THE UNIVERSITY OF CALGARY

Ion Trapping at Low Density Limits

by

Amy Alice Fisher

A DISSERTATION

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF M.Sc.

DEPARTMENT OF PHYSICS AND ASTRONOMY

CALGARY, ALBERTA

November, 2001

© Amy Alice Fisher 2001

THE UNIVERSITY OF CALGARY FACULTY OF GRADUATE STUDIES

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance, a dissertation entitled "Ion Trapping at Low Density Limits" submitted by Amy Alice Fisher in partial fulfillment of the requirements for the degree of M.Sc..

Supervisor, Dr. Robert I. Thompson Department of Physics and Astronomy

NASSER 1AH

Dr. Nasser Moazzen-Ahmadi Department of Physics and Astronomy

Dr. Eric Donovan Department of Physics and Astron-

omy

Dr. David Cramb Department of Chemistry

December 12,200/

Date

Abstract

Being able to trap an individual ion (or collection of ions) with electromagnetic fields allows for the observation of not only its statistical behaviour, but for the observation of chemical and physical processes as they occur on the atomic scale. In our laboratory, we implement this idea with a linear geometry quadrupole ion trap that was originally designed and constructed by Mark Welling at the Max-Planck-Institut für Quantenoptik in Garching bei München, Germany.

While we have yet to resolve all of the problems with the incorporation of this ion trap system, we have established a large working portion of the system. Our system is comprised of five distinct parts: the vacuum system, the ion sources, the detection system, the resonant circuit (which controls voltage allocation to the trap) and the ion trap itself (further detailed in Chapter 3). We have obtained encouraging results from preliminary tests. These tests indicate that the vacuum system, the ion sources, the detection system (for low count rates), and the resonant circuit (for low and high trapping voltages) all function properly.

Acknowledgements

I would like to thank first and foremost five of the people who are most important to me. I would not be who I am without them and I would never have finished this project without their support. I love each of them dearly. They are my family:

Ralph Fisher, Louise Fisher, Aaron Fisher, Krista MacIver, and Simon Strasser People of strong mind and good heart.

I would also like to especially thank at this time Lanny Murdoch, our laboratory technician, for not only his technical support, but for his encouragement, patience and guidance. Without his help, this project would never have been completed so thank you Lanny!

I would also like to thank my supervisor Dr. Robert Thompson for his knowledge and guidance over the course of this project.

I would like to sincerely thank my committee members, Dr. Nasser Moazzen-Ahmadi and Dr. Eric Donovan, for their support and encouragement.

Thank you as well to those who provided invaluable technical support such as the entire staff of the Science Workshop, the Department Office Staff, Brian Jackal, Pat Irwin, and Peter King.

There are many other people who deserve recognition. A very special thank you to my friends Aaron Szott and Andrew Bretz for their ear, their kindness and their good sense of humour.

Finally, I would like to thank sincerely Dr. Robert Hawkes, my former supervisor at Mount Allison University, for his contagious love of learning and advice at a time when I was unsure about where I was going.

Table of Contents

-

Approv	val Page	ii
Abstra	let	iii
Acknow	wledgements	\mathbf{iv}
Table of	of Contents	\mathbf{v}
1 Intr 1.1 1.2 1.3 1.4 1.5	oduction In the Beginning Endohedral versus Exohedral structures Determining the Relationship between the Photodissociation Cross-section and Energy Laser Cooling Goals and Motivations	1 4 6 15 16
2 The 2.1 2.2	How do we trap a charged particle?	19 19 28
3 Ion 3.1 3.2 3.3 3.4	Trap Laboratory ManualThe Vacuum System3.1.1 Problems We Encountered3.1.2 SolutionsThe Ion Trap Apparatus3.2.1 Problems We Encountered3.2.2 Solutions3.2.2 SolutionsThe Resonant Circuit3.3.1 Problems We Encountered3.3.2 SolutionsThe Electron Multiplier Tube3.4.1 Problems We Encountered3.4.2 Solutions	34 34 37 38 41 46 47 48 50 51 57 58 58
4 Ana 4.1 4.2 4.3	Alysis and ResultsUltrahigh Vacuum Chamber OperationIon Source and Detector OperationResults of Trials at Various He Pressures	62 62 66 75

,

.

	4.4	Result	s of Preliminary Trapping Tests		77
		4.4.1	High RF Voltage Trials and Results		79
		4.4.2	Results of Diagnostic tests	• • •	84
5	Con	clusio	n		90
Bi	bliog	graphy			92
\mathbf{A}	The	wave-	mechanical nature of the Franck-Condon Principle		97
в	Secu	ular Fr	equency Determination		101
\mathbf{C}	\mathbf{Exp}	erime	ntal Apparatus Components	1	104
D	Blac	ck box	circuit diagrams illustrating all external connection	ons to	
\mathbf{th}	e ion	trap			109
\mathbf{E}	Lab	View	Programming		117
F	Pro	be De	cating Curves		122
\mathbf{G}	\mathbf{Det}	ermina	ation of the Ion Trap Resonant Frequency		124

•

.

-

List of Tables

٠

4.1	Power Supply voltages used on September 2, 2001 to generate trapping	•
	fields in the vacuum chamber.	81
4.2	Results of ion trap tests at high input rf voltage (please note that a	
	$V_{fnp-p} = 0.17$ corresponds to a trap electrode voltage of $\approx 2000V$,	
	$V_{fnp-p} = 0.19$ corresponds to a trap electrode voltage of $\approx 2500V$ and	
	$V_{fnp-p} = 0.21$ corresponds to a trap electrode voltage of $\approx 3000V$).	82
4.3	EMT background count tests	83
C.1	List of Equipment and a description of its usage	107

*

1

List of Figures

•

1.1	One of the first fullerenes to be identified - C_{60} [10]	3
1.2	Potential energy versus distance from the center of C_{60} for the inter- action pair: C_{60} and Mg^+ . This is a modified version of the diagram	
	shown in figure 4, page 80 in [20]. \ldots \ldots \ldots \ldots \ldots	6
1.3	Energy versus distance from the center of C_{60} for an endohedral com- plex with Mg^+ in its ground state. This is a modified version of the	
1.4	diagram shown in figure 4, page 80 in [20]	8
	plex with Mg^+ in its ground state. This is a modified version of the	0
1.5	diagram shown in figure 4, page 80 in [20]	9
	in [20]	10
1.6	Upper state dissociating wavefunction of Mg^+ for an endohedral com- plex. This is a modified figure of the diagram shown in figure 4, page	10
	80 in [20]	12
1.7	Theoretical curves for photodissociation cross-section versus energy for an endohedral (A) and exohedral complex (B). This diagram is	
1.8	based on that shown in figure 4, page 80 in [20]	13
	energy. The solid line is a gaussian fit to the data. This is a modified version of the diagram shown in figure 10 in [3]	14
2.1	A plot of $\phi(x, y)$ - a hyperbolic paraboloid. This plot was generated in Maple V	21
2.2	A plot summarizing the stability characteristics of the solutions to the Mathieu differential equations in terms of the parameters a and q. This plot is a modified version of figure 2, page 501 in [1] and figure	
	2 30a page 47 in [28]	24
2.3	A plot of half of the largest area of intersection in q-a space. This plot is a modified version of figure 3, page 501 in [1] and figure 2.30b.	
	page 47 in $[28]$.	25
2.4	Diagram of the shape of the potential along the z-axis for each of the three segments of the ion trap. This diagram was generated in	
	Microsoft Powerpoint 97.	27
2.5	Diagram of a simple mass spectrometric apparatus	29

