# PERTURBATION THEORY AND RELATIVISTIC CORRECTION

Project report (part-1)

Submitted in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE
in
PHYSICS

By

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**DEPARTMENT OF PHYSICS**
**NATIONAL INSTITUTE OF TECHNOLOGY KARNATAKA**
**SURATHKAL, MANGALORE -575 025**
**DECEMBER 2014**
**PROJECT-I (PH 899)**

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Under the guidance of

**Dr.Deepak Vaid**


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## DECLARATION

I hereby declare that the report of P.G. Project Work entitled **PERTURBATION THEORY AND RELATIVISTIC CORRECTION** which is being submitted to the National Institute of Technology Karnataka, Surathkal, in partial fulfillment of the requirements for the award of the Degree of Master of Science in the Department of Physics, is a bonafide report of the work carried out by me. The material contained in this report has not been submitted to any University or Institution for the award of any Degree.

Place: NITK, Surathkal
Date:

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## CERTIFICATE

This is to certify that the P.G. project work entitled **PERTURBATION THEORY AND RELATIVISTIC CORRECTION** submitted by **SARATH.E (13450713PH14)** as the record of work carried out by him is accepted as the P.G.project work report submission in partial fulfilment of the requirements for the award of the Degree of Master of Science in the Department of Physics.

**Chairman-DPGC**

**Dr. Deepak Vaid**
Project Adviser

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## ABSTRACT

In this thesis time dependent and time independent perturbation theory is discussed.This is one of the approximate method using in Quantum Mechanics to solve the problem of small disturbed system.Then using first order time independent perturbation theory relativistic correction for energy is calculated.The perturbation method is most easily understood through a simple algebraic equation.The simple algebraic equation n is solved using approximate method.Two graphs are drawn by varying different parameter in the algebraic equation.

# Contents

# Chapter 1

# INTRODUCTION

Perturbation theory is the study of the effects of small disturbances. If the effects are small, the disturbances or perturbations are said to be regular; otherwise, they are said to be singular.In quantum mechanics, perturbation theory is a set of approximation schemes directly related to mathematical perturbation for describing a complicated quantum system in terms of a simpler one. The idea is to start with a simple system for which a mathematical solution is known, and add an additional "perturbing" Hamiltonian representing a weak disturbance to the system. If the disturbance is not too large, the various physical quantities associated with the perturbed system (e.g. its energy levels and eigenstates) can be calculated. Using perturbation theory, we can use the known solutions of these simple Hamiltonians to generate solutions for a range of more complicated systems. For example, by adding a perturbative electric potential to the quantum mechanical model of the hydrogen atom, we can calculate the tiny shifts in the spectral lines of hydrogen caused by the presence of an electric field (the Stark effect).

In Quantum mechanics the effects of external disturbance on a system could be obtained theoretically by solving Schrdinger equation. In most cases, the resulting equation is, too complex to be solved exactly. Assuming that a small change in the Hamiltonian produces a correspondingly small change in the wave function. And successive approximations are made using perturbation theory to get an approximate solution for the Schrdinger equation of the perturbed system.In the last section we are correcting the energy term by using relativistic method.[1]

# Chapter 2

# TIME INDEPENDENT PERTURBATION THEORY

## 2.1 General Formalism

Suppose we have solved the (time-independent) Schrodinger equation for some potential (say, the one-dimensional infinite square well):

$$H^0\psi_n^0 = E_n^0\psi_n^0 \tag{2.1}$$

obtaining a complete set of orthonormal eigenfunctions, $\psi_n^0$

$$\langle\psi_n^0|\psi_m^0\rangle = \delta_{nm} \tag{2.2}$$

and the corresponding eigenvalues$E$ Now we perturb the potential slightly. We'd like to solve for the new eigenfunctions and eigenvalues:

$$H\psi_n = E_n\psi_n \tag{2.3}$$

but unless we are very lucky, we're unlikely to be able to solve the Schrodinger equation exactly, for this more complicated potential. Perturbation theory is a systematic procedure for obtaining approximate solutions to the perturbed problem by building on the known exact solutions to the unperturbed case. The new Hamiltonian transform as

the sum of two terms,

$$H = H^0 + \lambda H^{'} \tag{2.4}$$

where $H^{'}$ indicate perturbation and the super script 0 always identifies the unperturbed quantity.If we take $\lambda$ is small number:later we will crank it upto 1,and H will be the true Hamiltonian.
We can write $\psi_n$ and $E_n$ as power series in $\lambda$

$$\psi = \psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + .... \tag{2.5}$$

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + ..... \tag{2.6}$$

Here $E_n^1$ is the first-order correction to the nth eigenvalue, and $\psi_n^1$ is the first-order correction to the $n^{th}$ eigenfunction; $E_n^2$ and $\psi_n^2$ are the second-order corrections, and so on. Substitute the above power series expansion in new Hamiltonian,

$$(H^0+\lambda H^{'})[\psi_n^0+\lambda\psi_n^1+\lambda^2\psi_n^2+....] = (E_n^0+\lambda E_n^1+\lambda^2 E_n^2+....)[\psi_n^0+\lambda\psi_n^1+\lambda^2\psi_n^2+....] \tag{2.7}$$

collecting same powers of $\lambda$,

$$H^0\psi_n^0 + \lambda(H^0\psi_n^1 + H^{'}\psi_n^0) + \lambda^2(H^0\psi_n^2 + H^{'}\psi_n^1) + ....$$

$$= E_n^0\psi_n^0 + \lambda(E_n^0\psi_n^1 + E_n^1\psi_n^0) + \lambda^2(E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0) + .... \tag{2.8}$$

the lowest order implies

$$H^0\psi_n^0 = E_n^0\psi_n^0 \tag{2.9}$$

To first order

$$H^0\psi_n^1 + H^{'}\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0 \tag{2.10}$$

to second order

$$H^0\psi_n^2 + H^{'}\psi_n^1 = E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0 \tag{2.11}$$

and so on.[1]

