

TIME-DEPENDENT PERTURBATION THEORY  
APPROACH TO THE QUANTUM  
MOTION OF A PARTICLE  
IN A PAUL TRAP

By

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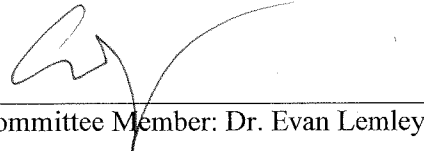
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**Abstract:**

The main objective of this study is to investigate the quantum mechanical lifetime of a trapped ion in a Paul trap. The motivation for this research is that there are several applications of trapped ion devices such as mass spectrometers, atomic clocks, and quantum computers. Active research is presently ongoing in the subject of an ion trapping by electric and magnetic fields. There are many classical studies of the characteristics of trapped ions, however there have been relatively few done quantum mechanically. It might be expected that purely quantum effects could play an important role in describing the trapped ions. So, those are the main factors behind the research on this topic.

Time-dependent perturbation theory was used in this study which is to find the quantum mechanical lifetime of trapped ion in a Paul trap because time-dependent perturbation theory allows describing the complex system with the help of a simple system that can be calculated easily. It is shown that the lifetime of a trapped ion depends on its transition frequency and the transition between two allowed quantum states of the ion. The transition frequency of an ion has to be very close to the applied frequency of alternating current (AC). The results show that the lifetime of a trapped ion can be adjusted as desired for experimentation.

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## CHAPTER I

### INTRODUCTION

#### 1.1 Literature Review

How long a trapped ion is confined in a Paul trap is one of the important pieces of information that trap designers need to know and Wolfgang Paul gave the first detailed information about the Paul trap based on classical mechanics in his paper “*Electromagnetic Traps for Charged and Neutral Particles*” [1]. As a consequence there have been many classical studies in the theory of trapped ions. An important detail that has been less studied is the quantum mechanical lifetime of the trapped ion in a Paul trap. The Paul trap allows an ion to be trapped inside a quadrupole potential that varies with time. A detailed knowledge of this movement is critical since the ion could escape if the frequency and amplitude of the applied voltage is not correctly set for a given charge- mass ratio of an ion with a fixed Paul trap. The purpose of this study is to determine quantum mechanically how stable the trapped ion is in a Paul trap when the transition frequency is very close to the applied frequency of alternating current (AC).

The research in the field of trapped ion to find the quantum mechanical lifetime of a trapped ion is relatively recent but the previous research in quantum computers and atomic clocks has addressed some similar ideas [2]. The ideas behind those technologies are not solely based on the lifetime of trapped ion; there are many other factors that need to be considered in addition.



To our knowledge, the study of quantum mechanical lifetime of a trapped ion in a Paul trap has not previously been investigated using the methodology of this study where time-dependent perturbation theory is used.

Considerable research literatures in mass spectrometers, quantum computers and atomic clocks are available but few of these addresses specifically the quantum mechanical lifetime of trapped ions. Much has been done that are associated with the quantum mechanics of laser cooled trapped ions. Haroche, S. and Wineland, D. J. [2012], have developed methods for measuring and manipulating individual particles in a quantum world [3]. Blatt, R., Leibfried, D., Monroe, C., and Wineland, D. J. [2003], have studied the quantum dynamics of a trapped ion [4]. Jelezko, F., Ladd, T. D., Laflamme, R., Monroe, C., Nakamura, Y., and O'Brien, J. [2010], have described the leading approaches to quantum computers [5]. HolzScheiter, M.H., [2002] described the quantum computation in ion trap [6]. Roseband, T., Hume, D. B., Wineland, D.J., et al., [2008] has studied about the single- ion optical clocks [7]. There are also many papers on mass spectrometry and one of them is "*An Introduction to Mass Spectrometry*" by Ashcroft, A.E [8]. March, R.E. and Todd, J.F.J. [2005] presented detailed information about mass spectrometry in their book "*Quadrupole Ion Trap Mass Spectrometry*" [9].

## 1.2 Applications

The Paul trap has been used in mass spectrometry, atomic clocks and quantum computers therefore the study of the quantum mechanical lifetime of trapped ion in a Paul trap might help in improving such technologies. It is not the purpose here to go into the details of those applications but some background of those technologies is helpful in understanding the motivation for this study.

### 1.2.1 Mass Spectrometry

Mass spectrometry is a device that is used to study the physical characteristics of atoms, molecules and compounds such as mass, structure and chemical composition of materials. These spectrometers are used today for proteins and peptides analysis, forensic analysis, drug testing and analytical chemistry. The mass spectrometer has three main components- the ionizer, the analyzer and the detector. The Paul trap is one of the main components of the mass spectrometers and it is used as the mass analyzer. The configuration of a mass spectrometer is shown in Figure 1. A sample is fed into the ionizer where it breaks down the sample into ions and the ions pass through the mass analyzer where only the right kinds of ions are trapped based on the stability region and then finally it goes to the detector. The invention of the Paul trap revolutionized the field of atomic mass filters and the study of the quantum mechanical lifetime of a trapped ion in a Paul trap might help to improve this technology [1, 2, 8, and 9].

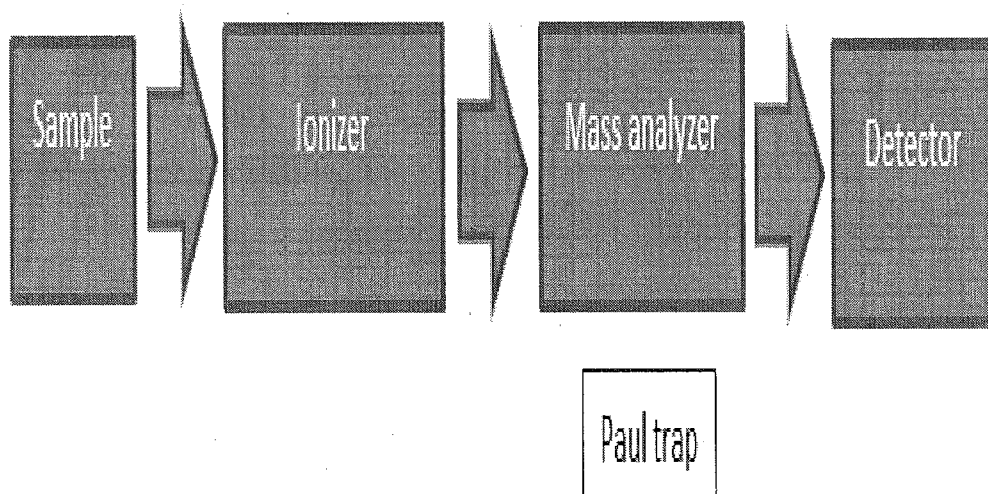


Figure 1: Schematic of Mass Spectrometry

### 1.2.2 Atomic Clocks

The atomic clock uses the transition frequency of an electron jumping from one quantum state to another state as a time keeping element. The idea that hydrogen and sodium atoms could be used in this way for time keeping was suggested by Lord Kelvin in 1879 [10]. Isidor Issac Rabi developed the idea of molecular beam magnetic resonance in 1930 and discussed publicly applying molecular beam magnetic resonance technique as a time and frequency standard in 1945. It is the basis of the modern cesium-atomic clocks and these clocks are the most accurate commercially produced time and frequency standards. Atomic clocks are used as primary standards for international time distribution services and play an important role in Global Positioning System (GPS) and digital communication [11]:

Research is active in building the optical and quantum clock that uses the forbidden transitions frequency of an electron from one quantum state to another state as a time keeping element. These clocks maintain an accuracy of one part in  $10^{19}$  to just one part in  $10^{14}$  in current Cesium atomic clocks. If one can build this type of clock then there will be better and more secure communication systems, more-precise GPS systems, and it might also help to understand the fabric of time- space and matter. A scheme for an optical clock is shown in Figure 2. A laser that has frequency slightly below than the allowed transition frequency is used to cool trapped ions and ions in the cooling transition jump to the upper state. If an ion in the cooling transition goes to another state other than a metastable stable state, then repumping laser is used to drive the ion back up to the upper state. A photon is emitted when an ion jumps from the upper states to lower states. Then another probe laser (very narrow linewidth laser) is used to investigate the forbidden transition of the metastable state which is used as a clock transition [11-13].

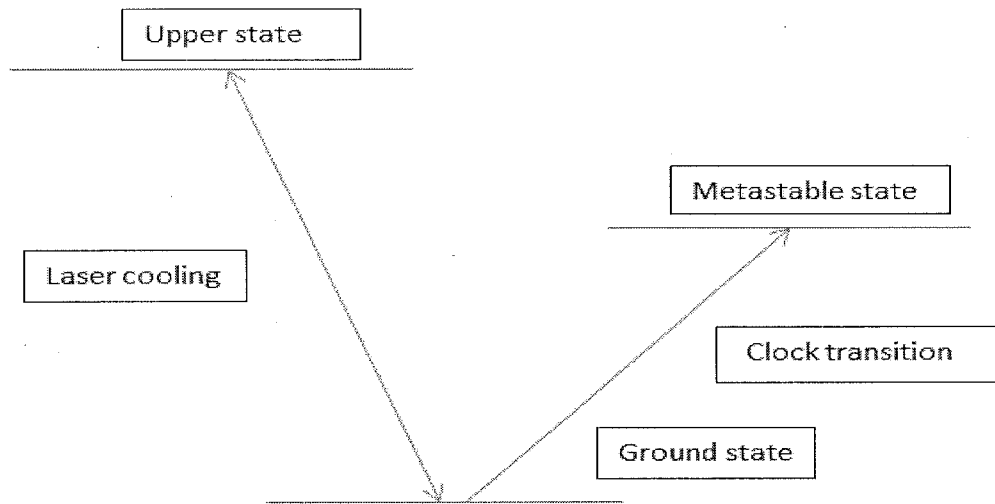


Figure 2: Scheme of Atomic Clock [12]

### 1.2.3 Quantum Computers

Ignacio Cirac and Peter Zoller in 1995 first proposed the ion-trap quantum computer where the ions served as physical qubits of the quantum computers [6, 14]. A qubit is the smallest unit of information in quantum computers just like a bit in the classical computer. Classical computers are based on the transistors whereas the quantum computer relies on the quantum mechanics of qubits where the data are processed differently than classical computers. A quantum computer with two qubits was first demonstrated by Wineland et al [3, 6].

A quantum computer is based on manipulating the states of a particle such as electron and photon. Here the mechanics of a quantum computer that uses electrons as qubits is explained. All electrons have magnetic fields and a property called spin. It is called spin up (1 state) if the electron spins clockwise and it is called spin down (0 state) if the electron spins anticlockwise. The spin up and spin down representation in 1 and 0 similar to classical computer as shown in Figure 3a. Quantum computers exploit the fact of quantum mechanics that the electron spins both

directions at the same time which sounds strange but is true, that means a quantum computer can do many computations at the same time. This quantum concept gives superior computing power to the quantum computer [3, 6].

For two bits it can be 00 or 01, 10 or 11 but for two qubits, it is the superposition of all four possible classical states which are  $|00\rangle$ ,  $|01\rangle$ ,  $|10\rangle$ ,  $|11\rangle$ , and the picture is shown in Figure 3b and 3c respectively. It is possible to have  $2^n$  states for  $n$  qubits so a computer with only 300 qubits could hold  $2^{300}$  classical values simultaneously which are more than the numbers of atoms in the universe. Considerable progress has been made in this field and if one can build the quantum computer then it will change society enormously as the classical computers did in the last century [3, 5, and 6].

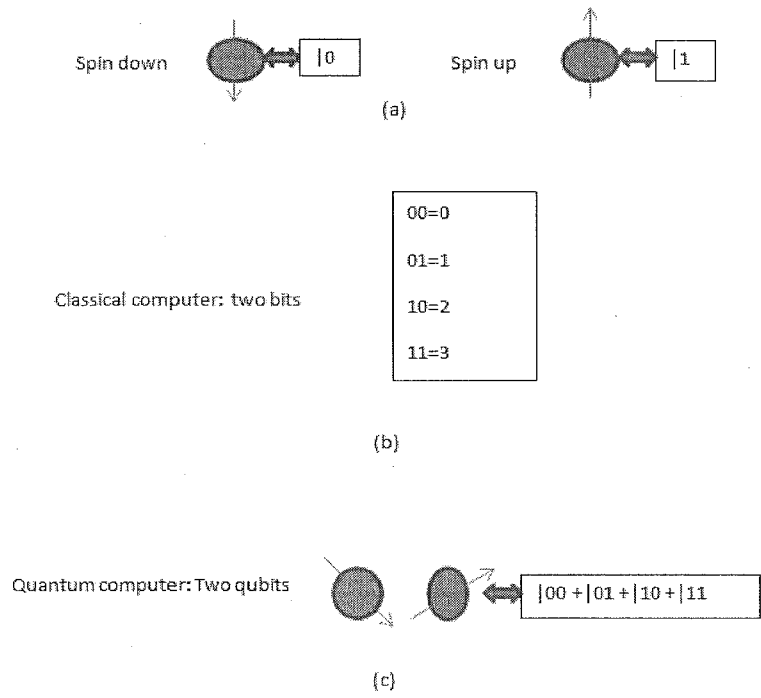


Figure 3: Data Storage in Classical and Quantum Computers

### 1.3 Discussion of Research Procedure

The procedure to find the lifetime of trapped ion quantum mechanically in a Paul trap started with the multipole expansion of the electrostatic potential, then the results from the multipole expansion is used to find the potential in the Paul trap. The ion in the Paul trap undergoes harmonic oscillation similar to the simple harmonic oscillator with the difference being that the potential is time-dependent. Since, it is very hard to find the exact solution of Schrödinger equation for such a potential, time-dependent perturbation theory is used to find the approximate solution based upon the solution that is already known from the unperturbed theory. Using this method, the lifetime of trapped ion is found in the present study.

