QM-23 Lecture Notes
Approximation Scheme for Time Independent Problems*
23.1 Non degenerate perturbation theory

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§1 Time Independent Problems

We shall discuss the perturbation theory method for time independent problems. Our aim is to compute the eigenvalues and eigenfunctions of a time independent Hamiltonian. In this approximation scheme the starting point is to split the Hamiltonian of the system, H, into two parts

$$H = H_0 + H'$$

in such a way that the eigenvalues and eigenfunctions of H_0 can be found exactly. We further assume that the additional part $\lambda H'$ has small in matrix elements as compared to H_0.

The approximate solution is obtained by assuming that the exact eigenvalues and eigenfunctions have an expansion in powers of λ and that it is sufficient to keep first few terms of the expansion in powers of λ.

We shall be interested in first and second order perturbation theory (terms up order λ^2) for the following two cases

- Eigenvalues of H_0 are non-degenerate.
- Eigenvalues of H_0 may have degeneracy.

Notation: We shall write

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

where λ is introduced for book keeping purposes and at the end of all computations λ will be set equal to one. Eigenfunctions of H_0 will be

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denoted by u_n and eigenvalues by E_n

$$H_0 u_n = E_n u_n \tag{2}$$

Eigenfunctions of the full Hamiltonian will be denoted by ψ and the corresponding eigenvalues by W.

$$H\psi = W\psi \tag{3}$$

Further, it will be assumed that, ψ and W can be expanded in powers of λ

$$\psi = \psi_0 + \lambda\psi_1 + \lambda^2\psi_2 + \cdots \tag{4}$$
$$W = W_0 + \lambda W_1 + \lambda^2 W_2 + \cdots \tag{5}$$

The eigenfunctions u_n of the unperturbed Hamiltonian will be assumed to be orthonormal

$$(u_n, u_m) = \delta_{nm} \tag{6}$$

We start with Eq.(1) and substitute the expansions for ψ and W from Eq.(4)-Eq.(5) in the eigenvalue equation

$$H\psi = W\psi \tag{7}$$

for the full Hamiltonian giving

$$(H_0+\lambda H')(\psi_0+\lambda\psi_1+\lambda^2\psi_2+\cdots) = (W_0+\lambda W_1+\lambda^2 W_2+\cdots)(\psi_0+\lambda\psi_1+\lambda^2\psi_2+\cdots) \tag{8}$$

Comparing powers of λ on both sides we get

$$H_0\psi_0 = W_0\psi_0 \tag{9}$$
$$H_0\psi_1 + H'\psi_0 = W_0\psi_1 + W_1\psi_0 \tag{10}$$
$$H_0\psi_2 + H'\psi_1 = W_0\psi_2 + W_1\psi_1 + W_2\psi_0 \tag{11}$$
$$\tag{12}$$

These equations will be utilized and corrections to the energy levels and wave functions for different cases, degenerate and nondegenerate levels, will be obtained in the first and second orders in perturbation.

§2 Nondegenerate Case

We shall obtain corrections, (assumed to be small), to eigenvalue and eigenfunctions corresponding to a fixed level n. Let u_n and E_n be the corresponding energy eigenfunction and eigenvalue, so that

$$H_0 u_n = E_n u_n \tag{13}$$

where n is a given, fixed number throughout this discussion and refers to a particular energy level of H_0. In this section we assume that the energy level E_n is nondegenerate.

The equation (9) shows that ψ_0 is an eigenfunction of H_0 with eigenvalue W_0. Since we are interested in finding corrections to energy and eigenfunctions of the n-th energy level (assumed to nondegenerate), we take

$$W_0 = E_n \qquad \psi_0 = u_n \tag{14}$$

where n is fixed number. Thus, (10) and (11) take form

$$H_0\psi_1 + H'u_n = E_n\psi_1 + W_1 u_n \tag{15}$$
$$H_0\psi_2 + H_1'\psi_1 = W_0\psi_2 + W_1\psi_1 + W_2 u_n \tag{16}$$

§3 First Order Perturbation Corrections

Take scalar product of (10) with u_k gives

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

The first term in Eq.(17), using the hermiticity of H_0, can be written as $(u_k, H_0\psi_1) = (H_0u_k, \psi_1) = (E_ku_k, \psi_1) = E_k(u_k, \psi_1)$ and hence

$$E_k(u_k, \psi_1) + (u_k, H'u_n) = E_n(u_k, \psi_1) + W_1(u_k, u_n) \tag{18}$$

We write Eq.(18) for two cases $k = n$ and $k \neq n$ separately.

Case $k = n$

For $k = n$ Eq.(18) takes the form

$$E_n + (u_n, H'u_n) = E_n + W_1\|u_n\|^2 \tag{19}$$

The first terms on the two sides cancel, noting $(u_n, u_n) = \|u_n\|^2 = 1$, because u_n are assumed to be normalized, we get from Eq.(19)

$$W_1 = (u_n, H'u_n) \tag{20}$$

This equation gives then first order correction to the energy eigenvalue E_n.

