The truncated matrix would be diagonal: i.e.,

$$\begin{pmatrix} E_1 & & & \\ & E_2 & & 0 \\ & & \ddots & \\ 0 & & & E_N \end{pmatrix}$$

and the eigenvectors would have only <u>one</u> non-zero element.

As $\lambda H_1 = H - H_0$

grows from <u>zero</u>, the off diagonal elements grow and perturbation theory then tells us they lead to more mixing of states (see p. 6-36a) and including states remoter in energy — which makes the truncation of matrix a poorer approximation.

outside of the region of truncation,

6-86

From ~~the argument of p. 6-36d there is a tendency for states~~

By the way we expect the truncate matrix to be diagonalish

This follows from the p. 6-36d argument that $\langle \chi_{0j} | H | \chi_{0i} \rangle$ should tend to be small as $|E_{0j} - E_{0j}|$ grows

there the argument was for H_1,
but the same ~~argument~~ argument
applies to H also.

~~Mathematically this means far off~~

This means far-off-diagonal elements tend to have less influence on the solution than ~~near~~-near-diagonal elements

How does this Manifest itself mathematically?

Well $\det|H - E\,1_{op}|$

$= \det|A|$

$= \sum_{\mathcal{P}} (-1)^{\mathcal{P}} A_{11'} A_{22'} A_{33'} \cdots$

$\mathcal{P}$ stands for permutation of the primed indices.

The more off-diagonal

elements a term contains, the smaller it tends to be and the less influence on the solution for E; it tends to have.

Concrete Examples

a) 3×3

$$\det\begin{pmatrix} H_{11}-E & H_{12} & H_{13} \\ H_{21} & H_{22}-E & H_{23} \\ H_{31} & H_{32} & H_{33}-E \end{pmatrix}$$

$$= (H_{11}-E)(H_{22}-E)(H-E_{33})$$

$$\left.\begin{array}{l} +H_{12}H_{23}H_{31} \\ +H_{13}H_{21}H_{32} \end{array}\right\}\text{ 2-permutation terms}$$

$$\text{1-permutation terms}\left\{\begin{array}{l} -H_{31}(H_{22}-E)H_{13} \\ -H_{32}H_{23}(H_{11}-E) \\ \cancel{-H_{33}H_{21}H_{12}}\ -(H_{33}-E)H_{21}H_{12} \end{array}\right.$$

Using the trick

$$\left(\begin{array}{ccc} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{array}\right)\begin{array}{cc} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{array}$$

add down diagonal products subtract up diagonal products.

See Wiki: determinant

rule of Sarrus

So we get a cubic in E.

If the tendency for ~~off~~ far-off-diagonal terms to ~~be~~ be small holds true, then the 2-permutation terms are least important.

Again remoteness in energy ~~sh~~ tends to less influence on solutions.

Do the eigenvectors show the some weak coupling ~~for remote~~ between states remote in energy? Perturbation theory suggests this must be so, but it takes more matrix skill than I have to show it.

6-90)

There is, of course, a general solution for cubics, but ~~we~~ it's beyond us.

Special cases of 3 × 3 's are easy to solve

b) 2 X 2 Case

- Very important since a ~~simple~~ case with simple general solution.

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \underset{\sim}{c} = E \underset{\sim}{c}$$

$$0 = \det |H - E 1_{op}| = (H_{11} - E)(H_{22} - E) - H_{21} H_{12}$$

$$0 = E^2 + E(-H_{11} - H_{22}) + H_{11} H_{22} - |H_{12}|^2$$

Since $H_{mat} = H^{\dagger}_{mat}$

$H_{21} = H^{*}_{12}$

$$E_\pm = \frac{(H_{11}+H_{22}) \pm \sqrt{(H_{11}+H_{22})^2 - 4(H_{11}H_{22} - |H_{12}|^2)}}{2}$$

$$= \frac{1}{2}(H_{11}+H_{22}) \pm \sqrt{\left(\frac{H_{11}-H_{22}}{2}\right)^2 + |H_{12}|^2}$$

In this case $\begin{pmatrix} H_{11} & 0 \\ 0 & H_{11} \end{pmatrix} c = E_\pm c$ and $E_\pm = H_1$

$c_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$c_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

simplest choice of eigenvectors

but $c_+ = \begin{pmatrix} a \\ b \end{pmatrix}$, $c_- = \begin{pmatrix} b^* \\ -a^* \end{pmatrix}$ with $|a|^2 + |b|^2 = 1$ works too so continuum infinity of choices.