## 2.2 First order Theory

### 2.2.1 First Order Energies

Taking the inner product of the equation first order $\lambda$(multiplying by $(\psi_n^0)^*$ and integrating)

$$\langle\psi_n^0|H^0\psi_n^1\rangle + \langle\psi_n^0|H^{'}\psi_n^0\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle + E_n^1\langle\psi_n^0|\psi_n^0\rangle \tag{2.12}$$

Here $H^0$ is Hermitian,

$$\langle\psi_n^0|H^0\psi_n^1\rangle = \langle H^0\psi_n^0|\psi_n^1\rangle = \langle E_n^0\psi_n^0|\psi_n^1\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle \tag{2.13}$$

and the above cancels with first term on the right side of the equation. We have

$$\langle\psi_n^0|\psi_n^0\rangle = 1 \tag{2.14}$$

$$E_n^1 = \langle\psi_n^0|H^{'}|\psi_n^0\rangle \tag{2.15}$$

This equation is the most fundamental equation in Quantum Mechanics and it has many practical applications.
It says that the first order correction to the energy is the expectation value of the perturbation in unperturbed states.[2]

### 2.2.2 First Order Wave function

Here unperturbed wave function forms complete set, so $\psi_n^1$ can be expressed as linear combination of them.

$$\psi_n^1 = \sum_{m\neq n} c_m^{(n)}\psi_m^0 \tag{2.16}$$

To find the first order correction to the wave function we first rewrite the equation in the form

$$(H^0 - E_n^0)\psi_n^1 = -(H^{'} - E_n^1)\psi_n^0 \tag{2.17}$$

There is no need to include $m \neq n$ in the sum, because $\psi_n^1$ satisfies the above equation; so $(\psi_n^1 + \alpha\psi_n^0)$,for any constant we can subtract $\psi_n^0$ term.Here our aim is to determine the coefficients $c_m^n$.
So putting $\psi_n^1$ in the first order correction of wave function

$$\sum_{m\neq n}(E_m^0 - E_n^0)c_m^n\psi_m^0 = -(H^{'} - E_n^1)\psi_n^0 \tag{2.18}$$

Take inner product with $\psi_l^0$

$$\sum_{m\neq n}(E_m^0 - E_n^0)c_m^n\langle\psi_l^0|\psi_m^0\rangle = -\langle\psi_l^0|H^{'}|\psi_n^0\rangle + E_n^1\langle\psi_l^0|\psi_n^0\rangle \tag{2.19}$$

suppose $l = n$ the left side is zero, so

$$(E_l^0 - E_n^0)c_l^{(n)} = -\psi_l^0|H^{'}|\psi_n^0\rangle \tag{2.20}$$

$$c_m^n = \frac{\langle\psi_m^0|H^{'}|\psi_n^0\rangle}{E_n^0 - E_m^0} \tag{2.21}$$

Which implies

$$\psi_n^1 = \sum_{m\neq n}\frac{\langle\psi_m^0|H^{'}|\psi_n^0\rangle}{E_n^0 - E_m^0}\psi_m^0 \tag{2.22}$$

As long as the system is non-degenerate the equation holds good.But if two different unperturbed states share same energy, in that case we need to degenerate perturbation theory.

We should remember that perturbation theory often yields surprisingly accurate energies , the wave functions are weak.[2]

## 2.3 Second Order Theory

### 2.3.1 Second Order correction in energy

Proceeding like above, take the inner product of the second order equation with $\psi_n^0$

$$\langle\psi_n^0|H^0\psi_n^2\rangle + \langle\psi_n^0|H^{'}\psi_n^1 = E_n^0\langle\psi_n^0|\psi_n^2\rangle + E_n^1\langle\psi_n^0|\psi_n^1\rangle + E_n^2\langle\psi_n^0|\psi_n^0\rangle \tag{2.23}$$

Then we get

$$\langle\psi_n^0|H^0\psi_n^2\rangle = \langle H^0\psi_n^0|\psi_n^2\rangle = E_n^0\langle\psi_n^0|\psi_n^2\rangle \tag{2.24}$$

So the first terms on the left and right cancel. And we know that wave function is normalised

$$\langle\psi_n^0|\psi_n^0\rangle = 1$$

$$E_n^2 = \langle\psi_n^0|H^{'}|\psi_n^1 - E_n^1\langle\psi_n^0|\psi_n^1\rangle \tag{2.25}$$

and

$$\langle \psi_n^0 | \psi_n^1 \rangle = \sum_{m \neq n} c_m^{(0)} \langle \psi_n^0 | \psi_m^0 \rangle = 0 \tag{2.26}$$

Here we exclude $m \neq n$ because we are considering non-degenerate case

$$E_n^2 = \langle \psi_n^0 | H^{'} | \psi_n^1 \rangle = \sum_{m \neq n} c_m^{(n)} \langle \psi_n^0 | H^{'} | \psi_m^0 \rangle \tag{2.27}$$

$$E_n^2 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H^{'} | \psi_n^0 \rangle \langle \psi_n^0 | H^{'} | \psi_m^0 \rangle}{E_n^0 - E_m^0} \tag{2.28}$$

$$E_n^2 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H^{'} | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0} \psi_m^0 \tag{2.29}$$

[4]

