Phys 487 Discussion 7 – Degenerate Perturbation Theory

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

• The New Stuff : **The Procedure** for dealing with **degenerate states** is as follows :

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 ε << 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 { α1, α2, α3, …, αn }. 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 $\left(\mathbf{H}_0\right)_{mn} \equiv \left\langle m^{(0)}\right| \hat{H}_0 \left|n^{(0)}\right\rangle$:

$$\mathbf{H}_0 = \begin{pmatrix} E_1^{(0)} & & & & & \\ & E_2^{(0)} & & & & \\ & & \boldsymbol{E_\alpha} & & & \\ & & & \boldsymbol{E_\alpha} & & \\ & & & & E_5^{(0)} & \\ & & & & & \ddots \end{pmatrix}$$ 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 $\left\{ \left|\alpha_1^{(0)}\right\rangle, ..., \left|\alpha_n^{(0)}\right\rangle \right\}$, 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 | α_i >'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 | α_i 〉's, i.e. within the degenerate subspace, that **diagonalizes the perturbation matrix** $\left(\mathbf{H}'\right)_{ij} \equiv \left\langle i^{(0)}\right| \hat{H}' \left| j^{(0)}\right\rangle$.

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

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

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 that we will immediately set to 1 for convenience and ε is a small number << 1.

Part the First : The Exact Spectrum

(a) Calculate the exact eigenvalues E_1, E_2, and E_3 of the Hamiltonian **H** without using any perturbation-theory formulae at all. As shown in class, wolframalpha will readily do this for you using the command

`eigenvalues { { a, b, c}, { d, e, f }, { g, h, i} }`

where the letters are the matrix elements. Next, expand each of them as a power series in ε, up to second order. Of course Taylor expansions are so! enjoyable! that you will have no need for the command

`expand` *function_of_x* `around x=0`

Part the Second : The Perturbative Approximation

Now use first- and second-order non-degenerate perturbation theory (formulae on the back page) to find the approximate eigenvalues of the Hamiltonian **H**. You will proceed in steps:

(b) Separate **H** into a dominant "unperturbed" part $\mathbf{H_0}$ plus a small perturbation $\mathbf{H'}$. Next, write down the eigenvalues $E_1^{(0)}, E_2^{(0)}, E_3^{(0)}$ and eigenvectors $|1^{(0)}\rangle, |2^{(0)}\rangle, |3^{(0)}\rangle$ of the unperturbed Hamiltonian.

(c) Those were the "0th order" terms in the energy spectrum. Now use 1st- and 2nd-order non-degenerate perturbation theory (formulae are on the back page) to find the approximate eigenvalue for state #3. Does it match the exact value from (a) to 2nd order in the small quantity ε?

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[1] **Q1** (a) exact eigenvalues of H Taylor-approximated to order ε^2 are : $E_1 = 1 - \varepsilon$, $E_2 \approx 1 - \varepsilon^2$, $E_3 \approx 2 + \varepsilon^2$

(b) $\mathbf{H}_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$, $\mathbf{H'} = \begin{pmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{pmatrix}$. Since $\mathbf{H}_0$ is diagonal, it is written in terms of its own eigenvectors.

Turning those words around, the eigenvectors of $\mathbf{H}_0$ are the basis vectors in terms of which $\mathbf{H}_0$ is written:

$$\begin{matrix}\text{eigen-}\\\text{vector}\end{matrix} |1^{(0)}\rangle \text{ of } H_0 = \begin{matrix}\text{basis}\\\text{vector}\end{matrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |2^{(0)}\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |3^{(0)}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

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

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

(d) Correcting to 1st order only, $E_1^{(0)+(1)} = E_1^{(0)} + H'_{11} = 1 - \varepsilon$ ✔ and $E_2^{(0)+(1)} = E_2^{(0)} + H'_{22} = 1 + 0 = 1$ ✔

(e) State #3 is NON-degenerate at 0th order, while states #2 and #1 are degenerate. The 2nd order correction formula for energy #1 or energy #2 would involve a term with $E_1^{(0)} - E_2^{(0)} = 0$ in the denominator → a divide-by-zero error.

