Lecture 21

Time Independent Perturbation Theory – II
Finite Basis Expansion
Block Diagonalization
Degenerate Perturbation Theory

In this lecture you will learn:

- Time independent perturbation theory
- Solution by matrix diagonalization

Statement of the Problem

Consider a problem for which the Hamiltonian is:

$$\hat{H}_o$$

The eigenstates are:

$$\hat{H}_o \left| e_j \right\rangle = E_j \left| e_j \right\rangle$$

The eigenstates form a complete orthonormal set:

$$\sum_j \left| e_j \right\rangle \left\langle e_j \right| = \hat{1} \qquad \left\langle e_j \middle| e_k \right\rangle = \delta_{jk}$$

Now suppose a small perturbation $\hat{O}$ is added to the Hamiltonian:

$$\hat{H} = \hat{H}_o + \hat{O}$$

Question: How do we find the new energies and the new eigenstates?

$$\hat{H} \left| e_j^{new} \right\rangle = E_j^{new} \left| e_j^{new} \right\rangle$$

The Original Hamiltonian

Since the eigenstates of the Hamiltonian $\hat{H}_o$ form a complete orthonormal set:

$$\sum_j |e_j\rangle\langle e_j| = \hat{1}$$

We can write the Hamiltonian $\hat{H}_o$ as:

$$\hat{H}_o = \hat{1}\,\hat{H}_o\,\hat{1} = \left(\sum_j |e_j\rangle\langle e_j|\right)\hat{H}_o\left(\sum_k |e_k\rangle\langle e_k|\right)$$

$$= \sum_{j,k} E_k \langle e_j|e_k\rangle\, |e_j\rangle\langle e_k| = \sum_j E_j |e_j\rangle\langle e_j|$$

Let:

$$|e_1\rangle \to \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix} \quad |e_2\rangle \to \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix} \quad \cdots \quad |e_j\rangle \to \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ \vdots \end{bmatrix} \; j\text{-th row}$$

$$\hat{H}_o \to \begin{bmatrix} E_1 & 0 & 0 & \cdots & 0 & \cdots \\ 0 & E_2 & 0 & \cdots & \cdots & \cdots \\ 0 & 0 & E_3 & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ 0 & \cdots & \cdots & \cdots & E_j & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix}$$

Original Hamiltonian matrix is diagonal in the representation defined by its own eigenbasis

The Full Hamiltonian

Since the eigenstates of the Hamiltonian $\hat{H}_o$ form a complete orthonormal set:

$$\sum_j |e_j\rangle\langle e_j| = \hat{1}$$

We can write the Hamiltonian $\hat{H}$ as:

$$\hat{H} = \hat{1}\,\hat{H}_o\,\hat{1} + \hat{1}\,\hat{O}\,\hat{1} =$$

$$= \sum_j E_j\,|e_j\rangle\langle e_j| \quad + \quad \left(\sum_j |e_j\rangle\langle e_j|\right)\hat{O}\left(\sum_k |e_k\rangle\langle e_k|\right)$$

$$= \sum_j E_j\,|e_j\rangle\langle e_j| \quad + \quad \sum_{j,k} \langle e_j|\hat{O}|e_k\rangle\; |e_j\rangle\langle e_k|$$

$$= \sum_j E_j\,|e_j\rangle\langle e_j| \quad + \quad \sum_{j,k} O_{jk}\; |e_j\rangle\langle e_k|$$

Note that:

$$O_{jk} = \langle e_j|\hat{O}|e_k\rangle = \langle e_k|\hat{O}|e_j\rangle^* = O_{kj}^*$$

The Full Hamiltonian

$$\hat{H} = \sum_j E_j \left|e_j\right\rangle\left\langle e_j\right| \quad + \quad \sum_{j,k} O_{jk} \left|e_j\right\rangle\left\langle e_k\right|$$

Again let:

$$\left|e_1\right\rangle \rightarrow \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix} \quad \left|e_2\right\rangle \rightarrow \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ \vdots \\ \vdots \end{bmatrix} \quad \cdots\cdots\cdots \left|e_j\right\rangle \rightarrow \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ \vdots \end{bmatrix} \begin{matrix} \\ \\ \\ j\text{-th row} \\ \\ \\ \end{matrix}$$