### 2.3.2 Second Order Correction to Wave function

$\psi_n^2$ can be write in terms of unperturbed wave functions,

$$\psi_n^2 = \sum_k b_k \psi_k^0 \tag{2.30}$$

substitute in 2.12 and multiply by $\langle \psi_l^0 |$

$$\sum_m^{'} a_m \langle \psi_l^0 | H^{'} | \psi_m^0 \rangle + \sum_k b_k \langle \psi_l^0 | H^0 \psi_k^0 \rangle \tag{2.31}$$

$$= E_n^2 \langle \psi_l^0 | \psi_n^0 \rangle + E_n^1 a_m \sum_m \langle \psi_l^0 | \psi_m^0 \rangle + E_n^0 \sum_k b_k \langle \psi_l^0 | \psi_k^0 \rangle \tag{2.32}$$

consider

$$m = l$$

$$k = l$$

$$\sum_m a_m \langle \psi_l^0 | H^{'} | \psi_m^0 + b_l E_l^0 = E_n^1 a_l + E_n^0 b_l \tag{2.33}$$

$$b_l (E_l^0 - E_n^0 = E_n^1 a_l - \sum_m a_m \langle \psi_l^0 | H^{'} | \psi_m^0 \tag{2.34}$$

$$b_l = \frac{E_n^1 a_l}{E_l^0 - E_n^0} - \frac{\sum_m a_m \langle \psi_l^0 | H^{'} | \psi_m^0 \rangle}{E_l^0 - E_n^0} \tag{2.35}$$

$$= \frac{\langle\psi_n^0|H^{'}|\psi_n^0\rangle\langle\psi_l^0|H^{'}|\psi_n^0\rangle}{(E_l^0 - E_n^0)(E_n^0 - E_l^0)} - \sum_m \frac{\langle\psi_m^0|H^{'}|\psi_n^0\rangle\langle\psi_l^0|H^{'}|\psi_m^0\rangle}{(E_n^0 - E_m^0)(E_l^0 - E_n^0)} \tag{2.36}$$

$$b_l = \sum_m \frac{\langle\psi_m^0|H^{'}|\psi_n^0\rangle\langle\psi_l^0|H^{'}|\psi_m^0\rangle}{(E_n^0 - E_m^0)(E_n^0 - E_l^0)} - \frac{\langle\psi_n^0|H^{'}|\psi_n^0\rangle\langle\psi_l^0|H^{'}|\psi_n^0\rangle}{(E_n^0 - E_l^0)^2} \tag{2.37}$$

The energy and wave function corrected to second order in the perturbation is

$$E_n = E_n^0 + \langle\psi_n^0|H^{'}|\psi_n^0\rangle + \sum_m \frac{(\langle\psi_n^0|H^{'}|\psi_n^0\rangle))^2}{E_n^0 - E_m^0)} \tag{2.38}$$

$$\psi_n = \psi_n^0 + \sum_m a_m\psi_m^0 + \sum_l b_l\psi_l^0 \tag{2.39}$$

In Quantum mechanics as in Classical mechanics exactly solvable problems are rare and one most frequently resort to approximation.Approximations are therefore expected to play an important role.So various methods of approximation solutions of the wave equation has been derived.Of these methods the first and in many respect the most interesting is perturbation theory.The above discussed is non-degenerate perturbation theory.We can apply perturbation on degenerate case also.[4]

## 2.4 Perturbation Theory for degenerate states

If the unperturbed states are degenerate, two or more distinct state share the same energy.In that case ordinary perturbation theory will not work.

Suppose $\psi_a^0$ and$\psi_b^0$ are degenerate states then there is a chance to become the denominator zero in non-degenerate case equation.

Consider two fold degeneracy

$$H^0\psi_a^0 = E^0\psi_a^0 \tag{2.40}$$

$$H^0\psi_b^0 = E^0\psi_b^0 \tag{2.41}$$

Suppose the states are normalised

$$\langle\psi_a^0|\psi_b^0\rangle = 0$$

The linear combination of these two states can be written as

$$\psi^0 = \alpha\psi_a^0 + \beta\psi_b^0 \tag{2.42}$$

and we have

$$H^0\psi^0 = E^0\psi^0 \tag{2.43}$$

Perturbation breaks the unperturbed energy into two.When we turn of the perturbation the upper state coming back to one linear combination of $\psi_a^0$ and $\psi_b^0$ and lower reduces to some orthogonal linear combination.

We want to solve the schrodinger equation

$$H\psi = E\psi$$

$$H = H^0 + \lambda H^{'} \tag{2.44}$$

and

$$E = E^0 + \lambda E^1 + \lambda^2 E^2 + ....$$

$$\psi = \psi^0 + \lambda\psi^1 + \lambda^2\psi^2...$$

$$(H^0 + \lambda H^{'})(\psi = \psi^0 + \lambda\psi^1 + \lambda^2\psi^2...)$$

$$= (E = E^0 + \lambda E^1 + \lambda^2 E^2 + ....)(\psi = \psi^0 + \lambda\psi^1 + \lambda^2\psi^2..) \tag{2.45}$$

$$H^0\psi^0 + H^0\lambda\psi^1 + H^0\lambda^2\psi^2 + \lambda H^{'}\psi^0 + \lambda^2 H^{'}\psi^1 + ..$$

$$= E^0\psi^0 + E^0\lambda\psi^1 + \lambda^2 E^0\psi^2 + \lambda\psi^0 E^1 + \lambda^2 E^1\psi^1 + \lambda^2 E^2\psi^0 \tag{2.46}$$

Collecting the terms $\lambda^2$

$$H^0\psi^1 + H^{'}\psi^0 = E^0\psi^1 + E^1\psi^0 \tag{2.47}$$

Taking the inner product with $\langle\psi_a^0\rangle$

$$\langle\psi_a^0|H^0|\psi^1\rangle + \langle\psi_a^0|H^{'}|\psi^0\rangle = E^0\langle\psi_a^0|\psi^1\rangle + E^1\langle\psi_a^0|\psi^0\rangle \tag{2.48}$$