(d) Now apply the 1st-order non-degenerate PT formula to find the approximate eigenvalues for states #1 & #2. (Don't calculate the 2nd order correction this time.) Do the non-degenerate formulae work give the correct energy corrections for states #1 and #2 to 1st order in ε?

If you are surprised at your result, hang on, we'll revisit it in the next question.

(e) What is special about state #3 that allows us to compute its 2nd-order energy correction using the back-page formulae, while we cannot do so for states #1 & #2?

Problem 2 : That was kind of surprising … now try this: *Checkpoints* [2]

Here is a slightly 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. Feel free to use wolframalpha.

(c) Apply the 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?

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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. In contrast, in question 1 the perturbation H′ was already diagonal 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 that subspace were zero.
(e) Focus on the degenerate subspace D=$\{ |2\rangle, |3\rangle \}$ … Within this subspace, the perturbing matrix H' is $\begin{pmatrix} H'_{22} & H'_{23} \\ H'_{32} & H'_{33} \end{pmatrix} = \begin{pmatrix} 0 & \varepsilon \\ \varepsilon & 0 \end{pmatrix}$
… 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 $H'_D = \begin{pmatrix} 0 & \varepsilon \\ \varepsilon & 0 \end{pmatrix}$ are ~$\begin{pmatrix} \pm 1 \\ 1 \end{pmatrix}$ with eigenvalues $2 \pm \varepsilon$
… When the matrix $\begin{pmatrix} 0 & \varepsilon \\ \varepsilon & 0 \end{pmatrix}$ 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 $\begin{pmatrix} \varepsilon & 0 \\ 0 & -\varepsilon \end{pmatrix}$
… 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's the Hamiltonian 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)

(d) No they do not! WHY NOT? And why did the 1st order formulae work just fine in Question 1, where we ALSO had a pair of degenerate levels. What was different there?

(e) So this time, we must apply our degenerate-PT prescription to obtain 1st order corrections for the degenerate states #2 and #3. Do that! Your first task is to immediately **extract the degenerate subspace** from the full problem --> extract rows & columns #2 & #3 from the matrices H_0 and H', producing 2×2 sub-matrices. Once you have those two sub-matrices, follow the procedure we went through in the 2×2 example in class (see the lecture notes), or as described on the first page of this discussion. A list of progressive hints / steps is also provided in the footnote for this question. If you *really* don't want to do any matrix manipulations by hand, you might try out the wolframalpha command `diagonalize`; if you compare its output to the matrix-transformation formulae from the lecture notes, you will see that the matrix "S" it spits out is the "R^{-1}" matrix from the notes, with columns equal to the eigenvectors of the input matrix (which it calls "M"). At the end of your work, you should have 1st-order energy corrections for states #2 and #3 that do match the exact values.

(f) We have so far only on tested the PT corrections to the *eigenvalues* against the exact results we obtained from wolframalpha. What about the *eigenvectors*? The new basis vectors you found in (e) by diagonalizing H' within the degenerate subspace $\{\#2, \#3\}$ should be the actual eigenvectors of the full $H = H_0 + H'$, accurate to first order in ε. Let's check. When you use wolframalpha's `eigenvalues` command, it usually gives you both eigenvalues and eigenvectors; otherwise, try the `eigenvectors` command. Verify that your new basis from part (e) does indeed match the exact eigenvectors of H, at least to 1st order in ε.

Problem 3 : 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 change in the ground state energy to order $O(U^2)$. Use without proof all the results you like from the 1D SHO → see **Formulae-SHO-reference.pdf** on our website for the full collection.

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

- "zeroth-order" Hamiltonian H_0 has exact 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 small correction to H_0 (a "perturbation", $H' \ll H_0$)
- 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

- $\boxed{E_n^{(1)} = \left\langle n^{(0)}\middle|H'\middle|n^{(0)}\right\rangle = H'_{nn}}$ = expectation value of H' in the n^{th} unperturbed state
- $\boxed{\left|n^{(1)}\right\rangle = \sum_{m\neq n}\frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}}\left|m^{(0)}\right\rangle}$ 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 $\boxed{E_n^{(2)} = \sum_{m\neq n}\frac{\left|H'_{mn}\right|^2}{E_n^{(0)} - E_m^{(0)}}} = \left\langle n^{(0)}\middle|H'\middle|n^{(1)}\right\rangle$