3.1	Schematic diagram of the connections between the six way cross, vac- uum pumps, and sensors. This figure was generated in Microsoft	
	Powerpoint.	36
3.2	Schematic diagram of the buffer gas injection mechanism. This figure was generated in Microsoft Powerpoint.	37
3.3	Schematic diagram of the four rods comprising the ion trap. This figure was generated in Microsoft Powerpoint.	41
3.4	Artist's illustration of the ion trap located within the six way cross. This figure was generated in Microsoft Powerpoint.	42
3.5	Diagram showing the four locations for ion generation, namely the atomic ovens and their corresponding electron gun assemblies. This figure was generated in Microsoft Powerpoint.	43
3.6	Schematic diagram of the atomic oven and electron gun assembly with an enlarged diagram of the electron gun assembly. This figure was generated in Microsoft Powerpoint.	44
3.7	Schematic diagram of the Mg ion injection system. This figure was generated in Microsoft Powerpoint.	45
3.8	Diagram illustrating the two unconnected sides of the ion trap system. This figure was generated in Microsoft Powerpoint.	46
3.9	Circuit diagram of the resonant control circuit. This figure was gen- erated in Microsoft Powerpoint.	49
3.10	Block diagram of the rf trapping field power supplies and set-up. This figure was generated in Microsoft Powerpoint.	51
3.11	Graph of resonant frequency versus temperature of the tank capacitor. This figure was generated by data collected with Labview in Microsoft	51
3.12	Diagram of the resonant frequency of the ion trap/resonant circuit system. This figure was generated by data collected through a Tie-pie 2 channel handyscope interface package in Microsoft Excel	54 59
3.13	Diagram of the internal connections in an electron multiplier tube. This figure is a modified version of the figure on page 599 in [40].	60
3.14	Diagram of the external electron multiplier tube connections. This figure was made in Microsoft Powerpoint.	61
4.1	Logarithmic plot of the amount of time it takes for the vacuum cham- ber to be evacuated by the rotary pump to pressures on the order of 10^{-2} Torr. The logarithmic data has been fitted with an exponential curve. This figure was made in Origin, Version 6.0.	63

.

An enlarged region of graph 4.1 for the amount of time it takes for the vacuum chamber to be evacuated by the rotary pump to pressures on the order of 10^{-2} Torr. The logarithmic data has been fitted with an	
exponential curve. This figure was made in Origin, Version 6.0 Graph of the amount of time it takes for the vacuum chamber to be evacuated by a turbo molecular pump to pressures on the order of 10^{-7} Torr. The data has been fitted with an exponential curve. This	64
figure was made in Origin, Version 6.0	65
together (please note that the connecting line has been added to ald the eye only). This figure was made in Microsoft Excel	67
that the connecting line has been added to aid the eye only). This figure was made in Microsoft Excel	68
added to aid the eye only). This figure was made in Microsoft Excel. Semi-logarithmic plot showing the frequency of particle detection as a function of time for the C_{60} oven (operated at 1.3 A) source alone, the C_{60} electron gun (operated at 1.4 A) alone, and the when the C_{60} oven source and electron gun operate together after having flushed the chamber with He gas (please note that the connecting line has been	70
added to aid the eye only). This figure was made in Microsoft Excel. Semi-logarithmic plot showing the frequency of particle detection as a function of time for the Mg e-gun with He being injected into the chamber ≈ 60 s after the e-gun was first enabled. This figure was made in Microsoft Excel.	73 76
	An enlarged region of graph 4.1 for the amount of time it takes for the vacuum chamber to be evacuated by the rotary pump to pressures on the order of 10^{-2} Torr. The logarithmic data has been fitted with an exponential curve. This figure was made in Origin, Version 6.0 Graph of the amount of time it takes for the vacuum chamber to be evacuated by a turbo molecular pump to pressures on the order of 10^{-7} Torr. The data has been fitted with an exponential curve. This figure was made in Origin, Version 6.0

4.9	Semi-logarithmic plot showing the frequency of particle detection as a function of time for the Mg e-gun with He being injected into the chamber ≈ 60 s after the e-gun was first enabled and then evacuated from the chamber ≈ 60 s later (please note that the connecting line has been added to eid the evacuate). This forms was made in Microsoft	
4.10	Excel	77
	was made in Microsoft Excel.	78
4.11	Reflected voltage and forward voltage as functions of time for $V_{fnp-p} = 0.06V$. This figure was made in Microsoft Excel	86
4.12	Reflected voltage as a function of time for various low input amplifier rf voltages. This figure was made in Microsoft Excel.	88
4.13	Reflected voltage as a function of time after having been in operation for 15 minutes at $V_{fnp-p} = 0.06V$. This figure was made in Microsoft Excel	89
D.1	This figure shows the ion trap in block format along with the various electrical connections made to it. This figure was made in Microsoft	
D.2	Powerpoint	110
D.3	Block diagram of the dc power supplies used to bias the three trap	111
D.4	segments. This figure was made in Microsoft Powerpoint Block diagram of the rf trapping field power supplies. This figure was	112
D.5	made in Microsoft Powerpoint	113
D.6	Powerpoint	114
D.7	figure was made in Microsoft Powerpoint	115
	figure was made in Microsoft Powerpoint	116
E.1	This is a reproduction of the graphical interface window as seen by the user. This figure was generated by the National Instruments software, LabView	118
E.2	This is a reproduction of the labview code which interfaces and oper- ates the HP54600B digital oscilloscope. This figure was generated by	
	the National Instruments software, LabView	119

•

E.3	A list of all of the interface controls used in the program and their function. This figure was generated by the National Instruments software, LabView.	120
E.4	A list of the interface commands used that are specific to the HP54600B digital oscilloscope. This figure was generated by the National Instruments software, LabView.	121
F.1	Figure showing the high voltage probe derating curves. This figure was taken directly from [41]	122
F.2	Technical information on the tektronix oscilloscope probe used in our experiments as obtained from the P6013 User Manual. This figure was taken directly from [41].	123
G.1	Diagram of the resonant frequency of the ion trap/resonant circuit system. The scale of this figure is 1 cm : 0.405 MHz. This figure was created by the x-y plot function on the spectrum analyzer	125
G.2	Diagram of the resonant frequency of the ion trap/resonant circuit system. The scale of this figure is 1 cm : 1.61 MHz. This figure was	196
	created by the x-y plot function on the spectrum analyzer	120

.

Chapter 1

Introduction

"Until a few years ago all measurements were performed on an ensemble of particles. Therefore, the measured value - for example, the transition probability between two eigenstates of an atom - is a value averaged over many particles. Tacitly one assumes that all atoms show exactly the same statistical behaviour if one attributes the result to a single atom. On a trapped single atom, however, one can observe its interaction with a radiation field and its own statistical behaviour alone."

W. Paul [p. 497 [1]]¹

1.1 In the Beginning

The notion of ion trapping evolved from the fields of "molecular-beam physics, mass spectrometry, and particle accelerator physics" [1]. Two scientists, W. Paul and H. G. Dehmelt, were involved in its inception and subsequently awarded the Nobel Prize in 1989² for their research into the spatial isolation of charged particles.