Because $H^0$ is hermitian first terms on left and right cancel out

$$\langle\psi_a^0|H^{'}|\psi^0\rangle = E^1\langle\psi_a^0|\psi^0\rangle \tag{2.49}$$

$$\alpha\langle\psi_a^0|H^{'}|\psi_a^0\rangle + \beta\langle\psi_a^0|H^{'}|\psi_b^0\rangle = \alpha E^1\langle\psi_a^0|H^{'}|\psi_a^0\rangle + \beta\langle\psi_a^0|H^{'}|\psi_b^0\rangle \tag{2.50}$$

And we can write it in the following form

$$\alpha W_{aa} + \beta W_{ab} = \alpha E^1 \tag{2.51}$$

Taking the inner product with $\langle\psi_b^0|$

$$\langle\psi_b^0|H^0|\psi^1\rangle + \langle\psi_b^0|H^{'}|\psi^0\rangle = E^0\langle\psi_b^0|\psi^1\rangle + E^1\langle\psi_b^0|\psi^0\rangle \tag{2.52}$$

Because $H^0$ is Hermitian first term on left and right cancels out

$$\langle\psi_b^0|H^{'}|\psi^0\rangle = E^1\langle\psi_b^0|\psi^0\rangle \tag{2.53}$$

And proceed as before

$$\alpha\langle\psi_b^0|H^{'}|\psi_a^0\rangle + \beta\langle\psi_b^0|H^{'}|\psi_b^0\rangle = \alpha E^1\langle\psi_b^0|\psi_a^0\rangle + \beta E^1\langle\psi_b^0|\psi_b^0\rangle \tag{2.54}$$

We can write above equation in the following manner

$$\alpha W_{ba} + \beta W_{bb} = \beta E^1 \tag{2.55}$$

From equation 2.63

$$W_{ab} = \frac{\alpha E^1 - \alpha W_{aa}}{\beta} \tag{2.56}$$

Multiply this equation 2.67

$$\alpha W_{ab}W_{ba} + \beta W_{ab}W_{bb} = \beta E^1 W_{ab} \tag{2.57}$$

$$\alpha W_{ab}W_{ba} + \beta W_{bb}(\frac{\alpha E^1 - \alpha W_{aa}}{\beta}) = \beta E^1(\frac{\alpha E^1 - \alpha W_{aa}}{\beta}) \tag{2.58}$$

$$\alpha W_{ab}W_{ba} + \alpha E^1 W_{bb} - \alpha W_{aa}W_{bb} = \alpha(E^1)^2 - \alpha E^1 W_{aa} \tag{2.59}$$

$$\alpha(W_{ab}W_{ba} + E^1 W_{bb} - W_{aa}W_{bb} - (E^1)^2 + E^1 W_{aa}) = 0 \tag{2.60}$$

$$\alpha[(W_{ab}W_{ba} + E^1 W_{bb}) - (E^1 - W_{aa})(E^1 - W_{bb})] = 0 \tag{2.61}$$

$$(W_{ab}W_{ba} + E^1 W_{bb}) - (E^1 - W_{aa})(E^1 - W_{bb}) = 0 \tag{2.62}$$

$$(E^1)^2 - E^1(W_{aa} + W_{bb}) + (W_{aa}W_{bb} - W_{ab}W_{ba}) \tag{2.63}$$

It is a quadratic equation,hence

$$E^1 = \frac{(W_{aa} + W_{bb}) \pm \sqrt{(W_{aa} + W_{bb})^2 - 4(W_{aa}W_{bb} - W_{ab}W_{ba})}}{2} \tag{2.64}$$

$$E^1 = \frac{(W_{aa} + W_{bb}) \pm \sqrt{W_{aa}^2 + W_{bb}^2 + 2W_{aa}W_{bb} - 4W_{aa}W_{bb} + 4W_{ab}W_{ba}}}{2}$$

$$E^1 = \frac{1}{2}[(W_{aa} + W_{bb}) \pm \sqrt{W_{aa}^2 + W_{bb}^2 - 2W_{aa}W_{bb} + 4W_{ab}W_{ba}}]$$

$$E^1 = \frac{1}{2}[(W_{aa} + W_{bb}) \pm \sqrt{(W_{aa} - W_{bb})^2 + |4W_{ab}|^2}] \tag{2.65}$$

We know that

$$W_{ab} = W_{ba}^* \tag{2.66}$$

And we will end up with the below equation

$$E_{\pm}^1 = \frac{1}{2}[(W_{aa} + W_{bb}) \pm \sqrt{(W_{aa} - W_{bb})^2 + |4W_{ab}|^2}] \tag{2.67}$$

If

$$\alpha = 1$$

$$\beta = 0$$

$$E_+^1 = W_{aa} = \langle \psi_a^0 | H^{'} | \psi_a^0 \rangle \tag{2.68}$$

$$E_-^1 = W_{bb} = \langle \psi_b^0 | H^{'} | \psi_b^0 \rangle \tag{2.69}$$

The above result is same what we obtained with non-degenerate case

In the above discussed case we express the states with the linear combination of appropriate states.It helped us to find the energy correction more easily.If there is correct choice of linear combination we can apply non-degenerate theory also.[2]

### 2.4.1 Theorem

Let 'A' be the Hermitian Operator that commutates with $H^0$ and $H^{'}$. If $\psi_a^0$ and $\psi_b^0$ are (degenerate eigenfunctions of $H^0$) are also eigenfunctions of A with different eigenvalues.

$$A\psi_a^0 = \mu\psi_a^0 \tag{2.70}$$
$$A\psi_b^0 = \nu\psi_b^0 \tag{2.71}$$
$$\mu \neq \nu \tag{2.72}$$