The perturbation is due to the changing electric field produced by applying radio frequency (rf) voltage is assumed small so that time-dependent perturbation theory can be applied. For simplicity the transition of a trapped ion was assumed to occur between two states only. The driving frequency has to be close to the transition frequency of the trapped ion for this study. These are the limitations that were considered when the Schrödinger equation was solved in order to investigate the lifetime of a trapped ion in a Paul trap.

Perturbation theory is a methodical technique to acquire approximate solutions to the perturbed system, by a process of successive approximations based on the known exact solutions to the unperturbed system. The results of the first order perturbation theory are the most important equation in the quantum dynamics; the first-order correction to the energy is the expectation value of the perturbation in the unperturbed state ( $E_n^1 = \langle \Psi_n^0 | H' | \Psi_n^0 \rangle$ ) where the Hamiltonian is the sum of the unperturbed quantity ( $H^0$ ) and the perturbed quantity ( $H'$ ), i.e. ( $H = H^0 + H'$ ). Here, “the expectation value is the average of repeated measurements on an ensemble of identically prepared systems, not the average of repeated measurements on one and the same system” (Griffiths, 2005, p. 15). The notation in this study is same as in Griffith’s quantum mechanics book [15].

## CHAPTER II

### REVIEW OF PAUL TRAP

#### 2.1 Historical Background

The idea of an ion trap was developed accidentally from the research on electrical discharges and mass filters. K. H. Kingdon's research on the electrical discharge between a very thin filament cathode and a cylindrical anode led to the development of the earliest trap called the Kingdon trap. The Kingdon trap has been used in some precision spectrometry but due to its limited storage time, it was very hard to investigate the characteristics of a trapped ion. Another common ion trap is the Penning trap named afterward F. M. Penning whose work in 1936 studied the electrical discharge between coaxial cylinders in the presence of an axial magnetic field. The significant result of Penning's work was that the electron path between the two electrodes could be very long due to the tendency of magnetic field to force the electrons in circular orbits around the axis. The complete development of the Penning trap did not happened until the development of the Paul trap. The breakthrough of ion traps happened after Wolfgang Paul developed the Paul trap in 1959 when he was investigating the non-magnetic linear mass filter for atomic ions. The development of the Paul trap revolutionized mass spectrometry. Since, then many kinds of ion trap have been developed [16].

The Paul trap is one of the widely used ion traps to investigate the characteristics of trapped ions for different purposes that led to many new discoveries in the microscopic world.

For his work, Wolfgang Paul won the Nobel Prize in physics in 1989 along with Hans Dehmelt who developed the Penning trap [2, 16].

## 2.2 Classical Paul trap

A Paul trap is a device that is used for trapping charged particles and ions in a quadrupole potential and therefore it is known as quadrupole ion storage trap (QUISTOR). It uses static direct current (DC) and radio frequency oscillating alternating current (AC) to trap an ion. It creates the saddle-shaped electric field and isolates the trapped ion from interacting with outside environment. The motion of a trapped ion is described by the Mathieu equations and Paul solved the Mathieu equations for stability and instability regions of trapped ions within the framework of classical physics. The motion of a trapped ion is stable in stable region and one can manipulate the parameters in the stable region to find the critical range for applied voltage ( $V_0$ ) and radio frequency ( $\Omega$ ) for different charge- mass ratio ( $Q/m$ ) and radius ( $r$ ) of a Paul trap. Here the condition is  $0 < \frac{2QV_0}{mr^2\Omega^2} \leq 0.908$  in the classical Paul trap without any DC [1, 2, 6, 8, and 9].

Consider a positive ion is trapped in a free space inside a region surrounded by a four conducting cylindrical rods as shown in Figure 4.

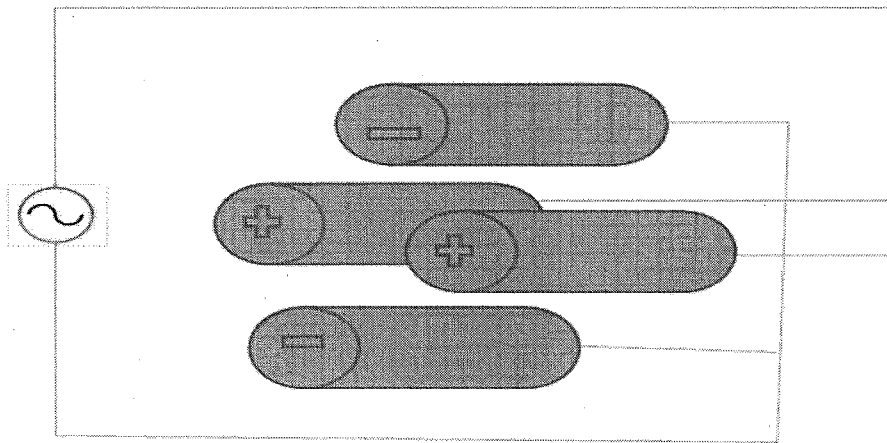


Figure 4: Linear Paul Trap



The configuration cross section of the linear Paul trap is shown in Figure 5 where a positive ion is trapped. The positive ion feels the repulsive force from the positively charged conducting rods and the attractive force from the negatively charged conducting rods as a result the ions motion looks like approaching and departing from a center similar to the simple harmonic oscillator. Therefore, the ion gets trapped forever at least in principle by applying the right voltage and frequency for same charge-mass ratio and fixed radius of the Paul trap [6, 17].

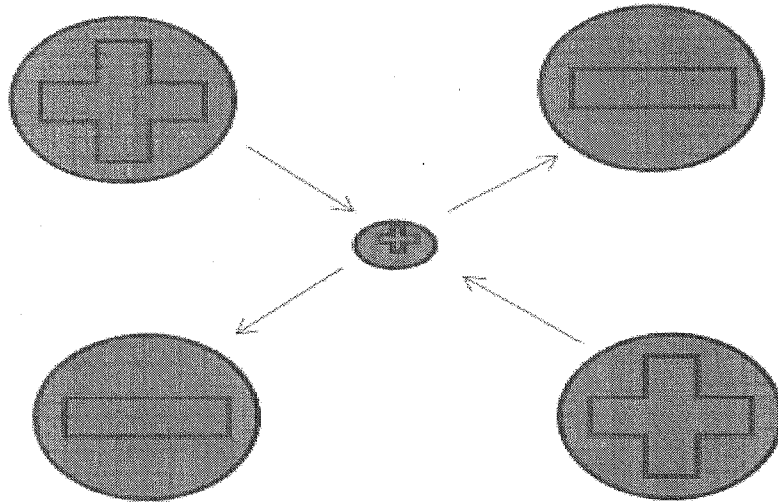


Figure 5: Cross Section of Linear Paul Trap [17]

The detailed information about the trapping conditions of a Paul trap is given in the “*Electromagnetic Traps for Charged and Neutral Particles*” by Wolfgang Paul [1]. The potential inside the region of a Paul trap as shown in the Figure 4 and derived in Appendix B is given by the Equation (B.7) which is shown below

$$\varphi(\vec{R}, t) = \frac{3V_0 \cos(\Omega t) (x^2 - y^2)}{r^2},$$

where  $V_0$  = applied voltage,

$\Omega$  = radio frequency of applied alternating current (AC),

$r$  = distance of the conductors from the center of the trap,

$x$  = the point in space how far away from the center in  $x$ -axis,

$y$  = the point in space how far away from the center in  $y$ -axis.

The configuration of the oscillating potential inside the Paul trap is shown below in Figure 6.

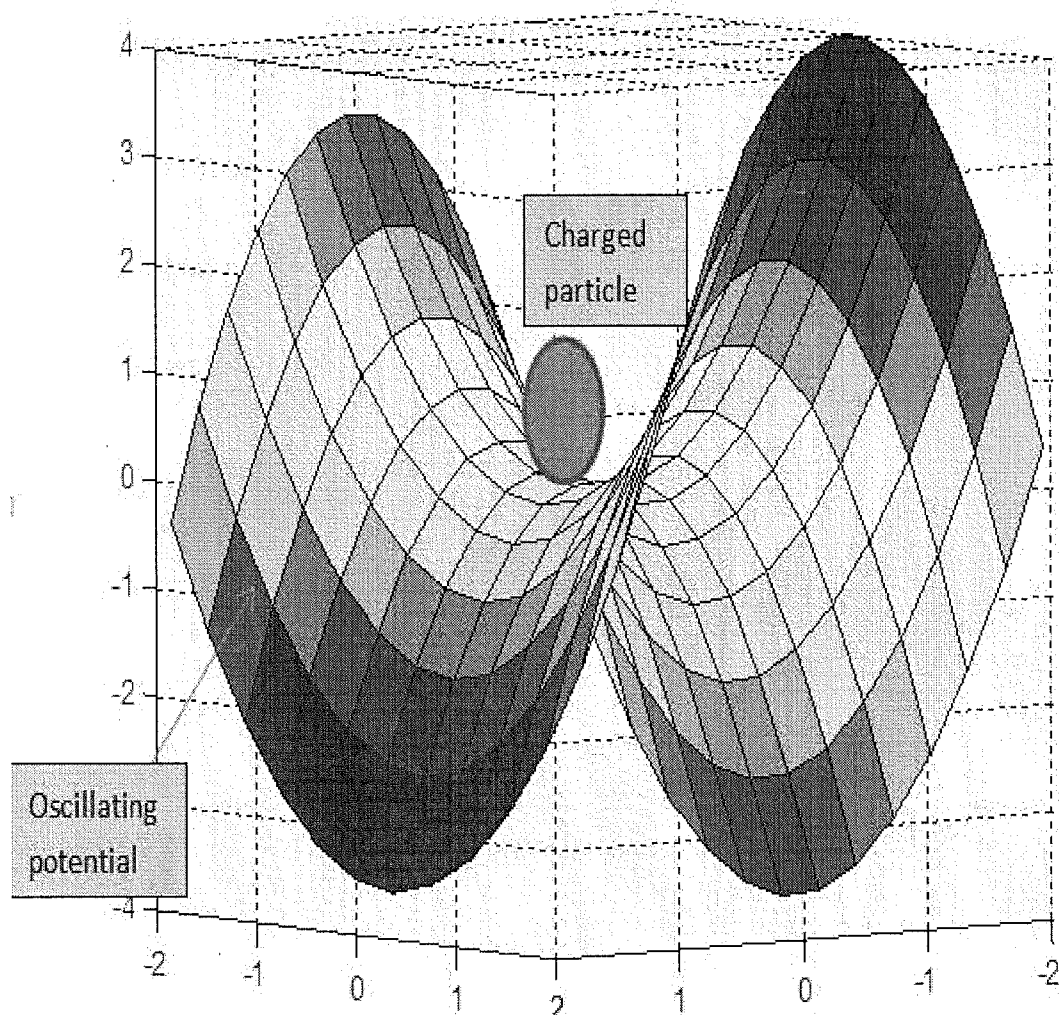


Figure 6: Oscillating Potential in a Paul Trap

### 2.3 Quantum Paul trap

Particles at the atomic level do not follow the classical physics so the trapped particles in a Paul trap needs to be treated quantum mechanically. Cook, Shankland and Wells [1985] were the first to investigate the Paul trap within the framework of quantum mechanics. They showed that the stable motion of a charge particle in a Paul trap as described classically is identical in the quantum- mechanical formulation [18]. The following chapters focus on quantum motion of trapped ion in a Paul trap.

## CHAPTER III

### QUANTUM MECHANICS IN A PAUL TRAP

The potential of a linear Paul trap in this study is given by Equation (B.7) which is

$\varphi(\vec{R}, t) = \frac{3V_0 \cos(\Omega t)(x^2 - y^2)}{r^2}$  and the schematic of oscillating potential is shown in Figure 6. The time dependent potential energy,  $V(r, t)$  of the trapped particle in a Paul trap is,

$$V(\vec{R}, t) = \frac{3qV_0 \cos(\Omega t)(x^2 - y^2)}{r^2}. \quad (3.1)$$

where,  $q$  is the charge of a trapped ion.

The right applied radio frequency voltage in a Paul trap produces harmonic potential with its minima located in center and the motion of a trapped ion undergoes harmonic oscillation, therefore in this study the motion of an ion is treated like a quantum harmonic oscillator. Since, the potential energy as shown in Equation (3.1) is time dependent so it is hard to get the exact solution for the Schrödinger time dependent equation. However, this system can be treated with time-dependent perturbation theory by assuming that the time dependent part of the Hamiltonian is small compared to the time independent part, so using perturbation theory; the solution for the Schrödinger equation for the potential energy as shown in Equation (3.1) can be found with the aid of the known solution of quantum harmonic oscillator. The solution of the quantum harmonic oscillator is already known and can be found in any quantum mechanics book.

