpha E^1 \langle \psi_0^0 | \psi_0^0 \rangle \]

\[ \alpha W_{aa} + \beta W_{ab} = \alpha E^1 \]
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi^0_a | \rangle \), substitute \( \psi^0 = \alpha\psi^0_a + \beta\psi^0_b \), and integrate through

\[
\begin{align*}
\langle \psi^0_a | H' | \psi^0_a \rangle + \langle \psi^0_a | H^0 | \psi^1 \rangle &= E^1 \langle \psi^0_a | \psi^0 \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \\
\langle \psi^0_a | H' | \alpha\psi^0_a \rangle + \langle \psi^0_a | H' | \beta\psi^0_b \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle &= E^1 \langle \psi^0_a | \alpha\psi^0_a \rangle + E^1 \beta \langle \psi^0_a | \psi^0_b \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \\
\alpha \langle \psi^0_a | H' | \psi^0_a \rangle + \beta \langle \psi^0_a | H' | \psi^0_b \rangle &= \alpha E^1 \langle \psi^0_a | \psi^0_a \rangle \\
\alpha W_{aa} + \beta W_{ab} &= \alpha E^1
\end{align*}
\]

where \( W_{ij} \equiv \langle \psi^0_i | H' | \psi^0_j \rangle \), \( (i, j = a, b) \)
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi^0_a | \rangle \), substitute \( \psi^0 = \alpha \psi^0_a + \beta \psi^0_b \), and integrate through

\[
\langle \psi^0_a | H' | \psi^0 \rangle + \langle \psi^0_a | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_a | \psi^0 \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle
\]

\[
\langle \psi^0_a | H' | \alpha \psi^0_a \rangle + \langle \psi^0_a | H' | \beta \psi^0_b \rangle + E^0 \langle \psi^0 | \psi^1 \rangle = E^1 \langle \psi^0_a | \alpha \psi^0_a \rangle + E^1 \beta \langle \psi^0_a | \psi^0_b \rangle + E^0 \langle \psi^0 | \psi^1 \rangle
\]

\[
\alpha \langle \psi^0_a | H' | \psi^0_a \rangle + \beta \langle \psi^0_a | H' | \psi^0_b \rangle = \alpha E^1 \langle \psi^0_a | \psi^0_a \rangle
\]

\[
\alpha W_{aa} + \beta W_{ab} = \alpha E^1
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where \( W_{ij} \equiv \langle \psi^0_i | H' | \psi^0_j \rangle \), \((i, j = a, b)\)

doing the same with \( \langle \psi^0_b | \rangle \)
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi^0_a | \), substitute \( \psi^0 = \alpha \psi^0_a + \beta \psi^0_b \), and integrate through

\[ \langle \psi^0_a | H' | \psi^0_a \rangle + \langle \psi^0_a | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_a | \psi^0_a \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \]
\[ \langle \psi^0_a | H' | \alpha \psi^0_a \rangle + \langle \psi^0_a | H' | \beta \psi^0_b \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle = E^1 \langle \psi^0_a | \alpha \psi^0_a \rangle + E^1 \beta \langle \psi^0_a | \psi^1 \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \]
\[ \alpha \langle \psi^0_a | H' | \psi^0_a \rangle + \beta \langle \psi^0_a | H' | \psi^0_b \rangle = \alpha E^1 \langle \psi^0_a | \psi^0_a \rangle \]
\[ \alpha W_{aa} + \beta W_{ab} = \alpha E^1 \]

where \( W_{ij} \equiv \langle \psi^0_i | H' | \psi^0_j \rangle, \quad (i, j = a, b) \)

doing the same with \( \langle \psi^0_b | \)

\[ \langle \psi^0_b | H' | \psi^0 \rangle + \langle \psi^0_b | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_b | \psi^0 \rangle + E^0 \langle \psi^0_b | \psi^1 \rangle \]
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi^0_a | \) substitute \( \psi^0 = \alpha\psi^0_a + \beta\psi^0_b \), and integrate through

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\langle \psi^0_a | H' | \psi^0_a \rangle + \langle \psi^0_a | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_a | \psi^0 \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \\
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\alpha \langle \psi^0_a | H' | \psi^0_a \rangle + \beta \langle \psi^0_a | H' | \psi^0_b \rangle = \alpha E^1 \langle \psi^0_a | \psi^0_a \rangle \\
\alpha W_{aa} + \beta W_{ab} = \alpha E^1 \\
\text{where } W_{ij} \equiv \langle \psi^0_i | H' | \psi^0_j \rangle, \quad (i, j = a, b)
\]

doing the same with \( \langle \psi^0_b | \)

\[
\langle \psi^0_b | H' | \psi^0 \rangle + \langle \psi^0_b | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_b | \psi^0 \rangle + E^0 \langle \psi^0_b | \psi^1 \rangle \\
\]