Then $W_{ab} = 0$
Hence $\psi_a^0$ and $\psi_b^0$ are best states to use in Perturbation Theory.Proof is given below

$$[A, H^{'}] = 0$$

$$\langle\psi_a^0|[A, H^{'}]|\psi_b^0\rangle = 0 \tag{2.73}$$

$$\langle\psi_a^0|AH^{'}\psi_b^0\rangle - \langle\psi_a^0|H^{'}A\psi_b^0\rangle = 0 \tag{2.74}$$
$$\langle A\psi_a^0|H^{'}\psi_b^0\rangle - \langle\psi_a^0|H^{'}\nu\psi_b^0\rangle = 0 \tag{2.75}$$
$$\mu\langle\psi_a^0|H^{'}|\psi_b^0\rangle - \nu\langle\psi_a^0|H^{'}|\psi_b^0\rangle = 0 \tag{2.76}$$

$$(\mu - \nu)(\langle\psi_a^0|H^{'}|\psi_b^0\rangle) = 0 \tag{2.77}$$
$$(\mu - \nu)W_{ab} = 0 \tag{2.78}$$

But $(\mu \neq \nu)$ so $W_{ab} = 0$ [4]

## 2.5 Higher Order Degeneracy

Previous section we used two fold degeneracy,

$$\begin{pmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Here $E^1$ are the eigenvalues of $W$ matrix.In the case of 'n' fold degeneracy we find eigenvalues for 'n' square matrix.[4]

$$W_{ij} = \langle\psi_i^0|H^{'}|\psi_j^0\rangle$$

# Chapter 3

# TIME DEPENDENT PERTURBATION THEORY

## 3.1 Introduction

Until now we worked with the potential that independent of time

$$V(r,t) = V(r)$$

In such cases we can solve the Schrodinger equation by

$$H\psi = i\hbar\frac{\partial\psi}{\partial x}$$

It may solve by separation of variables

$$\psi(r,t) = \psi(r)e^{(\frac{-iEt}{\hbar})} \tag{3.1}$$

Here $\psi(r)$ obey time independent schrodinger equation $H\psi = E\psi$

the time dependence factor is expressed by the exponential term,which can be eliminate using suitable $|\psi|^2$.If we want to know the quantum jumps,transition from one state to other we need to introduce time dependent potential.In the given Hamiltonian time independent part play small role compared to time dependent part.Hence it can be considered as perturbation.Here we are developing time dependent perturbation theory.The importance of time dependent perturbation theory is it allow us to understand the interaction

of radiation with matter.[1]

## 3.2 Two Level System

We start with two unperturbed system $\psi_a$ and $\psi_b$.There is an unperturbed Hamiltonian $H^0$.$\psi_a$ and $\psi_b$ are eigen states of the Hamiltonian.

$$H^0\psi_a = E_a\psi_a \tag{3.2}$$

$$H^0\psi_b = E_b\psi_b \tag{3.3}$$

If the states are orthonormal

$$\langle\psi_a|\psi_b\rangle = \delta_{ab} \tag{3.4}$$

So any state can be expressed as linear combination of these states.

$$\psi(t) = c_a\psi_a + c_b\psi_b \tag{3.5}$$

In time dependent perturbation each component have characteristic exponential form.

$$\psi(t) = c_a\psi_a e^{\frac{-iE_at}{\hbar}} + c_b\psi_b e^{\frac{-iE_bt}{\hbar}} \tag{3.6}$$

$|c_a^2|^2$represent probability of the particle to occupy in $\psi_a$. similarly $|c_b^2|^2$ represent probability to occupy in state $\psi_b$.By applying normalization condition we get

$$|c_a^2|^2 + |c_b^2|^2 = 1$$

## 3.3 The Perturbed System

Here we are introducing perturbation $H^{'}(t)$.Then also .$\psi_a$ and $\psi_b$ can be expressed as linear combinations.But $c_a(t)$ and $c_b(t)$ transformed to function of time.

$$\psi(t) = c_a(t)\psi_a e^{\frac{-iE_at}{\hbar}} + c_b(t)\psi_b e^{\frac{-iE_bt}{\hbar}} \tag{3.7}$$

Our ultimate aim is to find the $c_a$ and $c_b$.Assume that initially particle is in the state $\psi_a$ ($c_a(0) = 1$,$c_b(0) = 0$).later it on $c_a(t_1) = 0$,$c_b(t_1) = 1$ ,that mean particle undergo quantum transition from $\psi_a$ to $\psi_b$

The schrodinger equation for this case is given by

$$H\psi = i\hbar\frac{\partial\psi}{\partial x}$$

Where

$$H = H^0 + H^{'}(t) \tag{3.8}$$

$$c_a[H^0\psi_a]e^{\frac{-iE_at}{\hbar}} + c_b[H^0\psi_b]e^{\frac{-iE_bt}{\hbar}} + c_a[H^{'}\psi_a]e^{\frac{-iE_at}{\hbar}} + c_b[H^{'}\psi_b]e^{\frac{-iE_bt}{\hbar}} \tag{3.9}$$

$$= i\hbar\left[\dot{c_a}\psi_a e^{\frac{-iE_at}{\hbar}} + \dot{c_b}\psi_b e^{\frac{-iE_bt}{\hbar}} + c_a\psi_a(\frac{-iE_a}{\hbar})e^{\frac{-iE_at}{\hbar}} + c_b\psi_b(\frac{-iE_b}{\hbar})e^{\frac{-iE_bt}{\hbar}}\right] \tag{3.10}$$

$$c_a[H^{'}\psi_a]e^{\frac{-iE_at}{\hbar}} + c_b[H^{'}\psi_b]e^{\frac{-iE_bt}{\hbar}}$$
$$= i\hbar\left[\dot{c_a}\psi_a e^{\frac{-iE_at}{\hbar}} + \dot{c_b}\psi_b e^{\frac{-iE_bt}{\hbar}}\right]$$