### 3.1 Stationary States and Energy of the Quantum Harmonic Oscillator

The solution for a wave equation of Schrödinger equation for the quantum harmonic oscillator can be found in any quantum mechanics book. The normalized stationary states  $\Psi_{m_a}$ ,  $\Psi_{m_b}$  with energy  $E_{m_a}$ ,  $E_{m_b}$  for the one-dimensional harmonic oscillator are [Griffiths, 2005, p. 54, 56]

$$\Psi_a = \Psi_{m_a}(x) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^{m_a}m_a!}} H_{m_a}(\xi_x) e^{-\frac{\xi_x^2}{2}}, \quad (3.2-a)$$

$$E_{m_a} = \left(m_a + \frac{1}{2}\right) \hbar\omega_0. \quad (3.2-b)$$

$$\Psi_b = \Psi_{m_b}(x) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^{m_b}m_b!}} H_{m_b}(\xi_x) e^{-\frac{\xi_x^2}{2}}, \quad (3.2-c)$$

$$E_{m_b} = \left(m_b + \frac{1}{2}\right) \hbar\omega_0. \quad (3.2-d)$$

For the two-dimensional harmonic oscillator, the normalized stationary states  $\Psi_{m_a n_a}$ ,  $\Psi_{m_b n_b}$  and energy  $E_{m_a n_a}$ ,  $E_{m_b n_b}$  is represented as  $\Psi_a = \Psi_{m_a n_a} = \Psi_{m_a}(x)\Psi_{n_a}(y)$ . So the states are given by

$$\Psi_{m_a n_a} = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{2}} \frac{1}{\sqrt{2^{m_a}m_a!2^{n_a}n_a!}} H_{m_a}(\xi_x) H_{n_a}(\xi_y) e^{-\left(\frac{\xi_x^2}{2} + \frac{\xi_y^2}{2}\right)}, \quad (3.3-a)$$

$$E_{m_a n_a} = (m_a + n_a + 1) \hbar\omega_0, \quad (3.3-b)$$

$$\Psi_{m_b n_b} = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{2}} \frac{1}{\sqrt{2^{m_b}m_b!2^{n_b}n_b!}} H_{m_b}(\xi_x) H_{n_b}(\xi_y) e^{-\left(\frac{\xi_x^2}{2} + \frac{\xi_y^2}{2}\right)}, \quad (3.3-c)$$

$$E_{m_b n_b} = (m_b + n_b + 1) \hbar\omega_0, \quad (3.3-d)$$

where

$H_{m_a}(\xi_x)$  and  $H_{n_a}(\xi_y)$  are the Hermite polynomials,

$$\xi_x = \sqrt{\frac{m\omega_0}{\hbar}} x, \quad H_{n_a}(\xi_y) = \sqrt{\frac{m\omega_0}{\hbar}} y,$$

and

$\hbar$  = Planck constant ( $1.05457 \times 10^{-34}$  J s),

$\omega_0$  = angular frequency,

$m$  = mass of particle,

and  $m_a, n_a = 0, 1, 2, 3, \dots$

The first five Hermite polynomials are:

$$H_0(\xi) = 1,$$

$$H_1(\xi) = 2\xi,$$

$$H_2(\xi) = 4\xi^2 - 2,$$

$$H_3(\xi) = 8\xi^3 - 12\xi,$$

$$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12,$$

$$H_5(\xi) = 32\xi^5 - 160\xi^3 + 120\xi.$$

### 3.2 Two Level System

Focusing on transitions between the two states  $\Psi_a$  and  $\Psi_b$ ; any state of the system at time  $t$ ,  $\Psi(t)$  can be expressed in the absence of any perturbation as the linear combination of the two states which is given below [Griffiths, 2005, p.341],

$$\Psi(t) = C_a \Psi_a e^{\frac{-iE_a t}{\hbar}} + C_b \Psi_b e^{\frac{-iE_b t}{\hbar}}. \quad (3.4)$$

Normalization of  $\Psi(t)$  requires  $|C_a|^2 + |C_b|^2 = 1$ ,

where

$|C_a|^2$  = probability that a particle is in the state  $\Psi_a$ ,

$|C_b|^2$  = probability that a particle is in the state  $\Psi_b$ .

Now, for a time dependent perturbed system, the wave function  $\Psi(t)$  still can be expressed as a linear combination of the states which looks exactly like Equation (3.4) but the only difference is that  $C_a(t)$  and  $C_b(t)$  are now functions of time. Now the wave function  $\Psi(t)$  can be expressed as;

$$\Psi(t) = C_a(t)\Psi_a e^{\frac{-iE_a t}{\hbar}} + C_b(t)\Psi_b e^{\frac{-iE_b t}{\hbar}}. \quad (3.5)$$

### 3.3 Time-Dependent Perturbation Theory

Assuming that the particle started out in the state,  $\Psi_a$   $\{C_a(0) = 1, C_b(0) = 0\}$  and that is the state when there is no perturbation. The particle can be found some later time  $t$ , in the state  $\Psi_b$   $\{C_a(t) = 0, C_b(t) = 1\}$ , after the perturbation. That means the system undergoes a transition from state  $\Psi_a$  to state  $\Psi_b$ . Assuming the perturbation is small, Equation (3.6) can be solved by a process of successive approximation. The zeroth order approximation does not contain any factor of the perturbed Hamiltonian whereas the first order and second order approximation contains one factor and two factors of perturbed Hamiltonian respectively [Griffiths, 2005, p. 345, 345]. The first order approximation can be calculated as

$$C_a^1(t) = 1, \text{ and}$$

$$C_b^1(t) = -\frac{i}{\hbar} \int_0^t H'_{ba}(t') e^{i\omega_0 t'} dt', \quad (3.6)$$

where  $\omega_0 \equiv \frac{E_b - E_a}{\hbar}$  and  $H'_{ba} = \langle \Psi_b | H' | \Psi_a \rangle$ .

The quantum mechanics of a trapped particle in a Paul trap is investigated one-dimensionally and two-dimensionally in Chapters 4 and 5 respectively.

## CHAPTER IV

### ONE-DIMENSIONAL PAUL TRAP

#### 4.1 One-Dimensional Potential Energy

For the simplicity of mathematics and to envision the output, this chapter is limited to one-dimension to investigate the lifetime of trapped particle in a Paul trap. The schematic of one dimension Paul trap is shown below in Figure 7.

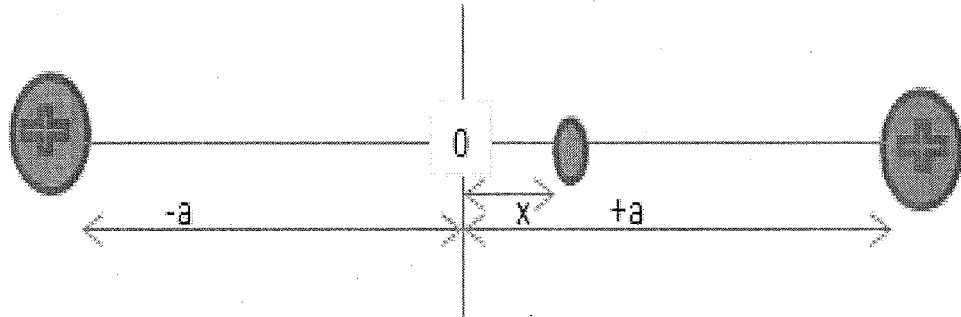


Figure 7: One-Dimensional Paul Trap

The potential energy,  $V(r)$  of a particle with charge ( $q$ ) at a distance  $x$  from the origin as shown in above Figure 7 can be found by the following equation,

$$V(r) = q\phi, \quad (4.1)$$

where  $\phi$  is the electric potential.



The electric potential produced ( $\varphi$ ) by the point charge (Q) at a distance from the charge is given

by  $= \frac{Q}{4\pi\epsilon_0}$ . Then substituting  $\varphi$  in Equation (4.1), it becomes  $V(r) = q \left[ \frac{1}{4\pi\epsilon_0} \left( \frac{-Q}{a+x} \right) + \right.$

$\left. \frac{1}{4\pi\epsilon_0} \left( \frac{+Q}{a-x} \right) \right]$  and simplifying, one gets Equation (4.2),

$$V(r) = \frac{qQ}{4\pi\epsilon_0 a} \left[ \frac{1}{1 + \frac{x}{a}} + \frac{1}{1 - \frac{x}{a}} \right],$$

$$V(r) = \frac{qQ}{4\pi\epsilon_0 a} \left[ \frac{-1 + \frac{x}{a} + 1 + \frac{x}{a}}{1 - \frac{x^2}{a^2}} \right],$$

$$V(r) = \frac{2qQ}{4\pi\epsilon_0 a} \left[ \frac{\frac{x}{a}}{1 - \frac{x^2}{a^2}} \right]. \quad (4.2)$$

For  $x \ll a$  or  $\frac{x^2}{a^2} \ll 1$  in the Equation (4.2), the potential energy can be calculated by the

Equation (4.3),

$$V(r) \approx \frac{2qQx}{4\pi\epsilon_0 a^2}. \quad (4.3)$$

But  $Q = Q_0 \cos(\Omega t)$  in Paul trap, therefore the Equation (4.3) becomes

$$V(r, t) = \frac{2qQ_0 \cos(\Omega t)x}{4\pi\epsilon_0 a^2}. \quad (4.4)$$

The motion in a Paul trap is harmonic, therefore the potential energy in the Paul trap could be

described by the time-dependent harmonic oscillator which is shown in Equation (4.5),

$$V(r, t) = \left\{ \begin{array}{l} \frac{1}{2} k \cos(\Omega t) x^2 \text{ for } x > 0 \\ -\frac{1}{2} k \cos(\Omega t) x^2 \text{ for } x < 0 \end{array} \right\}. \quad (4.5)$$

The potential given by the Equation (4.5) is shown in Figure 8,

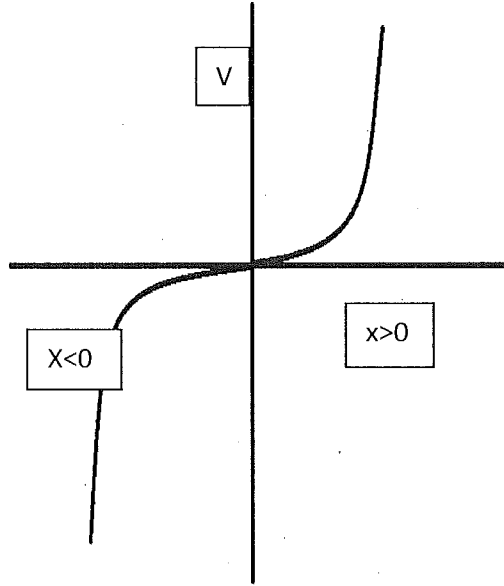


Figure 8: Harmonic potential

The electric potential in two-dimensional Paul trap is given by the Equation (B.6), therefore omitting the  $y$  part gives the one-dimension electric potential and the potential energy of an ion in a Paul trap is given by,

$$V(\vec{R}, t) = \frac{3qQ_0 \cos(\Omega t)(x^2)}{4\pi\epsilon_0 r^3}. \quad (4.6)$$

The potential energy given by the Equations (4.4), (4.5), and (4.6) are all true but the potential energy given by the Equation (4.6) is more convincing than other two. Therefore the potential described by the Equation (4.6) is used for further study. Adding and subtracting  $\frac{1}{2}kx^2$  in

Equation (4.6), it becomes  $V(\vec{R}, t) = \frac{1}{2}kx^2 - \frac{1}{2}kx^2 + \frac{3qQ_0 \cos(\Omega t)(x^2)}{4\pi\epsilon_0 r^3}$  and simplifying it,

one gets;

$$V(\vec{R}, t) = \frac{1}{2}kx^2 + \left[ \frac{1}{2}kx^2 \{ \cos(\Omega t) - 1 \} \right]. \quad (4.7)$$

where  $k = \frac{3qQ_0}{2\pi\epsilon_0 r^3}$ .

But the constant  $k$  in harmonic oscillator in terms of angular frequency is,  $k = m\omega_0^2$  and equaling

the constant  $k$  one gets, angular frequency  $\omega_0 = \sqrt{\frac{3qQ_0}{2\pi\epsilon_0 mr^3}}$ . The angular frequency in terms of

applied voltage ( $V_0$ ) is,

$$\omega_0 = \sqrt{\frac{6qV_0}{mr^2}}. \quad (4.8)$$

Substitute the Equation (4.7) in time-dependent Schrödinger equation  $H\Psi = i\hbar \frac{\partial\Psi}{\partial t}$ , where

$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(r, t)$ . Then the time-dependent Schrödinger equation becomes  $\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} +$

$\frac{1}{2}kx^2 + \frac{1}{2}kx^2\{\cos(\Omega t) - 1\}\right]\Psi = i\hbar \frac{\partial\Psi}{\partial t}$  and here the Hamiltonian ( $H$ ) is divided into

unperturbed ( $H^0$ ) and perturbed ( $H'$ ) system which is shown in Equation (4.9),

$$H = H^0 + H'(t). \quad (4.9)$$

where  $H^0 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2$  and  $H'(t) = \left[\frac{1}{2}kx^2\{\cos(\Omega t) - 1\}\right]$ .

Now, substitute Equation (3.5) and Equation (4.9) in the time-dependent Schrödinger equation

and solve for the first-order correction of  $C_a(t)$  and  $C_b(t)$  in Equation (3.5) assuming the particle

starts out in the lower state ( $C_a(0) = 1, C_b(0) = 0$ ). Then the first order approximation can be

calculated by the Equation (3.6), which is shown below and the detailed work is given in

[Griffiths, 2005, p. 344].

$$C_a^1(t) = 1,$$

$$C_b^1(t) = -\frac{i}{\hbar} \int_0^t H'_{ba}(t') e^{i\omega_0 t'} dt'.$$

where

$H'_{ba} = \langle\Psi_b|H'(t)|\Psi_a\rangle$ , and

$H'(t) = \left[\frac{1}{2}kx^2\{\cos(\Omega t) - 1\}\right]$ .

#### 4.2 Expectation Value of Perturbed system

Here, the expectation value of the perturbed system in the unperturbed state can be calculated as  $H'_{ba} = \langle \Psi_b | H'(t) | \Psi_a \rangle$  and substituting  $H'(t)$  one gets,

$H'_{ba} = \left\langle \Psi_b \left| \frac{1}{2} kx^2 \{ \cos(\Omega t) - 1 \} \right| \Psi_a \right\rangle$  and simplifying it gives;

$$H'_{ba} = \left[ \left\langle \Psi_b \left| \frac{1}{2} kx^2 \right| \Psi_a \right\rangle \{ \cos(\Omega t) - 1 \} \right]$$

$$H'_{ba} = [V_{ba} \{ \cos(\Omega t) - 1 \}], \quad (4.10)$$

where  $V_{ab} = \left\langle \Psi_a \left| \frac{1}{2} kx^2 \right| \Psi_b \right\rangle$  is the expectation value of the potential energy of a trapped ion (harmonic oscillator approximation).

