

Basics of Degenerate Perturbation Theory - Finite Dimensional Spaces

1 Definition

For a given \hat{H}^0 and \hat{H}' , a “good” basis consists of a set of eigenstates of \hat{H}^0 that diagonalizes \hat{H}' in the degenerate subspace of \hat{H}^0 (keeping \hat{H}^0 diagonal everywhere).

- Once you have a “good” basis for a given \hat{H}^0 and \hat{H}' , you can use the same expressions that you use in non-degenerate perturbation theory for the perturbative corrections to the energies and energy eigenstates.

2 Notes for this tutorial on Degenerate Perturbation Theory:

- * A Hermitian operator \hat{Q} must satisfy the property $Q_{ij} = (Q_{ji})^*$. Here * denotes the complex conjugate
- * For the matrix representation of a Hermitian operator \hat{Q} in a given basis, we will use “=” or “is equal to” instead of “ \doteq ” or “is represented by” as in the notation below

$$\hat{Q} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix} \text{ is equivalent to } \hat{Q} \doteq \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}.$$

- * Since both \hat{H}^0 and \hat{H}' correspond to physical observables, \hat{H}^0 and \hat{H}' must be Hermitian. For the matrix representations of the unperturbed Hamiltonian \hat{H}^0 and perturbing Hamiltonian \hat{H}' in a given basis, we have

$$\hat{H}^0 = V_0 \begin{pmatrix} a & b & c \\ b^* & e & f \\ c^* & f^* & i \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} a' & b' & c' \\ b'^* & e' & f' \\ c'^* & f'^* & i' \end{pmatrix}.$$

- * In this tutorial, “degeneracy” denotes degeneracy in the energy eigenvalue spectrum, i.e., the fact that more than one distinct energy eigenstate can have the same energy eigenvalue. For example, if

$$\hat{H}^0|\psi_a\rangle = E_1|\psi_a\rangle \quad \text{and} \quad \hat{H}^0|\psi_b\rangle = E_1|\psi_b\rangle,$$

$|\psi_a\rangle$ and $|\psi_b\rangle$ are degenerate eigenstates for the Hamiltonian \hat{H}^0 since they correspond to the same energy E_1 .

- * Assume that the initially chosen basis states $\{|\psi_1^0\rangle, |\psi_2^0\rangle, |\psi_3^0\rangle\}$ are always eigenstates of the unperturbed Hamiltonian \hat{H}^0 whether or not they are “good” basis states for a given pair \hat{H}^0 and \hat{H}' .
- * Assume that all basis states are orthonormal (normalized and orthogonal).

3 Objectives

Upon completion of this tutorial, you should be able to do the following:

1. For a given \hat{H}^0 and \hat{H}' , describe why the expressions may fail for finding corrections to the energies and energy eigenstates from non-degenerate perturbation theory when there is degeneracy in the unperturbed energy if the basis states are not chosen correctly.
 - (a) For a given \hat{H}^0 and \hat{H}' , describe the problem that may occur when the expressions from non-degenerate perturbation theory are used if the basis states are not chosen carefully and how the problem can be addressed by choosing a “good” basis.
 - (b) Identify the degenerate subspace of the unperturbed Hamiltonian \hat{H}^0 .
 - (c) Show that the off-diagonal matrix elements of \hat{H}' must be zero in the degenerate subspace of \hat{H}^0 when “good” basis states are chosen.
2. For a given \hat{H}^0 and \hat{H}' , determine “good” states for finding corrections to the unperturbed energy.
 - (a) Show that in the subspace in which \hat{H}^0 does not have a degeneracy, the originally chosen basis states are “good” basis states since the eigenstates of \hat{H}^0 are unique in the subspace in which there is no degeneracy.
 - (b) Show that the basis states in the subspace in which \hat{H}^0 has degeneracy may or may not be “good” basis states for a given \hat{H}' .
 - i. Show that if \hat{H}' is already diagonal in the degenerate subspace of \hat{H}^0 , the initially chosen energy eigenstates of the unperturbed Hamiltonian \hat{H}^0 already are “good” states.
 - ii. Show that if \hat{H}' is NOT diagonal in the degenerate subspace of \hat{H}^0 , the initially chosen energy eigenstates of the unperturbed Hamiltonian \hat{H}^0 are NOT “good” states.
 - A. Demonstrate that linear combinations of the eigenstates of \hat{H}^0 are still eigenstates of \hat{H}^0 in the degenerate subspace of \hat{H}^0 and we can make use of this fact to diagonalize both \hat{H}^0 and \hat{H}' in the degenerate subspace of \hat{H}^0 .
 - B. Find “good” basis states by diagonalizing \hat{H}' in the degenerate subspace of \hat{H}^0 .
 - C. Show that in a “good” basis (in which \hat{H}' is diagonal in the degenerate subspace of \hat{H}^0), \hat{H}^0 remains diagonal.
 - D. Explain why it is necessary to choose a basis that keeps the unperturbed Hamiltonian \hat{H}^0 diagonal (basis states are eigenstates of \hat{H}^0 , i.e. we need to find perturbative corrections to the energies using a basis in which \hat{H}^0 is diagonal).
 - (c) Calculate corrections to the unperturbed energies and energy eigenstates when \hat{H}^0 has degeneracy.
 - (d) Describe why we must diagonalize \hat{H}' only in the degenerate subspace of \hat{H}^0 (instead of diagonalizing the entire \hat{H}' matrix).
 - i. Demonstrate that diagonalizing the entire \hat{H}' matrix makes the \hat{H}^0 matrix non-diagonal if \hat{H}^0 and \hat{H}' don't commute (we cannot find a complete set of simultaneous eigenstates of \hat{H}^0 and \hat{H}' when they don't commute).
 - Note that if two operators commute, in the basis consisting of a complete set of simultaneous eigenstates of both, each operator is diagonal (however, if there is degeneracy in the eigenvalue spectrum of one or both operators then all eigenstates of one operator may not be eigenstates of another and both operators may not be diagonal in that basis, but it is possible to find a complete set of simultaneous eigenstates of both).

4 Review of Non-Degenerate Perturbation Theory

In perturbation theory, for the case in which the unperturbed Hamiltonian \hat{H}^0 has NO degeneracy:

- the first order corrections to the energies are

$$E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle \quad (1)$$

- the first order corrections to the energy eigenstates are

$$|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} |\psi_m^0\rangle \quad (2)$$

in which $\{|\psi_n^0\rangle\}$ is the set of energy eigenstates of the unperturbed Hamiltonian \hat{H}^0 .

5 Degenerate Perturbation Theory

5.1 Degeneracy in the Eigenvalue Spectrum of \hat{H}^0 Requires Finding a “GOOD” Basis to Determine Corrections to the Energies and Energy Eigenstates

If there is degeneracy in the eigenvalue spectrum of \hat{H}^0 , are equations (1) and (2) still valid for a given perturbation \hat{H}' ? If so, in which situations are they valid? Explain any constraints on the basis states.

Use the following two examples to help answer these questions.

5.1.1 CASE 1: First Order Corrections to the Energy when \hat{H}' IS DIAGONAL IN THE DEGENERATE SUBSPACE of \hat{H}^0

EXAMPLE 1: Consider the following example, in which the Hilbert space is three dimensional and ϵ is a small parameter ($\epsilon \ll 1$). Answer questions 1-6.

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} \epsilon & 2\epsilon & 0 \\ 2\epsilon & \epsilon & 0 \\ 0 & 0 & 3\epsilon \end{pmatrix} \quad (3)$$

The normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (4)$$

1. The basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ are eigenstates of

- (A) \hat{H}^0 only
- (B) \hat{H}' only
- (C) Both \hat{H}^0 and \hat{H}'
- (C) Neither \hat{H}^0 nor \hat{H}'

Explain your reasoning.

2. Does \hat{H}^0 have degeneracy? Why or why not?

3. Choose one of the following options to fill in the blank. In the degenerate subspace of \hat{H}^0 , the matrix representation of \hat{H}^0 is _____ and the matrix representation of \hat{H}' is _____, respectively.

(A)

$$V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad V_0 \begin{pmatrix} \epsilon & 2\epsilon \\ 2\epsilon & \epsilon \end{pmatrix}$$

(B)

$$V_0 \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}, \quad V_0 \begin{pmatrix} \epsilon & 0 \\ 0 & 3\epsilon \end{pmatrix}$$

(C)

$$V_0 \begin{pmatrix} \epsilon & 2\epsilon \\ 2\epsilon & \epsilon \end{pmatrix}, \quad V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$

(D)

$$V_0 \begin{pmatrix} \epsilon & 0 \\ 0 & 3\epsilon \end{pmatrix}, \quad V_0 \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

4. Do the basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ form a “good” basis? Explain.

Consider the following conversation regarding whether the initially chosen basis is a “good” basis in EXAMPLE 1.

Student 1: In EXAMPLE 1, in the degenerate subspace of \hat{H}^0 , the perturbing Hamiltonian \hat{H}' is $V_0 \begin{pmatrix} \epsilon & 0 \\ 0 & 3\epsilon \end{pmatrix}$. So we can use equations (1) and (2) from non-degenerate perturbation theory to find the corrections to the energies and energy eigenstates.

Student 2: How can we use equation (2) when the unperturbed energies are degenerate with $E_2^0 = E_3^0 = 2V_0$? In equation (2), the first order corrections to the energy eigenstates $|\psi_2^0\rangle$ and $|\psi_3^0\rangle$ is undefined as the denominator is zero!

Student 3: Since \hat{H}' is diagonal in the degenerate subspace of \hat{H}^0 in equation (3), we can use equations (1) and (2). Since $\langle \psi_2^0 | \hat{H}' | \psi_3^0 \rangle = 0$ and $\langle \psi_3^0 | \hat{H}' | \psi_2^0 \rangle = 0$, the undefined terms that “blow up” do not appear in equation (2).¹

Explain why you agree or disagree with each student.

¹Please note that once we have a good basis, we do not have 0/0 terms present in Eq. 2.

5. The first order corrections to the energies are

(A) $E_1^1 = \epsilon V_0$, $E_2^1 = \epsilon V_0$, and $E_3^1 = 3\epsilon V_0$.

(B) $E_1^1 = \epsilon V_0$, $E_2^1 = 2\epsilon V_0$, and $E_3^1 = 0$.

(C) $E_1^1 = 2\epsilon V_0$, $E_2^1 = \epsilon V_0$, and $E_3^1 = 3\epsilon$.

(D) $E_1^1 = 0$, $E_2^1 = 0$, and $E_3^1 = 0$.

(E) None of the above

6. The first order corrections to the energy eigenstates are

(A) $|\psi_1^1\rangle = 2\epsilon V_0|\psi_2^0\rangle + 0|\psi_3^0\rangle$, $|\psi_2^1\rangle = 2\epsilon V_0|\psi_1^0\rangle + \epsilon V_0|\psi_3^0\rangle$, and $|\psi_3^1\rangle = 0|\psi_1^0\rangle + \epsilon V_0|\psi_2^0\rangle$.

(B) $|\psi_1^1\rangle = -2\epsilon|\psi_2^0\rangle + 0|\psi_3^0\rangle$, $|\psi_2^1\rangle = 2\epsilon|\psi_1^0\rangle + 0|\psi_3^0\rangle$ and $|\psi_3^1\rangle = 0$.

(C) $|\psi_1^1\rangle = 0$, $|\psi_2^1\rangle = 0$, and $|\psi_3^1\rangle = \epsilon V_0|\psi_1^0\rangle$.

(D) None of the above.

**** Check your answers to questions 1-6 in EXAMPLE 1. ****

1. A ($|\psi_3^0\rangle$ is an eigenstate of both \hat{H}^0 and \hat{H}' , however $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ are only eigenstates of \hat{H}^0 .)
2. Yes. $\hat{H}^0|\psi_2^0\rangle = 2V_0|\psi_2^0\rangle$ and $\hat{H}^0|\psi_3^0\rangle = 2V_0|\psi_3^0\rangle$.
3. B
4. Yes.
5. A
6. B

If your answers to questions 1-6 do not match with the checkpoint for EXAMPLE 1, go back and reconcile any differences.

Checkpoint

- In order to find the first order corrections to the energies and energy eigenstates using equations (1) and (2), **the basis set $\{|\psi_n^0\rangle\}$ in equations (1) and (2) must be “good” states** (\hat{H}^0 is diagonal everywhere since the basis states are eigenstates of \hat{H}^0 and \hat{H}' must be diagonal in the degenerate subspace of \hat{H}^0 in that basis).

