Phys 487 Discussion 6 – Degenerate Perturbation Theory

The Old Stuff : Formulae for perturbative corrections to **non-degenerate states** are on last page.

The New Stuff : **The Procedure** for dealing with **degenerate states**

Perturbation theory always starts with an "unperturbed" Hamiltonian H_0 whose eigenstates $\left\{ \left|n^{(0)}\right\rangle \text{ or } \psi_n^{(0)} \right\}$ and eigenvalues $\left\{ E_n^{(0)} \right\}$ can be obtained exactly. A small perturbing Hamiltonian $H' << H_0$ is then added to H_0 to produce the full Hamiltonian $H = H_0 + \varepsilon H'$. This is the Hamiltonian whose eigen-things we would like to obtain. I have attached a dimensionless scale factor $\varepsilon << 1$ to H' so that I can easily keep track of orders of smallness. (Sometimes such a small scale factor is an intrinsic part of the problem, sometimes not.)

Suppose that a subset of the unperturbed eigen-energies $\left\{ E_n^{(0)} \right\}$ are **degenerate**, i.e. have the same value E_α. Let the quantum numbers of these degenerate eigenstates be { $\alpha 1, \alpha 2, \alpha 3, \ldots, \alpha n$ }. If we write H_0 in matrix form using as basis the unperturbed eigenstates $\left\{ \left|n^{(0)}\right\rangle \right\}$, we get the diagonal matrix $(\mathbf{H}_0)_{mn} \equiv \left\langle m^{(0)} \middle| \hat{H}_0 \middle| n^{(0)} \right\rangle$:

$$\mathbf{H}_0 = \begin{pmatrix} E_1^{(0)} & & & & & \\ & E_2^{(0)} & & & & \\ & & \boldsymbol{E_\alpha} & & & \\ & & & \boldsymbol{E_\alpha} & & \\ & & & & E_5^{(0)} & \\ & & & & & \ldots \end{pmatrix}$$ where all the empty elements are 0.

I have bold-faced the degenerate energies and left off the superscript (0) so that you can spot them easily. The degenerate states $\left\{ \left|\alpha_1^{(0)}\right\rangle, \ldots, \left|\alpha_n^{(0)}\right\rangle \right\}$, which are just $\left\{ \left|3^{(0)}\right\rangle, \left|4^{(0)}\right\rangle \right\}$ here, form a **degenerate subspace** where any linear combination of the $|\,\alpha_i\,\rangle$'s is *also* an eigenstate of H_0 with the same eigenvalue E_α.

Degenerate perturbation theory is accomplished by finding a **particular set of linear combinations** of the $|\,\alpha_i\,\rangle$'s, i.e. within the degenerate subspace, that **diagonalizes the perturbation matrix** $(\mathbf{H}')_{ij} \equiv \left\langle i^{(0)} \middle| \hat{H}' \middle| j^{(0)} \right\rangle$.

Once you have found these linear combinations $\left\{ \left|\beta_1^{(0)}\right\rangle, \ldots, \left|\beta_n^{(0)}\right\rangle \right\}$, i.e. the eigenvectors of H' within the degenerate subspace, find their corresponding eigenvalues and you will have your first-order corrections :

$$E_{\beta i}^{(1)} = \left\langle \beta_i^{(0)} \middle| H' \middle| \beta_i^{(0)} \right\rangle$$

These are the expectation values of H' in the new basis states $\left|\beta_i^{(0)}\right\rangle$, i.e. *it is exactly our normal formula for* $E_i^{(1)}$, just using the new basis.

Problem 1 : A Perturbed Hamiltonian in Matrix Form *adapted from Griffiths 6.9, Checkpoints* [1]

Consider a quantum system with only three linearly independent states. We label these states $|1\rangle, |2\rangle, |3\rangle$. The system's Hamiltonian, expressed in the ordered basis $\{\ |1\rangle, |2\rangle, |3\rangle\ \}$, is

$$\mathbf{H} = V_0 \begin{pmatrix} (1-\varepsilon) & 0 & 0 \\ 0 & 1 & \varepsilon \\ 0 & \varepsilon & 2 \end{pmatrix}$$

where V_0 is a constant <u>that we will immediately set to 1 for convenience</u> and ε is a small number << 1.

(a) Write down the eigenvectors and eigenvalues of the **unperturbed Hamiltonian** , i.e. the Hamiltonian you obtain by setting the small parameter ε to <u>zero</u>.

(b) Solve for the *exact* eigenvalues of **H** without using any perturbation-theory formulae at all. Expand each of them as a power series in ε, up to second order.

(c) Use first- and second-order non-degenerate perturbation theory to find the approximate eigenvalue for the state that grows out of the non-degenerate eigenvector of H_0. Does it match the exact value from (b)?

(d) Now apply the <u>1st-order non-degenerate</u> PT formula to find the approximate eigenvalues for the states that grow out of the <u>degenerate</u> eigenvectors of H_0. You have the exact results from (b) … do the non-degenerate formulae work give the correct energy corrections for states #1 and #2?

