

Degenerate perturbation theory





- 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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- 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**

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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



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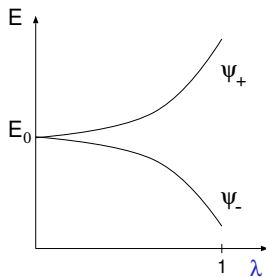
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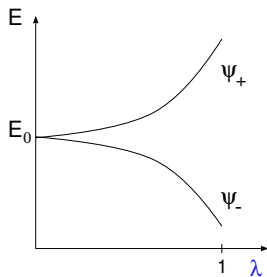
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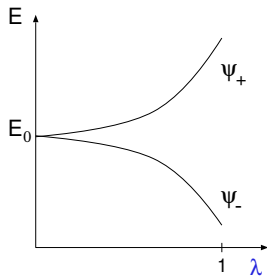
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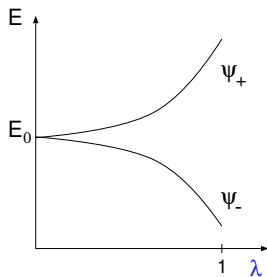
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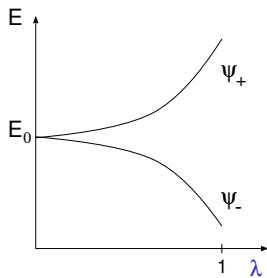
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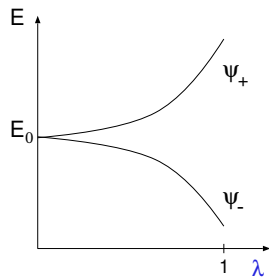
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$$\alpha W_{aa} + \beta W_{ab} = \alpha E^1$$

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Determining equations



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Determining the energies



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

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$$\begin{aligned} 0 &= (E^1)^2 - E^1(W_{aa} + W_{bb}) + (W_{aa}W_{bb} - W_{ab}W_{ba}) \\ E_{\pm}^1 &= \frac{1}{2} \left[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} + W_{bb})^2 - 4(W_{aa}W_{bb} - W_{ab}W_{ba})} \right] \\ &= \frac{1}{2} \left[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2} \right] \end{aligned}$$

Ideal energies



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

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these are simply the non-degenerate first order perturbation results and it means that ψ_a^0 and ψ_b^0 are already the “ideal” states

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these are simply the non-degenerate first order perturbation results and it means that ψ_a^0 and ψ_b^0 are already the “ideal” states

It is often possible to choose the “ideal” linear combination through use of a convenient theorem

Determining α and β



Theorem: If A is a hermitian operator which commutes with both H^0 and H' and ψ_a^0 and ψ_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 $W_{ab} = W_{ba} = 0$

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

$$\begin{aligned} \langle \psi_a^0 | [A, H'] | \psi_b^0 \rangle &= 0 \\ &= \langle \psi_a^0 | AH' | \psi_b^0 \rangle - \langle \psi_a^0 | H'A | \psi_b^0 \rangle = \langle A\psi_a^0 | H' | \psi_b^0 \rangle - \langle \psi_a^0 | H' \nu \psi_b^0 \rangle \\ &= \langle \mu\psi_a^0 | H' | \psi_b^0 \rangle - \langle \psi_a^0 | H' \nu \psi_b^0 \rangle = (\mu - \nu) \langle \psi_a^0 | H' | \psi_b^0 \rangle = (\mu - \nu) W_{ab} \end{aligned}$$

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

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Recall the two defining equations

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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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$$H^0 \psi_i^0 = E^0 \psi_i^0, \quad \langle \psi_i^0 | \psi_j^0 \rangle = \delta_{ij}$$

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$$\psi^0 = \sum_{i=1}^n \alpha_i \psi_i^0$$