- If \hat{H}' is already diagonal in the degenerate subspace of \hat{H}^0 :
 - The initially chosen basis states make up a “good” basis.

 - The expression $E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle$ CAN be used to find corrections to the energies since $\{|\psi_n^0\rangle\}$ are “good” states.

 - The expression $|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{E_n^0 - E_m^0} |\psi_m^0\rangle$ CAN be used to find the first order corrections $|\psi_n^1\rangle$ to the energy eigenstates $|\psi_n^0\rangle$ since $\{|\psi_n^0\rangle\}$ are “good” states and the divergent terms (that “blow up”) do not appear in equation (2).

5.1.2 CASE 2: Corrections to the Energies and Energy Eigenstates when \hat{H}' is not Diagonal in the Degenerate Subspace of \hat{H}^0

EXAMPLE 2: Consider a second example, in which ϵ is a small parameter ($\epsilon \ll 1$), and answer questions 7-10:

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & -4\epsilon \\ \epsilon & 2\epsilon & 0 \\ -4\epsilon & 0 & 2\epsilon \end{pmatrix} \quad (5)$$

The normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (6)$$

7. The basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ are eigenstates of

- (A) \hat{H}^0 only
- (B) \hat{H}' only
- (C) Both \hat{H}^0 and \hat{H}'
- (C) Neither \hat{H}^0 nor \hat{H}'

Explain your reasoning.

8. Does \hat{H}^0 have degeneracy? Why or why not?

9. Choose one of the following options to fill in the blank. In the degenerate subspace of \hat{H}^0 , the matrix representation of \hat{H}^0 is _____ and the matrix representation of \hat{H}' is _____, respectively.

(A)

$$V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad V_0 \begin{pmatrix} 2\epsilon & 0 \\ 0 & 2\epsilon \end{pmatrix}$$

(B)

$$V_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad V_0 \begin{pmatrix} 0 & \epsilon \\ \epsilon & 2\epsilon \end{pmatrix}$$

(C)

$$V_0 \begin{pmatrix} 0 & \epsilon \\ \epsilon & 2\epsilon \end{pmatrix}, \quad V_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(D)

$$V_0 \begin{pmatrix} 2\epsilon & 0 \\ 0 & 2\epsilon \end{pmatrix}, \quad V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$

10. Do the basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ form a “good” basis? Explain.

Consider the following conversation regarding whether the initially chosen basis is or is not a “good” basis in EXAMPLE 2.

Student 1: In EXAMPLE 2, we can use equations (1) and (2) obtained from non-degenerate perturbation theory.

Student 2: We cannot use equation (2) when the unperturbed states are degenerate with $E_1^0 = E_2^0 = V_0$. In the degenerate subspace of \hat{H}^0 , the perturbing Hamiltonian \hat{H}' is $V_0 \begin{pmatrix} 0 & \epsilon \\ \epsilon & 2\epsilon \end{pmatrix}$. The first order corrections to the energy eigenstates $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ “blow up” because the denominators are zero! However, we can use equation (1) to calculate the corrections to the energies since nothing in that equations “blows up.”

Student 3: If \hat{H}' is not diagonal in the degenerate subspace of \hat{H}^0 , we can neither use equation (1) nor (2) in the chosen basis $\{|\psi_1^0\rangle, |\psi_2^0\rangle, |\psi_3^0\rangle\}$. The initially chosen basis is not a “good” basis. We need to find a “good” basis in order to use equations (1) and (2).

Student 4: Student 3 is right. The first order corrections to the energy eigenstates $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ “blow up”, we cannot use these basis states to find even the first order corrections to the energies using equation (1).

Explain why you agree or disagree with each student.

**** Check your answers to questions 7-10 in EXAMPLE 2. ****

7. A
8. Yes. $\hat{H}^0|\psi_1^0\rangle = V_0|\psi_1^0\rangle$ and $\hat{H}^0|\psi_2^0\rangle = V_0|\psi_2^0\rangle$.
9. B
10. No.

If your answers to questions 7-10 do not match with the checkpoint for EXAMPLE 2, go back and reconcile any differences.

EXAMPLE 2 Revisited

For the following four conversations, consider Example 2 again in which equations (1) and (2) could not be used with the initial basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$. Recall that in EXAMPLE 2, the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}'$ is given by:

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & -4\epsilon \\ \epsilon & 2\epsilon & 0 \\ -4\epsilon & 0 & 2\epsilon \end{pmatrix} \quad (7)$$

and the basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, for which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (8)$$

Consider the following conversation regarding whether the basis states are “good” in EXAMPLE 2.

Student 1: In this case, we can calculate the first order corrections to the energies as $E_1^1 = \langle \psi_1^0 | \hat{H}' | \psi_1^0 \rangle = 0$ and $E_2^1 = \langle \psi_2^0 | \hat{H}' | \psi_2^0 \rangle = 2\epsilon V_0$.

Student 2: I disagree. \hat{H}^0 has a two-fold degeneracy, since $\hat{H}^0|\psi_1^0\rangle = V_0|\psi_1^0\rangle$ and $\hat{H}^0|\psi_2^0\rangle = V_0|\psi_2^0\rangle$. We cannot use the basis states $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ to calculate even the first order corrections to the energies because \hat{H}' is not diagonal in the degenerate subspace of \hat{H}^0 . $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ are not “good” basis states.

Student 1: I see. If \hat{H}^0 has a degenerate eigenvalue spectrum, the expression $E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle$ requires that the chosen basis states are “good” basis states, which is not the case for the initially chosen eigenstates $\{|\psi_1^0\rangle, |\psi_2^0\rangle, \text{ and } |\psi_3^0\rangle\}$ of \hat{H}^0 .

Explain why you agree or disagree with the students.

Consider the following conversation regarding finding the corrections to energy eigenstates using “good” basis states in EXAMPLE 2.

Student 1: In EXAMPLE 2, \hat{H}^0 has a two-fold degeneracy since $\hat{H}^0|\psi_1^0\rangle = V_0|\psi_1^0\rangle$ and $\hat{H}^0|\psi_2^0\rangle = V_0|\psi_2^0\rangle$. We cannot calculate the first order corrections to the energy eigenstates using $|\psi_1^0\rangle$, $|\psi_2^0\rangle$ or $|\psi_3^0\rangle$ in equation (2).

Student 2: I agree that we cannot calculate first order corrections to the energy eigenstates $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$. The first order corrections to the energy eigenstates in equation (2) “blow up”, i.e.,

$$|\psi_1^1\rangle = \frac{\langle\psi_2^0|\hat{H}'|\psi_1^0\rangle}{(E_1^0 - E_2^0)}|\psi_2^0\rangle + \frac{\langle\psi_3^0|\hat{H}'|\psi_1^0\rangle}{(E_1^0 - E_3^0)}|\psi_3^0\rangle = \frac{\epsilon V_0}{0}|\psi_2^0\rangle + \frac{-4\epsilon V_0}{-V_0}|\psi_3^0\rangle$$

and

$$|\psi_2^1\rangle = \frac{\langle\psi_1^0|\hat{H}'|\psi_2^0\rangle}{(E_2^0 - E_1^0)}|\psi_1^0\rangle + \frac{\langle\psi_3^0|\hat{H}'|\psi_2^0\rangle}{(E_2^0 - E_3^0)}|\psi_3^0\rangle = \frac{\epsilon V_0}{0}|\psi_1^0\rangle + \frac{0}{-V_0}|\psi_3^0\rangle.$$

Student 3: I agree with both Student 1 and Student 2. But we can calculate the first order corrections to the energy eigenstates if we first select “good” basis states. $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ are not “good” states since the \hat{H}' matrix is not diagonal in the degenerate subspace of \hat{H}^0 . So $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ cannot be used to find the first order corrections to the energy eigenstates using equation (2). We need to first choose a different basis that is “good” so terms that “blow up” in the corrections $|\psi_1^1\rangle$ and $|\psi_2^1\rangle$ are not present.

Explain why you agree or disagree with each student.

Summarize in one to three sentences what you learned from the previous two conversations.

Consider the following conversation regarding whether one can trust the corrections to the non-degenerate eigenvalues of \hat{H}^0 if some of the basis states are not “good” basis states in EXAMPLE 2.

Student 1: What about the first order correction to E_3 in EXAMPLE 2? Can we trust $E_3^1 = \langle \psi_3^0 | \hat{H}' | \psi_3^0 \rangle$ even if \hat{H}' is not diagonal in the degenerate subspace of \hat{H}^0 ?

Student 2: No, we cannot trust it because \hat{H}^0 has degeneracy in EXAMPLE 2. We must find a “good” basis first before finding any corrections to any of the energies.

Student 3: Actually, in EXAMPLE 2 we can trust $E_3^1 = \langle \psi_3^0 | \hat{H}' | \psi_3^0 \rangle = 2\epsilon V_0$ to yield the first order correction to energy $E_3 = 2V_0$. Since $|\psi_3^0\rangle$ corresponds to the non-degenerate subspace of \hat{H}^0 , it is unique. $|\psi_3^0\rangle$ must already be a “good” state.

Do you agree with Student 2 or Student 3? Explain.

Consider the following conversation regarding first order corrections to the energy eigenstates in the non-degenerate subspace.

Student 1: For EXAMPLE 2, can we use the expression $|\psi_3^1\rangle = \frac{\langle \psi_1^0 | \hat{H}' | \psi_3^0 \rangle}{(E_3^0 - E_1^0)} |\psi_1^0\rangle + \frac{\langle \psi_2^0 | \hat{H}' | \psi_3^0 \rangle}{(E_3^0 - E_2^0)} |\psi_2^0\rangle = \frac{-4\epsilon V_0}{V_0} |\psi_1^0\rangle + \frac{0}{V_0} |\psi_2^0\rangle$ from non-degenerate perturbation theory to find the correction $|\psi_3^1\rangle$?

Student 2: Yes, that is correct. However, we can also determine the first order correction $|\psi_3^1\rangle$ by determining a “good” basis and using the “good” basis states in Eq. 2 **to find the first order correction to the energy eigenstate.**

Student 3: I agree with Student 2. In EXAMPLE 2, “good” basis states in the degenerate subspace of \hat{H}^0 will be the non-degenerate state $|\psi_3^0\rangle$ and two linear combinations of $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$. So a “good” basis will be

$$|\phi_1^0\rangle = \alpha_1 |\psi_1^0\rangle + \alpha_2 |\psi_2^0\rangle, \quad |\phi_2^0\rangle = \beta_1 |\psi_1^0\rangle + \beta_2 |\psi_2^0\rangle, \quad \text{and} \quad |\phi_3^0\rangle = |\psi_3^0\rangle$$

in which $\alpha_1, \alpha_2, \beta_1,$ and β_2 are the coefficients for obtaining a “good” orthonormal basis states which diagonalize \hat{H}' in the degenerate subspace of \hat{H}^0 . $\{|\phi_n^0\rangle\}$ are still eigenstates of \hat{H}^0 .

Student 4: I agree with Student 2 and Student 3. To find first order corrections to $|\phi_3^0\rangle = |\psi_3^0\rangle$, we must use a “good” basis. $|\psi_3^0\rangle$ is a “good” basis state. However, $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ are not “good” basis states. We must find “good” basis states $|\phi_1^0\rangle$ and $|\phi_2^0\rangle$ by diagonalizing the \hat{H}' matrix in the degenerate subspace of \hat{H}^0 to calculate the first order correction to $|\psi_3^0\rangle$. Once we have the “good” basis, we use equation (2) to find the first order correction to $|\psi_3^0\rangle$:

$$|\psi_3^1\rangle = \frac{\langle \phi_1^0 | \hat{H}' | \phi_3^0 \rangle}{(E_3^0 - E_2^0)} |\phi_1^0\rangle + \frac{\langle \phi_2^0 | \hat{H}' | \phi_3^0 \rangle}{(E_3^0 - E_1^0)} |\phi_2^0\rangle.$$

Explain why you agree or disagree with Student 2, Student 3, and Student 4.

Summarize in one to three sentences what you learned from the previous two conversations.

Summarize why care should be exercised in using perturbation theory if the unperturbed Hamiltonian \hat{H}^0 possesses degeneracy in the eigenvalue spectrum.