— The energy levels are ~~only~~ only degenerate if $H_{11} = H_{22}$ and $H_{12} = 0$

— There are no complex solutions — as there shouldn't be for a Hermitian operator eigenvalue problem.

Eigenvectors?

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \underset{\sim}{c} = E_\pm \underset{\sim}{c}$$

Art-159

We only need one equation. Actually $\begin{pmatrix} H_{11}-E & H_{12} \\ H_{21} & H_{22}-E \end{pmatrix} \underset{\sim}{c} = 0$ a homogeneous matrix equation. A nontrivial solution only if determinant vanishes which we have arranged.

$$H_{11}c_1 + H_{12}c_2 = E_\pm c_1$$

$$c_2 = \frac{(E_\pm - H_{11})}{H_{12}} c_1$$

Solved for $c_1 = H_{12}$

$c_2 = (E_\pm - H_{11})$

6-92

Homogenous problems have only $N-1$ independent equations.

So we need one more equation for a full solution. Normalization provides that.

$$C_{\pm} = \frac{1}{\sqrt{(E_{\pm}-H_{11})^2 + |H_{12}|^2}} \begin{pmatrix} H_{12} \\ E_{\pm} - H_{11} \end{pmatrix}$$

normalized

actually dimensionless as it should be.

~~Note 1 the solutions are~~

$$C_{+}^{\dagger} C_{-} = \frac{1}{\sqrt{(E_{+}-H_{11})^2 + |H_{12}|^2}} \frac{1}{\sqrt{(E_{-}-H_{11})^2 + |H_{12}|^2}}$$

$$* \left(|H_{12}|^2 + (E_{+} - H_{11})(E_{-} - H_{11}) \right)$$

$$= \ldots \left[|H_{12}|^2 + \left(\tfrac{1}{2}(H_{22} - H_{11}) + \sqrt{} \right) \right.$$

$$\left. * \underbrace{\left(\tfrac{1}{2}(H_{22} - H_{11}) - \sqrt{} \right)}_{\text{a difference of squares case}} \right]$$

$$= \ldots \left[|H_{12}|^2 + \tfrac{1}{4}(H_{22} - H_{11})^2 - \tfrac{1}{4}(H_{11} - H_{22})^2 - |H_{12}|^2 \right]$$

$$= 0$$

and so the eigenvectors are orthogonal as they should be for a non-degenerate case.

[Note the eigenvectors can be written in many different equivalent ways by

6-94

dividing components and normalization by common factors.

Also one can multiply by an arbitrary phase factor $e^{i\theta}$ (e.g., i or $-i$)

A global phase factor has **NO** effect on the physics.

So people who solve problems in different ways or with different tastes end up different equivalent solutions

Caveat Marker

omit in lecture very tedious

Proof of 2nd order perturbation theory energy for 2-d Hilbert Space

The results for 1st order states are too hard?

Our solutions are exact for a 2-d space.

But say

$$H = H^0 + \lambda H^1$$

and in the representation

$$H^0_{mat} = \begin{pmatrix} H^0_{11} & 0 \\ 0 & H^0_{22} \end{pmatrix}$$

It is diagonal with eigenenergies H^0_{11} and H^0_{22}

Now $$H = \begin{pmatrix} H^0_{11} + \lambda H^1_{11} & \lambda H^1_{12} \\ \lambda H^1_{21} & H^0_{22} + \lambda H^1_{22} \end{pmatrix}$$

$$E_\pm = \frac{1}{2}(H_{11} + H_{22}) \pm \frac{1}{2}\sqrt{(H_{11} - H_{22})^2 + 4|H_{12}|^2}$$

$$= \frac{1}{2}(H_{11} + H_{22}) \pm \frac{1}{2}\sqrt{(H^0_{11} - H^0_{22})^2 + \lambda^2(H^1_{11} - H^1_{22})^2 + 2\lambda(H^0_{11} - H^0_{22})(H^1_{11} - H^1_{22}) + 4\lambda^2|H^1_{12}|^2}$$