Being able to trap an individual ion (or collection of ions) allows for the examination of not only its statistical behaviour, but for the observation of chemical and

¹from a slightly modified version of his Nobel winning lecture entitled "Electromagnetic Traps for Charged and Neutral Particles".

²In 1989 Paul and Dehmelt actually only received one half of the Nobel prize, each receiving a quarter. The other half of the Nobel prize was awarded to Norman Ramsey for "the invention of the separated oscillatory fields method and its use in the hydrogen maser and other atomic clocks" [2].

physical processes as they occur on the atomic scale. From these studies, fundamental characteristics of complexes, such as bond length, bond strength and ro-vibrational and electronic states, may be determined [3, 4, 5, 6].

In our laboratory, we hope to determine such characteristics for a variety of complexes with the use of a linear geometry quadrupole ion trap (see section 3.1) that was originally designed and constructed by Mark Welling at the Max-Planck-Institut für Quantenoptik in Garching bei München, Germany [6]. This apparatus has been used to explore and analyze the results of collision experiments between alkali metals and fullerene molecules [5]. In the future, we hope to not only perform new collision experiments with this apparatus, but observe various species, in particular simple fullerene complexes, at low temperatures via laser cooling techniques.

Fullerenes, defined as any carbon structure made up of pentagons and hexagons³ [7], were first identified in 1985 [8]. R. Smalley, H. Kroto, and R. Curl received the nobel Prize in Chemistry in 1996 for their discovery of the first fullerene, C_{60}^4 , a three dimensional cage comprised of 60 carbon atoms (figure 1.1) [9].

Fullerenes exhibit interesting properties. C_{60} , the most famous of the fullerene family, has been found to be a superconductor, to have potential biomedical applications, and can be readily transformed into other substances [11]. Fullerenes are also thought to be present in the interstellar medium (possible sources of some of the diffuse interstellar bands) [12, 13, 14].

More relevant to this work is the possibility of more complicated fullerene structures containing embedded atoms or molecules (e.g an atom locked inside a cage

³They were named after the architect of Montreal's geodesic dome Buckminister Fuller

 $^{{}^{4}}C_{60}$ is just one of the many fullerene molecules. It is sometimes referred to as the "buckyball".



Figure 1.1: One of the first fullerenes to be identified - C_{60} [10]

of carbon atoms). Molecules of this kind are not just important theoretically, but may have applications both biological (such as to explain transport of hormones and proteins throughout the body) and technological (for example in nanomachine development) [11]. As a result of the diversity of these molecules, research is being done to further our understanding of how they behave and interact with other chemical species.

1.2 Endohedral versus Exohedral structures

endo combining form inside; within; endocrine [from Greek endon within]

exo combining form external, outside or beyond: exobiology; exothermal. [from Greek $ex\bar{o}$ outside]

hedron n. *combining form* indicating a geometric solid having a specified number of faces or surfaces: *tetrahedron* [from Greek -*edron* sided, from *hedra* seat, base] - hedral *adj. combining form.*

The Collins English Dictionary [15]

The internal diameter of a C_{60} complex is ≈ 5.5 Å, just large enough to fit an atom or even a small molecule [16]. R. Smalley and his co-workers were the first to observe an endohedral structure (La (lanthanum) inside of C_{60}) [17] and since then many endohedral species have been synthesized (by building the carbon cage around an already existing metal atom) [18]. Fairly recently however endohedral complexes have also been formed through collision reactions [4].

Specifically in our laboratory, we hope to further the understanding of the following reaction:

$$Mg^+ + C_{60} \longrightarrow MgC_{60}^+$$

One of the questions we hope to answer is: through collision processes what is the ratio of exohedral to endohedral complexes formed (meaning, as a function of collision energy, how likely is it that the Mg ion bonds to the inside of the cage rather than to the outside of C_{60} ?

Using Ion Trap Mass Spectrometry, we can observe the formation of MgC_{60}^+ and determine how much has been formed within the trapping volume, however, this method of detection fails to provide information on the structure of the complex. The placement of the Mg ion with respect to the C_{60} molecule must be determined in order to ascertain the structure of MgC_{60}^+ . This can be done by analyzing the photodissociaton⁵ cross-section spectrum of complexes formed within the ion trap.

If the complex formed is exposed to laser radiation, it may become excited and as a result fragment or dissociate. The rate at which a molecule dissociates, R, is a function of the average light intensity incident on the complex, I_{ν} , the frequency of the laser, ν , and the photodissociation cross-section, σ , a quantity unique to each molecule [19]. Mathematically this is expressed as:

$$R = \frac{I_{\nu}}{\hbar\nu}\sigma$$

R, the rate of dissociation, can be determined experimentally by plotting the fraction of MgC_{60}^+ remaining as a function of laser exposure time [19]. From this result, the quantity of interest, σ (normally expressed in units of cm^2), may be calculated [19].

The relationship between photodissociation cross-section and the radiation frequency (or photon energy) of the laser beam is unique for each molecular structure. By comparing experimental results, obtained as described above, to those determined theoretically, one can discern the structure of the complex in question.

⁵photodissociation refers to how a given molecule breaks apart or fragments at a particular photon energy value (the energy for dissociation in this case coming from a laser source).

1.3 Determining the Relationship between the Photodissociation Cross-section and Energy



Figure 1.2: Potential energy versus distance from the center of C_{60} for the interaction pair: C_{60} and Mg^+ . This is a modified version of the diagram shown in figure 4, page 80 in [20].

Looking at the qualitative energy curve as a function of distance from the center of the molecule for C_{60} combined with Mg^+ (see figure 1.2)⁶, there is a large peak in energy ($\approx 10eV$) due to the carbon nuclei at $\approx 3.5 \text{\AA}$ [5]. This carbon cage creates a

⁶The potential energy curve shown in figure 1.2 is for Mg^+ AND C_{60} and that the potential energy curve changes with the interaction species. For example the potential energy curve for manganese and C_{60} is quite different in shape [4].

large potential barrier as the Mg ions are too large to get through the cage without breaking C-C bonds.

As the distance from the carbon nuclei increases, we see a second potential barrier much lower in energy. This activation barrier has been observed experimentally (Mg ions travelling with low thermal energies do not bond with C_{60} molecules to form new complexes), but has yet to be explained theoretically [3].⁷

Figure 1.3 illustrates a wavefunction for an endohedral complex, with the Mg ion inside the carbon cage. The qualitative energy curve versus distance from the center of the molecule shows the wavefunction representing the ground state of the Mg ion located inside the radius of the carbon nuclei⁸. The amount of energy therefore required to dissociate this molecule is quite large since C-C bonds must be broken to remove the internally located Mg ion. This is illustrated by the vertical transition arrow. This arrow must clear the top of the potential barrier in order for the Mg ion to reach a free particle state. In comparison to an exohedral structure, illustrated in figure 1.4, the wave function of the Mg ion is located between the potential barrier due to the carbon cage and the outermost barrier. The amount of energy required to dissociate this molecule is much smaller since the outermost potential barrier is smaller than the potential energy barrier to the carbon cage. This is represented by the vertical transition arrow.

Since the importance of photodissociation processes has been alluded to, we should consider what would happen if either the exohedral or endohedral structure

⁷This activation barrier is currently known to be unique only to collisions between Mg^+ and C_{60} . Manganese, a transition metal, for example will bond with C_{60} at thermal velocities to form $\operatorname{Mn} C_{60}^{+}$ [4].