Describe the procedure to deal with the difficulty that arises when we can't use the initially chosen basis states to find perturbative corrections. What must we ensure about \hat{H}^0 and \hat{H}' to find the corrections to the energies (including first order corrections to the energies for the cases in which the given basis is not good even though the first order correction to the energies do not “blow up”)?

Checkpoint

- If the first-order corrections to the energy eigenstates “blow up,” we cannot even trust the first order corrections to the energies because the basis states are not “good.”

- If \hat{H}' is **NOT** diagonal in a degenerate subspace of \hat{H}^0 :
 - The initially chosen basis states do not make up a “good” basis (even though they are eigenstates of \hat{H}^0).

 - The expression $E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle$ **CANNOT** be used to find the corrections to energies if $|\psi_n^0\rangle$ is **NOT** a “good” basis state.

 - The expression $|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{E_n^0 - E_m^0} |\psi_m^0\rangle$ **CANNOT** be used in the degenerate subspace to find corrections to energy eigenstates if $\{|\psi_n^0\rangle\}$ are **NOT** “good” basis states.

5.1.3 A “good” basis depends on both \hat{H}^0 and \hat{H}' .

Consider the following conversation regarding whether choosing a “good” basis requires consideration of both \hat{H}^0 and \hat{H}' .

Student 1: In degenerate perturbation theory, for a given \hat{H}' , “good” basis states must be the eigenstates of the unperturbed Hamiltonian, \hat{H}^0 .

Student 2: I disagree. A “good” basis should diagonalize the \hat{H}' matrix but \hat{H}^0 need not be diagonal in that basis. The diagonal elements of the \hat{H}' matrix in a “good” basis give us the first order corrections to the energies.

Student 3: Actually, we need to consider both \hat{H}^0 and \hat{H}' when determining a “good” basis. A “good” basis will diagonalize \hat{H}' in the degenerate subspace of \hat{H}^0 while simultaneously keeping \hat{H}^0 diagonal. The entire \hat{H}^0 matrix must be diagonal in a “good” basis since the basis states must be eigenstates of \hat{H}^0 .

Explain why you agree or disagree with each student.

In the following example, note that the unperturbed Hamiltonian \hat{H}^0 is the same as the \hat{H}^0 given in EXAMPLE 2. However, the perturbing Hamiltonian \hat{H}' is not the same as the \hat{H}' given in EXAMPLE 2.

EXAMPLE 3: Consider the following example in a three dimensional Hilbert space, in which ϵ is a small parameter ($\epsilon \ll 1$):

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} \epsilon & 0 & 2\epsilon \\ 0 & -3\epsilon & \epsilon \\ 2\epsilon & \epsilon & -3\epsilon \end{pmatrix} \quad (9)$$

The normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (10)$$

Now consider the following conversation about EXAMPLE 3 focusing on the Degenerate Subspace of \hat{H}^0 .

Student 1: In EXAMPLE 3, the \hat{H}^0 matrix is the same as in EXAMPLE 2, so we will not be able to use equation (1) with the initial basis states $\{|\psi_n^0\rangle\}$ that are given to find the first order corrections to the energies. We also cannot use equation (2) to find the first order corrections to the energy eigenstates.

Student 2: I disagree. Actually, you must consider both \hat{H}^0 and \hat{H}' before deciding whether the basis is good and whether we can use equations (1) and (2) with that basis. Since \hat{H}' is diagonal in the degenerate subspace of \hat{H}^0 in EXAMPLE 3, equations (1) and (2) can be used with the given basis to find the first order corrections to the energies and energy eigenstates, respectively. This is just like EXAMPLE 1!

Do you agree with Student 1 or Student 2? Why?

11. What are the first order corrections to the unperturbed energies in EXAMPLE 3? (HINT: Refer to EXAMPLE 1.)

**** Check your results to question 11 in EXAMPLE 3: ****

11. $E_1^1 = \epsilon V_0$, $E_2^1 = -3\epsilon V_0$, and $E_3^1 = -3\epsilon V_0$

If your first order corrections to the energies do not match the checkpoint for EXAMPLE 3, go back and reconcile any differences you may have.

Checkpoint

- When determining a “good” basis, we need information about **both \hat{H}^0 and \hat{H}'** .
 - A “good” basis is one that diagonalizes \hat{H}' in the degenerate subspace of \hat{H}^0 while keeping \hat{H}^0 diagonal.

SUMMARY: To Find Corrections to the Energies and Energy Eigenstates
You Must Choose a “Good” Basis

- If the first-order corrections to the eigenstates “blow up,” we cannot even trust the first order corrections to the energies because the basis states may not be “good.”
- Choosing a “good” basis requires information about **both \hat{H}^0 and \hat{H}'** .
- In order to find the first order corrections to the energies and energy eigenstates using equations (1) and (2), **the basis set $\{|\psi_n^0\rangle\}$ used in equations (1) and (2) must be “good” states** (in such a basis, \hat{H}' must be diagonal in a degenerate subspace of \hat{H}^0 and \hat{H}^0 must be entirely diagonal).

CASE 1: \hat{H}' IS DIAGONAL IN THE DEGENERATE SUBSPACE OF \hat{H}^0 IN THE INITIAL BASIS.

- If \hat{H}' is **already diagonal in the degenerate subspace of \hat{H}^0** :
 - The initial basis states make up a “good” basis (note that since we choose basis states to be eigenstates of \hat{H}^0 , \hat{H}^0 is diagonal in the basis everywhere).
 - The expression $E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle$ **CAN** be used to find corrections to energies since all $\{|\psi_n^0\rangle\}$ are “good” states.
 - The expression $|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{E_n^0 - E_m^0} |\psi_m^0\rangle$ **CAN** be used to find the first order corrections to the energy eigenstates $|\psi_n^0\rangle$ as all $\{|\psi_n^0\rangle\}$ are “good” states.

CASE 2: \hat{H}' IS NOT DIAGONAL IN THE DEGENERATE SUBSPACE OF \hat{H}^0 IN THE INITIAL BASIS.

- If \hat{H}' is **NOT diagonal in the degenerate subspace of \hat{H}^0** :
 - The initially chosen basis states do not make up a “good” basis (even though they are eigenstates of \hat{H}^0).
 - The expression $E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle$ **CANNOT** be used to find corrections to energies associated with the degenerate states since $\{|\psi_n^0\rangle\}$ does **NOT** form a complete set of “good” basis states.
 - The expression $|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{E_n^0 - E_m^0} |\psi_m^0\rangle$ **CANNOT** be used to find corrections to energy eigenstates associated with the degenerate states since $\{|\psi_n^0\rangle\}$ is **NOT** a “good” set of basis states.
 - We must first choose a “good” basis!
- As you will demonstrate shortly, in the degenerate subspace of \hat{H}^0 , “good” basis states will be made up of linear combinations of the initially chosen eigenstates of \hat{H}^0 that diagonalize \hat{H}' in the degenerate subspace of \hat{H}^0 .

5.2 Ensuring a “good” basis and determining corrections to the energies and energy eigenstates.

5.2.1 CASE 1: First Order Corrections to the Energies when \hat{H}' IS DIAGONAL IN THE DEGENERATE SUBSPACE of \hat{H}^0

EXAMPLE 4: Answer the following questions for this example:

$$\hat{H}^0 = V_0 \begin{pmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} -\epsilon & 0 & 2\epsilon \\ 0 & -\epsilon & 3\epsilon \\ 2\epsilon & 3\epsilon & 0 \end{pmatrix} \quad (\epsilon \ll 1) \quad (11)$$

and the basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (12)$$

12. Does \hat{H}^0 have degeneracy? If so, circle the part of \hat{H}^0 and \hat{H}' in the degenerate subspace of \hat{H}^0 .
13. Use your answer to the previous part to explain whether the basis states chosen in equation (12), which are used to write \hat{H}^0 and \hat{H}' in equation (11), are “good” basis states or not.
14. If the given basis is not a “good” basis, find a “good” basis.
15. Determine the first order corrections to the unperturbed energies.
16. Find the first order corrections to the unperturbed energy eigenstates.

Consider the following conversation regarding \hat{H}' already being diagonal in the degenerate subspace of \hat{H}^0 in EXAMPLE 4.

Student 1: If we are given an \hat{H}' matrix that is already diagonal in the degenerate subspace of \hat{H}^0 as in equation (11), the basis is already “good.” We can simply read off the matrix elements of \hat{H}' along the diagonal in the degenerate subspace of \hat{H}^0 to obtain the first order corrections to the degenerate energies.

Student 2: I disagree. You must still diagonalize \hat{H}' in equation (11) in the degenerate subspace of \hat{H}^0 to find the first order corrections to the energies.

Student 3: It does not make sense to diagonalize \hat{H}' in the degenerate subspace of \hat{H}^0 if \hat{H}' is already diagonal in that subspace. You would be doing unnecessary work. Since \hat{H}' is already diagonal in that subspace, if you chose to diagonalize \hat{H}' , you would simply obtain the same matrix back with the same eigenvalues as long as you didn't make any mistakes along the way.

Student 1: I agree with Student 3. And when \hat{H}' is also diagonal in the degenerate subspace of \hat{H}^0 as in equation (11), “good” basis states are the initially chosen energy eigenstates of \hat{H}^0 , i.e., the basis states used to write \hat{H}^0 and \hat{H}' in equation (11).

Explain why you agree or disagree with each student.

**** Check your answers to questions 12-16 pertaining to EXAMPLE 4.****

12. \hat{H}^0 has a two-fold degeneracy. In the degenerate subspace of \hat{H}^0 , \hat{H}^0 is $V_0 \begin{pmatrix} 4 & 0 \\ 0 & 4 \end{pmatrix}$ and the

perturbation \hat{H}' is $V_0 \begin{pmatrix} -\epsilon & 0 \\ 0 & -\epsilon \end{pmatrix}$

13. Since \hat{H}' is already diagonal in the degenerate subspace of \hat{H}^0 , the set of initially chosen energy eigenstates of \hat{H}^0 in equation (11) form a “good” basis.

14 “Good” basis states are the initially chosen eigenstates of \hat{H}^0 , $\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$.

15. The first order corrections to the energies are $E_1^1 = -\epsilon V_0$, $E_2^1 = -\epsilon V_0$, and $E_3^1 = 0$.

16 The first order corrections to the energy eigenstates are $|\psi_1^1\rangle = \frac{2}{3}\epsilon|\psi_3^0\rangle$, $|\psi_2^1\rangle = \epsilon|\psi_3^0\rangle$, and $|\psi_3^1\rangle = -\frac{2}{3}\epsilon|\psi_1^0\rangle - \epsilon|\psi_2^0\rangle$.

If your “good” basis states and first order corrections to the energies and energy eigenstates for EXAMPLE 4 do not match with the checkpoint answers, go back and reconcile any differences you may have.

For the case in which \hat{H}' is diagonal in the degenerate subspace of \hat{H}^0 and basis states are eigenstates of \hat{H}^0 , summarize in one to two sentences why we can simply use equations (1) and (2) to find the first order corrections to the energies and energy eigenstates.

Consider the following conversation regarding whether the first order corrections to the energies will remove all the degeneracy in the eigenvalue spectrum of \hat{H}^0 .

Student 1: If \hat{H}^0 has a degenerate energy spectrum, the perturbation \hat{H}' will always remove the degeneracy when we find the first order corrections to the energies. The energy levels will split into distinct energy levels.

Student 2: This may be true for some \hat{H}^0 and \hat{H}' but not necessarily true for all cases. The symmetry of the unperturbed Hamiltonian \hat{H}^0 and the perturbing Hamiltonian \hat{H}' will dictate whether all the degeneracies will be removed in first order.

Student 3: I agree with Student 2. Consider EXAMPLE 4 in which the perturbing Hamiltonian was already diagonal in the degenerate subspace of \hat{H}^0 . We found the energies, including the first order corrections, to be $E_1 = 4V_0 - \epsilon V_0$ and $E_2 = 4V_0 - \epsilon V_0$. Sometimes, even a higher order correction to the energies may not lift a degeneracy.

