$$\therefore \begin{pmatrix} M_{11} & M_{12} & M_{13} & \dots & M_{1N} \\ M_{21} & M_{22} & M_{23} & \dots & M_{2N} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ M_{N1} & M_{N2} & M_{N3} & \dots & M_{NN} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} = m \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$$

(3) written in long form:

$$k = 1: (M_{11} - m)c_1 + M_{12}c_2 + M_{13}c_3 + \cdots + M_{1N}c_N = 0$$

$$k = 2: M_{21}c_1 + (M_{22} - m)c_2 + M_{23}c_3 + \cdots + M_{2N}c_N = 0$$

$$k = 3: M_{31}c_1 + M_{32}c_2 + (M_{33} - m)c_3 + \cdots + M_{3N}c_N = 0$$

$$\vdots$$

$$k = N: M_{N1}c_1 + M_{N2}c_2 + M_{N3}c_3 + \cdots + (M_{NN} - m)c_N = 0$$

This can be written as: $$\left(\tilde{M} - m\tilde{I}\right)\tilde{c} = 0$$

I is an N x N unit matrix where $I_{ij} = \delta_{ij}$

$$\Rightarrow \left[\begin{pmatrix} M_{11} & M_{12} & M_{13} & \dots & M_{1N} \\ M_{21} & M_{22} & M_{23} & \dots & M_{2N} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ M_{N1} & M_{N2} & M_{N3} & \dots & M_{NN} \end{pmatrix} - m\begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{pmatrix}\right]\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} = 0$$

Note: if m is known, can solve (3) for c_1, c_2,…,c_N. Get a non-trivial solution only if the determinant of the coefficients of the unknown $\{c_i\}$ is zero

(4) In matrix form: $$\left|\tilde{M} - m\tilde{I}\right| = 0$$

$$\begin{vmatrix} (M_{11}-m) & M_{12} & M_{13} & \dots & M_{1N} \\ M_{21} & (M_{22}-m) & M_{23} & \dots & M_{2N} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ M_{N1} & M_{N2} & M_{N3} & \dots & M_{NN} \end{vmatrix} = 0$$

This is called a **SECULAR EQUATION** for the eigenvalues m; that is, it yields the m's.

Return to the eigenvalue problem: $\widetilde{M}\widetilde{c} = m\widetilde{c} \qquad (a)$

Let **M** be block diagonal and partition the column vector **c**

$$\widetilde{M} = \begin{pmatrix} \widetilde{M}^{(1)} & 0 & 0 \\ 0 & \widetilde{M}^{(2)} & 0 \\ 0 & 0 & \widetilde{M}^{(3)} \end{pmatrix} \quad \widetilde{c} = \begin{pmatrix} \widetilde{c}^{(1)} \\ \widetilde{c}^{(2)} \\ \widetilde{c}^{(3)} \end{pmatrix} \qquad (b)$$

Then (a) becomes:

$$\begin{pmatrix} \widetilde{M}^{(1)} & 0 & 0 \\ 0 & \widetilde{M}^{(2)} & 0 \\ 0 & 0 & \widetilde{M}^{(3)} \end{pmatrix} \begin{pmatrix} \widetilde{c}^{(1)} \\ \widetilde{c}^{(2)} \\ \widetilde{c}^{(3)} \end{pmatrix} = m \begin{pmatrix} \widetilde{c}^{(1)} \\ \widetilde{c}^{(2)} \\ \widetilde{c}^{(3)} \end{pmatrix} \qquad (c)$$

Using the usual rules of matrix multiplication one obtains:

$$\widetilde{M}^{(1)}\widetilde{c}^{(1)} = m\widetilde{c}^{(1)}$$
$$\widetilde{M}^{(2)}\widetilde{c}^{(2)} = m\widetilde{c}^{(2)} \qquad (d)$$
$$\widetilde{M}^{(3)}\widetilde{c}^{(3)} = m\widetilde{c}^{(3)}$$

Therefore, if **M** involves a N x N problem where N is large, (a) can be simplified into (this case) three eigenvalue problems of smaller dimensions given by (d).

→ 3 secular equations of smaller dimension to solve. This is easiest (and trivial) to do if **M** is completely diagonal. There are ways to diagonalize **M**, using the eigenfunctions of **M**, but we won't be covering that in this course.

Procedure

Given: $\left|\tilde{M} - m\tilde{I}\right| = 0$ = secular equation that yields m_i

1.) Take one solution for m, say m_1 and substitute into the set of equations given by:

$$\left(\tilde{M} - m\tilde{I}\right)\tilde{c} = 0 \qquad (1)$$

Solve for c_{n1}, n = 1,2,…,N

Since the solutions to (1) can only be solved within a constant; that is, for c_{n1}/c_{11}, the expansion coefficients can be completely specified by requiring $\Psi_1 = \Sigma_{n=1,..,N}\, c_{ni}\Omega_n$ to be normalized; that is, $<\Phi_i|\Phi_i> = 1 = \Sigma_{n=1,..,N}\, |c_{n1}|^2$.

Repeat steps above for next m_j, solving for the $\{c_{nj}\}$, and requiring Φ_j to be normal. The procedure is repeated for j = 1,2,…,N.

2.4: Time-independent degenerate perturbation theory

A. Getting the solution in principle: Procedure is effectively similar to non-degenerate case but needs modification for 2 reasons.