Take the inner product with $\psi_a$

$$c_a\langle\psi_a|H^{'}|\psi_a\rangle e^{\frac{-iE_at}{\hbar}} + c_b\langle\psi_a|H^{'}|\psi_b\rangle e^{\frac{-iE_bt}{\hbar}} = i\hbar\dot{c_a}e^{\frac{-iE_at}{\hbar}} \tag{3.11}$$

Here we define a shorthand notation

$$H^{'}_{ij} = \langle\psi_i|H^{'}|\psi_j\rangle$$

Multiply through out by $-(\frac{i}{\hbar})e^{\frac{-iE_at}{\hbar}}$
we will get

$$\dot{c_a} = -\frac{i}{\hbar}\left[H_{aa} + c_bH^{'}_{ab}e^{\frac{-i(E_a-E_b)t}{\hbar}}\right] \tag{3.12}$$

Similarly take the inner product with $\psi_b$

$$c_a\langle\psi_b|H^{'}|\psi_a\rangle e^{\frac{-iE_at}{\hbar}} + c_b\langle\psi_b|H^{'}|\psi_b\rangle e^{\frac{-iE_bt}{\hbar}} = i\hbar\dot{c_b}e^{\frac{-iE_bt}{\hbar}} \tag{3.13}$$

so

$$\dot{c_b} = -\frac{i}{\hbar}\left[c_bH_{bb} + c_aH^{'}_{ba}e^{\frac{-i(E_b-E_a)t}{\hbar}}\right] \tag{3.14}$$

The diagonal elements vanishes,Hence

$$\dot{c_a} = -\frac{i}{\hbar}c_bH^{'}_{ab}e^{-i\omega_0t} \tag{3.15}$$

and

$$\dot{c_b} = -\frac{i}{\hbar}c_aH^{'}_{ba}e^{-i\omega_0t} \tag{3.16}$$

We define

$$\omega_0 = \frac{E_b - E_a}{\hbar}$$

## 3.4 Time Dependent Perturbation Theory

In the starting particles in lower state

$$c_a^{(0)}(t) = 1 \qquad c_b(0) = 0 \tag{3.17}$$

If it free from disturbance of Perturbation it stay in same state.

### 3.4.1 Zeroth Order

$$c_a^{(0)}(t) = 1 \qquad c_b^{(0)}(t) = 0 \tag{3.18}$$

### 3.4.2 First Order

To get first order approximation substitute the above values in equation 3.16

$$\frac{dc_a^{(1)}(t)}{dt} = 0 \Longrightarrow c_a^{(1)} = 1$$

$$\frac{dc_b}{dt} = -\frac{i}{\hbar} c_a H_{ba}^{'} e^{-i\omega_0 t}$$

$$c_b^{(1)} = -\frac{i}{\hbar}\int_0^t H_{ba}^{'}(t^{'}) e^{-i\omega_0 t^{'}}\, dt^{'} \tag{3.19}$$

### 3.4.3 second Order

$$c_b^{(2)}(t) = c_b^{(1)}(t)$$

$$\frac{dc_a^{(2)}}{dt} = -\frac{i}{\hbar} H_{ab}^{'} e^{-i\omega_0 t}(-\frac{i}{\hbar})\int_0^t H_{ba}^{'}(t^{'}) e^{-i\omega_0 t^{'}}\, dt^{'}$$

$$c_a^{(2)}(t) = 1 - \frac{1}{\hbar^2}\int_0^t H_{ab}^{'}(t^{'}) e^{-i\omega_0 t^{'}} \left[\int_0^{t^{'}} H_{ba}^{'}(t^{''}) e^{-i\omega_0 t^{''}}\, dt^{''}\right] \tag{3.20}$$

To get the$(n+1)^{th}$ approximation we substituting $(n)^{th}$ in the equation. We proceed the same technique for higher order approximation.[2][4][8]

# Chapter 4

# RELATIVISTIC CORRECTION

The Hamiltonian for a free particle is given by

$$H = T = \frac{1}{2}mv^2 = \frac{p^2}{2m} \tag{4.1}$$

The momentum $p$ can be replaced by operator

$$p \to \frac{\hbar}{i}\nabla$$

$$T = -\frac{\hbar^2}{2m}\nabla^2$$

the relativistic equation for Kinetic Energy

$$T = \frac{mc^2}{\sqrt{1-\frac{v^2}{c^2}}} - mc^2 \tag{4.2}$$

Here the first term represent total energy and second term represent rest mass energy. suppose momentum is given by

$$p = \frac{mv}{\sqrt{1-\frac{v^2}{c^2}}}$$

so we can write it in the form

$$p^2c^2 + m^2c^4 = \frac{m^2v^2c^2 + m^2c^4(1-\frac{v^2}{c^2})}{(1-\frac{v^2}{c^2})}$$

$$\frac{m^2c^4}{(1-\frac{v^2}{c^2})} = (T + mc^2)^2$$

$$T = \sqrt{p^2c^2 + m^2c^4} - mc^2 \tag{4.3}$$

$$T = mc^2[\sqrt{1 + (\frac{p}{mc})^2} - 1 \tag{4.4}$$

This can be expressed by power series expansion

$$T = mc^2 \left[\sqrt{1 + (\frac{p}{mc})^2} - 1\right]$$

$$T = mc^2 \left[1 + \frac{1}{2}(\frac{p}{mc})^2 - \frac{1}{8}(\frac{p}{mc})^4 ....\right]$$