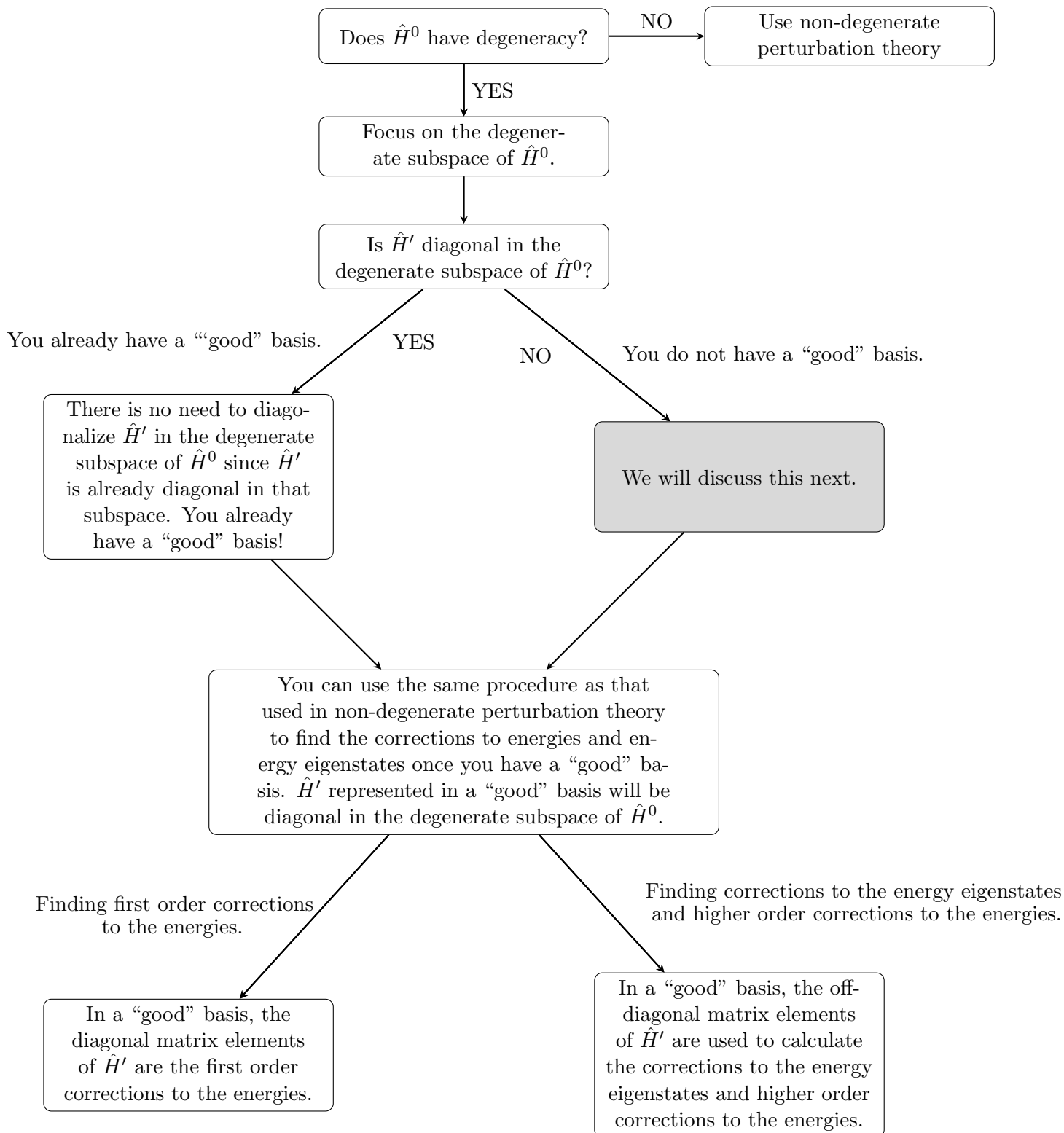
Explain why you agree or disagree with each student.

Checkpoint - Finding a “good” basis for Case 1

- If \hat{H}' is already diagonal in a degenerate subspace of \hat{H}^0 (and basis states are eigenstates of \hat{H}^0):
 - The initially chosen basis states make up a “good” basis.
 - The expression $E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle$ **CAN** be used to find corrections to the energies since $\{|\psi_n^0\rangle\}$ are “good” basis states.
 - ◇ These first order corrections to the energies correspond to the diagonal matrix elements of \hat{H}' in a “good” basis.
 - The expression $|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{E_n^0 - E_m^0} |\psi_m^0\rangle$ **CAN** be used to find the first order corrections to the energy eigenstates $\{|\psi_n^0\rangle\}$ as $\{|\psi_n^0\rangle\}$ are “good” basis states.
 - ◇ For a given \hat{H}^0 and \hat{H}' , these first order corrections to the energy eigenstates can be determined making use of equation (2) using the off-diagonal matrix elements of \hat{H}' in a “good” basis.
- Calculating the first order corrections to the energies may not be enough to lift all the degeneracy in many cases.

Review the flowchart for the steps to determine the corrections to the energies and energy eigenstates when \hat{H}' is diagonal in the degenerate subspace of \hat{H}^0 .

Finding First Order Corrections to the Energies and Energy Eigenstates



5.2.2 CASE 2: Corrections to the Energies and Energy Eigenstates when \hat{H}' is not Diagonal in the Degenerate Subspace of \hat{H}^0

- If \hat{H}' is not diagonal in the degenerate subspace of \hat{H}^0 then the initially chosen set of eigenstates of \hat{H}^0 does **NOT** form a complete set of “good” basis states.
- In this case, we must find a “good” basis first. To find “good” basis states, we must choose a basis that diagonalizes \hat{H}' in the degenerate subspace of \hat{H}^0 and simultaneously keeps \hat{H}^0 diagonal everywhere.
- Since the “good” basis states are still eigenstates of \hat{H}^0 , \hat{H}^0 will remain diagonal in a “good” basis.

Consider the following conversation regarding diagonalizing \hat{H}' in the degenerate subspace of \hat{H}^0 when \hat{H}^0 and \hat{H}' don't commute.

Student 1: I thought we cannot simultaneously diagonalize \hat{H}^0 and \hat{H}' unless they commute.

Student 2: Yes that's true! The entire \hat{H}^0 and \hat{H}' matrices cannot be diagonalized simultaneously unless they commute. But in the degenerate subspace of \hat{H}^0 , we can always diagonalize both \hat{H}^0 and \hat{H}' simultaneously.

Do you agree with Student 2? Explain your reasoning.

17. Can we find a linear combination of the eigenstates of \hat{H}^0 in the degenerate subspace of \hat{H}^0 that diagonalizes \hat{H}' in that subspace? If so, will a linear combination of eigenstates of \hat{H}^0 in the degenerate subspace remain an eigenstate of \hat{H}^0 ? Explain your reasoning.

Use the following example to help check your answers to question 17.

EXAMPLE 5: Consider the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}'$ in which

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & \epsilon \\ \epsilon & 0 & \epsilon \\ \epsilon & \epsilon & 0 \end{pmatrix} \quad (\epsilon \ll 1) \quad (13)$$

and the normalized eigenstates of \hat{H}^0 given by $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, are

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (14)$$

18. Fill in the blanks using equations (13) and (14).

$$\hat{H}^0 |\psi_1^0\rangle = \underline{\hspace{4cm}}$$

$$\hat{H}^0 |\psi_2^0\rangle = \underline{\hspace{4cm}}$$

$$\hat{H}^0 |\psi_3^0\rangle = \underline{\hspace{4cm}}$$

$$\hat{H}^0 (a |\psi_1^0\rangle + b |\psi_2^0\rangle) = \underline{\hspace{4cm}}$$

$$\hat{H}^0 (e |\psi_1^0\rangle + f |\psi_3^0\rangle) = \underline{\hspace{4cm}}$$

19. Is $a |\psi_1^0\rangle + b |\psi_2^0\rangle$ a normalized eigenstate of \hat{H}^0 , where a and b are arbitrary complex numbers that satisfy $|a|^2 + |b|^2 = 1$? Explain.

20. Can \hat{H}^0 still be diagonal if $a |\psi_1^0\rangle + b |\psi_2^0\rangle$ and $c |\psi_1^0\rangle + d |\psi_2^0\rangle$ are used as new basis states instead of $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$? Suppose that a, b, c and d are chosen such that $a |\psi_1^0\rangle + b |\psi_2^0\rangle$ and $c |\psi_1^0\rangle + d |\psi_2^0\rangle$ are orthonormal and \hat{H}' is diagonal in the degenerate subspace of \hat{H}^0 , is \hat{H}^0 diagonal if these new basis states are chosen? Explain.

21. Is $e |\psi_1^0\rangle + f |\psi_3^0\rangle$ a normalized eigenstate of \hat{H}^0 , where e and f are arbitrary complex numbers that satisfy $|e|^2 + |f|^2 = 1$?

(a) Will the \hat{H}^0 matrix remain diagonal if $e |\psi_1^0\rangle + f |\psi_3^0\rangle$ is chosen as one of the basis states to write the \hat{H}^0 matrix? Explain your answer.

(b) Based upon whether your answer to the preceding question is yes or no, can $e |\psi_1^0\rangle + f |\psi_3^0\rangle$ be used as a basis state to calculate corrections to the energies and energy eigenstates in perturbation theory? Explain.

Consider the following conversation regarding whether a linear combination of energy eigenstates of \hat{H}^0 that includes non-degenerate eigenstates of \hat{H}^0 (in EXAMPLE 5 in equation (13)) is an energy eigenstate of \hat{H}^0 .

Student 1: I don't see why we cannot have $e |\psi_1^0\rangle + f |\psi_3^0\rangle$ as a basis state for using perturbation theory.

Student 2: I disagree. \hat{H}^0 is not diagonal if $e |\psi_1^0\rangle + f |\psi_3^0\rangle$ is one of the basis states because the \hat{H}^0 matrix can only be diagonal if all basis states are eigenstates of \hat{H}^0 . As we showed in questions 18 and 21, since \hat{H}^0 acting on $e |\psi_1^0\rangle + f |\psi_3^0\rangle$ does not return a number times the same state $e |\psi_1^0\rangle + f |\psi_3^0\rangle$, this state is not an eigenstate of \hat{H}^0 .

Explain why you agree with Student 1 or Student 2.

Consider the following conversation regarding choosing orthonormal linear combinations of eigenstates of \hat{H}^0 that diagonalize the \hat{H}' matrix in the degenerate subspace of \hat{H}^0 as basis states for EXAMPLE 5.

Student 1: We showed in question 20 that any linear combination of eigenstates of \hat{H}^0 in the degenerate subspace of \hat{H}^0 , such as $a |\psi_1^0\rangle + b |\psi_2^0\rangle$ and $c |\psi_1^0\rangle + d |\psi_2^0\rangle$, remains an eigenstate of \hat{H}^0 . Can we choose any two linear combinations of the eigenstates of \hat{H}^0 , $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$, to form two of the “good” basis states?

Student 2: As long as the basis states are orthonormal, they form a “good” basis. Any two linear combinations of $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ whose inner product is zero forms a pair of “good” orthogonal basis states.

Student 3: I disagree with Student 2. There are many possible linear combinations of $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ that are orthogonal that will not form “good” basis states. The linear combination of the initial eigenstates must diagonalize \hat{H}' in the degenerate subspace of \hat{H}^0 . Diagonalizing \hat{H}' in the degenerate subspace of \hat{H}^0 provides the only pair, neglecting overall phase factors, of orthonormal linear combinations that form a “good” basis set.

Explain why you agree with Student 2 or Student 3.

**** Check your answers to questions 18-21 in EXAMPLE 5. ****

18.

$$\begin{aligned}\hat{H}^0|\psi_1^0\rangle &= V_0|\psi_1^0\rangle \\ \hat{H}^0|\psi_2^0\rangle &= V_0|\psi_2^0\rangle \\ \hat{H}^0|\psi_3^0\rangle &= 2V_0|\psi_3^0\rangle \\ \hat{H}^0(a|\psi_1^0\rangle + b|\psi_2^0\rangle) &= V_0(a|\psi_1^0\rangle + b|\psi_2^0\rangle) \\ \hat{H}^0(e|\psi_1^0\rangle + f|\psi_3^0\rangle) &= V_0(e|\psi_1^0\rangle + 2f|\psi_3^0\rangle)\end{aligned}$$

19. Yes. $a|\psi_1^0\rangle + b|\psi_2^0\rangle$ is an eigenstate of \hat{H}^0 .

20. Yes. \hat{H}^0 will still be diagonal if $a|\psi_1^0\rangle + b|\psi_2^0\rangle$ and $c|\psi_1^0\rangle + d|\psi_2^0\rangle$ are used as new basis states instead of $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$.

21. No. $e|\psi_1^0\rangle + f|\psi_3^0\rangle$ is not an eigenstate of \hat{H}^0 .

21a. No. \hat{H}^0 will no longer be diagonal if $e|\psi_1^0\rangle + f|\psi_3^0\rangle$ is chosen as one of the basis states.