#### 4.3 Expectation Value of Potential Energy

The expectation value of potential energy of the trapped ion in one-dimensional Paul trap when a particle makes the transition from state  $\Psi_a$  to state  $\Psi_b$  is

$$V_{ab} = \frac{1}{2} k \langle \Psi_a | x^2 | \Psi_b \rangle,$$

where  $\langle \Psi_a | x^2 | \Psi_b \rangle = \int \Psi_a x^2 \Psi_b dx$  is the expectation value of  $x^2$ .

The operator 'x' can be expressed in terms of the raising and lowering operators as  $x =$

$$\sqrt{\frac{\hbar}{2m\omega_0}} (a_+ + a_-), \text{ and the square of the operator } x \text{ (} x^2 \text{) becomes } x^2 = \frac{\hbar}{2m\omega_0} [(a_+)^2 + (a_+ a_-) +$$

$$(a_- a_+) + (a_-)^2]. \text{ Here } a_+ \Psi = \sqrt{n+1} \Psi_{n+1}, \quad a_- \Psi = \sqrt{n} \Psi_{n-1}, \quad a_+ a_- \Psi = n \Psi_n \text{ and } a_- a_+ \Psi =$$

$$(n+1) \Psi_n. \text{ The detailed information about the operators is given in the [Griffiths, 2005, p. 48].}$$

Then, evaluating the expectation value of  $x^2$  as follows,

$$\langle \Psi_a | x^2 | \Psi_b \rangle = \frac{\hbar}{2m\omega_0} \left[ \int \Psi_a \{ (a_+)^2 + (a_+ a_-) + (a_- a_+) + (a_-)^2 \} \Psi_b dx \right],$$

$$\langle \Psi_a | x^2 | \Psi_b \rangle = \frac{\hbar}{2m\omega_0} \left[ \left( \sqrt{m_b^2 + 3m_b + 2} \right) \delta_{m_a, m_b+2} + (2m_b + 1) \delta_{m_a, m_b} + \left( \sqrt{m_b^2 - m_b} \right) \delta_{m_a, m_b-2} \right].$$

In order to make a transition from state  $\Psi_a$  to  $\Psi_b$ ,  $m_b > m_a$  and with that condition, the first two terms vanishes from the above equation. So, the above equation becomes  $\langle \Psi_a | x^2 | \Psi_b \rangle =$

$$\frac{\hbar}{2m\omega_0} \left[ \left( \sqrt{m_b^2 - m_b} \right) \delta_{m_a, m_b-2} \right] \text{ and substituting this value in } V_{ab} \text{ one}$$

gets  $V_{ab} = \frac{1}{2} m \omega_0^2 \frac{\hbar}{2m\omega_0} \left[ \left( \sqrt{m_b^2 - m_b} \right) \delta_{m_a, m_b-2} \right]$ . Therefor the expectation value of potential

energy of trapped ion is,

$$V_{ab} = \frac{1}{4} \hbar \omega_0 \left[ \left( \sqrt{m_b^2 - m_b} \right) \delta_{m_a, m_b-2} \right]. \quad (4.11)$$

#### 4.4 Perturbation Theory

Now, the first order approximation of perturbed system can be calculated by the Equation

(3.6) which is  $C_a^1(t) = 1$ , and  $C_b^1(t) = -\frac{i}{\hbar} \int_0^t H'_{ba}(t') e^{i\omega_0 t'} dt'$  assuming the ion starts out in the

lower state ( $C_a(0) = 1, C_b(0) = 0$ ). Substituting the value of perturbation, one gets  $C_b^1(t) =$

$-\frac{i}{\hbar} \int_0^t [V_{ba} \{\cos(\Omega t') - 1\}] e^{i\omega_0 t'} dt'$  and taking out the factor  $V_{ba}$  and writing cosine in terms of

exponential functions using Euler's formula, it becomes  $C_b^1(t) = -\frac{i}{\hbar} V_{ba} \int_0^t \left\{ \frac{e^{i\Omega t'} + e^{-i\Omega t'}}{2} -$

$1 \right\} e^{i\omega_0 t'} dt'$ . Expanding  $e^{i\omega_0 t'}$  one gets  $C_b^1(t) = -\frac{i}{\hbar} V_{ba} \int_0^t \left\{ \frac{e^{i(\omega_0+\Omega)t'} + e^{i(\omega_0-\Omega)t'}}{2} - e^{i\omega_0 t'} \right\} dt'$

and simplifying, it becomes;

$$C_b^1(t) = -\frac{i}{2\hbar} V_{ba} \left[ \frac{e^{i(\omega_0+\Omega)t} - 1}{i(\omega_0 + \Omega)} + \frac{e^{i(\omega_0-\Omega)t} - 1}{i(\omega_0 - \Omega)} - 2 \frac{e^{i\omega_0 t} - 1}{i(\omega_0)} \right],$$

$$C_b^1(t) = -\frac{V_{ba}}{2\hbar} \left[ \frac{e^{i(\omega_0+\Omega)t} - 1}{(\omega_0 + \Omega)} + \frac{e^{i(\omega_0-\Omega)t} - 1}{(\omega_0 - \Omega)} - 2 \frac{e^{i\omega_0 t} - 1}{(\omega_0)} \right]. \quad (4.12)$$

#### 4.5 Transition Probability

The probability of a transition is greater when the driving frequency  $\Omega$ , is close to the natural frequency  $\omega_0$ , ( $\omega_0 \cong \Omega$ ) that gives  $|\omega_0 + \Omega| \gg |\omega_0| \gg |\omega_0 - \Omega|$ , then the second term in Equation (4.12) dominates, so the above Equation (4.12) can be written as,

$$C_b^1(t) = -\frac{V_{ba}}{2\hbar} \left[ \frac{e^{i(\omega_0 - \Omega)t} - 1}{(\omega_0 - \Omega)} \right]. \quad (4.13)$$

Now taking out the factor  $e^{i(\frac{\omega_0 - \Omega}{2})t}$  from the Equation (4.13), one gets

$$C_b^1(t) = -\frac{V_{ba}}{2\hbar} e^{i(\frac{\omega_0 - \Omega}{2})t} \left[ \frac{e^{i(\frac{\omega_0 - \Omega}{2})t} - e^{-i(\frac{\omega_0 - \Omega}{2})t}}{(\omega_0 - \Omega)} \right] \text{ and multiplying and dividing by the complex}$$

number (i) in the numerator and denominator it becomes

$$C_b^1(t) = -\frac{iV_{ba}}{2\hbar(\omega_0 - \Omega)} e^{i(\frac{\omega_0 - \Omega}{2})t} \left[ 2 \frac{e^{i(\frac{\omega_0 - \Omega}{2})t} - e^{-i(\frac{\omega_0 - \Omega}{2})t}}{2i} \right]. \text{ Here the exponential terms in the bracket}$$

can be written in terms of sine as  $C_b^1(t) = -\frac{iV_{ba}}{2\hbar(\omega_0 - \Omega)} e^{i(\frac{\omega_0 - \Omega}{2})t} \left[ 2 \sin\left(\frac{\omega_0 - \Omega}{2}t\right) \right]$  and simplifying

it more one finds,

$$C_b^1(t) = -\frac{iV_{ba}}{2\hbar} e^{i(\frac{\omega_0 - \Omega}{2})t} \left[ \frac{2 \sin\left(\frac{\omega_0 - \Omega}{2}t\right)}{(\omega_0 - \Omega)} \right]. \quad (4.14)$$

The probability of finding the particle in the state  $\Psi_b$  at time t, that started out in the state  $\Psi_a$  is

$$P_{a \rightarrow b}(t) = |C_b^1(t)|^2 = \frac{|V_{ba}|^2}{(2\hbar)^2} \left[ \frac{4 \sin^2\left(\frac{\omega_0 - \Omega}{2}t\right)}{(\omega_0 - \Omega)^2} \right] \text{ and it can be written in terms of delta functions as}$$

$$P_{a \rightarrow b}(t) = |C_b^1(t)|^2 = \frac{|V_{ba}|^2}{(2\hbar)^2} \{2\pi t \delta(\omega_0 - \Omega)\}, \quad (4.15)$$

where  $\lim_{\Omega \rightarrow \omega_0} \frac{4 \sin^2\left(\frac{\omega_0 - \Omega}{2}t\right)}{(\omega_0 - \Omega)^2} = 2\pi t \delta(\omega_0 - \Omega)$ .

#### 4.5.1 Transition Rate

The transition rate ( $R_{a \rightarrow b}(t)$ ) of the particle from state  $\Psi_a$  to state  $\Psi_b$  is given by

$$R_{a \rightarrow b}(t) = \frac{dP_{a \rightarrow b}(t)}{dt} \text{ [Griffiths, 2005, p. 353]. Therefore the transition rate is } R_{a \rightarrow b}(t) = \frac{dP_{a \rightarrow b}(t)}{dt} = \frac{|V_{ba}|^2}{(2\hbar)^2} \{2\pi\delta(\omega_0 - \Omega)\} \text{ and writing the transition rate in terms of energy states one gets,}$$

$$R_{a \rightarrow b}(t) = \frac{|V_{ba}|^2}{(2\hbar)^2} \{2\pi\delta(E_b - E_a - \hbar\Omega)\}. \quad (4.16)$$

There is an infinite number of final state instead of one final state, so the Equation (4.16) can be written as,

$$R_{a \rightarrow b}(t) = \frac{|V_{ba}|^2}{4\hbar} \{2\pi\rho_f(E)\}, \quad (4.17)$$

where

$$|V_{ba}|^2 = |V_{ab}|^2 = \frac{\hbar^2\omega_0^2}{16} (m_b^2 - m_a) \delta_{m_a, m_b-2}$$

and  $\rho_f(E)$  is the density of the final state.

Assuming non degenerate states, the density of final state can be found as  $\rho = \frac{\# \text{ states}}{\text{energy}} = \frac{dn}{dE}$  and

the energy of the quantum harmonic oscillator in  $n^{\text{th}}$  state is  $E_n = \hbar\omega_0 \left(n + \frac{1}{2}\right)$ . Then, taking the derivative of energy with respect to  $n$ , one gets  $dE = \hbar\omega_0 dn$  and reordering it becomes,

$$\frac{dn}{dE} = \frac{1}{\hbar\omega_0}. \quad (4.18)$$

Now substituting the corresponding values of  $V_{ba}$  and  $\rho_f(E)$  in Equation (4.17), one gets

$R_{a \rightarrow b}(t) = \left[ \frac{\hbar^2\omega_0^2}{16} \{(m_b^2 - m_a)\delta_{m_a, m_b-2}\} \frac{1}{4\hbar} \left\{ 2\pi \frac{1}{\hbar\omega_0} \right\} \right]$  and simplifying it one finds,

$$R_{a \rightarrow b}(t) = \left[ \frac{\pi\omega_0}{32} \{(m_b^2 - m_a)\delta_{m_a, m_b-2}\} \right]. \quad (4.19)$$

#### 4.6 Lifetime

Now, the lifetime ( $\tau_{a \rightarrow b}$ ) of the trapped ion in state  $\Psi_a$  before it makes transition to the state  $\Psi_b$  is  $\tau_{a \rightarrow b} = \frac{1}{R_{a \rightarrow b}(t)}$  and it can be written in terms of allowed transition and transition frequency as follows,

$$\tau_{a \rightarrow b} = \frac{32}{\pi \omega_0 \{(m_b^2 - m_b) \delta_{m_a, m_b - 2}\}}. \quad (4.20)$$

From the above Equation it can be seen that the lifetime depends upon the transition frequency and the allowed state. The lifetime of a particle decreases as a particle makes a transition to higher allowed states. So, the longest lifetime of a trapped particle is in the ground state before the particle makes a transition from the ground state to state 2.



## CHAPTER V

### TWO-DIMENSIONAL PAUL TRAP

#### 5.1 Two-Dimensional Potential Energy

A more realistic model for the Paul trap is two dimensional and the two -dimensional potential in a Paul trap is given by the Equation (B.7) which is  $\varphi(\vec{R}, t) = \frac{3V_0 \cos(\Omega t)(x^2 - y^2)}{r^2}$ . The potential energy of a trapped ion in a Paul trap is  $V(\vec{R}, t) = \frac{3qV_0 \cos(\Omega t)(x^2 - y^2)}{r^2}$  where  $q$  is the charge of a trapped ion and the potential energy in terms of constant  $k$  is  $V(\vec{R}, t) = \frac{1}{2}k(x^2 - y^2) \cos(\Omega t)$  where  $k = \frac{6qV_0}{r^2}$ . But the constant  $k$  in harmonic oscillator is  $k = m\omega_0^2$  and equaling the constant  $k$  one gets, angular frequency  $\omega_0 = \sqrt{\frac{6qV_0}{mr^2}}$ . Since this study tried to get the approximate solutions of the quantum motion of a trapped ion based on harmonic oscillator so adding and subtracting two-dimensional harmonic potential energy  $\frac{1}{2}kx^2$  and  $\frac{1}{2}ky^2$  in the potential energy of trapped ion one gets  $V(\vec{R}, t) = \frac{1}{2}kx^2 - \frac{1}{2}kx^2 + \frac{1}{2}ky^2 - \frac{1}{2}ky^2 + \frac{1}{2}k(x^2 - y^2) \cos(\Omega t)$  and simplifying it one finds,

$$V(\vec{R}, t) = \frac{1}{2}kx^2 + \frac{1}{2}ky^2 + \frac{1}{2}kx^2\{\cos(\Omega t) - 1\} - \frac{1}{2}ky^2\{\cos(\Omega t) + 1\}. \quad (5.1)$$

The time-dependent Schrödinger equation is  $H\Psi = i\hbar \frac{\partial \Psi}{\partial t}$ , where  $H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + V(t)$ .