6-96

$$E_\pm = \frac{1}{2}\left(H_{11}^0 + H_{22}^0 + \lambda(H_{11}^1 + H_{22}^1)\right)$$

$$\pm \frac{1}{2}\sqrt{(H_{11}^0 - H_{22}^0)^2}$$

$$* \sqrt{1 + 2\lambda\frac{(H_{11}^1 - H_{22}^1)}{(H_{11}^0 - H_{22}^0)} + \lambda^2\left(\frac{(H_{11}^1 - H_{22}^1)^2}{(H_{11}^0 - H_{22}^0)^2} + 4|H_{12}^1|^2\right)}$$

Without loss of generality assume $H_{22}^0 \geq H_{11}^0$

and expand to 2^{nd} order in λ

$$= \frac{1}{2}\left(H_{11}^0 + H_{22}^0 + \lambda(H_{11}^1 + H_{22}^1)\right)$$

$$\pm \frac{1}{2}(H_{22}^0 - H_{11}^0)\left[1 + \lambda\frac{(H_{11}^1 - H_{22}^1)}{(H_{11}^0 - H_{22}^0)} + \lambda^2\left[\frac{1}{2}\frac{(H_{11}^1 - H_{22}^1)^2}{(H_{11}^0 - H_{22}^0)^2} + \frac{2|H_{12}^1|^2}{(H_{11}^0 - H_{22}^0)^2} - \frac{1}{2}\frac{(H_{11}^1 - H_{22}^1)^2}{(H_{11}^0 - H_{22}^0)^2}\right]\right]$$

$$\frac{1}{2!}\left(-\frac{1}{2}\right)\left(\frac{1}{2}\right)2^2 = -\frac{1}{2}$$

$$= \frac{1}{2}\left(H^0_{11} + H^0_{22} + \lambda\left(H'_{11} + H'_{22}\right)\right)$$

$$\pm \frac{1}{2}\left[H^0_{22} - H^0_{11} \right.$$

$$\cancel{+}\ \lambda\left(H'_{11} - H'_{22}\right)$$

$$\left. \cancel{+}\ \lambda^2 \,(2)\, \frac{|H'_{12}|^2}{H^0_{11} - H^0_{22}} \right]$$

$$= \begin{cases} H^0_{11} + \lambda H'_{11} + \lambda^2 \dfrac{|H'_{21}|^2}{H^0_{11} - H^0_{22}} & \text{-ve case} \\[3em] H^0_{22} + \lambda H'_{22} + \lambda^2 \dfrac{|H'_{12}|^2}{H^0_{22} - H^0_{11}} & \text{+ve case} \end{cases}$$

Comparing to p 6-40,
we see this is exactly
what 2nd order perturbation
theory predicts.
(which is sort of a miracle of algebra)

Let's do the states too

$$\begin{pmatrix} H_{11}^0 + \lambda H_{11}^1 & \lambda H_{12}^1 \\ \lambda H_{21}^1 & H_{22}^0 + \lambda H_{22}^1 \end{pmatrix} \underset{\sim}{C}_\pm = E_\pm \underset{\sim}{C}_\pm$$

For -ve case

$$(H_{11}^0 + \lambda H_{11}^1) c_1 + \lambda H_{12}^1 c_2$$

$$= \left(H_0^{11} + \lambda H_{11}^1 + \lambda^2 \frac{|H_{12}^1|^2}{H_{11}^0 - H_{22}^0} \right) c_1$$

$$H_{12}^1 c_2 = \lambda \frac{|H_{12}^1|^2}{H_{11}^0 - H_{22}^0} c_1$$

$$c_2 = \lambda \frac{H_{21}^1}{H_{11}^0 - H_{22}^0} c_1$$

$$\underset{\sim}{C}_- = \begin{pmatrix} 1 \\ \lambda \dfrac{H_{21}^1}{H_{11}^0 - H_{22}^0} \end{pmatrix}$$

$$\underset{\sim}{C}_-^+ \underset{\sim}{C}_- = 1 + O(\lambda^2)$$

which is Normalized to 1st order in λ and this agrees with the 1st order perturbation result on p. 6-36a