21b. No. $e|\psi_1^0\rangle + f|\psi_3^0\rangle$ cannot be used as a basis state to calculate corrections to the energies and energy eigenstates in perturbation theory.

If your answers do not match the checkpoints for questions 18 - 21 in EXAMPLE 5, go back and reconcile any differences you may have.

Now let us determine values of $a, b, c,$ and d that correspond to a “good” basis for EXAMPLE 5, for which \hat{H}^0 and \hat{H}' given below are represented in the initially chosen basis.

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & \epsilon \\ \epsilon & 0 & \epsilon \\ \epsilon & \epsilon & 0 \end{pmatrix} \quad (\epsilon \ll 1)$$

We will only focus on \hat{H}' in the two-dimensional degenerate subspace of \hat{H}^0 for now.

22. Diagonalize \hat{H}' in equation (13) in the degenerate subspace of \hat{H}^0 and find the eigenstates and eigenvalues of \hat{H}' in that two-dimensional subspace.

Consider the following conversation regarding extending the eigenstates of \hat{H}' in the degenerate subspace of \hat{H}^0 from a two-dimensional to the three-dimensional Hilbert space.

Student 1: When we diagonalize \hat{H}' in the degenerate subspace of \hat{H}^0 in equation (13), we find two eigenstates of both \hat{H}' and \hat{H}^0 in the two-dimensional subspace. How can we use these states to find “good” basis states in the three dimensional Hilbert space?

Student 2: In EXAMPLE 5, the eigenstates found by diagonalizing \hat{H}' in the degenerate subspace of \hat{H}^0 are $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$. “Good” basis states must be $|\phi_1^0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ c_1 \end{pmatrix}$ and $|\phi_2^0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ c_2 \end{pmatrix}$ when we extend them to the three-dimensional Hilbert space. To determine the values c_1 and c_2 , we must satisfy the orthogonality conditions $\langle \phi_1^0 | \phi_3^0 \rangle = 0$ and $\langle \phi_2^0 | \phi_3^0 \rangle = 0$.

Student 3: From equation (13), $|\phi_3^0\rangle = |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ is already a “good” basis state and any vector orthogonal to $|\phi_3^0\rangle$ must have zero as its third component. Since $\langle \phi_1^0 | \phi_3^0 \rangle = c_1$ and $\langle \phi_2^0 | \phi_3^0 \rangle = c_2$, extending the states found from diagonalizing \hat{H}' in the two-dimensional degenerate subspace of \hat{H}^0 to find basis states in three dimensions requires adding a zero as the third component to ensure $\langle \phi_1^0 | \phi_3^0 \rangle = 0$ and $\langle \phi_2^0 | \phi_3^0 \rangle = 0$. Also, the condition $\langle \phi_1^0 | \phi_2^0 \rangle = 0$ is satisfied when we extend to three dimensions the states in two dimensions obtained by diagonalizing \hat{H}' in the degenerate subspace of \hat{H}^0 .

Explain why you agree with Student 2, Student 3, or both.

23. Extend the states you found in the preceding problem (question 22) to the three dimensional space, making use of the preceding conversation, to obtain the two “good” basis states $|\phi_1^0\rangle$ and $|\phi_2^0\rangle$.

24. Express the “good” basis states or eigenstates of \hat{H}^0 (obtained by diagonalizing \hat{H}' in the degenerate subspace of \hat{H}^0) as a linear combination of the initially chosen eigenstates of \hat{H}^0 , $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$, used in equation (13).

25. In the preceding question (question 24), $a|\psi_1^0\rangle + b|\psi_2^0\rangle$ and $c|\psi_1^0\rangle + d|\psi_2^0\rangle$ are “good” orthonormal basis states written in terms of the initially chosen basis states $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$. The constants that diagonalize \hat{H}' in the degenerate subspace of \hat{H}^0 must be:

$$a = \underline{\hspace{4cm}}$$

$$b = \underline{\hspace{4cm}}$$

$$c = \underline{\hspace{4cm}}$$

$$d = \underline{\hspace{4cm}}$$

26. Using your values of a, b, c , and d in the preceding question, find the matrix elements of \hat{H}^0 in the “good” basis.

$$\hat{H}^0 = \begin{matrix} a^* \langle \psi_1^0 | + b^* \langle \psi_2^0 | \\ c^* \langle \psi_1^0 | + d^* \langle \psi_2^0 | \\ \langle \psi_3^0 | \end{matrix} \left(\begin{array}{ccc} a |\psi_1^0\rangle + b |\psi_2^0\rangle & c |\psi_1^0\rangle + d |\psi_2^0\rangle & |\psi_3^0\rangle \\ & & \\ & & \end{array} \right)$$

Summarize your results in one to two sentences.

**** Check your answers to questions 22-26 in EXAMPLE 5. ****

22. Diagonalizing \hat{H}' in the degenerate subspace of \hat{H}^0 , the eigenvalues of \hat{H}' are ϵV_0 with corresponding eigenstate $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $-\epsilon V_0$ with corresponding eigenstate $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

NOTE: The eigenstates are unique up to a constant multiple (e.g., the eigenstate corresponding to the eigenvalue $-\epsilon V_0$ can be equivalently expressed as $\frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}$).

23. Using orthogonality with $|\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$, we can extend $\left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \right\}$ to the three dimensional space, so that the other “good” basis states are $\left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \right\}$.

24. Therefore, the “good” basis states (in terms of the initially chosen basis states in equation (13)) for the entire three-dimensional state space will be $\left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$, or equivalently

$\left\{ \frac{1}{\sqrt{2}} |\psi_1^0\rangle + \frac{1}{\sqrt{2}} |\psi_2^0\rangle, \frac{1}{\sqrt{2}} |\psi_1^0\rangle - \frac{1}{\sqrt{2}} |\psi_2^0\rangle, |\psi_3^0\rangle \right\}$. These basis states are eigenstates of \hat{H}^0 (\hat{H}^0 is still diagonal in this basis) as it should be in perturbation theory, but \hat{H}' is also diagonal in the degenerate subspace of \hat{H}^0 .

25. For the given perturbing Hamiltonian \hat{H}' in equation (13), a “good” orthonormal basis that diagonalizes \hat{H}' in the degenerate subspace of \hat{H}^0 is obtained with the constants $a = b = c = \frac{1}{\sqrt{2}}$ and $d = -\frac{1}{\sqrt{2}}$.

NOTE: The values of a, b, c , and d are unique up to overall phase factors.

26. The entire \hat{H}^0 matrix remains diagonal as it must be for an appropriately chosen “good” basis.

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

If your answers do not match the checkpoint for questions 22-26 in EXAMPLE 5, go back and reconcile any differences you may have.

Consider the following conversation regarding whether in the degenerate subspace of \hat{H}^0 , linear combinations of eigenstates of \hat{H}^0 remain eigenstates of \hat{H}^0 due to degeneracy.

Student 1: Consider EXAMPLE 5. Since any linear combination of the basis states $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ in the degenerate subspace of \hat{H}^0 keeps \hat{H}^0 diagonal, any linear combination of eigenstates of \hat{H}^0 in the degenerate subspace of \hat{H}^0 will be an eigenstate of \hat{H}^0 .

Student 2: But how can that be? In the context of a one-dimensional infinite square well, a linear combination of the ground state and the first excited state is no longer an energy eigenstate.

Student 1: You are correct, a linear combination of the ground state and the first excited state is not an energy eigenstate of the one-dimensional infinite square well. There is no degeneracy in the energy eigenvalue spectrum for the one-dimensional infinite square well. It is the degeneracy that guarantees that any linear combination of eigenstates of \hat{H}^0 in the degenerate subspace of \hat{H}^0 will be an eigenstate of \hat{H}^0 .

Explain why you agree or disagree with each student.

EXAMPLE 6: Interpreting the Matrix Elements of the \hat{H}' Matrix in a Given Representation

Answer the following questions for this example:

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} -3\epsilon & 2\epsilon & 0 \\ 2\epsilon & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix} \quad (\epsilon \ll 1) \quad (15)$$

and the normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

If we express \hat{H}^0 and \hat{H}' in a “good” basis, we have

$$\hat{H}_G^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}'_G = V_0 \begin{pmatrix} \epsilon & 0 & \frac{2\epsilon}{\sqrt{5}} \\ 0 & -4\epsilon & \frac{\epsilon}{\sqrt{5}} \\ \frac{2\epsilon}{\sqrt{5}} & \frac{\epsilon}{\sqrt{5}} & 0 \end{pmatrix} \quad (\epsilon \ll 1) \quad (16)$$

and the “good” basis states, respectively, are

$$|\phi_1^0\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}, \quad |\phi_2^0\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\phi_3^0\rangle = |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (17)$$

in which \hat{H}_G^0 is the matrix representation of \hat{H}^0 expressed in the “good” basis, \hat{H}'_G is the matrix representation of \hat{H}' expressed in a “good” basis, and $\{|\phi_n^0\rangle\}$ are the “good” basis states.

27. Using only the matrix elements in equation (16), find the first order corrections to the energies. **No matrix manipulation required!**

28. Using only the matrix elements in equation (16), find the first order corrections to the energy eigenstates. **No matrix manipulation required!**

**** Check your answers to questions 27-28 pertaining to EXAMPLE 6. ****

27. $E_1^1 = \epsilon V_0$, $E_2^1 = -4\epsilon V_0$, and $E_3^1 = 0$

28. $|\psi_1^1\rangle = -\frac{2\epsilon}{\sqrt{5}}|\phi_3^0\rangle$, $|\psi_2^1\rangle = -\frac{\epsilon}{\sqrt{5}}|\phi_3^0\rangle$, $|\psi_3^1\rangle = \frac{2\epsilon}{\sqrt{5}}|\phi_1^0\rangle + \frac{\epsilon}{\sqrt{5}}|\phi_2^0\rangle$ (Please note the values of the first order corrections to the energy eigenstates are not unique.)

If your answers to the first order corrections to the energies or energy eigenstates do not match EXAMPLE 6, go back and reconcile any differences.

Consider the following conversation regarding the matrix elements of \hat{H}' .

Student 1: For the corrections to the energies, we need the diagonal matrix elements of \hat{H}' . The matrix elements of \hat{H}' along the diagonal correspond to the first order corrections to the energy.

Student 2: But the diagonal elements of \hat{H}' correspond to the first order corrections to the energies only if the \hat{H}' matrix is written in a “good” basis.

Student 3: I agree with Student 2. The off-diagonal elements of \hat{H}' must be zero in the degenerate subspace of \hat{H}^0 for the basis states to be “good”.

Student 4: I agree with Student 2 and Student 3. Once we find a “good” basis, the diagonal matrix elements of \hat{H}' can be used to find the first order corrections to the energies. Also, the off-diagonal matrix elements of \hat{H}' are needed when calculating the second or higher order corrections to the energies and any corrections to the energy eigenstates.

Explain why you agree or disagree with each student.

EXAMPLE 7: Consider the Hamiltonian $\hat{H} = \hat{H}^0 + \hat{H}'$, in which

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} -\epsilon & 2\epsilon & 0 \\ 2\epsilon & -\epsilon & 3\epsilon \\ 0 & 3\epsilon & \epsilon \end{pmatrix} \quad (\epsilon \ll 1) \quad (18)$$

and the normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

29. Choose one of the following options to fill in the blank. In the degenerate subspace of \hat{H}^0 , the matrix representation of \hat{H}^0 is _____ and the matrix representation of \hat{H}' is _____, respectively.

(A)

$$V_0 \begin{pmatrix} -\epsilon & 2\epsilon \\ 2\epsilon & -\epsilon \end{pmatrix}, \quad V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$

(B)

$$V_0 \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}, \quad V_0 \begin{pmatrix} -\epsilon & 3\epsilon \\ 3\epsilon & \epsilon \end{pmatrix}$$

(C)

$$V_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad V_0 \begin{pmatrix} -\epsilon & 0 \\ 0 & \epsilon \end{pmatrix}$$

(D)

$$V_0 \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad V_0 \begin{pmatrix} -\epsilon & 2\epsilon \\ 2\epsilon & \epsilon \end{pmatrix}$$

30. Do the basis states $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$ form a “good” basis? Explain.

31. The first order corrections to the energies are

(A) $E_1^1 = -\epsilon V_0$, $E_2^1 = -\epsilon V_0$, and $E_3^1 = \epsilon V_0$.