⁸The shape of the ground state wavefunction of magnesium, or more generally any particle in its ground state in a potential well, can be approximated by a gaussian function [21].



Figure 1.3: Energy versus distance from the center of C_{60} for an endohedral complex with Mg^+ in its ground state. This is a modified version of the diagram shown in figure 4, page 80 in [20].

was excited out of their ground state by a laser source. Would the MgC_{60}^+ molecule break apart or exist in a new, stable, excited state? Does the outcome depend on whether its structure is exohedral or endohedral?

The answer to the latter question is yes.

Theoretically the relationship between photodissociation cross-section and energy (average photon energy of the laser beam) for a given molecule is determined by the Franck-Condon⁹ wavefunction overlap integral (= $\int \psi^*_{excited}(r)\psi_{ground}(r)d^3r$, please

⁹Franck and Condon developed the notion and wave mechanical model to describe the following



Figure 1.4: Energy versus distance from the center of C_{60} for an exohedral complex with Mg^+ in its ground state. This is a modified version of the diagram shown in figure 4, page 80 in [20].

see Appendix A). This is done by mathematically analyzing the probability of a dipole transition between the ground and any excited state of the MgC_{60}^+ complex. Figure 1.5 shows the upper state unbound wavefunction for the interaction pair C_{60}

principle: "the electron jump in a molecule takes place so rapidly in comparison to the vibrational motion that immediately afterwards the nuclei still have very nearly the same relative position and velocity as before the "jump"." (p.194 [22]) For example if in a diatomic molecule a given transition from one state, $\nu'' = 0$, to a second excited state, $\nu' = 1$, results in a substantial increase in the bond length between the two atoms, then the transition is less likely to happen (a substantial increase in bond length could result in large amplitude vibrational oscillations or even break the molecule apart). On the other hand, a transition that preserves the relative distance between the two nuclei would be much more probable.



Figure 1.5: Upper state unbound wavefunction of Mg^+ for an exohedral complex. This is a modified version of the diagram shown in figure 4, page 80 in [20].

and Mg^+ in the form of an exohedral molecule. Looking at how the C_{60} potential energy curve changes from the ground state to the excited state (please note that the excited state potential energy curve is not quantitatively known, but is here hypothesized), it is clear that in the ground state, the Mg ion is trapped in a small potential well between two barriers (exohedral structure). In order for the Mg ion to break free from C_{60} , it would need enough energy to climb over the outer barrier. In the excited C_{60} state however, there is no apparent potential well. From figure 1.5 it is clear that there is not a second potential barrier beyond the radius of the carbon cage. Therefore in the excited state, the Mg ion would have enough energy to escape or leave the C_{60} molecule and enter the continuum.

Also from figure 1.5, the vast majority of the Mg^+ wavefunction is concentrated at (or near) the boundary of the potential energy curve (or turning point) for C_{60} . The concentration of the upper state wavefunction near the turning point is a characteristic of "semi-free" particles.

Looking at the classical analogy, the potential energy curve of the excited state interaction between C_{60} and Mg^+ is higher than the potential energy curve of the ground state. Since the potential energy is high, the kinetic energy is low, and therefore Mg^+ is slow to leave this area. This is why the vast majority of the Mg^+ wavefunction is concentrated here, and it is in the excited state that one can think of the wavefunction of the Mg ion as behaving similarly to a delta function centered at the turning point. At the instant the Mg ion enters the excited state, it is free to go so to speak and thus is no longer bound to the molecule.

As a result of this transition, from the Mg ion being bound to the molecule (forming an exohedral structure) at one instant to it being released into the continuum at the next, the original ground state wavefunction of Mg^+ is effectively mirrored by the Franck-Condon overlap integral or translated directly from position space into energy space. This means that the photodissociation cross section should increase and then decrease smoothly (in the form of a gaussian since this is the shape of the ground state wave function) for exohedral complexes.

Figure 1.6 illustrates a transition to an upper state dissociating wavefunction of Mg^+ for an endohedral molecule. At low energies, the Mg ion remains trapped inside the C_{60} molecule. It is only when the activation barrier (due to the carbon cage itself



Figure 1.6: Upper state dissociating wavefunction of Mg^+ for an endohedral complex. This is a modified figure of the diagram shown in figure 4, page 80 in [20].

which is present in both the ground and excited states) is overcome that the Mg ion escapes to the continuum. This means that there should be a sharp increase in the photodissociation cross-section at this energy value. At higher energies, due to a decrease in the density of states, the photodissociation cross-section should gradually decline. Looking at the theoretical cross-section curves for an endohedral complex versus an exohedral complex as a function of energy (figure 1.7), the endohedral structure, as postulated, has a much sharper cut-off point at the dissociation energy (before this the molecule cannot break apart). This is because the energy required to



Figure 1.7: Theoretical curves for photodissociation cross-section versus energy for an endohedral (A) and exohedral complex (B). This diagram is based on that shown in figure 4, page 80 in [20].

remove a Mg ion from inside C_{60} is at least as great as the energy required to break a C-C bond (for example it takes $\approx 22eV/molecule$ to break apart a C_{58} molecule [4]). This dissociation energy is much larger than the energy required to break the bond¹⁰ between Mg^+ and a carbon atom located within C_{60} (C - Mn bond energy $\approx 2 - 3eV/molecule$ [4]). Intuitively, it seems reasonable that it is easier to remove an external object than an internal object. Using this logic then, if one could analyze

¹⁰it is not clear in the exohedral structure whether or not the bond that forms between C_{60} and Mg is a covalent bond or simply caused by van der Waal's forces (induced dipole).



Figure 1.8: Graph of the relationship between photodissociation cross section and energy. The solid line is a gaussian fit to the data. This is a modified version of the diagram shown in figure 10 in [3].

the photodissociation cross section of complexes formed within the ion trap, it would be possible to deduce whether or not these structures were endohedral or exohedral in nature.

Experiments in determining whether MgC_{60}^+ was endohedral or exohedral in structure were begun at the Max-Planck-Institut für Quantenoptik. Their results, for complexes formed at low collision energy, are shown in figure 1.8.

While these results are consistent with the predicted theoretical curve associated with exohedral complexes, only part of the energy spectrum has been explored to date, thus there remains significant work to be carried out on this system.

1.4 Laser Cooling

As mentioned very briefly in Section 1.1, we hope to determine fundamental characteristics of complexes, such as bond length, bond strength, ro-vibrational and electronic states, etc. Sections 1.2 and 1.3 detail the importance of photodissociation in determining the spatial structure of a given complex like MgC_{60}^+ , but also of interest is the energy spectrum such a molecule would absorb or produce. This would be another way to "fingerprint" or identify a chemical complex.

Molecular spectroscopy provides important information on the ro-vibrational and electronic states of a species, however, due to the nature of collision experiments, products are formed at relatively high temperatures¹¹. Since the gas present in the trapping volume is relatively hot and comprised of a number of different chemical

¹¹Ionic complexes formed in the trapping volume may be cooled to room temperature with the aid of a buffer gas. For example, if the ambient temperature of the Mg and C_{60} mixture is on the order of 300K, then the thermal velocity of a C_{60} molecule alone is on the order of 80m/s (from the relationship $\frac{1}{2}mv^2 \approx kT$).

complexes, the signal to noise ratio is very low for the various spectra.