For the +ve case

$$\lambda H'_{21} c_1 + \left(H^0_{22} + \lambda H'_{22}\right) c_2 = \left(H^0_{22} + \lambda H'_{22} + \lambda^2 \frac{|H'_{12}|^2}{H^0_{22} - H^0_{11}}\right) c_2$$

$$H'_{21} c_1 = \lambda \frac{|H'_{12}|^2}{H^0_{22} - H^0_{11}} c_2$$

$$c_1 = \lambda \frac{H'_{12}}{H^0_{22} - H^0_{11}} c_2$$

$$\underset{\sim}{c}_+ = \begin{pmatrix} \lambda \frac{H'_{12}}{H_{22} - H^0_{11}} \\ 1 \end{pmatrix}$$

which is normalized to 1st order in λ $\quad c_+^\dagger c_+ = O(\lambda^2) + 1$

and agrees with the 1st order perturbation result of p. 6-40

— golly.

6-100

But is there consistency?

When we solve for the eigen vectors c_i

— Do they ~~you~~ show the ~~weakle~~ weak coupling ~~we we~~ we believe exists from degenerate perturbation theory?

— Yes, but I'm not sure if we can prove it now. It probably takes more matrix solution skill than we've got.

6 + 2

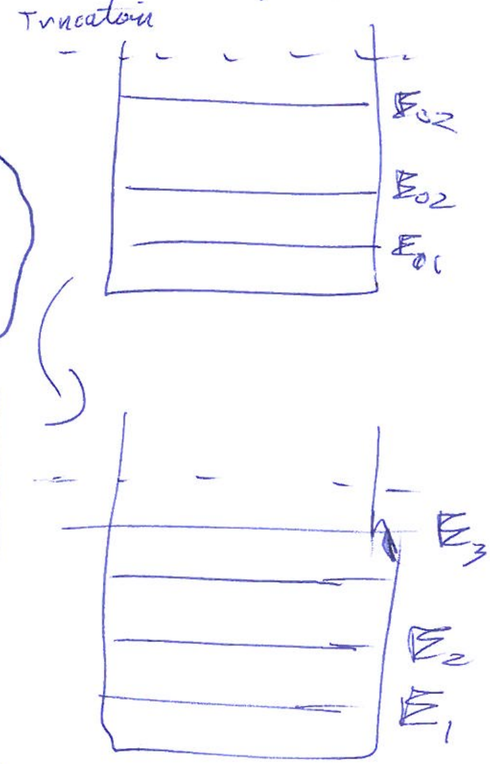
Ex — from set to be posted Hwk 6 (maybe)

Say we have a 3-d space with unperturbed Hamiltonian

Using dimensionless energy here.

$$H_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

For example



and perturbed Hamiltonian

$\varepsilon \ll 1$ but we don't need this restriction for parts (a) & (b).

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

Both matrices are in the H_0 representation

$$H_{0ij} = \langle \phi_{0i} | H_0^{op} | \phi_{0j} \rangle$$
$$= E_{0i} \delta_{ij}$$

$$H_{ij} = \langle \phi_{0i} | H^{op} | \phi_{0j} \rangle$$

a) Solve unperturbed

$$H_0 \underset{\sim}{c} = E \underset{\sim}{c}$$

problem by inspection.

$$E_1 = 1 \qquad \underset{\sim}{c}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$E_2 = \cancel{2}\,1 \,, \qquad \underset{\sim}{c}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$E_3 = \cancel{3}\,2 \,, \qquad \underset{\sim}{c}_{\cancel{3}} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

a general orthonormal pair are $c_1 = \begin{pmatrix} a \\ b \\ 0 \end{pmatrix}$ $c_2 = \begin{pmatrix} b^* \\ -a^* \\ 0 \end{pmatrix}$ subject to normalization constraint $|a|^2 + |b|^2 = 1$