(B) $E_1^1 = \epsilon V_0$, $E_2^1 = \epsilon V_0$, and $E_3^1 = \epsilon V_0$.

(C) $E_1^1 = -\epsilon V_0$, $E_2^1 = -\epsilon V_0$, and $E_3^1 = 0$.

(D) $E_1^1 = -\epsilon V_0$, $E_2^1 = 2\epsilon$, and $E_3^1 = 3\epsilon$.

(E) None of the above

**** Check your answers to questions 27-28 pertaining to EXAMPLE 7. ****

29. C
30. Yes.
31. A

If your answers to the first order corrections to the energies or energy eigenstates do not match the checkpoint answers for EXAMPLE 7, go back and reconcile any differences.

Consider the following conversation regarding writing the basis states in a different order so that the degenerate eigenvalues of \hat{H}^0 along the diagonal are adjacent. With that order, the degenerate subspace of \hat{H}^0 can be identified more easily.

Student 1: In equation (18), in the degenerate subspace of \hat{H}^0 , I don't see how the matrix representation of \hat{H}' is $V_0 \begin{pmatrix} -\epsilon & 0 \\ 0 & \epsilon \end{pmatrix}$.

Student 2: It is a little difficult to recognize the \hat{H}' matrix in the degenerate subspace of \hat{H}^0 because of the order in which the basis states are chosen. However, we are always free to choose the basis states in any order. In this case it may be helpful if we choose to express \hat{H}^0 and \hat{H}' with the basis states chosen in a different order than in the order $|\psi_1^0\rangle, |\psi_2^0\rangle$, and $|\psi_3^0\rangle$ selected in equation (18). If we choose the basis states in the order

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \text{ and } |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \text{ then}$$
$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} -\epsilon & 0 & 2\epsilon \\ 0 & \epsilon & 3\epsilon \\ 2\epsilon & 3\epsilon & -\epsilon \end{pmatrix} \quad (\epsilon \ll 1) \quad (19)$$

Now we can easily identify the matrix representation of \hat{H}^0 and \hat{H}' in the degenerate subspace of \hat{H}^0 .

Student 3: I disagree with Student 2. Since the first order corrections to the energies depend on the matrix elements of \hat{H}' , we cannot choose the basis states in a different order without affecting the first order corrections to each unperturbed energy.

Explain why you agree or disagree with each student.

Consider the following conversation regarding small corrections to the unperturbed energies and eigenstates of the unperturbed Hamiltonian \hat{H}^0 due to the perturbation \hat{H}' .

Student 1: When we use perturbation theory, we are assuming that the perturbation \hat{H}' is small compared to \hat{H}^0 . Therefore, we use the unperturbed eigenstates of \hat{H}^0 as basis states for our calculations of the corrections to the energies and the energy eigenstates.

Student 2: Yes, but a "good" basis is still needed to find corrections to the energies and energy eigenstates. We must choose as basis states a set of eigenstates of \hat{H}^0 that diagonalizes \hat{H}' in the degenerate subspace of \hat{H}^0 .

Do you agree with Student 1, Student 2, or both? Explain.

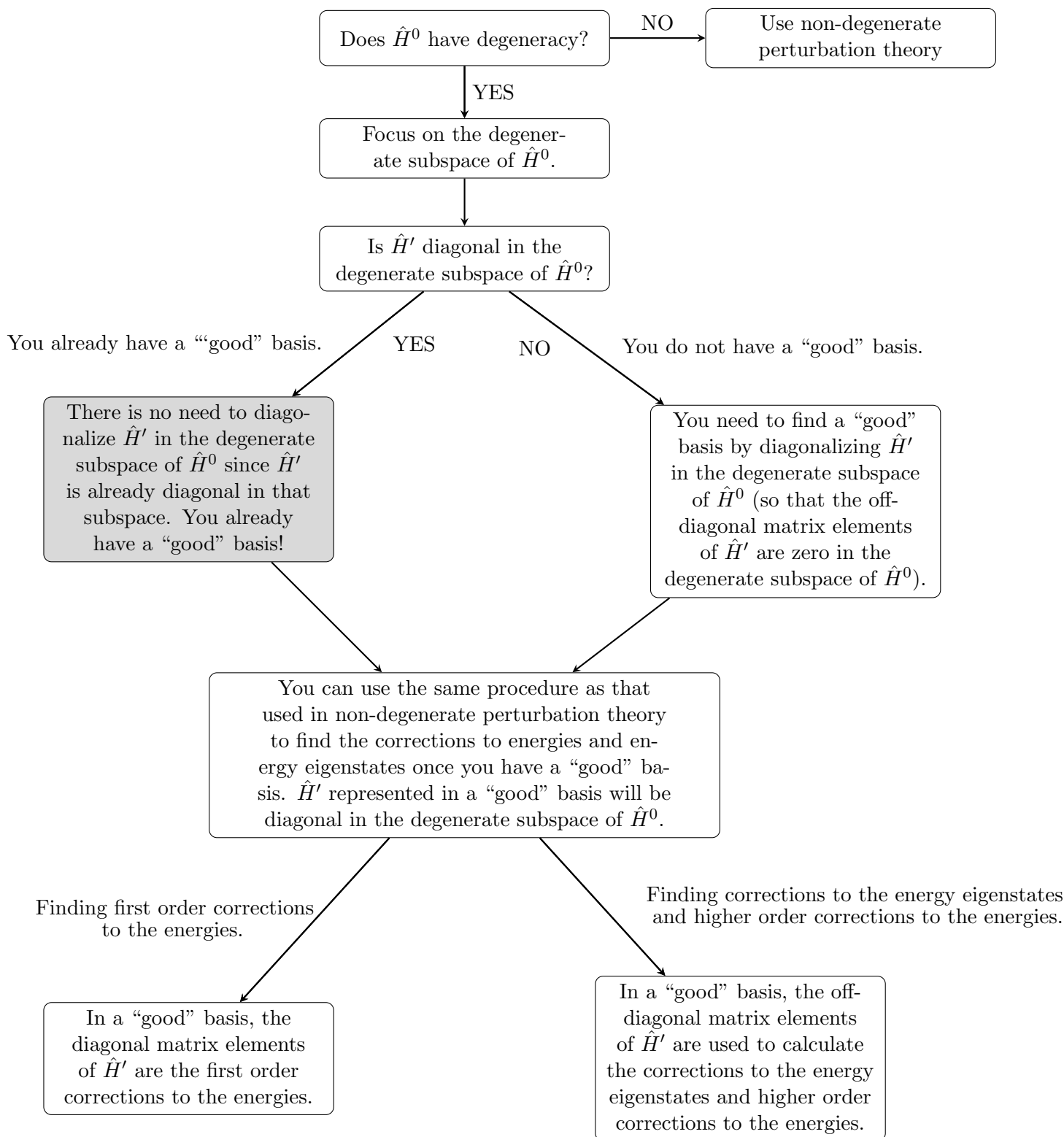
Checkpoint - Finding a “good” basis for Case 2

For the case in which the unperturbed Hamiltonian \hat{H}^0 has degeneracy, we must first ensure that we have a “good” basis before finding the corrections to the energies and energy eigenstates.

- If \hat{H}' is not diagonal in the degenerate subspace of \hat{H}^0 :
 - The initially chosen basis is not “good.”
 - We must **DIAGONALIZE** \hat{H}' in the degenerate subspace of \hat{H}^0 to find a “good” basis.
 - ◊ Diagonalizing \hat{H}' in the degenerate subspace of \hat{H}^0 gives a linear combination of eigenstates of \hat{H}^0 that form a “good” basis.
 - ◊ Any linear combination of energy eigenstates in the degenerate subspace of \hat{H}^0 remains an eigenstate of \hat{H}^0 .
 - ◊ In a “good” basis, \hat{H}^0 remains diagonal (i.e., “good” basis states are still eigenstates of \hat{H}^0).
 - The diagonal elements of \hat{H}' in a “good” basis are the first order corrections to the energies.
 - The off-diagonal matrix elements of \hat{H}' in a “good” basis are used to determine the first order corrections to the energy eigenstates.

Review the flowchart for the steps in determining corrections to the energies and energy eigenstates **when \hat{H}' is NOT diagonal in the degenerate subspace of \hat{H}^0 .**

Finding First Order Corrections to the Energies and Energy Eigenstates



5.2.3 If \hat{H}^0 and \hat{H}' do not commute, diagonalizing the entire \hat{H}' matrix makes \hat{H}^0 non-diagonal

Consider the following conversation regarding a “good” basis and diagonalizing \hat{H}' in the degenerate subspace of \hat{H}^0 .

Student 1: In degenerate perturbation theory, to find a “good” basis for a given \hat{H}^0 and \hat{H}' , we must diagonalize the \hat{H}' matrix.

Student 2: We should not diagonalize the entire \hat{H}' matrix, but rather only the part of \hat{H}' that corresponds to the degenerate subspace of \hat{H}^0 .

Student 3: I disagree. If we diagonalize part of the \hat{H}' matrix then we cannot guarantee that it will give us a “good” basis. We must diagonalize the entire \hat{H}' matrix.

Student 4: Actually, it is equally valid to diagonalize either the entire \hat{H}' matrix or only the \hat{H}' matrix in the degenerate subspace of \hat{H}^0 . We usually choose to diagonalize \hat{H}' in the degenerate subspace of \hat{H}^0 simply because it requires less work to diagonalize a matrix with a lower dimension.

Explain why you agree or disagree with each student.

EXAMPLE 8: Let’s see what happens when we diagonalize the entire \hat{H}' matrix. Consider the example

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{bmatrix} 5 & \epsilon & \epsilon \\ \epsilon & 1 & \epsilon \\ \epsilon & \epsilon & 1 \end{bmatrix}, \quad (\epsilon \ll 1). \quad (20)$$

Due to the degeneracy in the energy spectrum of \hat{H}' , the eigenstates of \hat{H}' are not unique. One possible set of eigenstates of \hat{H}' is

$$|\phi_1^0\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, |\phi_2^0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\phi_3^0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \quad (21)$$

in terms of the initially chosen basis states used to write equation (20).

If we use the eigenstates of \hat{H}' as the basis states, the \hat{H}^0 matrix becomes

$$\hat{H}^0 = \begin{bmatrix} \frac{7}{3} & -\frac{4}{\sqrt{6}} & -\frac{4}{\sqrt{6}} \\ -\frac{4}{\sqrt{6}} & 3 & \frac{5}{2} \\ -\frac{4}{\sqrt{6}} & \frac{5}{2} & 3 \end{bmatrix}. \quad (22)$$

32. Is \hat{H}^0 in equation (22) diagonal in the basis consisting of the eigenstates of \hat{H}' ?
33. Based upon your answer for whether \hat{H}^0 is diagonal in this basis or not, are these basis states, which are eigenstates of \hat{H}' , eigenstates of \hat{H}^0 ? Explain.
34. Can this basis be used for finding the corrections to the energies and energy eigenstates in perturbation theory for the Hamiltonian in equation (20)? Explain.

With this example in mind, summarize the student conversation on the previous page in one to two sentences and how would you help these students with the issues they are discussing.

**** Check your answers to questions 32-34 in EXAMPLE 8. ****

32. No. \hat{H}^0 is not diagonal in the basis consisting of the eigenstates of \hat{H}' .
33. No. \hat{H}^0 must be diagonal in a basis consisting of the eigenstates of \hat{H}^0 .
34. No. This is not a “good” basis as \hat{H}^0 is not diagonal in a basis consisting of the eigenstates of \hat{H}' .

If any of your answers do not match the checkpoint answers for EXAMPLE 8, go back and reconcile any differences you may have with the answers provided.

Checkpoint

If \hat{H}^0 and \hat{H}' do not commute:

- \hat{H}' **must be diagonalized only in the degenerate subspace of \hat{H}^0** in order to ensure that basis states remain eigenstates of \hat{H}^0 (i.e., \hat{H}^0 is diagonal in that basis).
- Diagonalizing the entire \hat{H}' matrix yields a basis that produces off-diagonal matrix elements in \hat{H}^0 when \hat{H}^0 and \hat{H}' do not commute, which is not valid for determining the perturbative corrections using perturbation theory (basis states must always be eigenstates of \hat{H}^0 since we are finding small corrections to the unperturbed energies).