Here, Hamiltonian is divided into unperturbed and perturbed system as  $H = H^0 + H'(t)$  and

Substituting the Equation (5.1) in time-dependent equation and comparing the Hamiltonian with

perturbed and unperturbed system one gets unperturbed system is  $H^0 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} kx^2 -$

$\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{1}{2} ky^2$ , and perturbed system is  $H'(t) = \frac{1}{2} kx^2 \{\cos(\Omega t) - 1\} - \frac{1}{2} ky^2 \{\cos(\Omega t) + 1\}$ .

Now, substitute Equation (3.5) and Equation (5.1) in the time-dependent Schrödinger equation and solve for the first-order correction of  $C_a(t)$  and  $C_b(t)$  in Equation (3.5) assuming the particle starts out in the lower state ( $C_a(0) = 1, C_b(0) = 0$ ). Then the first order approximation can be calculated by the Equation (3.6), which is shown below and the detailed work is given in [Griffiths, 2005, p. 344].

$$C_a^1(t) = 1,$$

$$C_b^1(t) = -\frac{i}{\hbar} \int_0^t H'_{ba}(t') e^{i\omega_0 t'} dt'.$$

Where  $H'_{ba} = \langle \Psi_b | H'(t) | \Psi_a \rangle$ .

## 5.2 Expectation Value of Perturbed system

The expectation value of the perturbed system in the unperturbed state is  $H'_{ba} =$

$\langle \Psi_b | H'(t) | \Psi_a \rangle$  and substituting the perturbed system and one finds

$H'_{ba} = \langle \Psi_b | \frac{1}{2} kx^2 \{\cos(\Omega t) - 1\} - \frac{1}{2} ky^2 \{\cos(\Omega t) + 1\} | \Psi_a \rangle$ . Now dividing the perturbed system

into x and y orientation then it becomes  $H'_{ba} = \langle \Psi_b | \frac{1}{2} kx^2 \{\cos(\Omega t) - 1\} | \Psi_a \rangle -$

$\langle \Psi_b | \frac{1}{2} ky^2 \{\cos(\Omega t) + 1\} | \Psi_a \rangle$  and simplifying it one gets,

$$H'_{ba} = [V(x)_{ba} \{\cos(\Omega t) - 1\} - V(y)_{ba} \{\cos(\Omega t) + 1\}], \quad (5.2)$$

where

$$V_{ab}(x) = \langle \Psi_a | V(x) | \Psi_b \rangle = \frac{1}{2} k \langle \Psi_a | x^2 | \Psi_b \rangle,$$

$$V_{ab}(y) = \langle \Psi_a | V(y) | \Psi_b \rangle = \frac{1}{2} k \langle \Psi_a | y^2 | \Psi_b \rangle.$$

Here the state  $\Psi_a$  and  $\Psi_b$  is represented by the stationary states of the quantum harmonic oscillator and is given by the Equations (3.3-a) and (3.3-c) which are  $\Psi_a = \Psi_{m_a n_a} = \Psi_{m_a}(x) \Psi_{n_a}(y)$  and  $\Psi_b = \Psi_{m_b n_b} = \Psi_{m_b}(x) \Psi_{n_b}(y)$ .

### 5.3 Expectation Value of Potential Energy

The expectation value of the potential energy of the trapped ion in a two-dimensional Paul trap as a particle makes transition from  $\Psi_a$  to  $\Psi_b$  is studied into two parts: potential energy in the  $x$  direction and potential energy in the  $y$  direction.

#### 5.3.1 Potential Energy in $x$ Direction

The expectation value of potential energy in the  $x$  direction is  $V_{ab}(x) = \frac{1}{2} k \langle \Psi_a | x^2 | \Psi_b \rangle$  and the operator 'x' can be expressed in terms of the raising and lowering operators as  $x = \sqrt{\frac{\hbar}{2m\omega_0}} (a_+ + a_-)$ , and the square of the operator  $x$  ( $x^2$ ) becomes  $x^2 = \frac{\hbar}{2m\omega_0} [(a_+)^2 + (a_+ a_-) + (a_- a_+) + (a_-)^2]$ . Here  $a_+ \Psi = \sqrt{n+1} \Psi_{n+1}$ ,  $a_- \Psi = \sqrt{n} \Psi_{n-1}$ ,  $a_+ a_- \Psi = n \Psi_n$  and  $a_- a_+ \Psi = (n+1) \Psi_n$ . The detailed information about the operators is given in the [Griffiths, 2005, p. 48]. Now replacing  $x$  with operator one gets  $V_{ab}(x) = \frac{1}{2} m \omega_0^2 \frac{\hbar}{2m\omega_0} \iint \Psi_a [(a_+)^2 + (a_+ a_-) + (a_- a_+) + (a_-)^2] \Psi_b dx dy$  and simplifying the potential one finds,

$$V_{ab}(x) = \frac{\hbar \omega_0}{4} \left[ \int \{ \Psi_{m_a}(x) [(a_+)^2 + (a_+ a_-) + (a_- a_+) + (a_-)^2] \Psi_{m_b}(x) dx \} \int \{ \Psi_{n_a}(y) \Psi_{n_b}(y) dy \} \right].$$

Now evaluating the potential one gets  $V_{ab}(x) = \frac{\hbar\omega_0}{4} \left[ \left( \sqrt{m_b^2 + 3m_b + 2} \right) \delta_{m_a, m_b+2} + (2m_b + 1) \delta_{m_a, m_b} + \left( \sqrt{m_b^2 - m_b} \right) \delta_{m_a, m_b-2} \right] \delta_{n_a, n_b}$ . In order to make a transition from state  $\Psi_a$  to  $\Psi_b$ ,  $m_b > m_a$  and  $n_a = n_b$ , with that condition, the first two terms vanishes from the above Equation and it becomes,

$$V_{ab}(x) = \frac{\hbar\omega_0}{4} \left[ \left( \sqrt{m_b^2 - m_b} \right) \delta_{m_a, m_b-2} \right] \delta_{n_a, n_b}. \quad (5.3)$$

### 5.3.2 Potential Energy in y Direction

The expectation value of potential energy in the y direction is

$V_{ab}(y) = \langle \Psi_a | V(y) | \Psi_b \rangle = \frac{1}{2} k \langle \Psi_a | y^2 | \Psi_b \rangle$  and the operator 'y' can be expressed in terms of

the raising and lowering operators as  $y = \sqrt{\frac{\hbar}{2m\omega_0}} (a_+ + a_-)$ , and the square of the operator y

( $y^2$ ) is  $y^2 = \frac{\hbar}{2m\omega_0} [(a_+)^2 + (a_+ a_-) + (a_- a_+) + (a_-)^2]$ . Here  $a_+ \Psi = \sqrt{n+1} \Psi_{n+1}$ ,

$a_- \Psi = \sqrt{n} \Psi_{n-1}$ ,  $a_+ a_- \Psi = n \Psi_n$  and  $a_- a_+ \Psi = (n+1) \Psi_n$ . The detailed information about

the operators is given in the [Griffiths, 2005, p. 48]. Now replacing y with operator one gets

$V_{ab}(y) = \frac{1}{2} m \omega_0^2 \frac{\hbar}{2m\omega_0} \iint \Psi_a [(a_+)^2 + (a_+ a_-) + (a_- a_+) + (a_-)^2] \Psi_b dx dy$  and

simplifying it becomes  $V_{ab}(y) = \frac{\hbar\omega_0}{4} \left[ \int \{ \Psi_{n_a}(y) [(a_+)^2 + (a_+ a_-) + (a_- a_+) + \right.$

$(a_-)^2] \Psi_{n_b}(y) dy \} \int \{ \Psi_{m_a}(x) \Psi_{m_b}(x) dx \} ]$ . Then evaluating it one gets  $V_{ab}(y) =$

$\frac{\hbar\omega_0}{4} \left[ \left( \sqrt{n_b^2 + 3n_b + 2} \right) \delta_{n_a, n_b+2} + (2n_b + 1) \delta_{n_a, n_b} + \left( \sqrt{n_b^2 - n_b} \right) \delta_{n_a, n_b-2} \right] \delta_{m_a, m_b}$ .

In order to make a transition from state  $\Psi_a$  to  $\Psi_b$ ,  $n_b > n_a$  and  $m_a = m_b$ , with that condition, the first two terms vanishes from the above equation and it becomes,

$$V_{ab}(y) = \frac{\hbar\omega_0}{4} \left[ \left( \sqrt{n_b^2 - n_b} \right) \delta_{n_a, n_b-2} \right] \delta_{m_a, m_b}. \quad (5.4)$$

#### 5.4 Perturbation Theory

The first order approximation of perturbed system can be calculated by the Equation

(3.6), which is  $C_a^1(t) = 1$  and  $C_b^1(t) = -\frac{i}{\hbar} \int_0^t H'_{ab}(t') e^{i\omega_0 t'} dt'$ . Now substituting the

perturbed system one gets  $C_b^1(t) = -\frac{i}{\hbar} \int_0^t [V_{ba}(x)\{\cos(\Omega t) - 1\} - V_{ba}(y)\{\cos(\Omega t) +$

$1\}] e^{i\omega_0 t'} dt'$  and simplifying it one finds  $C_b^1(t) = -\frac{i}{\hbar} \left[ \int_0^t V_{ba}(x)\{\cos(\Omega t) -$

$1\} e^{i\omega_0 t'} dt' \right] - \left[ -\frac{i}{\hbar} \left\{ \int_0^t V_{ba}(y)\{\cos(\Omega t) + 1\} e^{i\omega_0 t'} dt' \right\} \right]$ . Let

$\beta = -\frac{i}{\hbar} \int_0^t [V_{ba}(x)\{\cos(\Omega t') - 1\} e^{i\omega_0 t'} dt']$  and  $\Phi = -\frac{i}{\hbar} \int_0^t [V_{ba}(y)\{\cos(\Omega t') +$

$1\} e^{i\omega_0 t'} dt']$  then the above equation becomes

$$C_b^1(t) = \beta - \Phi. \quad (5.5)$$

Here,  $\beta = -\frac{i}{\hbar} V_{ab}(x) \int_0^t \left\{ \frac{e^{i(\omega_0+\Omega)t'} + e^{i(\omega_0-\Omega)t'}}{2} - e^{i\omega_0 t'} \right\} dt'$  and expanding the exponential one

gets  $\beta = -\frac{i}{2\hbar} V_{ab}(x) \left[ \frac{e^{i(\omega_0+\Omega)t} - 1}{i(\omega_0+\Omega)} + \frac{e^{i(\omega_0-\Omega)t} - 1}{i(\omega_0-\Omega)} - 2 \frac{e^{i\omega_0 t} - 1}{i\omega_0} \right]$ . Simplifying one finds  $\beta =$

$-\frac{V_{ab}(x)}{2\hbar} \left[ \frac{e^{i(\omega_0+\Omega)t} - 1}{(\omega_0+\Omega)} + \frac{e^{i(\omega_0-\Omega)t} - 1}{(\omega_0-\Omega)} - 2 \frac{e^{i\omega_0 t} - 1}{(\omega_0)} \right]$ . Similarly  $\Phi = -\frac{i}{\hbar} V_{ab}(y) \left[ \int_0^t \left\{ \frac{e^{i\Omega t'} + e^{-i\Omega t'}}{2} +$

$1 \} e^{i\omega_0 t'} dt' \right]$  and expanding the exponential one gets  $\Phi = -\frac{i}{\hbar} V_{ab}(y) \int_0^t \left\{ \frac{e^{i(\omega_0+\Omega)t'} + e^{i(\omega_0-\Omega)t'}}{2} +$

$e^{i\omega_0 t'} \right\} dt'$ . Then simplifying one finds  $\Phi = -\frac{i}{2\hbar} V_{ab}(y) \left[ \frac{e^{i(\omega_0+\Omega)t} - 1}{i(\omega_0+\Omega)} + \frac{e^{i(\omega_0-\Omega)t} - 1}{i(\omega_0-\Omega)} +$

$2 \frac{e^{i\omega_0 t} - 1}{i\omega_0} \right]$  and writing in order one gets  $\Phi = -\frac{V_{ab}(y)}{2\hbar} \left[ \frac{e^{i(\omega_0+\Omega)t} - 1}{(\omega_0+\Omega)} + \frac{e^{i(\omega_0-\Omega)t} - 1}{(\omega_0-\Omega)} + 2 \frac{e^{i\omega_0 t} - 1}{(\omega_0)} \right]$ .