$$T = mc^2 + \frac{p^2}{2m} + \frac{p^4}{8m^3c^2} + ... \tag{4.5}$$

So perturbed Hamiltonian is given by

$$H_r^{'} = -\frac{p^4}{8m^3c^2} \tag{4.6}$$

Apply First order time dependent Perturbation Theory

$$E_r^{'} = -\frac{1}{8m^3c^2}\langle\psi|p^4\psi\rangle \tag{4.7}$$

$$E_r^{'} = -\frac{1}{8m^3c^2}\langle p^2\psi|p^2\psi\rangle \tag{4.8}$$

In the case Schrodinger equation acquires the form

$$p^2\psi = 2m(E - V)\psi \tag{4.9}$$

$$E_r^{'} = -\frac{1}{2mc^2}\langle(E_V)^2\rangle$$

$$E_r^{'} = -\frac{1}{2mc^2}\left[E_n^2 + 2E_n\frac{e^2}{4\pi\epsilon_0}\left\langle\frac{1}{r}\right\rangle + (\frac{e^2}{4\pi\epsilon_0})^2\left\langle\frac{1}{r^2}\right\rangle\right] \tag{4.10}$$

The expectation values are given by

$$\left\langle\frac{1}{r}\right\rangle = \frac{1}{n^2a}$$

$$\left\langle\frac{1}{r^2}\right\rangle = \frac{1}{(l + \frac{1}{2})n^3a^2}$$

$$E_r^{'} = -\frac{1}{2mc^2}\left\{E_n^2 + 2E_n\frac{e^2}{4\pi\epsilon_0}\frac{1}{n^2a} + (\frac{e^2}{4\pi\epsilon_0})^2\frac{1}{(l + \frac{1}{2})n^3a^2}\right\} \tag{4.11}$$

From the Bohr Formula

$$a = \frac{4\epsilon_0 \pi \hbar^2}{me^2}$$

Finally we end up with

$$E_r^{'} = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{(l+\frac{1}{2})} - 3\right] \tag{4.12}$$

It is clear from the result that relativistic correction is smaller than the energy of the state. [2]

# Chapter 5

# THE PERTURBATION METHOD EXPLAINED WITH AN ALGEBRAIC EQUATION

## 5.1 Perturbation Method on Algebraic Equation

The objective of this section is to study, learn and introduce the perturbation method with the support of simple algebraic equation.Perturbation methods find approximate solutions to problems by taking advantage of a small parameter that appears in the initial problem.Consider the small parameter here is $\epsilon$.The value of $\epsilon$ ranges from $0 < \epsilon << 1$.The perturbation method is most easily understood through a simple algebraic equation.

$$x^2 + \epsilon x - 1 = 0 \tag{5.1}$$

The main assumption of perturbation theory is $\epsilon$ should be small.The primary way to obtain an approximate solution is take $\epsilon = 0$ ie,

$$x^2 = 1$$

The leading order root is

$$x = \pm 1$$

First order Solution
First order solution is given by leading order root with some additional term.The important thing is the extra added term is very small compared to the original roots.The

second solution approximation is given by

$$x = 1 \pm \delta(x) \tag{5.2}$$

Substitute the above equation in 4.1 get

$$(1 + \delta(x))(1 + \delta(x)) + \epsilon(1 + \delta(x)) - 1 = 0$$

$$1 + \delta(x) + \delta(x) + \delta(x)^2 + \epsilon + \epsilon(1 + \delta(x)) - 1 = 0$$

Here $\delta(x)^2$ and $\epsilon\delta(x)$ produce extremely small contribution hence we can eliminate it from the equation.Finally we end up with the result

$$\delta(x) = -\frac{\epsilon}{2} \tag{5.3}$$

Substitution of $\delta(x)$ back into 4.2 is

$$x = 1 - \frac{\epsilon}{2} \tag{5.4}$$

The second order solution approximation is assumed to be

$$x = 1 - \frac{\epsilon}{2} + \beta(x) \tag{5.5}$$

Substitute the above equation in 4.1 so

$$(1 - \frac{\epsilon}{2} + \beta(x))(1 - \frac{\epsilon}{2} + \beta(x)) + \epsilon(1 - \frac{\epsilon}{2} + \beta(x)) - 1 = 0$$

$$1 - \frac{\epsilon}{2} + \beta(x) - \frac{\epsilon}{2} + (\frac{\epsilon}{2})^2 - \frac{\epsilon}{2}\beta(x) + \beta(x) - \frac{\epsilon}{2}\beta(x) + \beta(x)^2 + \epsilon - \frac{\epsilon^2}{2} + \epsilon\beta(x) - 1 = 0$$

Similarly $\beta(x)^2$ and $\epsilon$ are small.So we finally reach a solution in the form

$$\beta(x) = \frac{\epsilon^2}{8} \tag{5.6}$$

so

$$x = 1 - \frac{\epsilon}{2} + \frac{\epsilon^2}{8} \tag{5.7}$$

From here it is clear that each correction term is smaller than the preceding term.

## 5.2 Exact Solution of Algebraic Equation

The equation 4.1 is a quadratic equation.Hence the roots are given by

$$x = \frac{-\epsilon \pm \sqrt{\epsilon^2 + 4}}{2} \tag{5.8}$$

And we can calculate percentage of error also.