Lowering the ambient temperature of the mixture [23] by one dimensional sympathetic laser cooling is a way to improve the signal to noise ratio¹². This process uses a gas made-up of two different species, the first component composed of atoms, and the second component of more complicated compounds comprised of two or more elements. By lowering the temperature of the first component through Doppler cooling¹³ [24, 25, 26], the ambient temperature of the entire gas decreases as the mixture comes to thermal equilibrium.

Inside the trapping volume we can produce a two component gas, and therefore, in principle, cool complicated molecules such as fullerenes. Through sympathetic cooling, we can learn more about the behaviour of molecules, by carrying out high resolution gas phase laser induced fluorescence spectroscopy. This would provide information on both their physical and quantum mechanical structure.

1.5 Goals and Motivations

First, we hope to generate an operational linear quadrupole ion trap by mating the ion trap apparatus obtained from the Max-Planck-Institut für Quantenoptik with new and existing equipment. While there are still unresolved problems in areas of its operation, we have established a large working portion of the system.

Our system is comprised of five distinct parts: the vacuum system, the ion sources, the detection system, the resonant circuit (which controls voltage alloca-

¹²Lower temperatures increase the amount of absorption at a specific wavelength in the gas.

¹³This type of cooling occurs as a result of a momentum transfer between a photon (with a frequency near an optical resonance point of the atom (or molecule)) and an atom (or molecule).

tion to the trap) and the ion trap itself (further detailed in Chapter 3). We have obtained encouraging results from preliminary tests. These tests indicate that the vacuum system, the ion sources, the detection system (for low count rates), the resonant circuit (for low and high trapping voltages), and the ion trap (for low trapping voltages) all function properly. This is further discussed in Chapters 3 and 4 respectively.

This apparatus will facilitate a number of interesting experiments. These include the following:

1) Collision Experiments

The relationship between photodissociation cross-section and energy, as described in section 1.3, was never fully explored at the Max-Planck-Institut für Quantenoptik. This was due to technological limitations in laser wavelength generation at the laboratory in Germany. Here at the University of Calgary, a pulsed laser system provides a much wider range of available wavelengths and as such, it is possible to explore the relationship between photodissociation cross-section and energy more completely. In addition, only complexes generated at low collision energy have been studied spectroscopically to date. Further laser studies of high energy species are of great interest.

To perform collision experiments with high mass particles, like fullerenes, relatively high rf-amplitudes (see chapter 2) are required. Collision experiments, however, can be completed quickly (2 -3 minutes), so stable trap operation is only required for relatively short time periods.

As such, we are not limited to work with Mg and C_{60} . For us, it is just a "place to start". There are many other collision reactions that would be both possible and interesting to observe.

2) Laser cooling experiments

The idea of performing laser cooling experiments is a rather recent motivation for some of the trials we have performed (this is further detailed in chapter 4). The opportunity to perform laser cooling experiments appeared due to the acquisition of a CW laser system which is currently being installed in our laboratory. This system should be on line by 2002. While this technique has never been attempted with this particular apparatus, we have high hopes that once our system is operational laser cooling will become a realistic research method for further exploration into the nature of MgC_{60}^+ as well as a whole range of other complexes.

The requirements for laser cooling experiments are quite different from collision reactions. For initial investigations of sympathetic laser cooling, less massive particles will be used and therefore we will require low trapping voltages for relatively long time periods $(\frac{1}{2} - 1 \text{ hour})$.

3) Combined collision and laser cooling experiments

To carry out collision and laser cooling experiments simultaneously, a combination of things would be required. Our system would need to be able to operate at high trapping voltages for relatively long periods of time. Once our system is fully operational (currently we are having problems maintaining a stable high trapping voltage, please see Chapter 3), it should be possible to perform experiments in which complexes are first formed through collision reactions and then cooled. If this works, the results could be very exciting as this technique would allow for the formation and determination of fundamental properties of new molecules!

Chapter 2

Theory: Ion Traps and Mass Spectrometry

2.1 How do we trap a charged particle?

Sometimes I lie awake at night, and I ask, "Where did I go wrong?" Then a voice says to me, "This is going to take more than one night."

Charlie Brown.

In 1989, Wolfgang Paul and Hans G. Dehmelt won the Nobel Prize for the development of the ion trap. Their research into spatial isolation of charged particles began in the 1950's and was so successful that ion traps are now made commercially for experimental work in biology, chemistry and physics.

The theory behind ion trapping is straightforward and elegant. Since an ion has charge, they wanted to use an electric field to trap the particle. As a consequence of Gauss' Law

$$\nabla\cdot\overrightarrow{E}=\nabla\cdot\left[-\nabla\phi\right]=\frac{1}{4\pi\varepsilon_{o}}\rho$$

the potential, ϕ , created by the electric field can have no local minimum (from the first derivative test). This meant that a time dependent potential would be necessary in order to generate a potential with an "apparent" minimum to the particle!

By discussing the simplest scenario, the trapping of a particle in two dimensions, they recognized then that in order to confine a charged particle within a plane, the particle needed to experience a restoring force, a force that would bring it back towards the center of the plane each time it wandered, of the mathematical form:

$$\overrightarrow{F} = -bx\hat{x} - cy\hat{y} \tag{2.1}$$

where x and y are the relative displacements of the particle with respect to the origin, and b and c are constants. A force of this form has a magnitude directly proportional to the distance the ion moves with respect to the origin [1] (assuming no electric potential variation along the z-axis). A potential can be found by integrating the desired expression for force (equation 2.1). This results in the following:

$$\phi = \frac{\phi_o}{2r_o^2} [\alpha x^2 + \beta y^2]$$

$$b = \frac{\phi_o}{r_o^2} \alpha$$

$$c = \frac{\phi_o}{r_o^2} \beta$$
(2.2)

Here ϕ represents the electric scalar potential. ϕ_o is a function of the magnitude of the a.c. and d.c voltage required to capture an ion (it determines the height of the sides of the function or in other words the trap depth), r_o represents the radius of the trapping area, and α , β constants yet to be specified.

The values of α and β are restricted by Gauss' Law. Gauss' Law in differential form is:

$$\nabla\cdot\overrightarrow{E}=\nabla\cdot\left[-\nabla\phi\right]=\frac{1}{4\pi\varepsilon_{o}}\rho$$

Since there is no charge density, ρ , anywhere within the plane until a charged particle enters the region, it can be concluded that

$$\nabla^2 \phi = 0 \tag{2.3}$$

This implies that

$$\alpha + \beta = 0$$

Looking at the simplest possible solution for equation 2.3, $\alpha = 1$ and $\beta = -1$, equation 2.2 for the potential function becomes

$$\phi = \frac{\phi_o}{2r_o^2} [x^2 - y^2] \tag{2.4}$$

A plot of $\phi(x, y)$ from equation 2.4 (figure 2.1) illustrates that ϕ is in the shape of a hyperbolic-paraboloid or saddle. This means that while the particle can oscillate side to side in the harmonic well along the x-axis, it can also escape due to the lower potential created by the inverted parabola along the y axis!



Figure 2.1: A plot of $\phi(x, y)$ - a hyperbolic paraboloid. This plot was generated in Maple V.