Carlo Segre  (Illinois Tech)  
PHYS 406 - Fundamentals of Quantum Theory II  
Degenerate perturbation theory
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi^a_0 | \psi^0 \rangle \), substitute \( \psi^0 = \alpha\psi^a_0 + \beta\psi^b_0 \), and integrate through

\[ \langle \psi^a_0 | H' | \psi^0 \rangle + \langle \psi^a_0 | H^0 | \psi^1 \rangle = E^1 \langle \psi^a_0 | \psi^0 \rangle + E^0 \langle \psi^a_0 | \psi^1 \rangle \]
\[ \langle \psi^a_0 | H' | \alpha\psi^a_0 \rangle + \langle \psi^a_0 | H' | \beta\psi^b_0 \rangle + E^0 \langle \psi^a_0 | \psi^1 \rangle = E^1 \langle \psi^a_0 | \alpha\psi^a_0 \rangle + E^1 \beta \langle \psi^a_0 | \psi^b_0 \rangle + E^0 \langle \psi^a_0 | \psi^1 \rangle \]

\[ \alpha \langle \psi^a_0 | H' | \psi^a_0 \rangle + \beta \langle \psi^a_0 | H' | \psi^b_0 \rangle = \alpha E^1 \langle \psi^a_0 | \psi^a_0 \rangle \]
\[ \alpha W_{aa} + \beta W_{ab} = \alpha E^1 \]

where \( W_{ij} \equiv \langle \psi^i_0 | H' | \psi^j_0 \rangle \), \( i, j = a, b \)

doing the same with \( \langle \psi^b_0 | \psi^0 \rangle \)

\[ \langle \psi^b_0 | H' | \psi^0 \rangle + \langle \psi^b_0 | H^0 | \psi^1 \rangle = E^1 \langle \psi^b_0 | \psi^0 \rangle + E^0 \langle \psi^b_0 | \psi^1 \rangle \]
\[ \alpha \langle \psi^b_0 | H' | \psi^b_0 \rangle + \beta \langle \psi^b_0 | H' | \psi^a_0 \rangle = \beta E^1 \langle \psi^b_0 | \psi^b_0 \rangle \]
Determining equations

\[ H'\psi^0 + H^0\psi^1 = E^1\psi^0 + E^0\psi^1 \]

Apply \( \langle \psi^0_a \rangle \), substitute \( \psi^0 = \alpha \psi^0_a + \beta \psi^0_b \), and integrate through

\[ \langle \psi^0_a | H' | \psi^0_a \rangle + \langle \psi^0_a | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_a | \psi^0 \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \]

\[ \langle \psi^0_a | H' | \alpha \psi^0_a \rangle + \langle \psi^0_a | H' | \beta \psi^0_b \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle = E^1 \langle \psi^0_a | \alpha \psi^0_a \rangle + E^0 \beta \langle \psi^0_a | \psi^0_b \rangle + E^0 \langle \psi^0_a | \psi^1 \rangle \]

\[ \alpha \langle \psi^0_a | H' | \psi^0_a \rangle + \beta \langle \psi^0_b | H' | \psi^0_b \rangle = \alpha E^1 \langle \psi^0_a | \psi^0_a \rangle \]

\[ \alpha W_{aa} + \beta W_{ab} = \alpha E^1 \]

where \( W_{ij} \equiv \langle \psi^0_i | H' | \psi^0_j \rangle \), \( (i, j = a, b) \)

doing the same with \( \langle \psi^0_b \rangle \)

\[ \langle \psi^0_b | H' | \psi^0_b \rangle + \langle \psi^0_b | H^0 | \psi^1 \rangle = E^1 \langle \psi^0_b | \psi^0 \rangle + E^0 \langle \psi^0_b | \psi^1 \rangle \]

\[ \alpha \langle \psi^0_b | H' | \psi^0_a \rangle + \beta \langle \psi^0_b | H' | \psi^0_b \rangle = \beta E^1 \langle \psi^0_b | \psi^0_b \rangle \]

\[ \alpha W_{ba} + \beta W_{bb} = \beta E^1 \]
Determining the energies

Solve these two equations for the energies of the two “ideal” orthogonal states

\[ \alpha W_{aa} + \beta W_{ab} = \alpha E^1 \]
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if we assume that \( \alpha \neq 0 \), we can solve for the energies

\[ E_0 = \left( E^1 \right)^2 - E^1 \left( W_{aa} + W_{bb} \right) + \left( W_{aa} W_{bb} - W_{ab} W_{ba} \right) \]
\[ \pm \frac{1}{2} \left[ W_{aa} + W_{bb} \pm \sqrt{(W_{aa} + W_{bb})^2 - 4(W_{aa} W_{bb} - W_{ab} W_{ba})} \right] = \frac{1}{2} \left[ W_{aa} + W_{bb} \pm \left| W_{ab} \right|^2 \right] \]
Determining the energies