## 5.3 Data Analysis

| $\epsilon$ | Exact root | First order term | Second order term | Third order term |
|---|---|---|---|---|
| 0 | 1 | 1 | 1 | 0 |
| 0.000001 | 1 | 1 | 1 | 0 |
| 0.00001 | 0.999995 | 0.999995 | 0.999995 | 0 |
| 0.0001 | 0.99995 | 0.99995 | 0.99995 | $(1.11)10^{14}$ |
| 0.001 | 0.9995 | 0.9995 | 0.9995 | $(7.84)10^{13}$ |
| 0.01 | 0.995012 | 0.9995 | 0.999013 | $(7.85)10^{9}$ |
| 0.1 | 0.951249 | 0.95 | 0.95125 | $(8.2)10^{5}$ |
| 1 | 0.61803 | 0.5 | 0.625 | 0.625 |

Table 5.1: Fig (4.1)Perturbation and algebraic solution for the equation 1

Note that for any given value of $\epsilon$ the accuracy of the perturbation approximation increases with the amount of corrections that were determined. The exact, 2nd term and

| $\epsilon$ | Percentage error 2nd term | Percentage error 2nd term |
|---|---|---|
| 0 | 0 | 0 |
| 0.000001 | $(-1.3)10^{-11}$ | 0 |
| 0.00001 | $(-1.3)10^{-9}$ | 0 |
| 0.0001 | $(-1.3)10^{-7}$ | $(1.11)10^{-14}$ |
| 0.001 | $(-1.3)10^{-5}$ | $(7.89)10^{-13}$ |
| 0.01 | -0.00126 | $(7.85)10^{-9}$ |
| 0.1 | -0.13132 | $(8.2)10^{-5}$ |
| 1 | -19.0983 | 1.12724 |

Table 5.2: Fig (4.2)Percentage error forthe algebraic solution for the equation 1

3rd term approximations are nearly indistinguishable at this magnification. Perturbations approximations, unlike a typical series expansion, do not necessarily always become more precise as additional terms are added to the approximation. Perturbation solutions are developed in powers of $\epsilon$ (in the limit as  goes to zero), whereas series solutions are developed in powers of . This distinction leads to differences in solution convergence. Engineers and scientists should be wary that distinct limitations exist with the accuracy that can be achieved with perturbation approximations.[5]

One of the major limitations of the perturbation method is that as the value of  approaches a number on the order of 1 or larger; the accuracy of the perturbation approximation rapidly decreases.In this case we varied different parameter in the algebraic equation and found the numerical results.Two graphs are drawn according to the numerical value.

In Quantum mechanics the effects of external disturbance on a system could be obtained theoretically by solving Schrdinger equation. In most cases, the resulting equation is, too complex to be solved exactly. Assuming that a small change in the Hamiltonian produces a correspondingly small change in the wave function. And successive approximations are made using perturbation theory to get an approximate solution for the Schrdinger equation of the perturbed system.Here we took an algebraic equation and solved it explicitly by simple approximation method.It is the easy way to understand perturbation theory analytically. [5[7]

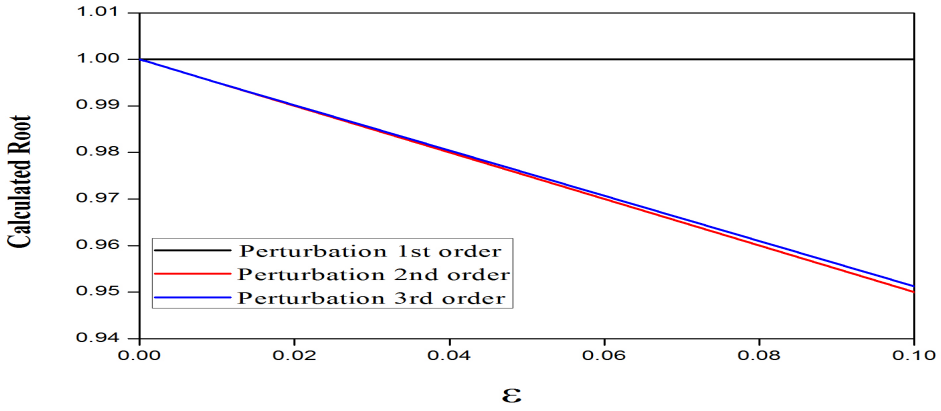


fig 5.1 Comparative solution plot for algebraic equation.

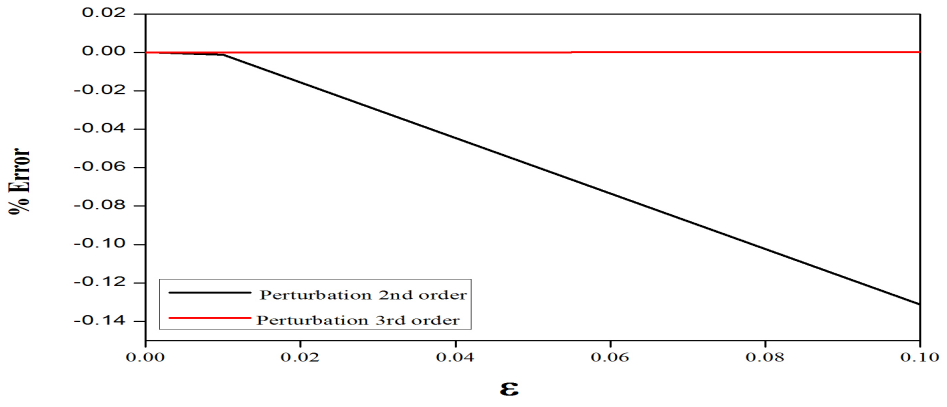


fig 5.2 Perturbation percentage plot for algebraic equation.

# FUTURE PLAN

Most problems in Quantum Mechanics cannot solve exactly.To solve general problems one must use approximation methods.The purpose of this project is to find approximate solution for the problem which cannot be solve common analytical method.Perturbation theory will then be applied to a linear ordinary differential equation boundary layer problem. The boundary layer problem demonstrates the technique required to match inner and outer solutions as well as the technique used to develop a composite solution.It can be used to find static and non oscillatory problem.The unforced Duffing and the Van Der Pol equations and the Poincare-Lindstedt and Multiple Scales methods will be study in next semester.

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