At first glance, this does not appear to be an effective way to confine an ion to a finite area in a given plane. As I mentioned earlier, the potential must be timedependent! If the saddle rotates faster than the particle can oscillate in any given direction, but not so fast as to introduce secondary undesired effects such as the generation of a magnetic field, then the time averaged electric potential effectively appears to be a "bowl like" structure to the particle. The particle in this structure would be at the bottom of the bowl, caught in a harmonic pseudopotential or well [1]. This rotation can be expressed as

$$\phi_o(t) = U + V \cos[\Omega t]$$

where U, V, and Ω are constants, and t is time.

To reiterate then, Paul developed a theory based on the notion that they could create a two dimensional potential well in which an ion would sit, trapped, with an electric field [1, 2]. This field is created by direct and alternating current potentials, the latter oscillating with frequency Ω .

In order to determine the physical values (i.e. the voltages needed, the appropriate angular frequency, etc.) we can analyze the forces acting on the particle in both the x and y directions:

$$\overrightarrow{F} = m\overrightarrow{a} = ze\overrightarrow{E} + ze\overrightarrow{v}\times\overrightarrow{B}$$

where the charge of the particle is ze. The electric field (and assuming $\vec{B} = 0$) can be determined from equation 2.4 and thus:

$$\overrightarrow{F} = m\overrightarrow{a} = ze(-\nabla\phi) = F_x\widetilde{x} + F_y\widetilde{y}$$

substituting in for ϕ and re-arranging:

$$\ddot{x} + \frac{ze}{mr_o^2} [U + V\cos[\Omega t]] x = 0$$
(2.5)

$$\ddot{y} - \frac{ze}{mr_o^2} [U + V\cos[\Omega t]] y = 0$$
(2.6)

These differential equations, known as Mathieu Differential Equations, have not to date been solved analytically¹ [27].

The equations (re-parameterized in terms of τ) appear in the following form:

$$\frac{\partial^2 x}{\partial \tau^2} + (a_x + 2q_x \cos[2\tau])x = 0 \tag{2.7}$$

$$\frac{\partial^2 y}{\partial \tau^2} - (a_y + 2q_y \cos[2\tau])y = 0 \tag{2.8}$$

where

$$-a_x = a_y = \frac{4zeU}{mr_o^2\Omega^2}$$
$$-q_x = q_y = \frac{2zeV}{mr_o^2\Omega^2}$$
$$\tau = \frac{\Omega t}{2}$$

These differential equations can be analyzed for solutions of the form $e^{\beta t}$. If, for given values of a and q, both of the allowed values of β are purely imaginary then the solution is oscillatory and bounded, and the solution is said to be stable. When β is real or complex then the solution tends towards infinity as t approaches infinity and the solutions are said to be unstable. This analysis must be carried out for the x-direction and for the y-direction.

As such, figure 2.2 indicates the results of this above analysis. It is important to note that there are regions where the solutions are stable in either the x or y direction alone and regions where these areas of stability overlap. To confine a particle to a

¹These equations were first studied in depth by a French mathematician named Mathieu. Mathieu, in the 1860's, was interested in trying to mathematically describe the vibrations of membranes and in his research numerically solved the above differential equations. They were subsequently named after him in his honour.



Figure 2.2: A plot summarizing the stability characteristics of the solutions to the Mathieu differential equations in terms of the parameters a and q. This plot is a modified version of figure 2, page 501 in [1] and figure 2.30a, page 47 in [28].

particular spatial area within the x-y plane, it is important that these regions of stability intersect.
The largest intersecting area (and thus the area generally chosen from which to determine the trapping parameters) occurs near the origin. This is shown in figure 2.3.

By setting the a coefficient to zero, a trap can operate solely on a specified q coefficient. From the diagram, noting that $|q| \leq 0.908$ for stable trapping, an appropriate value of q can be chosen and knowing the relative mass of the ion to be trapped, a corresponding a.c. voltage (V) and frequency value (Ω) can be calculated.



Figure 2.3: A plot of half of the largest area of intersection in q-a space. This plot is a modified version of figure 3, page 501 in [1] and figure 2.30b, page 47 in [28].

Also, from this q value, the frequency of the oscillatory motion of the particle (referred to as its "secular" motion) may be determined. Our charged particle, as you can imagine is not still. As a result of the trapping fields, it naturally oscillates inside the trap volume. The frequency of its motion is given by [5] (please see Appendix B):

$$\omega_{sec} = \frac{1}{\sqrt{8}}q\Omega \tag{2.9}$$

The depth of the trap (which is different for particles of different mass) is dependent upon the secular frequency of the particle² [5, 28]:

$$\Phi_o = \frac{1(2zeV)}{8(m\Omega^2 r_o^2)} V = \frac{ze}{8}qV$$
(2.10)

These two equations will become important when I discuss mass spectrometry.

These calculated quantities are the physical requirements for charged particles in the x-y plane. What happens to the particle as it travels along the z axis? In the laboratory we not only use a radio frequency (rf) field (to trap in the x-y plane), but several DC, non-quadrupolar fields (to manipulate the particle along the z-axis).

At this point, it is important to mention that the ion trap in our laboratory is a linear quadrupole trap segmented into three sections (details in section 4.2). By biasing each of these three segments differently, with a particular (non-quadrupole) d.c. voltage, a wall is effectively created (and therefore a potential well) along the z-axis over which the particle cannot "climb" [6]. This is more clearly illustrated in figure 2.4.

²This expression is determined when the force derived from the secular frequency (which is the time averaged analytical expression for the acceleration of the secular motion) is integrated between the limits [0, r_o] [28]. This assumes that the micromotion of the particles is much smaller than the macromotion.



Figure 2.4: Diagram of the shape of the potential along the z-axis for each of the three segments of the ion trap. This diagram was generated in Microsoft Powerpoint 97.

It is also important to note that there are many different types of trapping systems available 34 ⁵[29, 30, 31], but for our purposes the linear geometry ion trap I have described above, gives the ability to trap more atoms and allows more easily for the manipulation of ions inside the trap. This is required for collision experiments.

 $^{^{3}}http://entropy.davidson.edu/Projects/SuFischer/node11.html$

⁴http://www.chem.purdue.edu/cooks/trap/text/cross.html

⁵http://www.weizmann.ac.il/physics/molecule/ring.html

2.2 How do we determine what is in the trap? (Mass Spectrometry)

To see a World in a Grain of Sand And a Heaven in a Wild Flower, Hold Infinity in the palm of your hand And Eternity in an hour.

William Blake [32]⁶

The theory of mass spectrometry⁷, that different ionic species can be distinguished from one another on the basis of their charge to mass ratio (m/ze), was developed in the early 20th Century by J.J. Thomson [33]. This was done by injecting charged particles of fixed kinetic energy into a region containing a magnetic field of strength, B. If the particles have an initial velocity perpendicular to the region containing the applied magnetic field, they experience a force of the form:

$$\overrightarrow{F} = ze\overrightarrow{v} \times \overrightarrow{B}$$

This force causes the ion to experience a centripetal acceleration and as a result to undergo circular motion. This can be classically expressed by the following:

$$\overrightarrow{F} = z e \overrightarrow{v} \times \overrightarrow{B} = \frac{m v^2}{r} \hat{r}$$

⁶from Auguries of Innocence, 1803

⁷Spectrometry versus Spectroscopy: Spectrometry is the study of continuous spectra and is often associated with certain specific instrumentation whereas spectroscopy is the study of a localized part of a given spectra. This localized segment may be continuous over the interval of interest, but does not cover the complete spectral range (be it range of masses, wavelengths, etc.) possible for the source.

