Notes for Lectures in Quantum Mechanics *

Corrections to a degenerate level

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1 Setting Up Perturbation Theory

The total Hamiltonian H is split into two parts

$$H = H_0 + \lambda H' \tag{1}$$

Suppose we are looking for corrections to an energy eigenvalue E_n which is degenerate. Without loss of generality one may assume that the degeneracy is 2, the results derived can easily be generalized for any value of degeneracy. Thus assume that there are two linearly independent solutions $u_n^\alpha, \alpha = 1, 2$.

$$H_0 u_n^{(1)} = E_n u_n^{(1)} \tag{2}$$

$$H_0 u_n^{(2)} = E_n u_n^{(2)} \tag{3}$$

*Updated:Jul 15, 2021; Ver 0.x

We assume that exact eigenvalue, W, and eigenfunctions, $\psi(x)$, have expansions in powers of λ

$$\psi = \psi_0 + \lambda\psi_1 + \lambda^2\psi_2 + \cdots \tag{4}$$

$$W = W_0 + \lambda W_1 + \lambda^2 W_2 + \cdots \tag{5}$$

2 First Order Energy Level Splitting

Substituting the expansions of ψ and W from Eq.(4) and Eq.(5) in Eq.(1) we get

$$H_0\psi_0 = W_0\psi_0 \tag{6}$$

$$H_0\psi_1 + H'\psi_0 = W_0\psi_1 + W_1\psi_0 \tag{7}$$

$$H_0\psi_2 + H'\psi_1 = W_0\psi_2 + W_1\psi_1 + W_2\psi_0 \tag{8}$$

To find the corrections to the unperturbed solutions of Eq.(2)-Eq.(3) we set $W_0 = E_n$ the most general expression for the unpertubed eigenfunction s ψ_0 is

$$\psi_0(x) = \alpha_1 u_n^{(1)} + \alpha_2 u_n^{(2)} \tag{9}$$

Taking the scalar product of Eq.(7) with $u_n^{(1)}$ and using $W_0 = E_n$, Eq.(2) we get

$$(u_n^{(1)}, H_0\psi_1) + (u_n^{(1)}, H'\psi_0) = E_n(u_n^{(1)}, \psi_1) + W_1(u_n^{(1)}, \psi_0) \tag{10}$$

$$(u_n^{(1)}, H'\psi_0) = W_1(u_n^{(1)}, \psi_0) \tag{11}$$

Substiuting from Eq.(2) and Eq.(3) in Eq.(11) we get

$$(u_n^{(1)}, H'u_n(1))\alpha_1 + (u_n^{(1)}, H'u_n(2))\alpha_2 = W_1\alpha_1 \tag{12}$$

Similarly, taking the scalar product of Eq.(7) with $u_n^{[(2)}$ gives

$$(u_n^{(2)}, H'u_n(1))\alpha_1 + (u_n^{(2)}, H'u_n(2))\alpha_2 = W_1\alpha_2 \tag{13}$$

Now note that Eq.(12) and Eq.(13) can be rewritten in a matrix form

$$\begin{bmatrix} \langle n1|H'|n1\rangle & \langle n1|H'|n2\rangle \\ \langle n1|H'|n1\rangle & \langle n1|H'|n2\rangle \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} = W_1 \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} \tag{14}$$

This equation is recognized as an eigenvalue equation. Hence the first order correction, W_1, to the energy eigenvalue E_n is obtained by finding the eigenvalues of the matrix appearing in the left hand side of Eq.(14).

3 Lifting of Degeneracy

For the degenerate case, the diagonal elements are equal,

$$\langle n1|H'|n1\rangle = \langle n2|H'|n2\rangle \tag{15}$$

Therefore the eigenvalues W_1 appearing in Eq.(14) will be distinct if either the off diagonal elements are nonzero

$$\langle n1|H'|n2\rangle \neq 0 \tag{16}$$

If the eigenvalues are distinct,two sets of non-trivial values, one for each eigenvalue W_1, for the coefficients α_1, α_2 will can be found and Eq.(9) determines corresponding lowest order eigenfunctions,ψ_0.

However, when the off diagonal element is zero and the conditions in Eq.(16) is not satisfied, the constants α_1, α_2 remain undetermined and one must go to the second order perturbation theory to find the corrections to the energy levels and eigenfunctions.

4 First Order Eigenfunctions

We take the scalar product of Eq.(7) with u_k, with $k \neq n$, to get

$$(u_k, H_0\psi_1) + (u_k, H'\psi_0) = W_0(u_k, \psi_1) + W_1(u_k, \psi_0) \tag{17}$$

For $k \neq n$ $(u_k, \psi_0) = 0$ and

$$\begin{aligned}(u_k, H_0\psi_1) &= (H_0 u_k, \psi_1) && (18)\\ &= E_k(u_k, \psi_1) && (19)\end{aligned}$$

Making use of Eq.(18)-Eq.(19) in Eq.(17) gives

$$E_k(u_k, \psi_1) + (u_k, H'\psi_0) = E_n(u_k, \psi_1) \tag{20}$$

$$(u_k, \psi_1) = \frac{(u_k, H'\psi_0)}{E_k - En} \tag{21}$$

To determine ψ_1 we expand it in terms of the unperturbed solutions and write

$$\begin{aligned}\psi_1 &= \sum d_k u_k && (22)\\ &= d_n^{(1)}u_n^{(1)} + d_n^{(2)}u_n^{(2)} + \sum_{k\neq n} d_k u_k && (23)\end{aligned}$$

and the coefficients $d_n, n \neq k$ are just the constants given by $d_k = (u_k, \psi_1)$ and hence

$$\psi_1 = d_n^{(1)} u_n^{(1)} + d_n^{(2)} u_n^{(2)} + \sum_{k \neq n} \frac{(u_k, H' \psi_0)}{E_k - En} u_k \tag{24}$$

In case the matrix appearing in Eq.(14) is a multiple of identity then α_1, α_2 are not determined and one has to go to the next order of perturbation theory.

1. Assume that $\{\lambda_n, \phi_n\}$ are eigenvalues and eigenfunctions of a hermitian operator. $\hat{X}$.

   $$\hat{X}\phi_n = \lambda_n \phi_n.$$

   Also let the commutator of X with $\hat{H}'$, be zero. Prove that

   $$(\phi_n, \hat{H}'\phi_m) = 0 \text{ if } \lambda_n \neq \lambda_m \tag{25}$$

   We say that the operator $\hat{H}'$ cannot 'connect' eigenvectors of $\hat{X}$ with $\lambda_n \neq \lambda_m$

2. With $H' = I$, this above result reduces to a familiar theorem. Identify this theorem.

3. Show that the levels remain degenerate if the commutator of $[H, H']$ vanishes.

4. If we can find an hermitian operator $\hat{X}$ which commutes with both H_0, H', there exists a basis the matrix in which (14) is diagonal.

   Remark : This result means there will be no need to diagonalize the matrix if such an operator $\hat{X}$ can be found.