Degenerate Perturbation Theory

We start with an operator $\mathcal{A}$ such that

$$\mathcal{A} = \mathcal{A}^{(0)} + \epsilon\mathcal{A}^{(1)}$$

where $\mathcal{A}^{(0)}$ and $\mathcal{A}^{(1)}$ are both Hermitian, and given that we know the set of **orthogonal and normalized** eigenvectors and eigenvalues of the unperturbed system $\mathcal{A}^{(0)}$, that is, $\mathcal{A}|_{\epsilon=0}$.

$$\mathcal{A}^{(0)}x_{n,i}^{(0)} = \lambda_n^{(0)}x_{n,i}^{(0)}.$$

where there are μ_n eigenvectors associated with the eigenvalue $\lambda_n^{(0)}$ so that $i = 1, 2, \ldots \mu_n$. Note that some of the eigenvalues might *not* be degnenerate, so that for that eigenvalue $\mu_n = 1$). We wish to find the approximate eigenvectors and eigenvalues of $\mathcal{A}$:

$$\mathcal{A}y_{n,i} = \lambda_{n,i}\, y_{n,i}$$

To do so we seek a power series solution of the form

$$\begin{aligned} y_n &= y_n^{(0)} + \epsilon\, y_n^{(1)} + \epsilon^2\, y_n^{(2)} \ldots \\ \lambda_n &= \lambda_n^{(0)} + \epsilon\, \lambda_n^{(1)} + \epsilon^2\, \lambda_n^{(2)} \ldots \end{aligned}$$

where for the *non-degenerate eigenvalues* $\lambda_{n,1}^{(0)}$ we trivially have that

$$y_{n,1}^{(0)} = x_{n,1}^{(0)} \tag{1}$$

And the first order correction to their eigenvalues is calculated as before:

$$\lambda_{n,1}^{(1)} = \left(y_{n,1}^{(0)}\middle|\ \mathcal{A}^{(1)}y_{n,1}^{(0)}\right) \tag{2}$$

But we must handle the degenerate eigenvalues differently. For each degenerate $\lambda_n^{(0)}$ we associate a new (better) set of orthonormal eigenvectors made from the degenerate subspace spanned by the old $x_{n,i}^{(0)}$:

$$y_{n,i}^{(0)} = \sum_k a_{i,k}x_{n,k}^{(0)}$$

To find the expansion coefficients $a_{i,k}$, we construct the $\mu_n \times \mu_n$ matrix $\mathcal{M}$ (that is, smaller in rank than $\mathcal{A}$)

$$\mathcal{M}_{k,k'} = \left(x_{n,k}^{(0)}\middle|\ \mathcal{A}^{(1)}\, x_{n,k'}^{(0)}\right) \tag{3}$$

The $a_{i,k}$ giving the expansion coefficients for $y_{n,i}^{(0)}$ form a vector $\vec{a}_i$. We write it with an arrow to make it clear that is *not* the same dimension as x or y. It is an eigenvector of matrix $\mathcal{M}$ with an eigenvalue that gives the first order correction to the eigenvalue:

$$\mathcal{M}\vec{a}_i = \lambda_{n,i}^{(1)}\, \vec{a}_i$$

The first order correction to any *non-degenerate* eigenvector is calculated as before:

$$y_{n,1}^{(1)} = \sum_{k \neq n} \sum_{j=1}^{\mu_k} \frac{\left(y_{k,j}^{(0)} \middle| \mathcal{A}^{(1)} y_{n,1}^{(0)} \right)}{\lambda_n^{(0)} - \lambda_k^{(0)}} y_{k,j}^{(0)}$$

The first order correction to a *degenerate* eigenvector $y_{n,\ell}^{(0)}$ is broken into two parts: the part inside the degenerate subspace ($f_{n,\ell}$) and the part outside the degenerate subspace ($g_{n,\ell}$).

$$y_{n,\ell}^{(1)} = f_{n,\ell} + g_{n,\ell} \tag{4}$$

The $g_{n,\ell}$ is handled exactly as above:

$$g_{n,\ell} = \sum_{k \neq n} \sum_{j=1}^{\mu_k} \frac{\left(y_{k,j}^{(0)} \middle| \mathcal{A}^{(1)} y_{n,\ell}^{(0)} \right)}{\lambda_n^{(0)} - \lambda_k^{(0)}} y_{k,j}^{(0)} \tag{5}$$

The second order correction to *all* eigenvalues is:

$$\lambda_{n,\ell}^{(2)} = \sum_{k \neq n} \sum_{j=1}^{\mu_k} \frac{\left| \left(y_{k,j}^{(0)} \middle| \mathcal{A}^{(1)} y_{n,\ell}^{(0)} \right) \right|^2}{\lambda_n^{(0)} - \lambda_k^{(0)}} \tag{6}$$