Solve these two equations for the energies of the two “ideal” orthogonal states

\[ \alpha W_{aa} + \beta W_{ab} = \alpha E^1 \]
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\[ \alpha W_{aa} + \beta W_{ab} = \alpha E^1 \quad \rightarrow \quad \beta W_{ab} = \alpha [E^1 - W_{aa}] \]
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\]

\[
\alpha W_{aa} + \beta W_{ab} = \alpha E^1 \quad \rightarrow \quad \beta W_{ab} = \alpha [E^1 - W_{aa}]
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\[
\alpha W_{ab} W_{ba} + \beta W_{ab} W_{bb} = \beta E^1 W_{ab}
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\[ \alpha W_{ab} W_{ba} + \beta W_{ab} W_{bb} = \beta E^1 W_{ab} \quad \rightarrow \quad \alpha W_{ab} W_{ba} = \beta W_{ab} [E^1 - W_{bb}] \]
Determining the energies

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\[ \alpha W_{ab} W_{ba} = \alpha [E^1 - W_{aa}] [E^1 - W_{bb}] \]
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\[
\begin{align*}
\alpha W_{aa} + \beta W_{ab} &= \alpha E^1 \\
\alpha W_{ba} + \beta W_{bb} &= \beta E^1 \\
\alpha W_{ab} W_{ba} + \beta W_{ab} W_{bb} &= \beta E^1 W_{ab} \\
\alpha W_{ab} W_{ba} &= \alpha [E^1 - W_{aa}][E^1 - W_{bb}]
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if we assume that \( \alpha \neq 0 \), we can solve for the energies
Determining the energies

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\[ \alpha W_{ab} W_{ba} = \alpha [E^1 - W_{aa}] \]

\[ \alpha W_{ab} W_{ba} = \alpha [E^1 - W_{aa}] [E^1 - W_{bb}] \]

if we assume that \( \alpha \neq 0 \), we can solve for the energies

\[ 0 = (E^1)^2 - E^1 (W_{aa} + W_{bb}) + (W_{aa} W_{bb} - W_{ab} W_{ba}) \]
Determining the energies

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\alpha W_{aa} + \beta W_{ab} &= \alpha E^1 \\
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\begin{align*}
\alpha W_{aa} + \beta W_{ab} &= \alpha E^1 \quad \rightarrow \quad \beta W_{ab} = \alpha [E^1 - W_{aa}] \\
\alpha W_{ab} W_{ba} + \beta W_{ab} W_{bb} &= \beta E^1 W_{ab} \quad \rightarrow \quad \alpha W_{ab} W_{ba} = \beta W_{ab} [E^1 - W_{bb}] \\
\alpha W_{ab} W_{ba} &= \alpha [E^1 - W_{aa}] [E^1 - W_{bb}]
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\begin{align*}
0 &= (E^1)^2 - E^1 (W_{aa} + W_{bb}) + (W_{aa} W_{bb} - W_{ab} W_{ba}) \\
E^{\pm}_1 &= \frac{1}{2} \left[ W_{aa} + W_{bb} \pm \sqrt{(W_{aa} + W_{bb})^2 - 4(W_{aa} W_{bb} - W_{ab} W_{ba})} \right]
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Determining the energies

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if we assume that \( \alpha \neq 0 \), we can solve for the energies

\[ 0 = (E^1)^2 - E^1 (W_{aa} + W_{bb}) + (W_{aa} W_{bb} - W_{ab} W_{ba}) \]

\[ E^1_{\pm} = \frac{1}{2} \left[ W_{aa} + W_{bb} \pm \sqrt{(W_{aa} + W_{bb})^2 - 4(W_{aa} W_{bb} - W_{ab} W_{ba})} \right] \]

\[ = \frac{1}{2} \left[ W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2} \right] \]
Ideal energies

We assumed that $\alpha \neq 0$, but what if this is not the case?

Recall the two defining equations

Suppose we let $\alpha = 0$, then

$$\alpha W_{aa} + \beta W_{ab} = \alpha E_1$$

$$\alpha W_{ba} + \beta W_{bb} = \beta E_1$$

These are simply the non-degenerate first order perturbation results and it means that $\psi_0^a$ and $\psi_0^b$ are already the "ideal" states.