5.2.4 \hat{H}^0 and \hat{H}' do commute

In all the examples up to this point, we have considered systems such that \hat{H}^0 and \hat{H}' did not commute. Let's consider whether the same approach is valid for a system in which \hat{H}^0 and \hat{H}' do commute.

Consider the following conversation regarding diagonalizing \hat{H}' in each degenerate subspace of \hat{H}^0 for a system for which \hat{H}^0 and \hat{H}' commute.

Student 1: Even when $\hat{H} = \hat{H}^0 + \epsilon\hat{H}'$ ($\epsilon \ll 1$) for a system is such that \hat{H}^0 and \hat{H}' commute, we can use the same approach to find a “good” basis as when \hat{H}^0 and \hat{H}' do not commute. In particular, we can find a “good” basis by only diagonalizing \hat{H}' in each degenerate subspace of \hat{H}^0 .

Student 2: I disagree. Since \hat{H}^0 and \hat{H}' commute, we must diagonalize the entire \hat{H}' matrix. The “good” basis must consist of a complete set of simultaneous eigenstates of \hat{H}^0 and \hat{H}' .

Student 3: Actually, if \hat{H}^0 and \hat{H}' commute, then diagonalizing \hat{H}' in each degenerate subspace of \hat{H}^0 will diagonalize the entire \hat{H}' matrix. The first order corrections give the exact result.

Explain why you agree or disagree with each student.

Checkpoint

If \hat{H}^0 and \hat{H}' commute, i.e., $[\hat{H}^0, \hat{H}'] = 0$:

- \hat{H}^0 and \hat{H}' can be simultaneously diagonalized.
- Diagonalize \hat{H}' **in the degenerate subspace of \hat{H}^0** in order to find corrections to the energies and energy eigenstates.
- Diagonalizing \hat{H}' in each degenerate subspace of \hat{H}^0 will diagonalize the entire \hat{H}' matrix. The first order corrections (the diagonal matrix elements of \hat{H}') give the exact result.

SUMMARY: Finding First Order Corrections to the Energies and Energy Eigenstates Requires that You Choose a “Good” Basis

The perturbative Hamiltonian \hat{H}' in the degenerate subspace of \hat{H}^0 will dictate how we proceed to determine the first order corrections to the energies and the energy eigenstates.

CASE 1: \hat{H}' IS DIAGONAL IN THE DEGENERATE SUBSPACE OF \hat{H}^0 IN THE INITIAL BASIS.

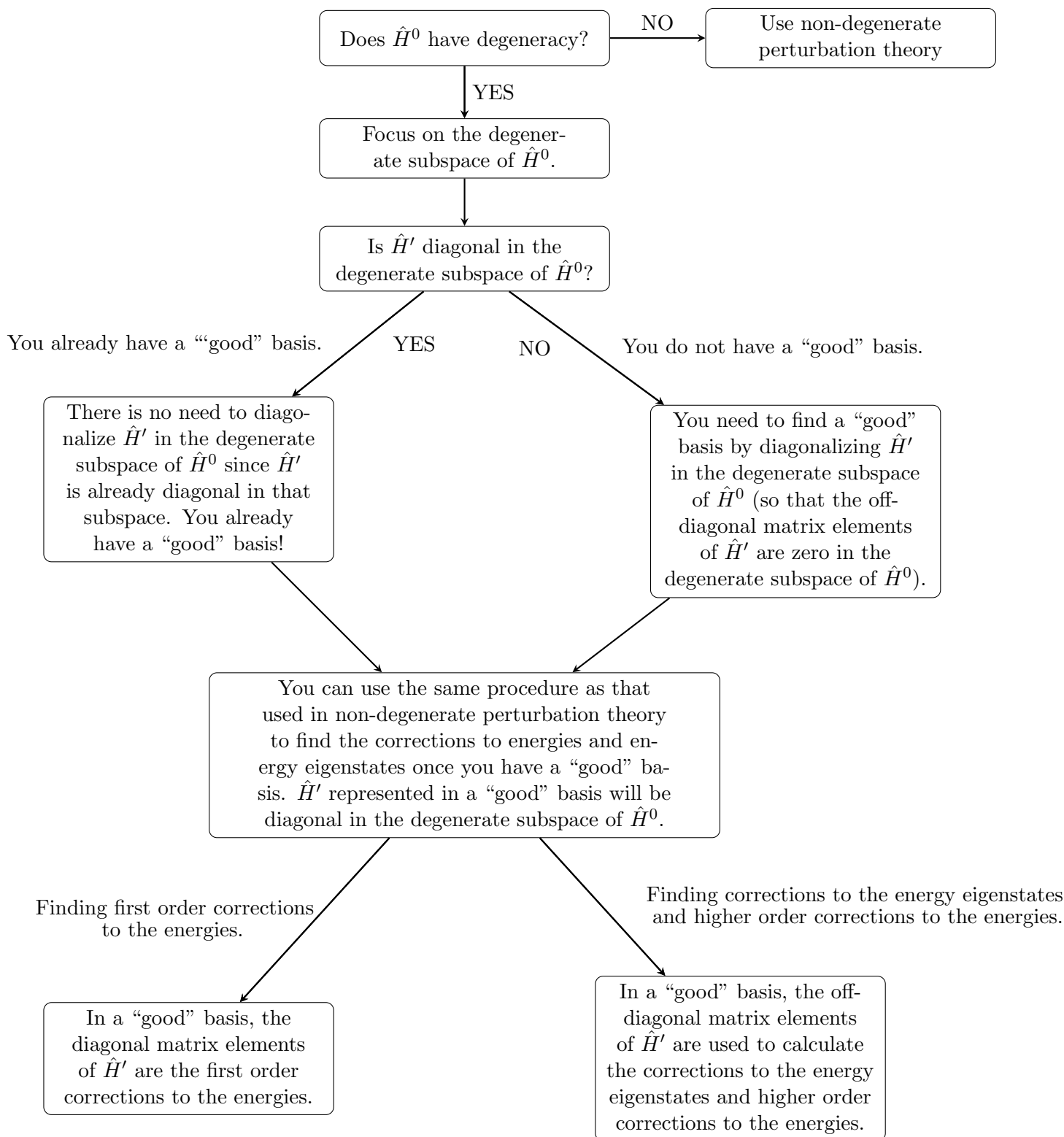
- If \hat{H}' is diagonal in the degenerate subspace of \hat{H}^0 :
 - The initially **chosen eigenstates of \hat{H}^0 already form a “good” basis** so the corrections to the energies and energy eigenstates can be found simply by **using the matrix elements of \hat{H}'** as in non-degenerate perturbation theory.
 - ◊ One can use equations (1) and (2) with the initial basis states.
 - ◊ The expression $E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle$ gives the first order correction to the energies.
 - ◊ The expression $|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} |\psi_m^0\rangle$ gives the first order corrections to the energy eigenstates since the numerator will be zero when $E_n^0 = E_m^0$ (if \hat{H}' is diagonal in the degenerate subspace of \hat{H}^0).
 - * The terms with $E_n^0 = E_m^0$ in the denominator will not appear in the first order correction to the energy eigenstates $|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} |\psi_m^0\rangle$.

CASE 2: \hat{H}' IS NOT DIAGONAL IN THE DEGENERATE SUBSPACE OF \hat{H}^0 IN THE INITIAL BASIS.

- In the initially chosen basis, if \hat{H}' has **non-zero off-diagonal matrix elements in the degenerate subspace of \hat{H}^0** :
 - The initially **chosen eigenstates of \hat{H}^0 do not form a “good” basis**.
 - One **CANNOT** use equations (1) and (2) with the initially chosen basis states (since they do not form a “good” basis).
 - In this case, a “good” basis must be found such that \hat{H}' is diagonal in the degenerate subspace of \hat{H}^0 while \hat{H}^0 remains diagonal.
 - To find a “good” basis $\{|\phi_n^0\rangle\}$, **diagonalize \hat{H}' in the degenerate subspace of \hat{H}^0** .
 - Once a “good” basis is found, the corrections to the energies and energy eigenstates can be found by **inspecting the matrix elements of \hat{H}'** as in non-degenerate perturbation theory.
 - ◊ The expression $E_n^1 = \langle \phi_n^0 | \hat{H}' | \phi_n^0 \rangle$ gives the first order corrections to the energies after finding a “good” basis $\{|\phi_n^0\rangle\}$.
 - ◊ The expression $|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \phi_m^0 | \hat{H}' | \phi_n^0 \rangle}{(E_n^0 - E_m^0)} |\phi_m^0\rangle$ gives the first order correction to the energy eigenstates after finding a “good” basis $\{|\phi_n^0\rangle\}$, since the numerator will be zero when $E_n^0 = E_m^0$ (if \hat{H}' is diagonal in the degenerate subspace of \hat{H}^0).
 - * So the terms with $E_n^0 = E_m^0$ will not appear in the first order corrections to the energy eigenstates $|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \phi_m^0 | \hat{H}' | \phi_n^0 \rangle}{(E_n^0 - E_m^0)} |\phi_m^0\rangle$.

For a given \hat{H}^0 and \hat{H}' , the following flowchart summarizes the steps required to find the corrections to the energies and energy eigenstates when \hat{H}^0 possesses a degeneracy.

Finding First Order Corrections to the Energies and Energy Eigenstates



5.3 Practice

EXAMPLE 9: Now let's apply these ideas to an example (question 35-39): Given

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{bmatrix} 1 + 11\epsilon & -8\epsilon & 4\epsilon \\ -8\epsilon & 2 - \epsilon & -2\epsilon \\ 4\epsilon & -2\epsilon & 2 - 4\epsilon \end{bmatrix}, \quad (\epsilon \ll 1). \quad (23)$$

The normalized basis states are $|\psi_1^0\rangle$, $|\psi_2^0\rangle$, and $|\psi_3^0\rangle$, respectively, in which

$$|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (24)$$

Answer the following questions.

35. Choose the unperturbed Hamiltonian, \hat{H}^0 , and the perturbing Hamiltonian, \hat{H}' from the choices below.

(A)

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 + 11\epsilon & 0 & 0 \\ 0 & 2 - \epsilon & 0 \\ 0 & 0 & 2 - 4\epsilon \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} 0 & -8\epsilon & 4\epsilon \\ -8\epsilon & 0 & -2\epsilon \\ 4\epsilon & -2\epsilon & 0 \end{pmatrix}$$

(B)

$$\hat{H}^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} 11\epsilon & -8\epsilon & 4\epsilon \\ -8\epsilon & -\epsilon & -2\epsilon \\ 4\epsilon & -2\epsilon & -4\epsilon \end{pmatrix}$$

(C)

$$\hat{H}^0 = V_0 \begin{pmatrix} 11\epsilon & -8\epsilon & 4\epsilon \\ -8\epsilon & -\epsilon & -2\epsilon \\ 4\epsilon & -2\epsilon & -4\epsilon \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

(D)

$$\hat{H}^0 = V_0 \begin{pmatrix} 11\epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & 4\epsilon \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} 1 & -8\epsilon & 4\epsilon \\ -8\epsilon & 2 & -2\epsilon \\ 4\epsilon & -2\epsilon & 2 \end{pmatrix}$$

36. Choose the unperturbed energies and the normalized eigenstates of \hat{H}^0 from the choices below.

(A) The unperturbed energies are V_0 , $4V_0$, and $11V_0$.

$$\text{The eigenstates are } \left\{ |\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}.$$

(B) The unperturbed energies are ϵV_0 , $4\epsilon V_0$, and $11\epsilon V_0$.

$$\text{The eigenstates are } \left\{ |\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}.$$

(C) The unperturbed energies are ϵV_0 , and $4\epsilon V_0$.

$$\text{The eigenstates are } \left\{ |\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}.$$

(D) The unperturbed energies are V_0 and $2V_0$ (twice).

$$\text{The eigenstates are } \left\{ |\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}.$$

37. Which one of the following is true about the degeneracy of \hat{H}^0 ?

(A) \hat{H}^0 has a two-fold degeneracy with energy eigenvalue of $2V_0$.

(B) \hat{H}^0 has a two-fold degeneracy with energy eigenvalues of $-\epsilon V_0$ and $-4\epsilon V_0$.

(C) \hat{H}^0 has a two-fold degeneracy with energy eigenvalue of V_0 .

(D) \hat{H}^0 has a two-fold degeneracy with energy eigenvalues of V_0 and $2V_0$.

38. Now you will diagonalize part of the \hat{H}' matrix in the degenerate subspace of \hat{H}^0 .

(i) What is the \hat{H}' matrix in the degenerate subspace of \hat{H}^0 ?