This means that r (the radius of curvature of the particle's path) is dependent upon the charge to mass ratio of the ion.

$$r = \frac{mv}{zeB}$$

By placing a phosphorous detector ninety degrees to the line of injection, an image of the projected ions can be obtained (please see figure 2.5). Charged particles with different charge to mass ratios will travel in circular orbits of different radii. By measuring these differences in displacement, the types of charged species present in the original sample may be determined [33].



Figure 2.5: Diagram of a simple mass spectrometric apparatus

The trapping system in our laboratory requires a different method of mass spectrometry, however, the basic principle of "fingerprinting" species through differences in charge to mass ratio (m/ze) remains the same.

A linear quadrupole trap uses r.f. (radio frequency) fields to confine a charged particle to a given region within the x-y plane. The design implemented in our laboratory applies three separate d.c. fields, one on each of three segments along the length of the trap, to control particle propagation along the z direction. By varying one (or more) of the trapping field parameters (and/or the addition of extra excitation fields), selection and expulsion from the trap of charged particles of a given mass (or of a range of masses) can be controlled. This is easily done as the trapping parameters are mass dependent. Once outside of the trapping volume, they are collected by a detector, an Electron Multiplier Tube with a negatively biased front cathode (see Section 4.4) thus producing a mass spectrum of the trap contents.

How do we select which masses are to be removed from the trap? The answer lies in the Mathieu differential equations (equations 2.6 and 2.7, Chapter 2.1). Massselection can be accomplished by three different methods [5]:

1. Unstable Regions of q-a space

As mentioned previously, the trap operates in the stability region a = 0 and $0.908 \ge |q| = \frac{2zeV}{mr_o^2 \Omega^2}$ (figure 2.3). This means that (by re-arranging):

$$\frac{m}{ze} < 2.203 \frac{V}{r_o^2 \Omega^2} \tag{2.11}$$

describes all masses expelled from the trapping region [5]. By either slowly increasing V or decreasing Ω , it is possible to scan through the range of masses present in the trapping region. This technique is used predominantly to set a lower limit on the masses present in the trapping region since there are other more common methods that produce higher resolution and/or a more complete mass spectra of the trapped

species.

2. Q-Scanning (A Perturbing Electric field)

Instead of slowly increasing V, consider what would happen if the trapping field amplitude was decreased. From figure 2.3, as we decrease q (a = 0), the masses within the trapping volume remain stable and trapped. It is also clear from the following equations:

$$0.908 \ge |q| = \frac{2zeV}{mr_o^2\Omega^2}$$

$$\frac{F}{m} = \ddot{x} + \frac{ze}{mr_o^2} [U + V\cos[\Omega t]] x = \frac{\partial^2 x}{\partial \tau^2} + (a_x + 2q_x)\cos[\Omega \tau] x$$

and equation 2.10, for the trap depth,

$$\Phi_o = \frac{ze}{8}qV = \frac{1(2zeV)}{\sqrt{8}(m\Omega^2 r_o^2)}V$$

that both Φ_o and q are functions of V. Therefore, as V changes so do $\Phi_o(V)$ and q(V). As V becomes smaller, the depth of the trap becomes smaller. As a result the force produced by the trapping field also decreases. It is important to note that different masses have different well depths as implied by the above equations.

Now introduce into the system an electrostatic field perpendicular to the z axis. This field is naturally produced in the system by the detector, an electron multiplier tube (Section 3.4), which has a negatively biased front cathode. This applied external electric field also produces a force that acts on the particles within the trap. As you can imagine, this force causes some sort of perturbation within the trapping volume. If this new applied field produces a force that exceeds the force produced by the trapping field on a particular mass, those particles of mass m will be effectively pulled from the trap by the detector into the detector. Theoretically, the presence of this applied electric field adds a great deal of complexity to the model presented in Chapter 2.1. We can, however, from a first order approximation, get an expression for the lower limit of masses expelled from the trap by [5]:

$$\frac{m}{ze} > \frac{0.5V^2}{\epsilon r_o^3 \Omega^2} \tag{2.12}$$

where ϵ represents the electric field strength created by the electron multiplier tube⁸.

By slowly reducing the amplitude of the trapping field, it is possible to scan through all of the masses present within the trapping volume. This technique is used most commonly because of our system design which allows for easy access to an electric field (Electron Multiplier Tube). This technique as such allows for quick and easy observation of a wide range of masses, however, it has poor resolution due to ion height in the well⁹.

3. Secular Scanning

This third, and final method, allows for the examination of a small portion of the masses present within the trapping volume in detail. Instead of altering the parameters of the trapping field, this technique manipulates the classical motion of our charged particle within the harmonic pseudopotential.

As you can imagine, our ion, sitting in the well generated by the trapping fields, is not stationary. It in fact oscillates and this oscillatory movement is called its

⁸This equation is determined by approximating when the time averaged force (from the rf field) is less then the force produced by the EMT's electric field [5].

⁹Ions of different mass have different trap depths as is implied by the equation $\Phi_o = \frac{1(2zeV)}{8(m\Omega^2 r_o^2)}V$. By lowering the amplitude of the trapping fields, many ions are released at once. Since the electric field strength of the EMT is fixed, we pull out the range of masses that are clustered in those energy levels accessible to the force produced by the EMT. As such, ions of different masses may be caught by the EMT. Since the EMT amplifies charge (see Section 4.4), no mass information is conveyed to the experimenter. This is why this technique has in general poor resolution.

"secular" motion as was alluded to in Section 2.1.

The frequency of this motion is dependent upon the mass of the particle and the parameters of the trapping field. It is mathematically, as in equation 2.9, expressed by the following [28]:

$$\omega_{sec} = \frac{1}{\sqrt{8}} q\Omega = \frac{zeV}{\sqrt{2}mr_o^2\Omega}$$
(2.13)

By applying to the trap a second oscillatory quadrupole field of frequency ω_{quad} , we can excite the secular motion of the ions. Using the theory of parametric excitation, this applied quadrupole field will excite masses oscillating at one half the applied frequency:

$$\omega_{sec} = rac{1}{2} \omega_{quad}$$

Therefore, from equation 2.13, we can solve for the expelled masses:

$$\frac{m}{ze} = \sqrt{2} \frac{V}{\omega_{guad} r_o^2 \Omega} \tag{2.14}$$

This result implies that high resolution spectra can be taken by slowly scanning through $2\omega_{sec}$ while simultaneously collecting the escaping ions in our detector¹⁰. This technique provides extremely high resolution, however, only a limited mass range may be explored in a finite time span.

¹⁰Here ω_{quad} is the applied frequency while ω_{sec} is the oscillatory frequency of a particular ion.

Chapter 3

Ion Trap Laboratory Manual

Do Not Meddle In The Affairs Of Dragons, For You Are Crunchy And Taste Good With Ketchup.

from Jokes and Quotes [34]

I have decided to present this section in a somewhat unorthodox manner. Since the vast majority of the work done this past year revolves around the laboratory and its equipment, I felt that it would be useful to write about some of the specific problems we have encountered and our solutions. I have done this in the hopes that a student may be able to use this chapter as a reference guide when working on this apparatus.

A comprehensive list of the equipment used in conjunction with the ion trap system may be found in Appendix C. Block diagrams of the system's electrical connections may be found in Appendix D.

3.1 The Vacuum System

In order to study charged atoms and molecules on the atomic scale, one must first establish a reasonably good vacuum on the order of $10^{-5} - 10^{-12}$ Torr. These pressures are obtained in this system with three different vacuum pumps and two pressure sensors.