It is often possible to choose the "ideal" linear combination through use of a convenient theorem.
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\alpha W_{ba} + \beta W_{bb} &= \beta E^1
\end{align*}
\]

suppose we let $\alpha = 0$, then

\[
W_{ab} = 0, \quad E^1_- = W_{bb}
\]

and if $\beta = 0$

\[
W_{ba} = 0, \quad E^1_+ = W_{aa}
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Ideal energies

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\alpha W_{ba} + \beta W_{bb} &= \beta E^1
\end{align*}
\]

suppose we let \( \alpha = 0 \), then

\[
\begin{align*}
W_{ab} &= 0, \quad E_{-}^1 = W_{bb} = \langle \psi_0^b | H' | \psi_0^b \rangle \\
W_{ba} &= 0, \quad E_{+}^1 = W_{aa} = \langle \psi_0^a | H' | \psi_0^a \rangle
\end{align*}
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these are simply the non-degenerate first order perturbation results and it means that $\psi_a^0$ and $\psi_b^0$ are already the “ideal” states

It is often possible to choose the “ideal” linear combination through use of a convenient theorem
Determining $\alpha$ and $\beta$

**Theorem:** If $A$ is a hermitian operator which commutes with both $H^0$ and $H'$ and $\psi_a^0$ and $\psi_b^0$ are also eigenfunctions of $A$ with distinct eigenvalues

$$A\psi_a^0 = \mu \psi_a^0, \quad A\psi_b^0 = \nu \psi_b^0, \quad \mu \neq \nu$$

then $W_{ab} = W_{ba} = 0$
### Theorem: If $A$ is a hermitian operator which commutes with both $H^0$ and $H'$ and $\psi^0_a$ and $\psi^0_b$ are also eigenfunctions of $A$ with distinct eigenvalues

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### Proof: Since $A$ and $H'$ commute, we have that $[A, H'] = AH' - H'A \equiv 0$
Determining $\alpha$ and $\beta$

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$$\langle \psi_a^0 | [A, H'] \psi_b^0 \rangle = 0$$

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$$\langle \psi^0_a | [A, H'] | \psi^0_b \rangle = 0$$

$$= \langle \psi^0_a | AH' \psi^0_b \rangle - \langle \psi^0_a | H' A \psi^0_b \rangle = \langle A \psi^0_a | H' \psi^0_b \rangle - \langle \psi^0_a | H' \nu \psi^0_b \rangle$$
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**Theorem:** If $A$ is a hermitian operator which commutes with both $H^0$ and $H'$ and $\psi_a^0$ and $\psi_b^0$ are also eigenfunctions of $A$ with distinct eigenvalues

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$$\langle \psi_a^0 | [A, H'] \psi_b^0 \rangle = 0$$

$$= \langle \psi_a^0 | AH' \psi_b^0 \rangle - \langle \psi_a^0 | H' A \psi_b^0 \rangle = \langle A \psi_a^0 | H' \psi_b^0 \rangle - \langle \psi_a^0 | H' \nu \psi_b^0 \rangle$$

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**Proof:** Since $A$ and $H'$ commute, we have that $[A, H'] = AH' - H'A \equiv 0$

$$\langle \psi^0_a | [A, H'] | \psi^0_b \rangle = 0$$

$$= \langle \psi^0_a | AH' | \psi^0_b \rangle - \langle \psi^0_a | H'A | \psi^0_b \rangle = \langle A\psi^0_a | H' | \psi^0_b \rangle - \langle \psi^0_a | H' \nu | \psi^0_b \rangle$$

$$= \langle \mu \psi^0_a | H' | \psi^0_b \rangle - \langle \psi^0_a | H' \nu | \psi^0_b \rangle = (\mu - \nu) \langle \psi^0_a | H' | \psi^0_b \rangle$$
Determining $\alpha$ and $\beta$

**Theorem**: If $A$ is a hermitian operator which commutes with both $H^0$ and $H'$ and $\psi_0^a$ and $\psi_0^b$ are also eigenfunctions of $A$ with distinct eigenvalues

$$A\psi_0^a = \mu\psi_0^a, \quad A\psi_0^b = \nu\psi_0^b, \quad \mu \neq \nu$$

then $W_{ab} = W_{ba} = 0$

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$$= \langle \mu \psi_0^a | H' \psi_0^b \rangle - \langle \psi_0^a | H' \nu \psi_0^b \rangle = (\mu - \nu)\langle \psi_0^a | H' \psi_0^b \rangle = (\mu - \nu)W_{ab}$$
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**Theorem:** If $A$ is a hermitian operator which commutes with both $H^0$ and $H'$ and $\psi_a^0$ and $\psi_b^0$ are also eigenfunctions of $A$ with distinct eigenvalues