Note these are degenerate, and the ~~eigenvalue~~ eigenvectors are NOT necessarily orthogonal. But we've chosen orthogonal ones by inspection

A general ~~orthogonal pair~~ are $\underset{\sim}{c}_2 = \begin{pmatrix} 0 \\ b \end{pmatrix}$ ~~c_b~~ $c_2 = \begin{pmatrix} 0 \\ b^* \\ -a^* \end{pmatrix}$ with constraint $|a|^2 + |b|^2 = 1$

$$\underset{\sim}{c}_{ab} = a\underset{\sim}{c}_1 + b\underset{\sim}{c}_2 \qquad \left\{ a^2 + b^2 = 1 \right.$$

~~this~~ is also an eigenvector

6 ~~14~~

but we don't need it for anything.

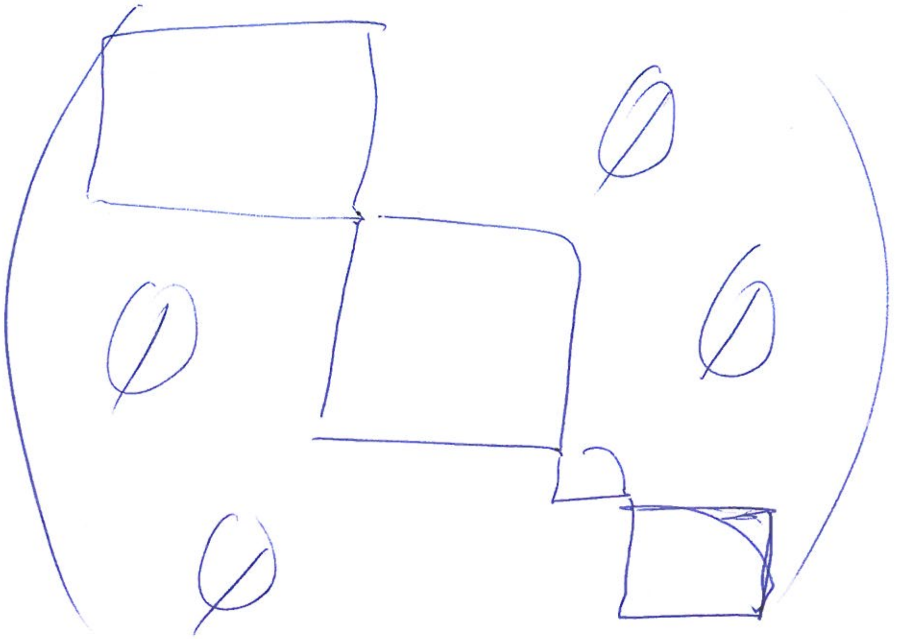
b) Solve the perturbed Hamilton eigenvalue problem.

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

— we ~~can~~ actually can sort of solve cubic equations, but this matrix equation ~~decouples~~ breaks into 2 simpler matrix equations.

The Matrix in Fact is a BLOCK DIAGONAL Matrix.

A =



- a square matrix where the only Non-zero elements are in square blocks that symmetrically straddle the diagonal
- the Blocks have no overlapping rows or columns.
- In an eigenvalue problem each block can be treated independently.

$\boxed{6}$

In our case

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

didn't need to show these explicitly.

$$\begin{pmatrix} 1-\varepsilon & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \underset{\sim}{c} = E \underset{\sim}{c}$$

$\therefore$ $E_1 = 1 - \varepsilon$

Call E_1 and $\underset{\sim}{c} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$.

and $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & \varepsilon \\ 0 & \varepsilon & 2 \end{pmatrix} \underset{\sim}{c} = E \underset{\sim}{c}$

or $$\begin{pmatrix} 1 & \varepsilon \\ \varepsilon & 2 \end{pmatrix} \underset{\sim}{c} = E \underset{\sim}{c}$$

