

Notes for Lectures on Quantum Mechanics *

How to Choose a Suitable Basis for A Degenerate Level?

A. K. Kapoor

<http://ospace.org/users/kapoor>

akkapoor@cmi.ac.in; akkhcu@gmail.com

Contents

1. 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

$$\hat{H}u_n^a = E_n u_n^a, \quad a = 1, 2, \dots$$

2. A perturbation H_0) is switched on and we want to compute corrections to energy levels using degenerate perturbation theory.
3. 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

$$(u_n^{(1)}, H' u_n^{(1)})\alpha_1 + (u_n^{(1)}, H' u_n^{(2)})\alpha_2 = W_1 \alpha_1 \quad (1)$$

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

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

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

*qm-lec-23010; Updated:Oct 6, 2021; Ver 1.x

5. 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?”
6. Suppose we can find an operator X which commutes with both H_0, H' . Then the set $\{v_n^{(a)} | a =, 1, 2, \dots\}$ should be selected to be simultaneous eigen vectors of H and X and will satisfy the eigen value equations

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

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

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

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

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

where $u^{(a)}$ are eigenvectors of X with eigen value λ_a

We say that the operator H' cannot 'connect' eigen vectors $u^{(a)}, u^{(b)}$ of \hat{X} with different eigenvalues $\lambda_a \neq \lambda_b$.