Once we know $\lambda_{n,\ell}^{(2)}$, we can calculate $f_{n,\ell}$ for the degenerate states. It can be written

$$f_{n,\ell} = \sum_{k=1}^{\mu_n} b_{\ell,k} x_{n,k}^{(0)} \tag{7}$$

The μ_n expansion coefficients $b_{\ell,k}$ of the first order correction to the eigenvector $y_{n,i}^{(0)}$ again form a vector $\vec{b}_\ell$ that will satisfy the matrix equation

$$\left(\mathcal{M} - \lambda_{n,\ell}^{(1)} \mathbb{1} \right) \vec{b}_\ell = \lambda_{n,\ell}^{(2)} \vec{a}_\ell - \vec{c}_\ell$$

Where the elements of the vector $\vec{c}_\ell$ are

$$c_{\ell,j} \equiv \left(x_{n,j}^{(0)} \middle| \mathcal{A}^{(1)} g_{n,\ell} \right) \tag{8}$$

If we have done everything correctly then we find $\vec{a}_\ell \cdot \vec{b}_\ell = 0$. (The first order correction to to $y_{n,i}^{(0)}$ is orthogonal to $y_{n,i}^{(0)}$).

"EXACT" ANSWER

Degenerate Perturbation Theory

In[980]:=
```
a0 = {{1, 2, 0}, {2, 1, 0}, {0, 0, -1}};
a1 = {{0, 0, 0}, {0, 0, 1}, {0, 1, 0}};
MatrixForm[a0]
MatrixForm[a1]
```

Out[982]//MatrixForm=

$$\begin{pmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Out[983]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

In[984]:=
```
atot = a0 + ϵ a1;
```

In[985]:=
```
eout = Eigensystem[atot];
evals = eout[[1]];
evecs = eout[[2]];
```

In[990]:=
```
TableForm[ToRadicals[evals]]
```

Out[990]//TableForm=

$$\frac{1}{3} - \frac{-16-3\,\epsilon^2}{3\left(64-9\,\epsilon^2+3\sqrt{3}\sqrt{-128\,\epsilon^2-13\,\epsilon^4-\epsilon^6}\right)^{1/3}} + \frac{1}{3}\left(64-9\,\epsilon^2+3\sqrt{3}\sqrt{-128\,\epsilon^2-13\,\epsilon^4-\epsilon^6}\right)^{1/3}$$

$$\frac{1}{3} + \frac{\left(1+i\sqrt{3}\right)\left(-16-3\,\epsilon^2\right)}{6\left(64-9\,\epsilon^2+3\sqrt{3}\sqrt{-128\,\epsilon^2-13\,\epsilon^4-\epsilon^6}\right)^{1/3}} - \frac{1}{6}\left(1-i\sqrt{3}\right)\left(64-9\,\epsilon^2+3\sqrt{3}\sqrt{-128\,\epsilon^2-13\,\epsilon^4-\epsilon^6}\right)^{1/3}$$

$$\frac{1}{3} + \frac{\left(1-i\sqrt{3}\right)\left(-16-3\,\epsilon^2\right)}{6\left(64-9\,\epsilon^2+3\sqrt{3}\sqrt{-128\,\epsilon^2-13\,\epsilon^4-\epsilon^6}\right)^{1/3}} - \frac{1}{6}\left(1+i\sqrt{3}\right)\left(64-9\,\epsilon^2+3\sqrt{3}\sqrt{-128\,\epsilon^2-13\,\epsilon^4-\epsilon^6}\right)^{1/3}$$