## 5.5 Transition Probability

The probability of a transition is greater when the driving frequency  $\Omega$ , is close to the natural frequency  $\omega_0$ , ( $\omega_0 \cong \Omega$ ), that gives  $|\omega_0 + \Omega| \gg |\omega_0| \gg |\omega_0 - \Omega|$ , and then the second

term  $\frac{e^{i(\omega_0 - \Omega)t} - 1}{(\omega_0 - \Omega)}$  dominates so the Equation (5.5) becomes  $C_b^1(t) = -\frac{V_{ab}(x)}{2\hbar} \left[ \frac{e^{i(\omega_0 - \Omega)t} - 1}{(\omega_0 - \Omega)} \right] +$

$\frac{V_{ab}(y)}{2\hbar} \left[ \frac{e^{i(\omega_0 - \Omega)t} - 1}{(\omega_0 - \Omega)} \right]$  and taking out the factor  $\frac{e^{i(\omega_0 - \Omega)t} - 1}{(\omega_0 - \Omega)}$  one gets

$C_b^1(t) = \frac{1}{2\hbar} \left[ \left\{ \frac{e^{i(\omega_0 - \Omega)t} - 1}{(\omega_0 - \Omega)} \right\} \{-V_{ab}(x) + V_{ab}(y)\} \right]$ . Again taking out the factor  $e^{i\left(\frac{\omega_0 - \Omega}{2}\right)t}$  one finds

$C_b^1(t) = \frac{1}{2\hbar} \left[ e^{i\left(\frac{\omega_0 - \Omega}{2}\right)t} \left\{ \frac{e^{i\left(\frac{\omega_0 - \Omega}{2}\right)t} - e^{-i\left(\frac{\omega_0 - \Omega}{2}\right)t}}{(\omega_0 - \Omega)} \right\} \{-V_{ab}(x) + V_{ab}(y)\} \right]$  and simplifying it one gets

$C_b^1(t) = \frac{i}{2\hbar(\omega_0 - \Omega)} e^{i\left(\frac{\omega_0 - \Omega}{2}\right)t} \left[ \{-V_{ab}(x) + V_{ab}(y)\} \left\{ 2 \frac{e^{i\left(\frac{\omega_0 - \Omega}{2}\right)t} - e^{-i\left(\frac{\omega_0 - \Omega}{2}\right)t}}{2i} \right\} \right]$ . Now writing the

exponential in terms of the sine functions one gets  $C_b^1(t) = \frac{i}{2\hbar(\omega_0 - \Omega)} e^{i\left(\frac{\omega_0 - \Omega}{2}\right)t} \left[ \{-V_{ab}(x) +$

$V_{ab}(y)\} \left\{ 2 \sin\left(\frac{\omega_0 - \Omega}{2} t\right) \right\} \right]$  and reordering it one finds,

$$C_b^1(t) = \frac{i}{2\hbar} e^{i\left(\frac{\omega_0 - \Omega}{2}\right)t} \left[ \{-V_{ab}(x) + V_{ab}(y)\} \left\{ \frac{2 \sin\left(\frac{\omega_0 - \Omega}{2} t\right)}{(\omega_0 - \Omega)} \right\} \right]. \quad (5.6)$$

The probability of finding the particle in the state  $\Psi_b$  at time  $t$  that started out in the state  $\Psi_a$  is

$P_{a \rightarrow b}(t) = |C_b^1(t)|^2 = \frac{|[V_{ab}(x) - V_{ab}(y)]|^2}{(2\hbar)^2} \left[ \frac{4 \sin^2\left(\frac{\omega_0 - \Omega}{2} t\right)}{(\omega_0 - \Omega)^2} \right]$  and the probability in terms of the delta

function is,

$$P_{a \rightarrow b}(t) = \frac{|[V_{ab}(x) - V_{ab}(y)]|^2}{(2\hbar)^2} \{2\pi t \delta(\omega_0 - \Omega)\} \quad (5.7)$$

where

$$\lim_{\Omega \rightarrow \omega_0} \frac{4 \sin^2\left(\frac{\omega_0 - \Omega}{2} t\right)}{(\omega_0 - \Omega)^2} = 2\pi t \delta(\omega_0 - \Omega).$$

### 5.5.1 Transition Rate

The transition rate ( $R_{a \rightarrow b}(t)$ ) of the particle from state  $\Psi_a$  to state  $\Psi_b$  is given by

$$R_{a \rightarrow b}(t) = \frac{dP_{a \rightarrow b}(t)}{dt} \text{ [Griffiths, 2005, p. 353] and the transition rate of the trapped ion}$$

is  $R_{a \rightarrow b}(t) = \frac{||V_{ab}(x) - V_{ab}(y)||^2}{(2\hbar)^2} \{2\pi\delta(\omega_0 - \Omega)\}$ . Writing the transition rate in terms of energy

states one gets,

$$R_{a \rightarrow b}(t) = \frac{||V_{ab}(x) - V_{ab}(y)||^2}{(2\hbar)^2} \{2\pi\delta(E_b - E_a - \hbar\Omega)\}. \quad (5.8)$$

Instead of one final state, there is infinite number of final states so the Equation (5.8) becomes

$$R_{a \rightarrow b}(t) = \frac{||V_{ab}(x) - V_{ab}(y)||^2}{4\hbar} \{2\pi\rho_f(E)\}, \quad (5.9)$$

where

$$||V_{ab}(x) - V_{ab}(y)||^2 = \frac{\hbar^2\omega_0^2}{16} [(m_b^2 - m_a) \delta_{m_a, m_b-2} \delta_{n_a, n_b} + (n_b^2 - n_a) \delta_{n_a, n_b-2} \delta_{m_a, m_b}],$$

$\rho_f(E) = \frac{1}{\hbar\omega_0}$  is the density of the final states.

Here, the transition of an ion happens either when  $m_b > m_a$  and  $n_a = n_b$  or  $n_b > n_a$

and  $m_a = m_b$ . That means the transition of a particle cannot happen in both direction, it can

happen in only one direction either in x direction or in y direction.

### 5.6 Lifetime

Therefore, the lifetime ( $\tau_{a \rightarrow b}$ ) of the trapped ion in state  $\Psi_a$  before it makes transition to

state  $\Psi_b$  is  $\tau_{a \rightarrow b} = \frac{1}{R_{a \rightarrow b}(t)}$  and the lifetime in terms of allowed states and transition frequency is,

$$\tau_{a \rightarrow b} = \frac{32}{\pi\omega_0 [(m_b^2 - m_a) \delta_{m_a, m_b-2} \delta_{n_a, n_b} + (n_b^2 - n_a) \delta_{n_a, n_b-2} \delta_{m_a, m_b}]} \quad (5.10)$$

Therefore, from the above equation, it is shown that the lifetime depends upon the transition frequency and the allowed state. The lifetime of a particle decreases as the particle makes transition to the higher states. So the longest lifetime of a trapped particle is in ground state before it makes transition from ground state to the state 2.



## CHAPTER VI

### RESULTS

The significant results that were found from this study are given by the Equations (4.8), (4.20), and (5.10). The transition frequency that corresponds with the charge-mass ratio of a trapped ion,

radius of the Paul trap and charge of the conductor is  $\omega_0 = \sqrt{\frac{3qQ_0}{2\pi\epsilon_0mr^3}}$  and the transition

frequency that corresponds with the charge-mass ratio of a trapped ion, radius of the Paul trap and

applied voltage is  $\omega_0 = \sqrt{\frac{6qV_0}{mr^2}}$ . The lifetime of a trapped ion in state  $\Psi_a$  before it makes

transition to state  $\Psi_b$  in one-dimensional and two-dimensional Paul trap are  $\tau_{a \rightarrow b} =$

$$\frac{32}{\pi\omega_0\{(m_b^2 - m_b)\delta_{m_a, m_b - 2}\}}, \text{ and } \tau_{a \rightarrow b} = \frac{32}{\pi\omega_0[(m_b^2 - m_b)\delta_{m_a, m_b - 2}\delta_{n_a, n_b} + (n_b^2 - n_b)\delta_{n_a, n_b - 2}\delta_{m_a, m_b}]} \text{ respectively.}$$

The lifetime of a trapped ion in state  $\Psi_a$  in two-dimensional would be the same as the lifetime of a trapped ion in one-dimensional when  $n_a = n_b$  or  $m_a = m_b$  and here just to verify it, hydrogen ion has been used. For a hydrogen ion, the mass (m) is  $1.673 \times 10^{-27}$  kilograms (Kg) and the charge (q) is  $1.61 \times 10^{-19}$  coulomb (C). Let's say the radius (r) of a Paul trap is 1.0 centimeters (cm) and the applied voltage ( $V_0$ ) is 3.0 kilovolts (kV).

*Note: this study has been limited to applied frequencies ( $\Omega$ ) that are very close to the transition frequency ( $\omega_0$ ) i. e.  $\omega_0 \cong \Omega$ .*

## 6.1 Transition Frequency

The transition frequency for a hydrogen ion in a Paul trap is

$$\omega_0 = \sqrt{\frac{6qV_0}{mr^2}}$$

$$\omega_0 = \sqrt{\frac{6 \times 1.61 \times 10^{-19} \times 3.0 \times 10^3}{1.673 \times 10^{-27} \times (1.0 \times 10^{-2})^2}}$$

or  $\omega_0 = 1.316 \times 10^8$  Rad/s or  $\frac{\omega_0}{2\pi} = 20.945 \times 10^6$  Hz.

## 6.2 Lifetime in a One-Dimensional Paul Trap

The lifetime for trapped hydrogen ion in a one-dimensional Paul trap when the ion makes transition from ground state to 2 is,

$$\tau_{0 \rightarrow 2} = \frac{32}{\pi \omega_0 \{(m_b^2 - m_b) \delta_{m_a, m_b - 2}\}}$$
$$\tau_{0 \rightarrow 2} = \frac{32}{\pi \times 1.316 \times 10^8 \times (4 - 2)}$$

or  $\tau_{0 \rightarrow 2} = 3.870 \times 10^{-8}$ s.

The lifetime for trapped hydrogen ion in a one-dimensional Paul trap when the ion makes transition from state 2 to 4 is,

$$\tau_{2 \rightarrow 4} = \frac{32}{\pi \times 1.316 \times 10^8 \times (16 - 4)}$$

or  $\tau_{2 \rightarrow 4} = 0.645 \times 10^{-8}$ s.

The lifetime for trapped hydrogen ion in a one-dimensional Paul trap when the ion makes transition from state 4 to 6 is,

$$\tau_{4 \rightarrow 6} = \frac{32}{\pi \times 1.316 \times 10^8 \times (36 - 6)}$$

or  $\tau_{4 \rightarrow 6} = 0.258 \times 10^{-8}$ s.

### 6.3 Lifetime in a Two-Dimensional Paul Trap

The lifetime for a trapped hydrogen ion in a two-dimensional Paul trap when the ion makes transition from ground state to 2 is, when  $n_a = n_b$  and  $m_a = 0$  and  $m_b = 2$  or when  $m_a = m_b$  and  $n_a = 0$  and  $n_b = 2$ .

$$\tau_{a \rightarrow b} = \frac{32}{\pi \omega_0 [(m_b^2 - m_b) \delta_{m_a, m_b - 2} \delta_{n_a, n_b} + (n_b^2 - n_b) \delta_{n_a, n_b - 2} \delta_{m_a, m_b}]}$$

$$\tau_{0 \rightarrow 2} = \frac{32}{\pi \times 1.316 \times 10^8 \times (4 - 2)}$$

or  $\tau_{0 \rightarrow 2} = 3.870 \times 10^{-8} \text{s}$ .

The lifetime for a trapped hydrogen ion in a two-dimensional Paul trap when the ion makes transition from state 2 to 4 is, when  $n_a = n_b$  and  $m_a = 2$  and  $m_b = 4$ , or when  $m_a = m_b$  and  $n_a = 2$  and  $n_b = 4$ .

$$\tau_{2 \rightarrow 4} = \frac{32}{\pi \times 1.316 \times 10^8 \times (16 - 4)}$$

or  $\tau_{2 \rightarrow 4} = 0.645 \times 10^{-8} \text{s}$ .

The lifetime for a trapped hydrogen ion in a two-dimensional Paul trap when the ion makes transition from state 4 to 6 is, when  $n_a = n_b$  and  $m_a = 4$  and  $m_b = 6$ , or when  $m_a = m_b$  and  $n_a = 4$  and  $n_b = 6$ .

$$\tau_{4 \rightarrow 6} = \frac{32}{\pi \times 1.316 \times 10^8 \times (36 - 6)}$$

or  $\tau_{4 \rightarrow 6} = 0.258 \times 10^{-8} \text{s}$ .

The graph of Figure 9 shows how the lifetime ( $\tau_{0 \rightarrow 2}$ ) of a trapped hydrogen ion in ground state changes with applied voltage, radius and mass as it make a transition to energy state 2. The top graph in Figure 9 shows that the lifetime decreases exponentially as the applied voltage increased from 0 to 500 volts then after the lifetime is almost same as voltage is increased. So the lifetime of a trapped hydrogen ion ( $\frac{m}{q} = 1.04 \times 10^{-8} \frac{kg}{c}$ ) in a Paul trap that has a radius of 1.0 cm can be adjusted with applied voltage as desired for experimentation. The middle graph in Figure 9 shows that the lifetime increases linearly as the radius of a Paul trap increased but typically radius of a Paul trap is fixed. The value of radius can be choose from the middle graph in Figure 9 to design a Paul trap to get a desired lifetime of a trapped hydrogen ion ( $\frac{m}{q} = 1.04 \times 10^{-8} \frac{kg}{c}$ ) for 3.0 kV applied voltage. The bottom graph in Figure 9 shows that the lifetime increases faster as the atomic mass unit (amu) of a trapped ion increases from 0 to 50 then after the lifetime increases linearly. Here, the radius of a Paul trap is 1.0 cm, applied voltage is 3.0 kV and mass-charge ratio is ( $\frac{m}{q} = 1.04 \times 10^{-8} \times amu \frac{kg}{c}$ ).