(e) It appears we don't need degenerate perturbation theory at all! How disappointing! WHY did non-degenerate formulae work for degenerate states #1 & #2 without any effort ?

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[1] **Q1** (a) Since H_0 is diagonal, it is written in terms of its own eigenvectors. … Turning those words around, the **eigenvectors** of H_0 are the basis vectors in terms of which H_0 is written: $\begin{matrix}\text{eigen-}\\\text{vector}\end{matrix}\ |1^{(0)}\rangle$ of $H_0 = \begin{matrix}\text{basis}\\\text{vector}\end{matrix} \begin{pmatrix}1\\0\\0\end{pmatrix}$, $|2^{(0)}\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix}$, $|3^{(0)}\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}$.

As always with a diagonal matrix, the diagonal elements are the **eigenvalues** : $E_1^{(0)} = 1$, $E_2^{(0)} = 1$, $E_3^{(0)} = 2$.

(b) exact eigenvalues of H Taylor-approximated to order ε^2 are : $E_1 = 1 - \varepsilon$, $E_2 = 1 - \varepsilon^2$, $E_3 = 2 + \varepsilon^2$

(c) non-degenerate state is #3 … sum of corrections to 2nd order is

$$E_3^{(0)+(1)+(2)} = E_3^{(0)} + H'_{33} + \left[\frac{|H'_{13}|^2}{E_3^{(0)} - E_1^{(0)}} + \frac{|H'_{23}|^2}{E_3^{(0)} - E_2^{(0)}} \right] = 2 + 0 + \left[\frac{0^2}{2-1} + \frac{\varepsilon^2}{2-1} \right] = 2 + \varepsilon^2 \ ✔ ☺$$

(d) degenerate states are #1 and #2 … correcting to 1st order, $E_1^{(0)+(1)} = E_1^{(0)} + H'_{11} = 1 - \varepsilon$ ✔ and $E_2^{(0)+(1)} = E_2^{(0)} + H'_{22} = 1 + 0 = 1$ ✔

(e) The perturbation H' is <u>already diagonal</u> in the degenerate subspace of $\{\ |\text{state}\,\#1\rangle, |\text{state}\,\#2\rangle\ \}$, i.e. the off-diagonal matrix elements H'_{12} and H'_{21} within this subspace are zero.

Problem 2 : Now let's *use* our new technique *Checkpoints* [2]

Now that we have a good idea of how this works, let's work with a system where we DO need to do something to obtain the energy corrections for a pair of degenerate states. Here is a different Hamiltonian for the same 3-level system:

$$\mathbf{H} = V_0 \begin{pmatrix} (1-\varepsilon) & 0 & 0 \\ 0 & 2 & \varepsilon \\ 0 & \varepsilon & 2 \end{pmatrix}$$ where V_0 is set to 1 (poof!) by an ingenious choice of units.

(a) Write down the eigenvalues of the unperturbed part, H_0, of the Hamiltonian.

(b) Find the exact eigenvalues E_1, E_2, and E_3 of the full Hamiltonian, H.

(c) Apply our standard, non-degenerate-PT formulae to read off the energy corrections to all three states at first order in ε. Do they give the correct results this time?

(d) No they do not! WHY NOT?

(e) This time, we *do* have to apply our degenerate-PT prescription to obtain 1st order corrections for the degenerate states #2 and #3. Do that!

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[2] **Q2** (a) $E^{(0)}_{1,2,3} = 1, 2, 2$ (b) exact eigenvalues are $E_{1,2,3} = 1-\varepsilon,\ 2-\varepsilon,\ 2+\varepsilon \rightarrow$ this time all corrections are exactly 1st order in ε

(c) correcting to 1st order, $E_1 \approx E_1^{(0)} + H'_{11} = 1-\varepsilon$ ✔ ... $E_2 \approx E_2^{(0)} + H'_{22} = 2+0 = 2$ ✘ ... $E_3 \approx E_3^{(0)} + H'_{33} = 2+0 = 2$ ✘

(d) The perturbation H' is not diagonal this time in the degenerate subspace of $\{ |\text{state}\,\#2\rangle, |\text{state}\,\#3\rangle \}$,
i.e. the off-diagonal matrix elements H'_{23} and H'_{32} within this subspace are NOT zero.

(e) Focus on the degenerate subspace D=$\{ |2\rangle, |3\rangle \}$ ... Within this subspace, the perturbing matrix H' is $\begin{pmatrix} H'_{22} & H'_{23} \\ H'_{32} & H'_{33} \end{pmatrix} = \begin{pmatrix} 2 & \varepsilon \\ \varepsilon & 2 \end{pmatrix}$
... We must find a **new basis** $\{ |\beta_2\rangle, |\beta_3\rangle \}$ for the subspace D that **diagonalizes** this 2×2 matrix ...

