Degenerate Perturbation Theory Tutorial

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1 Procedure for dealing with degeneracies

- Start by redefining H^0 to include elements of H' involving only the degenerate states. Now H' is whatever is left after the terms involving only degenerate states have been moved over to H^0.
- We want to use the eigenstates of our newly defined H^0 as basis vectors. Some of these eigenstates will be obvious (they are the non-degenerate eigenstates from our original basis). To find the others we must find the eigenvalues and eigenvectors of the sub-matrix that involves the degenerate states (this will be the only part of the matrix that has off-diagonal terms).
- The eigenvectors of the sub-matrix now become new basis vectors, replacing the degenerate basis vectors in your original basis of unperturbed eigenstates. We must now write H^0 and H' in this new basis. First construct the transformation matrix from the old basis ($|\phi_n\rangle$) to the new basis ($|\phi'_m\rangle$):

$$U = \begin{pmatrix} \langle\phi'_1|\phi_1\rangle & \langle\phi'_1|\phi_2\rangle & \langle\phi'_1|\phi_3\rangle & \cdots \\ \langle\phi'_2|\phi_1\rangle & \langle\phi'_2|\phi_2\rangle & \langle\phi'_2|\phi_3\rangle & \cdots \\ \langle\phi'_3|\phi_1\rangle & \langle\phi'_3|\phi_2\rangle & \langle\phi'_3|\phi_3\rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

  Now apply this transformation matrix to H^0 and H': $H^{0'} = UH^0U^\dagger$ and $H'' = UH'U^\dagger$.
- Repeat the above steps for all groups of degenerate states.
- Once the degeneracies have been addressed you can use non-degenerate perturbation theory.

2 An Example

1. Suppose we have an unperturbed Hamiltonian with three basis vectors. In the basis of unperturbed eigenstates we can represent this Hamiltonian as:

$$H^0 = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 5 \end{pmatrix}.$$

   This system is then perturbed by some new interaction. We can represent the perturbation (in the same basis of unperturbed eigenstates) as

$$H' = \begin{pmatrix} 0 & 2 & 2 \\ 2 & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix}.$$

   Is the matrix H' Hermitian?

2. Write the matrix for the full Hamiltonian $H = H^0 + H'$. Is this matrix Hermitian?

3. Redefine H^0 so that it incorporates the terms from H' that involve only the degenerate states. Write this new H^0 below. Is this matrix Hermitian?

4. Now write the new H', removing anything you moved over to H^0 in the previous step. Is this matrix Hermitian?

5. Find the eigenvalues and eigenvectors of the degenerate sub-matrix of H^0.

6. We will now use the eigenvectors of the sub-matrix, as well as any of your original basis vectors that were not degenerate, as our new basis vectors. Construct the transformation matrix to transform from the old basis to the new basis. Is this matrix Hermitian?

7. Transform H^0 into the new basis. Explain why this results makes sense.

8. Transform H' into the new basis. Is this matrix Hermitian?

9. Now use non-degenerate perturbation theory to find the first-order correction to the three energies.

10. Use non-degenerate perturbation theory to find the second-order correction to the three energies.

11. Calculate the corrected energies to second order.

12. In this case we could have just found the eigenvalues and eigenvectors of the full 3 by 3 Hamiltonian right from the start. If we do this we find the eigenvalues are 4.28242, 8.11694, and 12.6006 (to 6 significant figures). Compare these "exact" values to the values you found using perturbation theory.