How to Choose a Suitable Basis for A Degenerate Level?

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- Assume that $\{E_n, u_n\}$ are eigen values and eigen functions of unperturbed Hamiltonian operator H_0) and that level E_n is degenerate. So

$$\hat{H} u_n^a = E_n u_n^a, \qquad a = 1, 2, \ldots$$

- A perturbation H_0) is switched on and we want to compute corrections to energy levels using degenerate perturbation theory.

- For the first order corrections to the degenerate level we need to diagonalize the matrix and find its eigen values and eigen vectors. The matrix is

$$\begin{pmatrix} (u_n^{(1)}, H' u_n^{(1)}) & (u_n^{(1)}, H' u_n^{(2)}) & \ldots \\ (u_n^{(2)}, H' u_n^{(1)}) & (u_n^{(2)}, H' u_n^{(2)}) & \ldots \\ \ldots & \ldots & \ldots \end{pmatrix}. \tag{1}$$

- In stead of using $u_n^(a)$ as zeroth order eigen functions, we can start with their arbitrary linear combinations $v_n^{(a)}$

$$v^{(a)}(x) = \sum_a C_{ab} u_n^{(b)}(x) \tag{2}$$

  These will again be eigen functions of H_0 with the same energy E_n.

- We are interested in asking ," How to choose basis functions $v_n^{(a)}(x)$ so that the matrix to be diagonalized can be made to have as many as possible off diagonal matrix elements may vanish?"

Suppose we can find an operator X which commutes with both $H_0, H\,'$. Then the set $\{v_n^{(a)} | a =, 1, 2...\}$ should be selected to be simultaneous eigen vectors of H and X and will satisfy the eigen value equations

$$H_0 v_n^{(a)} = E_n v_n^{(a)}, \qquad X v_n^{(a)} = \lambda_a v_n^{(a)}. \tag{3}$$

The off diagonal terms $\left(v_n^{(b)}, H\,' \, v_n^{(a)}\right)$ will vanish when ever $\lambda \neq \lambda_b$.

The vanishing of matrix elements mentioned in the above is a follows from the proposition given below.

Let $v^{(a)}$ be eigenvector of X with eigen value λ_a

If the commutator of X with H', be zero, then

$$(v^{(a)}, H'v^{(b)}) = 0 \text{ if } \lambda_{a,n} \neq \lambda_{b,n}. \tag{4}$$

In this case, we say that the operator H' **cannot 'connect'** eigen vectors $v^{(a)}, v^{(b)}$ of $\hat{X}$ with different eigenvalues $\lambda_a \neq \lambda_b$.

On the other hand, if

$$(v^{(a)}, H'v^{(b)}) \neq 0 \text{ for } \lambda_{a,n} \neq \lambda_{b,n}. \tag{5}$$

we say that the operator $\hat{X}$ **connects the eigenvectors** of $\hat{X}$ with eigenvalues $\lambda_a \neq \lambda_b$