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$$= \langle \mu \psi_a^0 | H' \psi_b^0 \rangle - \langle \psi_a^0 | H' \nu \psi_b^0 \rangle = (\mu - \nu) \langle \psi_a^0 | H' \psi_b^0 \rangle = (\mu - \nu) W_{ab}$$

since $\mu \neq \nu$, $W_{ab} \equiv 0$
Higher order degeneracy

When there are more than two degenerate states, a matrix formulation is more useful

Recall the two defining equations:

They can be rewritten in the form of a matrix:

The $E_1$ are the eigenvalues of the $W$-matrix and the "good" linear combinations of the unperturbed states are the eigenvectors of $W$.

This is proven in problem 7.13 where you assume that the set of unperturbed eigenfunctions $\psi_0$ are $n$-fold degenerate and that $\psi_0$ is a general linear combination

$$W_{aa} \alpha + W_{ab} \beta = E_1 \alpha$$
$$W_{ba} \alpha + W_{bb} \beta = E_1 \beta$$

$$(W_{aa} W_{ab} W_{ba} W_{bb}) (\alpha \beta) = E_1 (\alpha \beta)$$

$$W_{ij} = \langle \psi_0 i | H | \psi_0 j \rangle$$

$H_0 \psi_0 i = E_0 \psi_0 i$

$\langle \psi_0 i | \psi_0 j \rangle = \delta_{ij}$

$\psi_0 = \sum_{i=1}^{n} \alpha_i \psi_0 i$, Carlo Segre (Illinois Tech) PHYS 406 - Fundamentals of Quantum Theory II Degenerate perturbation theory
Higher order degeneracy

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Higher order degeneracy

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\[ \alpha W_{aa} + \beta W_{ab} = \alpha E^1 \]
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\[
\begin{align*}
\alpha W_{aa} + \beta W_{ab} &= \alpha E^1 \\
\alpha W_{ba} + \beta W_{bb} &= \beta E^1
\end{align*}
\]

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$$\begin{align*}
\alpha W_{aa} + \beta W_{ab} &= \alpha E^1 \\
\alpha W_{ba} + \beta W_{bb} &= \beta E^1
\end{align*}$$

$$(W_{aa} \ W_{ab}) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$
Higher order degeneracy

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\[ \alpha W_{ba} + \beta W_{bb} = \beta E_1 \]

they can be rewritten in the form of a matrix

\[
\begin{pmatrix}
W_{aa} & W_{ab} \\
W_{ba} & W_{bb}
\end{pmatrix}
\begin{pmatrix}
\alpha \\
\beta
\end{pmatrix}
= E_1
\begin{pmatrix}
\alpha \\
\beta
\end{pmatrix}
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The \( E_1 \) are the eigenvalues of the \( W \)-matrix and the “good” linear combinations of the unperturbed states are the eigenvectors of \( W_{ij} \).
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W_{ba} & W_{bb}
\end{pmatrix}
\begin{pmatrix}
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\beta
\end{pmatrix}
= E^1
\begin{pmatrix}
\alpha \\
\beta
\end{pmatrix}
$$

$$W_{ij} = \langle \psi_0^i | H' | \psi_0^j \rangle$$
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\[ \alpha W_{aa} + \beta W_{ab} = \alpha E^1 \]
\[ \alpha W_{ba} + \beta W_{bb} = \beta E^1 \]

\[ \begin{pmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \]

\[ W_{ij} = \langle \psi_i^0 | H' | \psi_j^0 \rangle \]

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This is proven in problem 7.13 where you assume that the set of unperturbed eigenfunctions \( \psi_i^0 \) are n-fold degenerate
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\[
W_{ij} = \langle \psi_i^0 | H' | \psi_j^0 \rangle
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\[
H^0 \psi_i^0 = E^0 \psi_i^0,
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\[
\begin{align*}
\alpha W_{aa} + \beta W_{ab} &= \alpha E^1 \\
\alpha W_{ba} + \beta W_{bb} &= \beta E^1 \\
(W_{aa} & W_{ab}) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \\
W_{ij} &= \langle \psi^0_i | H' | \psi^0_j \rangle \\
H^0 \psi^0_i &= E^0 \psi^0_i, \quad \langle \psi^0_i | \psi^0_j \rangle = \delta_{ij}
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$$\psi^0 = \sum_{i=1}^{n} \alpha_i \psi_i^0$$