Then:

$$\hat{H} \rightarrow \begin{bmatrix} E_1 & 0 & 0 & \cdots & \cdots & \cdots \\ 0 & E_2 & 0 & \cdots & \cdots & \cdots \\ 0 & 0 & E_3 & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & E_j & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix} + \begin{bmatrix} O_{11} & O_{12} & O_{13} & \cdots & O_{1j} & \cdots \\ O_{21} & O_{22} & O_{23} & \cdots & \cdots & \cdots \\ O_{31} & O_{32} & O_{33} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ O_{j1} & \cdots & \cdots & \cdots & O_{jj} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix}$$

The Full Hamiltonian

$$\hat{H} \rightarrow \begin{bmatrix} E_1 + O_{11} & O_{12} & O_{13} & \cdots & O_{1j} & \cdots \\ O_{21} & E_2 + O_{22} & O_{23} & \cdots & \cdots & \cdots \\ O_{31} & O_{32} & E_3 + O_{33} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ O_{j1} & \cdots & \cdots & \cdots & E_j + O_{jj} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix}$$

Hamiltonian matrix is now NOT diagonal in the representation defined by the eigenbasis of the original Hamiltonian

But the Hamiltonian matrix is Hermitian and solving the problem amounts to diagonalizing this matrix by rotating the basis (similarity transformation)

$$\hat{S}\hat{H}\hat{S}^{-1} = \begin{bmatrix} E_1^{new} & 0 & 0 & \cdots & 0 & \cdots \\ 0 & E_2^{new} & 0 & \cdots & \cdots & \cdots \\ 0 & 0 & E_3^{new} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ 0 & \cdots & \cdots & \cdots & E_j^{new} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix}$$

Finite Basis Expansion

Since it is not possible to diagonalize an infinite matrix by hand or numerically, one needs to make approximations

STEP 1:

One first identifies a *NxN* block of the matrix that has the largest off-diagonal parts

For example, this block could be:

3x3 block

$$\hat{H} \rightarrow \begin{bmatrix} E_1 + O_{11} & O_{12} & O_{13} & \cdots & O_{1j} & \cdots \\ O_{21} & E_2 + O_{22} & O_{23} & \cdots & \cdots & \cdots \\ O_{31} & O_{32} & E_3 + O_{33} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ O_{j1} & \cdots & \cdots & \cdots & E_j + O_{jj} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix}$$

The block can be contiguous ….

Finite Basis Expansion

The *NxN* block need not be contiguous ……….

For example, this block could be:

2x2 block

$$\hat{H} \rightarrow \begin{bmatrix} E_1 + O_{11} & O_{12} & O_{13} & \cdots & O_{1j} & \cdots \\ O_{21} & E_2 + O_{22} & O_{23} & \cdots & \cdots & \cdots \\ O_{31} & O_{32} & E_3 + O_{33} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ O_{j1} & \cdots & \cdots & \cdots & E_j + O_{jj} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix}$$

The block can also be non-contiguous ….

Finite Basis Expansion

STEP 2:

One then diagonalizes the selected *N*x*N* block and obtain the new eigenvalues and eigenvectors

3x3 block

$$\hat{H} \rightarrow \begin{bmatrix} E_1 + O_{11} & O_{12} & O_{13} & \cdots & O_{1j} & \cdots \\ O_{21} & E_2 + O_{22} & O_{23} & \cdots & \cdots & \cdots \\ O_{31} & O_{32} & E_3 + O_{33} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ O_{j1} & \cdots & \cdots & \cdots & E_j + O_{jj} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix}$$

Ignoring

Ignoring

Ignoring

$$\hat{H} \rightarrow \begin{bmatrix} E_1 + O_{11} & O_{12} & O_{13} \\ O_{21} & E_2 + O_{22} & O_{23} \\ O_{31} & O_{32} & E_3 + O_{33} \end{bmatrix}$$

Diagonalize

$$\hat{H} \rightarrow \begin{bmatrix} E_1^{new} & 0 & 0 \\ 0 & E_2^{new} & 0 \\ 0 & 0 & E_3^{new} \end{bmatrix}$$

NOTES:

- **The bigger the size of the *NXN* block (i.e. larger the value of *N*), the better the accuracy of the end results**
- **End results typically converge as *N* increases**

Finite Basis Expansion

STEP 2:

One then diagonalizes the selected *N*x*N* block and obtain the new eigenvalues and eigenvectors