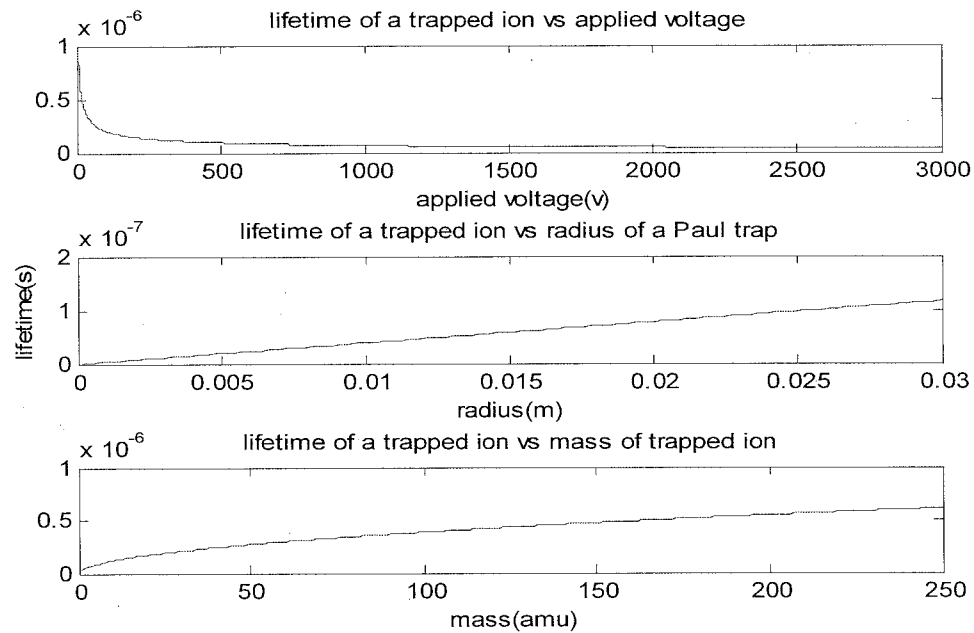


Figure 9: Plot of a Lifetime with Voltage, Radius and Mass.

The graph below shows how the resonance frequency needs to be adjusted when one changes applied voltage, radius of a Paul trap and mass of trapped ion. The top graph in Figure 10 shows that the resonance frequency increases faster as the applied voltage increased from 0 to 500 volts then after the resonance frequency increases linearly. So the resonance frequency of a trapped hydrogen ion ( $\frac{m}{q} = 1.04 \times 10^{-8} \frac{kg}{C}$ ) in a Paul trap that has a radius of 1.0 cm can be adjusted with applied voltage as desired for experimentation. The middle graph in Figure 10 shows that the resonance frequency decreases exponentially as the radius of a Paul trap increased from 1 to 7 mm but typically radius of a Paul trap is fixed. The value of radius can be choose from the middle graph in Figure 10 to design a Paul trap to get a desired resonance frequency of a trapped hydrogen ion ( $\frac{m}{q} = 1.04 \times 10^{-8} \frac{kg}{C}$ ) for 3.0 kV applied voltage. The bottom graph in Figure 10 shows that the resonance frequency decreases exponentially as the atomic mass unit (amu) of a trapped ion increases from 0 to 50 after then the resonance frequency is almost same for increased mass (amu). Here, the radius of a Paul trap is 1.0 cm, applied voltage is 3.0 kV and mass-charge ratio is ( $\frac{m}{q} = 1.04 \times 10^{-8} \times amu \frac{kg}{C}$ ).

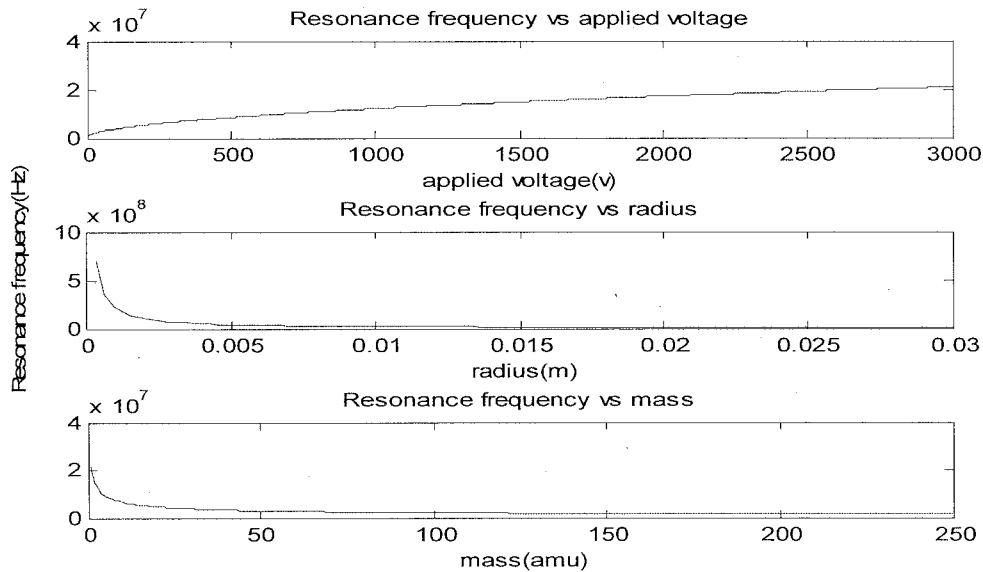


Figure 10: Plot of Resonance Frequency with Applied Voltage, Radius and Mass.

## CHAPTER VII

### CONCLUSIONS

Time-dependent perturbation theory has been used in study this research and this study is based on the approximation of quantum harmonic oscillator of a particle. The energies are quantized in quantum harmonic oscillator and the particle spends most of time at the bottom of the potential well (ground state) if there were no perturbation at all. The particle jumps to higher states as a particle absorbs the energy, so a trapped ion makes a transition to higher states as it gains the energy from the applied radio frequency voltage. The transition of a particle is greater when the applied frequencies are close to the transition frequency so this study is restricted the driving frequencies ( $\Omega$ ) close to transition frequency ( $\omega_0$ ) i.e. ( $\omega_0 \cong \Omega$ ).

Therefore, using time-dependent perturbation theory, the results from this study shows that transition frequencies ( $\omega_0$ ) of an ion can be controlled with the amplitude of applied voltage ( $V_0$ ), radius of a Paul trap ( $r$ ) and charge-mass ratio ( $q/m$ ). How the applied frequencies changes with those parameters is shown in Figure 10. The lifetime ( $\tau_{a \rightarrow b}$ ) of an ion depends upon the transition frequencies ( $\omega_0$ ) and also some specific allowed states ( $n_a, n_b, m_a, m_b$ ) i.e. when the difference in energy state is by two. A trapped ion in a linear Paul trap makes transition either in the  $x$ -direction or in the  $y$ -direction but not on both directions. The lifetime in a two-dimensional Paul trap would be the same in state  $\Psi_a$  as in state  $\Psi_a$  in one-dimensional Paul trap when  $n_a = n_b$  or  $m_a = m_b$  and it is shown in the previous chapter for hydrogen ion.

When an ion absorbs the energy, it makes a transition to higher energy states and eventually it gets lost from the trap. But not only that happens, it can also radiate the energy when an ion jumps from higher states to lower states which make possible trapping an ion for a longer period of time. This study shows that the Paul trap can be designed to get higher or lower lifetime of a trapped ion with the parameters that are given by the Equation (4.8) and the graph is shown in the Figures 9 and 10. If one wants to get the higher lifetime then the transition frequency should be small which one gets by decreasing the amplitude of applied radio frequency voltage and increasing the radius of the Paul trap for a specific ion. Similarly, if one wants to get the lower lifetime then the transition frequency should be large which one gets by increasing the amplitude of applied radio frequency voltage and decreasing the radius of the Paul trap for a particular ion.

Paul traps are used in many scientific researches so knowing the quantum mechanical lifetime of trapped particle in a Paul trap certainly aids in understanding the physics of trapped ions in the Paul trap. This paper gives an initial result; additional research needs to be done to fully understand the quantum motion of particles in a Paul trap.

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## APPENDIX A

### MULTIPOLE EXPANSION OF THE ELECTROSTATIC POTENTIAL

The electric potential  $\varphi$ , at the observation point P, due to the collection of number of point charges  $Q_1, Q_2, Q_3, Q_4, Q_5, \dots$  and  $Q_n$ , that are enclosed in volume V, is given by

$$\varphi(\vec{R}) = \sum_{i=1}^n \frac{Q_i}{4\pi\epsilon_0 |\vec{R} - \vec{r}_i|}, \quad (\text{A.1})$$

where

$\epsilon_0$  = permittivity of the free space,

$\vec{r}_i$  = position vector of the charges  $Q_i$ ,

$\vec{R}$  = position vector of observation point [19, 20].

The schematic figure of the multipole expansion of the potential due to point charges is shown below in Figure 11.

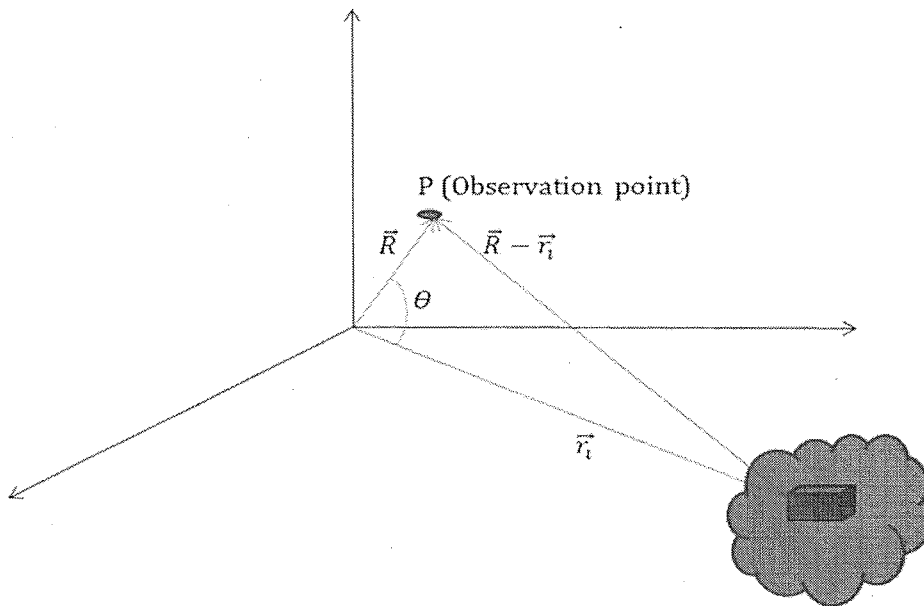


Figure 11: Potential due to the point charges

Let  $\theta_i$ , be the angle between the observation point P, and the point charges  $Q_i$ , then by the law of cosines, one gets

$$|\vec{R} - \vec{r}_i| = (R^2 + r_i^2 - 2Rr_i \cos \theta_i)^{1/2}, \quad (\text{A.2})$$

where  $\cos \theta_i = \frac{\vec{R} \cdot \vec{r}_i}{Rr_i}$ .

Now, assuming that observation point P, is close to the origin and the point charges  $Q_i$ , are far

from the origin so that  $R \ll r_i$  or  $\frac{R}{r_i} \ll 1$  for all i. The reciprocal of Equation (A.2) is  $\frac{1}{|\vec{R} - \vec{r}_i|} =$

$\frac{1}{(R^2 + r_i^2 - 2Rr_i \cos \theta_i)^{1/2}}$  and taking out the factors  $r_i$  in the denominator gives  $\frac{1}{|\vec{R} - \vec{r}_i|} =$

$\frac{1}{r_i \left\{ 1 + \left(\frac{R}{r_i}\right)^2 - 2\left(\frac{R}{r_i}\right) \cos \theta_i \right\}^{1/2}}$ . then simplifying gives the following Equation (A.3)

$$\frac{1}{|\vec{R} - \vec{r}_i|} = \frac{1}{r_i} \left\{ 1 + \left(\frac{R}{r_i}\right)^2 - 2\left(\frac{R}{r_i}\right) \cos \theta_i \right\}^{-1/2},$$

$$\frac{1}{|\vec{R} - \vec{r}_i|} = \frac{1}{r_i} (1 + \delta)^{-1/2}, \quad (\text{A.3})$$

where  $\delta = \left(\frac{R}{r_i}\right)^2 - 2\left(\frac{R}{r_i}\right) \cos \theta_i$ .