To diagonalize a matrix, find its **eigenvectors** and use them as your new basis ...

The eigenvectors of $H'_D = \begin{pmatrix} 2 & \varepsilon \\ \varepsilon & 2 \end{pmatrix}$ are $\sim \begin{pmatrix} \pm 1 \\ 1 \end{pmatrix}$ with eigenvalues $2 \pm \varepsilon$ ...

When the matrix $\begin{pmatrix} 2 & \varepsilon \\ \varepsilon & 2 \end{pmatrix}$ is expressed *in its own eigen-basis* $\{ |\beta_2\rangle, |\beta_3\rangle \} = \frac{1}{\sqrt{2}} \left\{ \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 1 \end{pmatrix} \right\}$, it will be diagonal with its eigenvalues as its diagonal elements (I hope this is becoming obvious; if not, ask!!!) ... it will become $\begin{pmatrix} 2+\varepsilon & 0 \\ 0 & 2-\varepsilon \end{pmatrix}$ ...

Now return to the full 3-dimensional space of our system, what basis vectors are we switching to? ...

Only the degenerate subspace D=$\{ |2\rangle, |3\rangle \}$ is altered, $|1\rangle$ is left unchanged ...

Our **new basis vectors** for the system are $\{ |1\rangle, |\beta_2\rangle, |\beta_3\rangle \} = \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix} \right\}$ ...

What is the Hamiltonian matrix in the new basis? ... $H = \begin{pmatrix} 1-\varepsilon & 0 & 0 \\ 0 & 2+\varepsilon & 0 \\ 0 & 0 & 2-\varepsilon \end{pmatrix} \rightarrow H_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$ & $H' = \begin{pmatrix} -\varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & -\varepsilon \end{pmatrix}$

What are the 1st-order energy corrections? ... $E_1 \approx E_1^{(0)} + H'_{11} = 1-\varepsilon$, similarly $E_2 \approx 2+\varepsilon$ and $E_3 \approx 2-\varepsilon$ ✔ matches exact (b)

Problem 3 : Qual Time! A Second-Order Perturbation Theory Problem

A particle moves in a 3D SHO with potential energy $V(r)$. A weak perturbation $\delta V(x,y,z)$ is applied:

$$V(r) = \frac{m\omega^2}{2}\left(x^2 + y^2 + z^2\right) \qquad \text{and} \qquad \delta V(x,y,z) = U\,xyz + \frac{U^2}{\hbar\omega}x^2y^2z^2$$

where U is a small parameter. Use perturbation theory to calculate the <u>change</u> in the <u>ground state energy</u> to order $O(U^2)$. Use without proof all the results you like from the 1D SHO → see supplementary file on website.

——————— **Formulae** for perturbative corrections to **non-degenerate states** ———————

- "zeroth-order" Hamiltonian H_0 has <u>exact</u> eigenvalues $\left\{E_n^{(0)}\right\}$ and eigenstates $\left\{\left|n^{(0)}\right\rangle\right\}$
- *actual* Hamiltonian $H = H_0 + H'$ where H' is a <u>small correction</u> to H_0 (a "<u>perturbation</u>", $H' \ll H_0$)
- series expansion of H eigenvalues: $E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \ldots$ for each n, where $E_n^{(0)} \gg E_n^{(1)} \gg E_n^{(2)} \gg \ldots$
- series expansion of H eigenstates: $|n\rangle = \left|n^{(0)}\right\rangle + \left|n^{(1)}\right\rangle + \left|n^{(2)}\right\rangle + \ldots$ for each n, where $\left|n^{(0)}\right\rangle \gg \left|n^{(1)}\right\rangle \gg \ldots$

As long as the unperturbed eigenstates $\left\{\left|n^{(0)}\right\rangle\right\}$ are **non-degenerate** and the Hamiltonian $H = H_0 + H'$ has **no explicit time-dependence**, the corrections to the energy eigenvalues E_n and eigenstates $|n\rangle$ are given by

- $\boxed{E_n^{(1)} = \left\langle n^{(0)}\middle|H'\middle|n^{(0)}\right\rangle}$ = expectation value of H' in the n^{th} unperturbed state = matrix element H'_{nn}
- $\boxed{\left|n^{(1)}\right\rangle = \sum_{m\neq n}\frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}}\left|m^{(0)}\right\rangle}$ where H'_{mn} is the matrix element $\left\langle m^{(0)}\middle|H'\middle|n^{(0)}\right\rangle$
- $\boxed{E_n^{(k)} = \left\langle n^{(0)}\middle|H'\middle|n^{(k-1)}\right\rangle}$ for higher orders ... which gives $E_n^{(2)} = \left\langle n^{(0)}\middle|H'\middle|n^{(1)}\right\rangle = \sum_{m\neq n}\frac{\left|H'_{mn}\right|^2}{E_n^{(0)} - E_m^{(0)}}$