2x2 block

$$\hat{H} \rightarrow \begin{bmatrix} E_1 + O_{11} & O_{12} & O_{13} & \cdots & O_{1j} & \cdots \\ O_{21} & E_2 + O_{22} & O_{23} & \cdots & \cdots & \cdots \\ O_{31} & O_{32} & E_3 + O_{33} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ O_{j1} & \cdots & \cdots & \cdots & E_j + O_{jj} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix}$$

Ignoring

Ignoring

Ignoring

Ignoring

$$\hat{H} \rightarrow \begin{bmatrix} E_1 + O_{11} & O_{1j} \\ O_{j1} & E_j + O_{jj} \end{bmatrix}$$

Diagonalize

$$\hat{H} \rightarrow \begin{bmatrix} E_1^{new} & 0 \\ 0 & E_j^{new} \end{bmatrix}$$

NOTES:

- The bigger the size of the *NXN* block (i.e. larger the value of *N*), the better the accuracy of the end results
- End results typically converge as *N* increases

Why the Name, "Finite Basis Expansion"?

Implicit in this process is the assumption that each new eigenstate of the selected finite-sized block can be adequately written as (or expanded in) a superposition of the old eigenstates of this same block alone:

ignoring

$$\left|e_1^{new}\right\rangle = \sum_{m=1,2,3} c_{1m}\left|e_m\right\rangle + \sum_{m>3} c_{1m}\left|e_m\right\rangle$$

ignoring

$$\left|e_2^{new}\right\rangle = \sum_{m=1,2,3} c_{2m}\left|e_m\right\rangle + \sum_{m>3} c_{2m}\left|e_m\right\rangle$$

ignoring

$$\left|e_3^{new}\right\rangle = \sum_{m=1,2,3} c_{3m}\left|e_m\right\rangle + \sum_{m>3} c_{3m}\left|e_m\right\rangle$$

3x3 block

$$\hat{H} \rightarrow \begin{bmatrix} E_1+O_{11} & O_{12} & O_{13} & \cdots & O_{1j} & \cdots \\ O_{21} & E_2+O_{22} & O_{23} & \cdots & \cdots & \cdots \\ O_{31} & O_{32} & E_3+O_{33} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ O_{j1} & \cdots & \cdots & \cdots & E_j+O_{jj} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix}$$

$$\hat{H} \rightarrow \begin{bmatrix} E_1+O_{11} & O_{12} & O_{13} \\ O_{21} & E_2+O_{22} & O_{23} \\ O_{31} & O_{32} & E_3+O_{33} \end{bmatrix}$$

Diagonalize

$$\hat{H} \rightarrow \begin{bmatrix} E_1^{new} & 0 & 0 \\ 0 & E_2^{new} & 0 \\ 0 & 0 & E_3^{new} \end{bmatrix}$$

Why the Name, "Degenerate Perturbation Theory"?

The technique works even if there are degeneracies:

Technique works if E_1 and E_2 are the same, for example

Technique works even if $E_1 + O_{11}$ and $E_2 + O_{22}$ are the same, for example

3x3 block

$$\hat{H} \rightarrow \begin{bmatrix} E_1 + O_{11} & O_{12} & O_{13} & \cdots & O_{1j} & \cdots \\ O_{21} & E_2 + O_{22} & O_{23} & \cdots & \cdots & \cdots \\ O_{31} & O_{32} & E_3 + O_{33} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ O_{j1} & \cdots & \cdots & \cdots & E_j + O_{jj} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix}$$

Ignoring

Ignoring

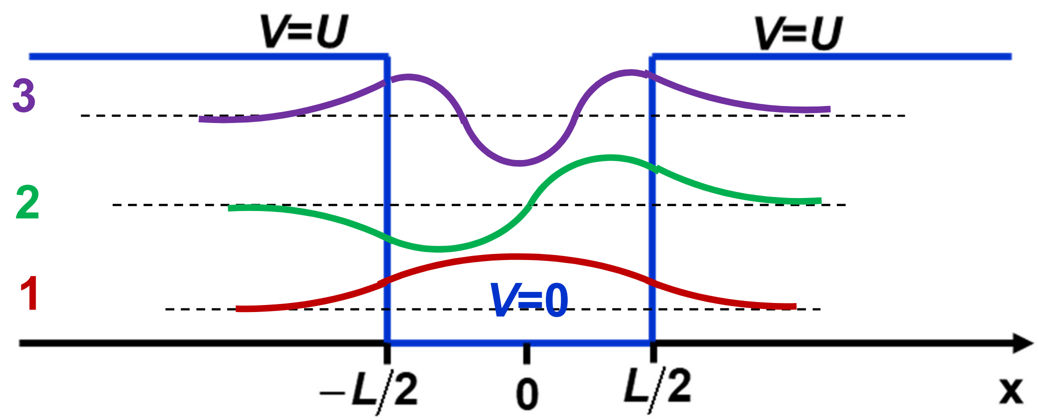
$$\hat{H} \rightarrow \begin{bmatrix} E_1 + O_{11} & O_{12} & O_{13} \\ O_{21} & E_2 + O_{22} & O_{23} \\ O_{31} & O_{32} & E_3 + O_{33} \end{bmatrix}$$