The power series for  $|x| < 1$  is given by the following Equation (A.4) [19, 20],

$$(1 + x)^n = 1 + nx + \frac{n(n-1)x^2}{2!} + \frac{n(n-1)(n-2)x^3}{3!} + \dots \quad (\text{A.4})$$

Here, substitute  $\delta$  for x in above Equation (A.4), then the Equation (A.4) becomes

$$(1 + \delta)^{-1/2} = 1 + (-1/2)\delta + \frac{(-1/2)(-3/2)\delta^2}{2} + \frac{(-1/2)(-3/2)(-5/2)\delta^3}{6} + \dots,$$

$$(1 + \delta)^{-1/2} = 1 - \frac{1}{2}\delta + \frac{3}{8}\delta^2 - \frac{5}{16}\delta^3 + \dots \quad (\text{A.5})$$

Now, substitute for  $\delta$  in above Equation (A.5), one gets

$$\begin{aligned}
(1 + \delta)^{-1/2} = & \left[ 1 - \frac{1}{2} \left\{ \left( \frac{R}{r_i} \right)^2 - 2 \left( \frac{R}{r_i} \right) \cos \theta_i \right\} + \frac{3}{8} \left\{ \left( \frac{R}{r_i} \right)^2 - 2 \left( \frac{R}{r_i} \right) \cos \theta_i \right\}^2 \right. \\
& \left. - \frac{5}{16} \left\{ \left( \frac{R}{r_i} \right)^2 - 2 \left( \frac{R}{r_i} \right) \cos \theta_i \right\}^3 + \dots \right].
\end{aligned}$$

Then, drop the higher terms such as  $\left(\frac{R}{r_i}\right)^3$  and  $\left(\frac{R}{r_i}\right)^4$  in above Equation one gets

$$(1 + \delta)^{-1/2} \approx \left[ 1 + \left( \frac{R}{r_i} \right) \cos \theta_i + \frac{1}{2} \left( \frac{R}{r_i} \right)^2 \{ 3 \cos^2 \theta_i - 1 \} + \dots \right] \quad (\text{A.6})$$

Substitute the Equation (A.6), in the Equation (A.3) one finds

$$\frac{1}{|\vec{R} - \vec{r}_i|} = \frac{1}{r_i} (1 + \delta)^{-1/2} = \left[ \frac{1}{r_i} + \frac{1}{r_i^2} R \cos \theta_i + \frac{1}{2r_i^3} R^2 \{ 3 \cos^2 \theta_i - 1 \} + \dots \right]$$

And replace  $\cos \theta_i$  with  $\frac{\vec{R} \cdot \vec{r}_i}{R r_i}$  in above Equation it becomes

$$\frac{1}{|\vec{R} - \vec{r}_i|} = \left[ \frac{1}{r_i} + \frac{\vec{R} \cdot \vec{r}_i}{r_i^3} + \frac{1}{2r_i^5} \{ 3(\vec{R} \cdot \vec{r}_i)^2 - R^2 r_i^2 \} + \dots \right]. \quad (\text{A.7})$$

Again, substitute the Equation (A.7) in the Equation (A.1), the electric potential due to point charges can be calculated by the following Equation (A.8) and the detailed information of multipole expansion is given in the [ Wangsness,1986] [19, 20],

$$\varphi(\vec{R}) = \left[ \frac{1}{4\pi\epsilon_0} \sum_{i=1}^n \frac{Q_i}{r_i} + \frac{1}{4\pi\epsilon_0} \sum_{i=1}^n \frac{Q_i}{r_i^3} \vec{R} \cdot \vec{r}_i + \frac{1}{8\pi\epsilon_0} \sum_{i=1}^n \frac{Q_i}{r_i^5} \{ 3(\vec{R} \cdot \vec{r}_i)^2 - R^2 r_i^2 \} + \dots \right] \quad (\text{A.8})$$

where

$$\text{Monopole } \varphi_m(\vec{R}) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^n \frac{Q_i}{r_i},$$

$$\text{Dipole } \varphi_d(\vec{R}) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^n \frac{Q_i}{r_i^3} \vec{R} \cdot \vec{r}_i,$$

$$\text{Quadrupole } \varphi_q(\vec{R}) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^n \frac{Q_i}{2r_i^5} \{ 3(\vec{R} \cdot \vec{r}_i)^2 - R^2 r_i^2 \}.$$

## APPENDIX B

### POTENTIAL IN A PAUL TRAP

The electrical potential close to the origin produced by multiple point charges that are far from the origin can be calculated by the Equation (A.8) which is shown in appendix A,

$$\varphi(\vec{R}) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^n \frac{Q_i}{r_i} + \frac{1}{4\pi\epsilon_0} \sum_{i=1}^n \frac{Q_i}{r_i^3} \vec{R} \cdot \vec{r}_i + \frac{1}{8\pi\epsilon_0} \sum_{i=1}^n \frac{Q_i}{r_i^5} \{3(\vec{R} \cdot \vec{r}_i)^2 - R^2 r_i^2\} + \dots$$

The electrical potential close to the center in the linear Paul trap as shown in Figure 12 can be approximately calculated by the Equation (B.1),

$$\varphi(\vec{R}) \cong \left[ \frac{1}{4\pi\epsilon_0} \sum_{i=1}^4 \frac{Q_i}{r_i} + \frac{1}{4\pi\epsilon_0} \sum_{i=1}^4 \frac{Q_i}{r_i^3} \vec{R} \cdot \vec{r}_i + \frac{1}{8\pi\epsilon_0} \sum_{i=1}^4 \frac{Q_i}{r_i^5} \{3(\vec{R} \cdot \vec{r}_i)^2 - R^2 r_i^2\} \right] \quad (\text{B.1})$$

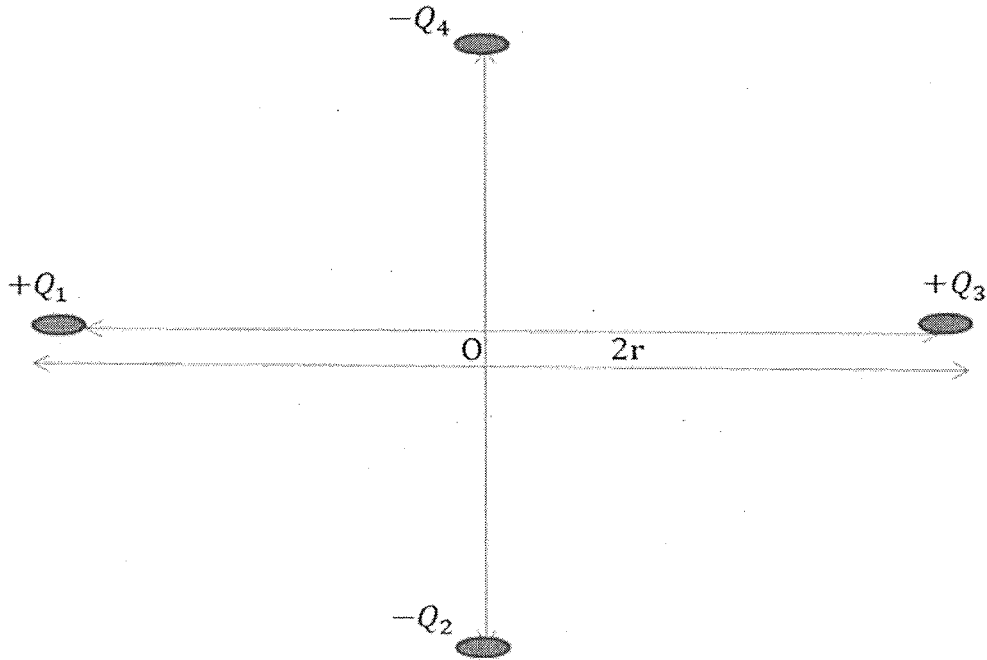


Figure 12: Side view of Linear Paul Trap

The charges  $Q_1, Q_2, Q_3$  and  $Q_4$  are at a distance  $r_1, r_2, r_3$  and  $r_4$  respectively from the origin. The position vector of charges  $Q_1, Q_2, Q_3, Q_4$  and observation field point P, are  $\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4$ , and  $\vec{R}$  respectively. Let, the magnitude of charges  $|Q_1|, |Q_2|, |Q_3|, |Q_4|$  on the Paul trap equal to  $Q$  and the radius  $r_1, r_2, r_3, r_4$ , are equal to  $r$ . here the positive (+) and negative (-) sign means that charges are connected to the positive and negative side of alternating current (AC) that oscillates with radio frequency. Then, the position vectors of charges and observation field point are  $\vec{r}_1 = -r\hat{x}$ ,  $\vec{r}_2 = -r\hat{y}$ ,  $\vec{r}_3 = r\hat{x}$ ,  $\vec{r}_4 = r\hat{y}$  and  $\vec{R} = x\hat{x} + y\hat{y} + z\hat{z}$  respectively. Then, the dot products of the vectors are;  $\vec{R} \cdot \vec{r}_1 = -rx$ ,  $\vec{R} \cdot \vec{r}_2 = -ry$ ,  $\vec{R} \cdot \vec{r}_3 = rx$ ,  $\vec{R} \cdot \vec{r}_4 = ry$  and  $|\vec{r}_1|^2 = |\vec{r}_2|^2 = |\vec{r}_3|^2 = |\vec{r}_4|^2 = r^2$ .

The Monopole term

The electric monopole potential of the Paul trap from the Equation (B.1) is,

$$\varphi_m(\vec{R}) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^4 \frac{Q_i}{r_i}$$

Now expand it,  $\varphi_m(\vec{R}) = \frac{1}{4\pi\epsilon_0} \left\{ \frac{Q_1}{r_1} + \frac{Q_2}{r_2} + \frac{Q_3}{r_3} + \frac{Q_4}{r_4} \right\}$  and substituting the corresponding values of charges ( $Q_i$ ) and the distances ( $r_i$ ), one gets

$$\varphi_m(\vec{R}) = \frac{1}{4\pi\epsilon_0} \left\{ +\frac{Q}{r} - \frac{Q}{r} + \frac{Q}{r} - \frac{Q}{r} \right\},$$

$$\varphi(\vec{R}) = 0. \quad (\text{B.2})$$

Here, the monopole term of the Paul trap is zero.

The Dipole term

The electric dipole potential of the Paul trap from the Equation (B.1) is,

$$\varphi_d(\vec{R}) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^4 \frac{Q_i}{r_i^3} \vec{R} \cdot \vec{r}_i$$

Now expand one gets,  $\varphi_d(\vec{R}) = \frac{1}{4\pi\epsilon_0} \left\{ \frac{Q_1}{r_1^3} (\vec{R} \cdot \vec{r}_1) + \frac{Q_2}{r_2^3} (\vec{R} \cdot \vec{r}_2) + \frac{Q_3}{r_3^3} (\vec{R} \cdot \vec{r}_3) + \frac{Q_4}{r_4^3} (\vec{R} \cdot \vec{r}_4) \right\}$

and substituting the corresponding values of charges ( $Q_i$ ), the distances ( $r_i$ ) and the dot

products  $\vec{R} \cdot \vec{r}_i$ . One gets  $\varphi_d(\vec{R}) = \frac{1}{4\pi\epsilon_0} \left[ \frac{Q}{r^3} \{(-rx) - (-ry) + (rx) - (ry)\} \right]$  and

simplifying it gives,

$$\varphi_d(\vec{R}) = \frac{1}{4\pi\epsilon_0} \left[ \frac{Q}{r^3} (-rx + ry + rx - ry) \right]$$

$$\varphi_d(\vec{R}) = 0. \quad (B.3)$$

Here, the dipole term of the Paul trap is also zero.

The Quadrupole term

The electric quadrupole potential of the Paul trap from the Equation (B.1) is,

$$\varphi_q(\vec{R}) = \frac{1}{8\pi\epsilon_0} \sum_{i=1}^4 \frac{Q_i}{r_i^5} \{3(\vec{R} \cdot \vec{r}_i)^2 - R^2 r_i^2\}.$$

Now expand one gets,  $\varphi_q(\vec{R}) = \frac{1}{8\pi\epsilon_0} \left[ \frac{Q_1}{r_1^5} \{3(\vec{R} \cdot \vec{r}_1)^2 - R^2 r_1^2\} + \frac{Q_2}{r_2^5} \{3(\vec{R} \cdot \vec{r}_2)^2 - R^2 r_2^2\} + \right.$

$\left. \frac{Q_3}{r_3^5} \{3(\vec{R} \cdot \vec{r}_3)^2 - R^2 r_3^2\} + \frac{Q_4}{r_4^5} \{3(\vec{R} \cdot \vec{r}_4)^2 - R^2 r_4^2\} \right]$  and substituting the corresponding

values of charges ( $Q_i$ ), the distances ( $r_i$ ) and the dot products  $\vec{R} \cdot \vec{r}_i$ . One gets  $\varphi_q(\vec{R}) =$

$$\frac{1}{8\pi\epsilon_0} \left[ + \frac{Q}{r^5} \{3(-rx)^2 - R^2 r^2\} - \frac{Q}{r^5} \{3(-ry)^2 - R^2 r^2\} + \frac{Q}{r^5} \{3(rx)^2 - R^2 r^2\} - \right.$$

$\left. \frac{Q}{r^5} \{3(ry)^2 - R^2 r^2\} \right]$  and simplifying it gives

$$\varphi_q(\vec{R}) = \frac{1}{8\pi\epsilon_0} \left[ \frac{Q}{r^5} (3r^2 x^2 - R^2 r^2 - 3r^2 y^2 + R^2 r^2 + 3r^2 x^2 - R^2 r^2 - 3r^2 y^2 + R^2 r^2) \right],$$

$$\begin{aligned}\varphi_q(\vec{R}) &= \frac{1}{8\pi\epsilon_0} \left[ \frac{Q}{r^5} (6r^2x^2 - 6r^2y^2) \right], \\ \varphi_q(\vec{R}) &= \frac{1}{8\pi\epsilon_0} \left[ \frac{Q}{r^5} 6r^2(x^2 - y^2) \right], \\ \varphi_q(\vec{R}) &= \frac{3Q(x^2 - y^2)}{4\pi\epsilon_0 r^3}.\end{aligned}\tag{B.4}$$

Here, the quadrupole term of the Paul trap is not zero.

Now substituting the values of Equations (B.2, B.3 and B.4) in Equation (B.1) gives

$$\varphi(\vec{R}) = \varphi_q(\vec{R}) = \frac{3Q(x^2 - y^2)}{4\pi\epsilon_0 r^3}\tag{B.5}$$

Therefore, the electric potential of the Paul trap is the quadrupole potential which is given by Equation (B.5). The Paul trap uses radio frequency alternating current (AC), so the charge on Q changes with AC that is oscillating with frequency  $\Omega$ . Then Q turns out to be  $Q = Q_0 \cos(\Omega t)$  and the potential in the linear Paul trap as shown in Figure 12 becomes,

$$\varphi(\vec{R}, t) = \frac{3Q_0 \cos(\Omega t)(x^2 - y^2)}{4\pi\epsilon_0 r^3},\tag{B.6}$$

where  $Q_0$  = charge of the conductors,

$\Omega$  = radio frequency of AC,

$r$  = distance of the conductor from the center or radius of the Paul trap,

$\epsilon_0$  = permittivity of the free space,

$x$  = the point in space how far away from the center in  $x$ -axis,

$y$  = the point in space how far away from the center in  $y$ -axis.

The potential in Paul trap (Equation B.6) in terms of applied voltage ( $V_0$ ) is

$$\varphi(\vec{R}, t) = \frac{3V_0 \cos(\Omega t)(x^2 - y^2)}{r^2},\tag{B.7}$$

where,  $V_0 = \frac{3Q_0}{4\pi\epsilon_0 r}$ .



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