(A) $V_0 \begin{pmatrix} 11\epsilon & -8\epsilon \\ -8\epsilon & -\epsilon \end{pmatrix}$

(B) $V_0 \begin{pmatrix} -8\epsilon & -\epsilon \\ 4\epsilon & -2\epsilon \end{pmatrix}$

(C) $V_0 \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$

(D) $V_0 \begin{pmatrix} -\epsilon & -2\epsilon \\ -2\epsilon & -4\epsilon \end{pmatrix}$

(ii) Choose the correct statement below.

- (A) In the degenerate subspace of \hat{H}^0 , the eigenvalues of \hat{H}' are $-5\epsilon V_0$ and $15\epsilon V_0$, and the normalized eigenstates of \hat{H}' are $\left\{ \begin{pmatrix} -2 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 2 \end{pmatrix} \right\}$, respectively.
- (B) In the degenerate subspace of \hat{H}^0 , the eigenvalues of \hat{H}' are $-5 - \sqrt{5}\epsilon V_0$ and $\sqrt{5} - 5\epsilon V_0$, and the normalized eigenstates of \hat{H}' are $\left\{ \frac{1}{4} \begin{pmatrix} -3 - \sqrt{5} \\ 1 \end{pmatrix}, \frac{1}{4} \begin{pmatrix} -3 + \sqrt{5} \\ 1 \end{pmatrix} \right\}$, respectively.
- (C) In the degenerate subspace of \hat{H}^0 , the eigenvalues of \hat{H}' are 0 and $-5\epsilon V_0$, and the normalized eigenstates of \hat{H}' are $\left\{ \frac{1}{\sqrt{5}} \begin{pmatrix} -2 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \end{pmatrix} \right\}$, respectively.
- (D) In the degenerate subspace of \hat{H}^0 , the eigenvalues of \hat{H}' are both $2V_0$ and the eigenstates of \hat{H}' are $\left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$.

(iii) Choose the true statement (among the following) about extending the eigenstates in the preceding problem to the three-dimensional Hilbert space using the orthogonality of the “good” basis states.

- (A) Extending the normalized eigenstates of \hat{H}' in the degenerate subspace of \hat{H}^0 to the three-dimensional Hilbert space, the “good” states are $\left\{ \frac{1}{\sqrt{5}} \begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} \right\}$, respectively.
- (B) Extending the normalized eigenstates of \hat{H}' in the degenerate subspace of \hat{H}^0 to the three-dimensional Hilbert space, the “good” states are $\left\{ \frac{1}{\sqrt{5}} \begin{pmatrix} -3 - \sqrt{5} \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{5}} \begin{pmatrix} -3 + \sqrt{5} \\ 1 \\ 0 \end{pmatrix} \right\}$, respectively.
- (C) Extending the normalized eigenstates of \hat{H}' in the degenerate subspace of \hat{H}^0 to the three-dimensional Hilbert space, the “good” states are $\left\{ \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{5}} \begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix} \right\}$, respectively.
- (D) Extending the normalized eigenstates of \hat{H}' in the degenerate subspace of \hat{H}^0 to the three-dimensional Hilbert space, the “good” states are $\left\{ \frac{1}{\sqrt{5}} \begin{pmatrix} 0 \\ -2 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{5}} \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix} \right\}$, respectively.

39. Now you will determine a “good” basis.

- (i) Express the “good” basis states as linear combinations of the initially chosen eigenstates of H^0 in equation (23).
- (A) The “good” states are $\left\{ -\frac{2}{\sqrt{5}}|\psi_1^0\rangle + \frac{1}{\sqrt{5}}|\psi_2^0\rangle, \frac{1}{\sqrt{5}}|\psi_1^0\rangle + \frac{2}{\sqrt{5}}|\psi_2^0\rangle, |\psi_3^0\rangle \right\}$.
- (B) The “good” states are $\left\{ |\psi_1^0\rangle, -\frac{2}{\sqrt{5}}|\psi_2^0\rangle + \frac{1}{\sqrt{5}}|\psi_3^0\rangle, \frac{1}{\sqrt{5}}|\psi_2^0\rangle + \frac{2}{\sqrt{5}}|\psi_3^0\rangle \right\}$.
- (C) The “good” states are $\left\{ |\psi_1^0\rangle, \frac{1}{4}(-3 - \sqrt{5})|\psi_2^0\rangle + \frac{1}{4}|\psi_3^0\rangle, \frac{1}{4}(-3 + \sqrt{5})|\psi_2^0\rangle + \frac{1}{4}|\psi_3^0\rangle \right\}$.
- (D) The “good” states are $\left\{ |\psi_1^0\rangle, |\psi_2^0\rangle, |\psi_3^0\rangle \right\}$.

(ii) The \hat{H}' matrix in the good basis is:

$$(A) \hat{H}'_G = V_0 \begin{pmatrix} 15\epsilon & 0 & 0 \\ 0 & -5\epsilon & 0 \\ 0 & 0 & -4\epsilon \end{pmatrix}$$

$$(B) \hat{H}'_G = V_0 \begin{pmatrix} 11\epsilon & \frac{20}{\sqrt{5}}\epsilon & 0 \\ \frac{20}{\sqrt{5}}\epsilon & 0 & 0 \\ 0 & 0 & -5\epsilon \end{pmatrix}$$

$$(C) \hat{H}'_G = V_0 \begin{pmatrix} 0 & -8\epsilon & 4\epsilon \\ -8\epsilon & 0 & -2\epsilon \\ 4\epsilon & -2\epsilon & 0 \end{pmatrix}$$

$$(D) \hat{H}'_G = V_0 \begin{pmatrix} 1 & -8\epsilon & 4\epsilon \\ -8\epsilon & 2 & 0 \\ 4\epsilon & 0 & 2 \end{pmatrix}$$

(iii) Choose the first order corrections to the energies from the choices below.

(A) The first order corrections to the energies are $E_1^1 = 15\epsilon V_0$, $E_2^1 = -5\epsilon V_0$, and $E_3^1 = -4\epsilon V_0$.

(B) The first order corrections to the energies are $E_1^1 = V_0$, $E_2^1 = 2V_0$ and $E_3^1 = 2V_0$.

(C) The first order corrections to the energies are $E_1^1 = 0$, $E_2^1 = -\epsilon V_0$ and $E_3^1 = -4\epsilon V_0$.

(D) The first order corrections to the energies are $E_1^1 = 11\epsilon V_0$, $E_2^1 = 0$ and $E_3^1 = -5\epsilon V_0$.

For a given \hat{H}^0 and \hat{H}' , when \hat{H}^0 has degeneracy, summarize in your own words, the steps necessary to find a “good” basis and the first order corrections to the energies and energy eigenstates.

**** Check your answers to questions 35-39 in EXAMPLE 9. ****

35. B

36. D

37. A

38. i. D

ii. C

iii. D

39. i. B

ii. B

iii. D

If any of your answers do not match the checkpoint for EXAMPLE 9, go back and reconcile any differences between your predictions and the answers in the checkpoint.

EXAMPLE 10: Another example:

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{bmatrix} 5 & \epsilon & \epsilon \\ \epsilon & 1 & \epsilon \\ \epsilon & \epsilon & 1 \end{bmatrix}, \quad (\epsilon \ll 1) \quad (25)$$

40. Identify the unperturbed Hamiltonian, \hat{H}^0 , and the perturbation Hamiltonian, \hat{H}' .
41. Find the unperturbed energies and the corresponding normalized eigenstates of \hat{H}^0 from equation (25).
42. How many fold degeneracy is there in the eigenvalue spectrum of \hat{H}^0 ?
43. Diagonalizing \hat{H}' in the degenerate subspace of \hat{H}^0 :
- (i) Write down \hat{H}' in the degenerate subspace of \hat{H}^0 in equation (25)?
 - (ii) Calculate the eigenvalues and normalized eigenstates of \hat{H}' in the degenerate subspace of \hat{H}^0 in the preceding question.

- (iii) Extend the states in the preceding question to the three-dimensional Hilbert space by making sure that the basis states found by diagonalizing \hat{H}' in the degenerate subspace of \hat{H}^0 are orthonormal to $|\psi_1^0\rangle$ (the basis states in equation (25) corresponding to the non-degenerate eigenvalue of \hat{H}^0).

44. Determine “good” basis states

- (i) Express the “good” states as a linear combination of the initially chosen eigenstates of \hat{H}^0 in equation (25).

- (ii) Find first order corrections to the energies.

**** Check your answers to questions 40-44 in EXAMPLE 10: ****

40.

$$\hat{H}^0 = V_0 \begin{pmatrix} 5 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \hat{H}' = V_0 \begin{pmatrix} 0 & \epsilon & \epsilon \\ \epsilon & 0 & \epsilon \\ \epsilon & \epsilon & 0 \end{pmatrix}$$

41. The unperturbed energies (eigenvalues of \hat{H}^0) are V_0 (which is two-fold degenerate) and $5V_0$.

The unperturbed energy eigenstates are $\left\{ |\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$.

42. \hat{H}^0 has a two-fold degeneracy with energy eigenvalue V_0 .

43. i. $V_0 \begin{pmatrix} 0 & \epsilon \\ \epsilon & 0 \end{pmatrix}$

ii. The eigenvalues of this matrix are $-\epsilon V_0$ and ϵV_0 , and the eigenvectors are $\left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right\}$ respectively.

iii. Extending to the three-dimensional Hilbert space the “good” states are $\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \right\}$.

44. i. The “good” basis states in terms of the initially chosen basis states in equation (25) are $\left\{ |\psi_1^0\rangle, \frac{1}{\sqrt{2}}(|\psi_2^0\rangle - |\psi_3^0\rangle), \frac{1}{\sqrt{2}}(|\psi_2^0\rangle + |\psi_3^0\rangle) \right\}$

ii. The first order corrections to the energies are $E_1^1 = 0$, $E_2^1 = \epsilon V_0$, and $E_3^1 = -\epsilon V_0$.

If any of your answers to EXAMPLE 10 do not match the checkpoint, go back and reconcile any difference you may have.

EXAMPLE 11: Consider the example:

$$\hat{H} = \hat{H}^0 + \hat{H}' = V_0 \begin{bmatrix} 4 + 2\epsilon & 0 & \epsilon \\ 0 & 1 - \epsilon & -2\epsilon \\ \epsilon & -2\epsilon & 1 - 4\epsilon \end{bmatrix}, \quad (\epsilon \ll 1). \quad (26)$$

45. Determine the first order corrections to the energies for \hat{H} given in equation (26).

**** Check your answers to questions 45 in EXAMPLE 11. ****

45. $E_1'' = 2\epsilon V_0$, $E_2' = 0$, $E_3' = -5\epsilon V_0$

If any of your answers for EXAMPLE 11 do not match the checkpoint, go back and reconcile any difference you may have with the answers provided.

EXAMPLE 12: Consider the unperturbed Hamiltonian

$$\hat{H}^0 = V_0 \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}. \quad (27)$$

46. Write an example of a perturbing Hamiltonian \hat{H}' in the same basis as \hat{H}^0 such that for that \hat{H}^0 and \hat{H}' , this basis forms a “good” basis (so that one can use the same expressions that one uses in non-degenerate perturbation theory for perturbative corrections). Use ϵ as a small parameter.

47. Write an example of a perturbing Hamiltonian \hat{H}' in the same basis as \hat{H}^0 such that for that \hat{H}^0 and \hat{H}' , this basis does NOT form a “good” basis (so that one can use the same expressions that one uses in non-degenerate perturbation theory for perturbative corrections). Use ϵ as a small parameter.

**** Check your answers to questions 46-47 in EXAMPLE 12. ****

46. Any \hat{H}' of the form $\hat{H}' = \epsilon V_0 \begin{bmatrix} a & b & 0 \\ b^* & c & d \\ 0 & d^* & e \end{bmatrix}$ in which a, b, c, d and e can be any value such that $a, c,$ and e are real and the product with ϵ remains small.

47. Any \hat{H}' of the form $\hat{H}' = \epsilon V_0 \begin{bmatrix} a & b & f \\ b^* & c & d \\ f^* & d^* & e \end{bmatrix}$ in which a, b, c, d, e and f can be any value such that $a, c,$ and e are real and the product with ϵ remains small and $f \neq 0$.

If any of your answers do not match the checkpoint for EXAMPLE 12, go back and reconcile any difference you may have with the answers provided.