Diagonalize

$$\hat{H} \rightarrow \begin{bmatrix} E_1^{new} & 0 & 0 \\ 0 & E_2^{new} & 0 \\ 0 & 0 & E_3^{new} \end{bmatrix}$$

Finite Basis Expansion Example: Stark Effect

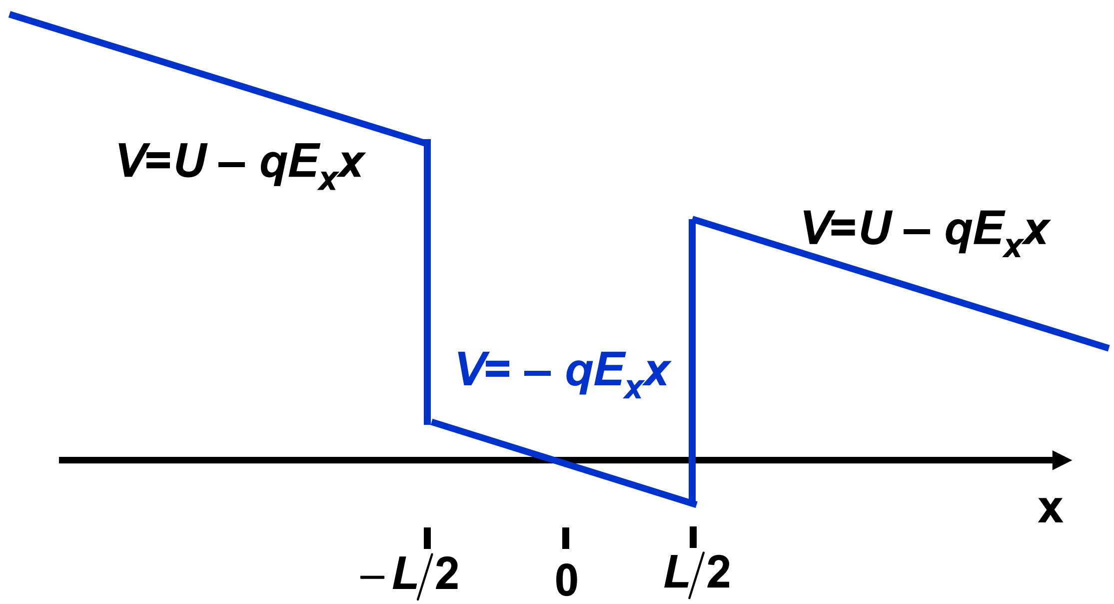
Finite Potential Well



$$\hat{H} = \hat{H}_o - qE_x\hat{x} = \hat{H}_o + \hat{O}$$

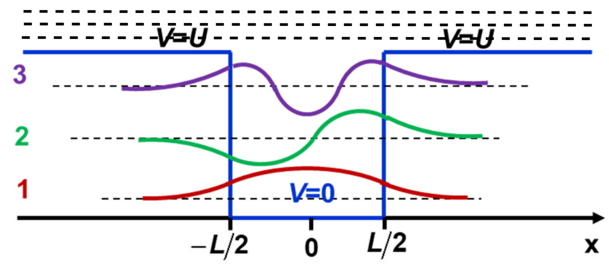
Finite Potential Well in a DC Electric Field