2×2 is ~~an~~ special case of the general 2×2 solved on p. 6-90 – 6-99

$$\det \begin{vmatrix} 1-E & \varepsilon \\ \varepsilon & 2-E \end{vmatrix} = 0$$

$$(1-E)(2-E) - \varepsilon^2 = 0$$

one can solve this or remember the general solution

$$E_{\pm} = \frac{1}{2}\left[H_{11} + H_{22} \pm \sqrt{(H_{11}-H_{22}) + 4|H_{12}|^2} \right]$$

(Gr - 257)

$$= \frac{1}{2}\left[3 \pm \sqrt{1 + 4\varepsilon^2} \right]$$

Now:

$$c_1 + \varepsilon c_2 = E_{\pm} c_1$$

$$c_2 = \frac{(E_{\pm} - 1) c_1}{\varepsilon}$$

which is satisfied by

$$c_1 = \varepsilon$$

$$c_2 = (E_{\pm} - 1)$$

6-108

$$\therefore \quad c_{\pm} = \left(\frac{1}{\sqrt{\varepsilon^2 + (E_{\pm} - 1)^2}} \right) \begin{pmatrix} \varepsilon \\ E_{\pm} - 1 \end{pmatrix}$$

Now to put the whole solution together

$$E_1 = 1 - \varepsilon \qquad E_2 = \tfrac{1}{2}\left[3 - \sqrt{1 + 4\varepsilon^2}\right]$$

$$c_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$c_2 = \frac{1}{\sqrt{\varepsilon^2 + (E_- - 1)^2}} \begin{pmatrix} 0 \\ \varepsilon \\ E_- - 1 \end{pmatrix}$$

$$E_3 = \frac{1}{2}\left[3 + \sqrt{1 + 4\varepsilon^2}\right]$$

$$c_3 = \left(\frac{1}{\sqrt{\varepsilon^2 + (E_+ - 1)^2}} \right) \begin{pmatrix} 0 \\ \varepsilon \\ E_+ - 1 \end{pmatrix}$$

Orthogonality

$\underset{\sim}{c}_1$ is clearly orthogonal to $\underset{\sim}{c}_2$ and $\underset{\sim}{c}_3$.

$$\underset{\sim}{c}_2^{\dagger}\, c_3 \propto \varepsilon^2 + (E_- - 1)(E_+ - 1)$$

Now $E_{\pm} - 1$

$$= \tfrac{1}{2}\left[1 \pm \sqrt{1+4\varepsilon^2}\,\right]$$

$$= \varepsilon^2 + \tfrac{1}{4}\left[1 - (1+4\varepsilon^2)\right]$$

using difference of squares

$$= 0$$

as it should be for non-degenerate eigenstates.

6-110

Taylor expansion of Energies to 2^{nd} order and states to 1^{st} order in ε

$$E_1^{(2)} = 1 - \varepsilon \quad \text{exactly}$$

$$E_2^{(2)} = \frac{1}{2}\left[3 - (1 + 2\varepsilon^2 \underbrace{- 2\varepsilon^4}_{-\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2!}\cdot 4^2 = -2})\right]$$

$$= \frac{1}{2}\left[2 - 2\varepsilon^2 + 2\varepsilon^4\right]$$

$$= 1 - \varepsilon^2 + \varepsilon^4$$

$$E_3^{(3)} = \frac{1}{2}\left[3 + (1 + 2\varepsilon^2 - 2\varepsilon^4)\right]$$

$$= \frac{1}{2}\left[4 + 2\varepsilon^2 - 2\varepsilon^4\right]$$

$$= 2 + \varepsilon^2 - \varepsilon^4$$

$$c_1^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad c_2^{(2)} = \frac{1}{\sqrt{\varepsilon^2 + (-\varepsilon^2 + \varepsilon^4)^2}} \begin{pmatrix} 0 \\ \varepsilon \\ -\varepsilon^2 + \varepsilon^4 \end{pmatrix}$$

$$= \begin{pmatrix} 0 \\ 1 \\ -\varepsilon \end{pmatrix}$$