In[991]:=
```
TableForm[Series[ToRadicals[evals], {ϵ, 0, 2}]]
```

Out[991]//TableForm=

$$3 + \frac{\epsilon^2}{8} + O[\epsilon]^3$$

$$-1 - \frac{\epsilon}{\sqrt{2}} - \frac{\epsilon^2}{16} + O[\epsilon]^3$$

$$-1 + \frac{\epsilon}{\sqrt{2}} - \frac{\epsilon^2}{16} + O[\epsilon]^3$$

In[995]:=
```
evecsRad = ToRadicals[evecs];
```

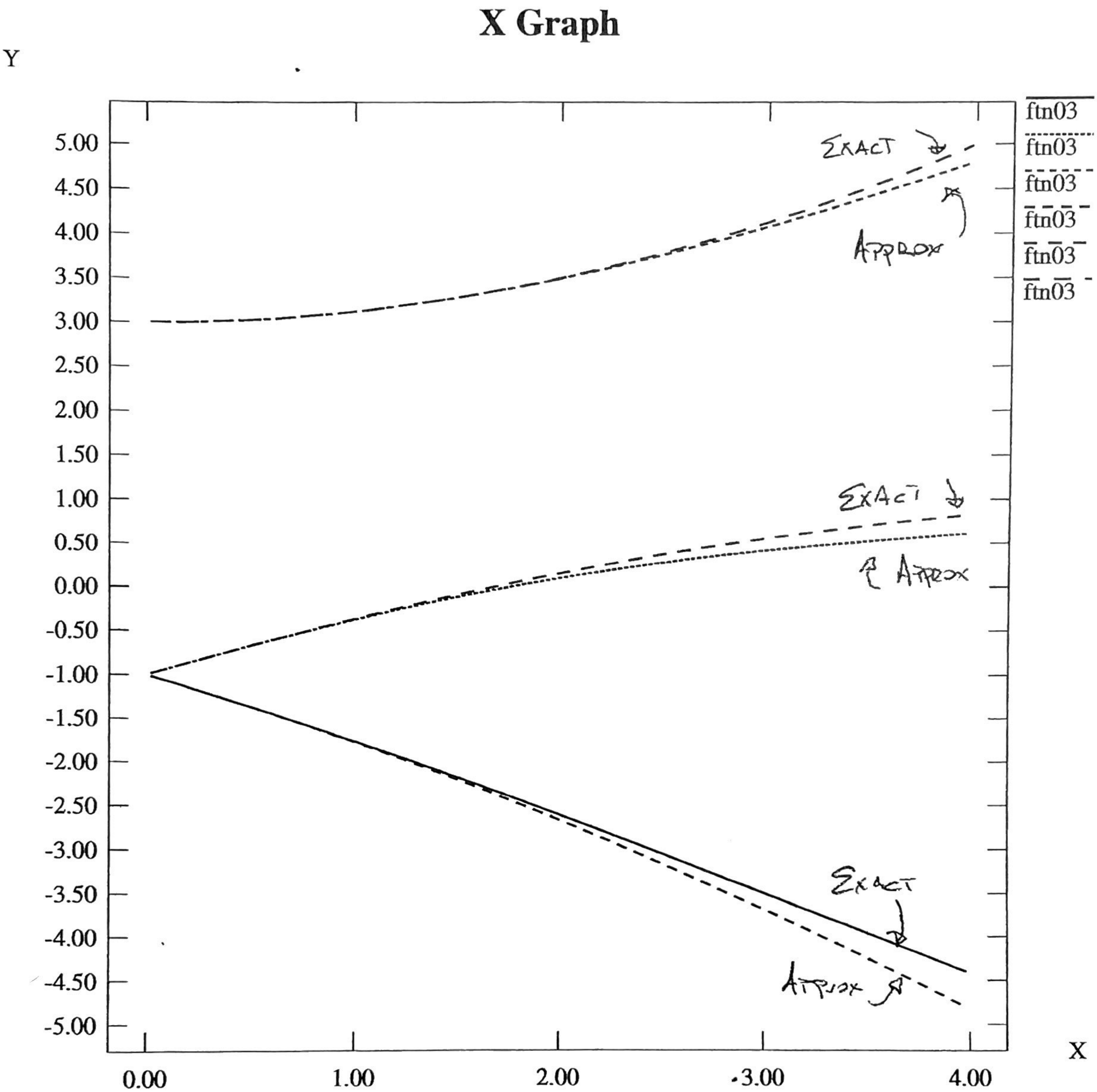
In[997]:=

$$\texttt{normEvecs} = \texttt{Table}\left[\frac{\texttt{evecsRad[[i]]}}{\sqrt{\texttt{evecsRad[[i]].evecsRad[[i]]}}}, \{i, 1, 3\}\right];$$

In[999]:=
```
Table[MatrixForm[Series[normEvecs[[i]], {ϵ, 0, 1}]], {i, 1, 3}]
```

Out[999]=

$$\left\{ \begin{pmatrix} \frac{1}{\sqrt{2}} + O[\epsilon]^2 \\ \frac{1}{\sqrt{2}} + O[\epsilon]^2 \\ \frac{\epsilon}{4\sqrt{2}} + O[\epsilon]^2 \end{pmatrix}, \begin{pmatrix} \frac{1}{2} - \frac{5\,\epsilon}{32\sqrt{2}} + O[\epsilon]^2 \\ -\frac{1}{2} - \frac{3\,\epsilon}{32\sqrt{2}} + O[\epsilon]^2 \\ \frac{1}{\sqrt{2}} + \frac{\epsilon}{32} + O[\epsilon]^2 \end{pmatrix}, \begin{pmatrix} -\frac{1}{2} - \frac{5\,\epsilon}{32\sqrt{2}} + O[\epsilon]^2 \\ \frac{1}{2} - \frac{3\,\epsilon}{32\sqrt{2}} + O[\epsilon]^2 \\ \frac{1}{\sqrt{2}} - \frac{\epsilon}{32} + O[\epsilon]^2 \end{pmatrix} \right\}$$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