Shifts in the eigenenergies are called Stark shifts

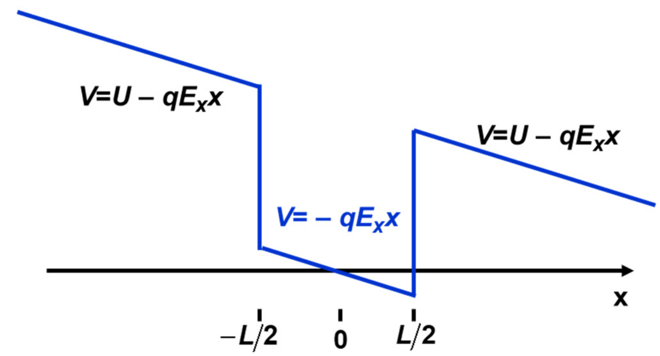


Finite Basis Expansion Example: Stark Effect

$$\hat{H} = \hat{H}_o - qE_x\hat{x} = \hat{H}_o + \hat{O}$$



$$\hat{H} \rightarrow \begin{bmatrix} E_1 + \cancelto{0}{O_{11}} & O_{12} & \cancelto{0}{O_{13}} & \cdots & O_{1j} & \cdots \\ O_{21} & E_2 + \cancelto{0}{O_{22}} & O_{23} & \cdots & \cdots & \cdots \\ \cancelto{0}{O_{31}} & O_{32} & E_3 + \cancelto{0}{O_{33}} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ O_{j1} & \cdots & \cdots & \cdots & E_j + \cancelto{0}{O_{jj}} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix}$$



3x3 block

$$\hat{H} \rightarrow \begin{bmatrix} E_1 & O_{12} & 0 & \cdots & O_{1j} & \cdots \\ O_{21} & E_2 & O_{23} & \cdots & \cdots & \cdots \\ 0 & O_{32} & E_3 & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots & \cdots \\ O_{j1} & \cdots & \cdots & \cdots & E_j & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \ddots \end{bmatrix}$$

Ignoring

Ignoring

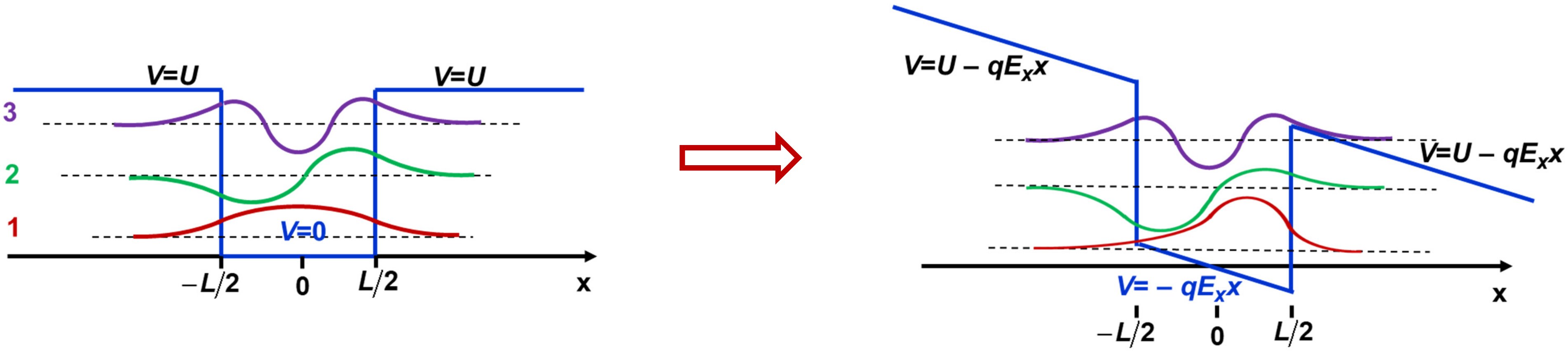
ignoring

$$\Rightarrow \hat{H} \rightarrow \begin{bmatrix} E_1 & O_{12} & 0 \\ O_{21} & E_2 & O_{23} \\ 0 & O_{32} & E_3 \end{bmatrix}$$

Diagonalize

$$\Rightarrow \hat{H} \rightarrow \begin{bmatrix} E_1^{new} & 0 & 0 \\ 0 & E_2^{new} & 0 \\ 0 & 0 & E_3^{new} \end{bmatrix}$$

Finite Basis Expansion: Stark Effect



Need to diagonalize this matrix:

$$\hat{H} = \begin{bmatrix} E_1 & -qE_x d_{12} & 0 \\ -qE_x d_{21} & E_2 & -qE_x d_{23} \\ 0 & -qE_x d_{32} & E_3 \end{bmatrix}$$