Case $k \neq n$

In this case $(u_k, u_n) = 0$ and the last term in Eq.(18) in the r.h.s. drops out and we get

$$E_k(u_k, \psi_1) + (u_k, H'u_n) = E_n(u_k, \psi_1) \tag{21}$$

which on a rearrangement gives

$$(E_n - E_k)(u_k, \psi_1) = (u_k, H'u_n) \tag{22}$$

which gives us an answer for (u_k, ψ_1)

$$(u_k, \psi_1) = \frac{(u_k, H'u_n)}{E_n - E_k}\ ,\ k \neq n. \tag{23}$$

Eq.(24) determines ψ_1 because $\{u_k\}$ form a complete orthonormal set, ψ_1 can be in terms of u_k as

$$\psi_1 = \sum_{k=1}^{\infty} c_ku_k = c_nu_n + \sum_{k\neq n}^{\infty} c_ku_k \tag{24}$$

where the expansion coefficients c_k, determined by using orthonormality of the unperturbed eigenfunction u_k are given by $c_k = (u_k, \psi_1)$. Thus for $k \neq n$ we get

$$c_k = \frac{(u_k, H'u_n)}{E_n - E_n} \qquad k \neq n \tag{25}$$

Thus Eq.(24) for ψ_1 takes the form

$$\psi_1 = c_nu_n + \sum_{k\neq n} c_ku_k \tag{26}$$

$$= c_nu_n + \sum_{k\neq n} \frac{< k|H'|n >}{E_n - E_k}u_k \tag{27}$$

To summarize the first order correction terms are given by

$$\boxed{W_1 =< n|H'|n >} \tag{28}$$

$$\boxed{\psi_1 = c_nu_n + \sum_{k=1}^{\infty}{}' \frac{< k|H'|n >}{E_n - E_k}u_k} \tag{29}$$

where $\sum'$ means sum over all values of k except $k = n$. Note that in the first order correction, Eq.(31), the constant c_n is not determined. Upto first order in λ the wave function becomes

$$\psi \approx \psi_0 + \lambda\psi_1 \tag{30}$$

$$\approx (1 + c_n)u_n + \lambda \sum_{\substack{k=1\\k\neq n}}^{\infty} \frac{< k|H'|n >}{E_n - E_k}u_k \tag{31}$$

The unknown constant c_n will be determined order by order by normalization requirement $(\psi, \psi) = 1$. Since the zeroth order approximation, u_n to ψ, is already assumed to be normalized, c_n is seen that $c_n \approx O(\lambda)$ holds, because c_n vanishes in the zeroth order.

§4 Second Order Nondegenerate Perturbation Theory

The total hamiltonian H is split into two parts

$$H = H_0 + \lambda H' \tag{32}$$

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 $u_n^\alpha, \alpha = 1, 2$.

$$\begin{aligned} H_0 u_n^{(1)} &= E_n u_n^{(1)} && (33)\\ H_0 u_n^{(2)} &= E_n u_n^{(2)} && (34) \end{aligned}$$

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

$$\begin{aligned} \psi &= \psi_0 + \lambda\psi_1 + \lambda^2\psi_2 + \cdots && (35)\\ W &= W_0 + \lambda W_1 + \lambda^2 W_2 + \cdots && (36) \end{aligned}$$

§5 First Order Energy Level Splitting

Substituting the expansions of ψ and W from Eq.(35) and Eq.(36) in Eq.(32) we get

$$\begin{aligned} H_0\psi_0 &= W_0\psi_0 && (37)\\ H_0\psi_1 + H'\psi_0 &= W_0\psi_1 + W_1\psi_0 && (38)\\ H_0\psi_2 + H'\psi_1 &= W_0\psi_2 + W_1\psi_1 + W_2\psi_0 && (39) \end{aligned}$$

To find the corrections to the unperturbed solutions of Eq.(33)-Eq.(34) we set $W_0 = E_n$ the most general expression for the unpertubed eigenfunction s ψ_0 is

$$\psi_0(x) = \alpha_1 u_n^{(1)} + \alpha_2 u_n^{(2)} \tag{40}$$

Taking the scalar product of Eq.(38) with $u_n^{(1)}$ and using $W_0 = E_n$, Eq.(33) we get

$$\begin{aligned} (u_n^{(1)}, H_0\psi_1) + (u_n^{(1)}, H'\psi_0) &= E_n(u_n^{(1)}, \psi_1) + W_1(u_n^{(1)}, \psi_0) && (41)\\ (u_n^{(1)}, H'\psi_0) &= W_1(u_n^{(1)}, \psi_0) && (42) \end{aligned}$$

Substiuting from Eq.(33) and Eq.(34) in Eq.(42) we get

$$(u_n^{(1)}, H'u_n(1))\alpha_1 + (u_n^{(1)}, H'u_n(2))\alpha_2 = W_1\alpha_1 \tag{43}$$

Similarly, taking the scalar product of Eq.(38) with $u_n^{[(2)}$ gives

$$(u_n^{(2)}, H'u_n(1))\alpha_1 + (u_n^{(2)}, H'u_n(2))\alpha_2 = W_1\alpha_2 \tag{44}$$

Now note that Eq.(43) and Eq.(44) can be rewritten in a matrix form

$$\begin{bmatrix} \langle n1|H'|n1\rangle & \langle n1|H'|n2\rangle \\ \langle n1|H'|n1\rangle & \langle n1|H'|n2\rangle \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} = W_1 \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} \tag{45}$$

This equation is recognised 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.(45).

Note that the eigenvlaues W_1 appearing in Eq.(45) will be distinct if either the off diagonal elements are nonzero

$$\langle n1|H'|n2\rangle \neq 0 \tag{46}$$

or if the diagonal elements are distinct,

$$\langle n1|H'|n1\rangle \neq \langle n2|H'|n2\rangle \tag{47}$$

If the eigenvalues are distinct,two sets of nontrivial values, one for each eigenvalue W_1, for the coefficients α_1, α_2 will can be found and Eq.(40) determines corresponding lowest order eigenfunctions,ψ_0. However, when the conditions in Eq.(46)-Eq.(47) are 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.

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