1.) $E_k^{(0)} - E_q^{(0)}$ can not be zero when we want to calculate a_k in the spectral expansion

2.) If there are 2 or more states with the same energy we don't know which state will arise in the expansion

Recall:

$$E_q = E_q^{(0)} + \lambda E_q^{(1)} + \lambda^2 E_q^{(2)} + \ldots.$$

$$\psi_q = \psi_q^{(0)} + \lambda \psi_q^{(1)} + \lambda^2 \psi_q^{(2)} + \ldots.$$

As $\lambda \rightarrow 0$, $E_q \rightarrow E_q^{(0)}$ and $\Psi_q \rightarrow \Psi_q^{(0)}$

But which state if there more than one with the same $E_q^{(0)}$?

In general therefore $$\lim_{\lambda \to 0} \psi_q = \sum_j c_j \psi_j^{(0)}$$ The sum is over the degenerate states, where the degeneracy is labeled g.

To solve this problem, we need two pieces of information:
a) superposition principle
b) orthonormalization procedure

a) Superposition Principle

All linear combinations of eigenfunctions of an operator **M** corresponding to the same degenerate eigenvalue, m, are also eigenfunctions of **M** with eigenvalue m.

That is: $$\hat{M}\psi_j = m\psi_j \qquad j = 1,2,\ldots,g$$

$$\therefore \hat{M}\left(\sum_j c_j\psi_j\right) = \sum_j c_j\hat{M}\psi_j = \sum_j c_j m\psi_j = m\left(\sum_j c_j\psi_j\right)$$

This means we can make linear combinations at will without altering the solutions to the problem.

Recall: eigenfunctions of a self-adjoint operator corresponding to different eigenvalues are orthogonal. Eigenfunctions which are degenerate may be but more than not are not orthogonal to one another

No problem: it is always possible to construct linear combinations of degenerate eigenfunctions which are orthogonal and normalized; that is orthonormal (point 2.)

b) Orthonormalization: Schmidt procedure

Consider a 3-fold degenerate set (Ψ_1, Ψ_2, Ψ_3).

$$\left\langle \psi_i \mid \psi_j \right\rangle \neq 0 \quad \text{necessarily.}$$

Therefore, construct three new functions ($\Phi_1^{(0)}$, $\Phi_2^{(0)}$, $\Phi_3^{(0)}$) from (Ψ_1, Ψ_2, Ψ_3) which are.

Procedure:

Let $\phi_1^{(0)} = \psi_1$

$$\phi_2^{(0)} = b_1\phi_1^{(0)} + b_2\psi_2 = b_1\psi_1 + b_2\psi_2$$

$$\phi_3^{(0)} = c_1\phi_1^{(0)} + c_2\phi_2^{(0)} + c_3\psi_3 = c_1\psi_1 + c_2(b_1\psi_1 + b_2\psi_2) + c_3\psi_3$$

and require $$\left\langle \phi_i^{(0)} \mid \phi_j^{(0)} \right\rangle = \delta_{ij}$$

Thus, for the example above:

i) $\phi_1^{(0)} = \psi_1$

ii) $\left\langle \phi_2^{(0)} \mid \phi_2^{(0)} \right\rangle = 1 = \left\langle b_1\psi_1 + b_2\psi_2 \mid b_1\psi_1 + b_2\psi_2 \right\rangle$

$$= b_1 b_1^* \left\langle \psi_1 \mid \psi_1 \right\rangle + b_2^* b_2 \left\langle \psi_2 \mid \psi_2 \right\rangle + b_1^* b_2 \left\langle \psi_1 \mid \psi_2 \right\rangle + b_2^* b_1 \left\langle \psi_2 \mid \psi_1 \right\rangle$$

$$= b_1^2 + b_2^2 + 2 b_1 b_2 \left\langle \psi_1 \mid \psi_2 \right\rangle$$

but $\left\langle \phi_1^{(0)} \mid \phi_2^{(0)} \right\rangle = 0 = \left\langle \psi_1 \mid b_1\psi_1 + b_2\psi_2 \right\rangle$

$$= b_1 + b_2 \left\langle \psi_1 \mid \psi_2 \right\rangle$$

This is 2 equations in 2 unknowns (b_1 and b_2) since $<\Psi_i|\Psi_j>$ can be calculated

iii) Similarly,use

$$\left\langle \phi_3^{(0)} \mid \phi_3^{(0)} \right\rangle = 1; \left\langle \phi_1^{(0)} \mid \phi_3^{(0)} \right\rangle = 0; \left\langle \phi_2^{(0)} \mid \phi_3^{(0)} \right\rangle = 0$$

to generate 3 equations in 3 unknowns to solve for (c_1, c_2, c_3).

These will be our starting wave functions! For state q, we will call these states $\{\Phi_{q,j}^{(0)}\}$

Now we can

1.) generate a complete orthonormal set of wave functions by linear combinations of the form

$$\phi_{q,j}^{(0)} = \sum_{j=1}^{g} c_j \psi_{q,j}^{(0)}$$

for all degenerate eigenvalues; that is, generate g Φ's with g sets of coefficients.

2. Use this new set of wave functions in a perturbation problem.

For the following be careful of the meaning of super- and subscripts

Will use: j for the degenerate level, j = 1,2,…,g
q for the level of interest
k for all levels, k=1,2,…,00, degenerate or not.