A roughing pump (a rotary compression mechanical pump with oil lubricated bearings) is used to achieve pressures on the order of 10^{-2} Torr. A second pump is then used with the roughing pump. This pump, called a turbo molecular pump, is a non-compressing mechanical pump with air cushioned bearings, similar to a small turbo fan jet engine! In comparison to a roughing pump, turbo molecular pumps are cleaner as fewer organic materials can back flow into and contaminate the vacuum chamber. As a result, the residual gas in the vacuum chamber consists of small, mainly inert atoms and diatomic molecules rather than large organic molecules. This is what is known as a clean vacuum. Turbo molecular pumps achieve pressures on the order of 10^{-9} Torr.

In order to work at ultra high vacuum (pressures on the order of 10^{-11} Torr), an ion getter pump is used. This pump generates electrons which are accelerated through a potential into a small chamber inside the pump near the junction between the vacuum chamber and the pump. Once inside this chamber, these electrons collide with in-falling atoms to form positive ions¹. These ions are then drawn back to and crash into the cathode, usually made of titanium (Ti), where they are chemically altered and stored. As these ions collide with the cathode, Ti ions are driven off the surface of the electrode. These Ti ions can also react with and trap neutrals inside the pump.

All pumps are attached to the chamber (a six way cross with 8'' connecting flanges) via an 8'' tee and sealed with copper gaskets (please see figure 3.1).

Not all experiments are performed at ultra high vacuum. In fact there are many

¹Electrons not involved in collisions with neutral atoms collide with and are absorbed by the surface of the ion getter pump.



Figure 3.1: Schematic diagram of the connections between the six way cross, vacuum pumps, and sensors. This figure was generated in Microsoft Powerpoint.

cases where a chemically inert gas such as xenon, argon or helium, is injected into the vacuum chamber to act as a buffer or as a cooling agent to increase loading efficiency for high velocity ions. Typical pressures for such experiments may range from 10^{-5} to 10^{-7} Torr. A buffer gas can be injected into our chamber via a valve located between the roughing and turbo molecular pump (please see figure 3.2). This gas then backflows through the turbo molecular pump into the chamber².

²While this may seem like a strange way to inject He into the vacuum chamber, it is actually quite safe and efficient. Turbo molecular pumps in general work well with heavier particles. He is an extremely light and small atom, therefore it does not interfere with the turbo molecular pump's function at all.



Figure 3.2: Schematic diagram of the buffer gas injection mechanism. This figure was generated in Microsoft Powerpoint.

The pressure in the chamber is monitored by a Pressure Gauge Controller³. This unit processes signals received from a thermocouple gauge (pressure range $10 - 10^{-3}$ Torr) and ionization gauge (pressure range $10^{-4} - 10^{-10}$ Torr) respectively.

3.1.1 Problems We Encountered

With regards to the vacuum system, there was one distinct issue that had to be resolved:

1. after first turning on either the roughing pump or the turbo molecular pump, there was no apparent decrease in pressure.

There were three causes for this problem:

a) the system was not closed due to a leak

³this unit is a Sentorr Gauge Controller purchased commercially from Varian Vacuum products.

b) the thermocouple gauge was not calibrated properly

c) the transition pressure (the point at which the thermocouple gauge turns off and the ionization gauge turns on) was lower than the minimum pressure capability of the thermocouple gauge

3.1.2 Solutions

a) Leak Detection - how to determine where air may be entering the system?

If the pressure in the chamber is not decreasing, it is likely that there is a leak somewhere in the system. A leak is most likely caused by an improper seal due to the misplacement of either a copper gasket or an o-ring in a metal/metal joint. It could be either very small or very large in size.

First, we determined whether or not there was any sort of audible leak (hissing sound).⁴ If the leak is not audible, a leak detector of some sort must be used⁵.

One type of leak detector is called a sniffer. It is used for fairly large leaks (pressures on the order of $10^{-2} - 10^{-5}$ Torr). The sniffer is sensitive to the thermal conductivity of various gases such as helium, nitrogen, sulphur dioxide, ammonia, etc. When it detects higher concentration levels than the background concentration of a particular gas (by comparing the thermal conductivity of the gas to that of air), a series of light emitting diodes light up with the number of illuminated diodes

⁴If you can not hear anything out of the ordinary, listen to the roughing pump. Does the pump sound as though it is working harder than usual? This may indicate a leak of substantial size.

⁵Never use abrasive chemicals such as methanol or acetone to determine if a joint is sealed properly. It is common practice to spray a chemical on a joint to see whether or not there is an increase in the overall pressure in the chamber. If the pressure increases after chemical exposure, this indicates that the joint in question had not been properly sealed and was the source of contamination. While this is a quick way to check for large leaks, chemicals (more specifically alcohols) cause the degradation of o-rings and metal gaskets. Joint exposure to such substances actually creates leaks overtime and should therefore be avoided [35]!

proportional to the concentration difference.

By over-pressuring the chamber (via a valve) with He, we can detect the presence of a leak. Typically, we use He in our laboratory because it is light in weight, inert, and inexpensive. Conveniently, He is also the gas for which the sniffer is most sensitive. By starting at the lowest joint in the chamber, we slowly move the needle sensor around the joint. It is important not to start at the topmost joint because He rises and therefore a leak at a lower joint may appear as a leak in an upper joint, thus masking the true source.

For leaks of smaller size, a high precision leak detector may be necessary. This black box device is composed of a turbo molecular pump, a rotary pump, and a sensitive He sensor (effectively a small mass spectrometer). This type of detector is far more invasive than the sniffer apparatus. It is attached directly into the system and evacuates the chamber itself. By slowly spraying He (via a needle nose hose attached to a small portable canister of He) around each joint, one can determine which joint is leaking based on concentration measurements made by the detector in the chamber [35].

b) The pressure may not change due to a calibration error of the thermocouple gauge.

On several occasions, we were confident that our system was sealed (due to the stability of the vacuum chamber pressure) and that no air was leaking into the chamber from the outside environment. This lead us to conclude that something was wrong with our actual pressure sensor.

It is important to note that thermocouple gauges have a safe operating pressure range. Our thermocouple gauge, for example, is only capable of determining pressure values less than 2 Torr [36]. When this maximum pressure level is exceeded, the gauge gives unreliable readings and may also need to undergo re-calibration. As such, it is important to make sure that the gauge controller is turned **off** before opening your chamber to atmospheric pressure.

Calibration requires a second vacuum chamber with known internal pressure. By comparing the reading on the gauge controller to the known pressure in this second system, you can calibrate your thermocouple gauge by following the instructions provided in the Sentorr Gauge Controller Instruction Manual [37].

c) Another source of difficulty we encountered when trying to determine the pressure of the system was activation of the ionization gauge.

Ionization gauges are used to measure very low pressures (on the order of $10^{-4} - 10^{-10}$ Torr). The Sentorr gauge controller determines, based on pressure readings supplied by the thermocouple gauge, whether or not the ionization gauge should be turned on. As such, there are two things to be careful of:

i) Is the thermocouple gauge calibrated properly?

•

ii) At what pressure will the controller actually turn the ionization gauge on? If the turning point is at a pressure lower than the minimum pressure sensitivity of the thermocouple gauge, then the controller will never switch the ionization gauge on. Similarly, if the pressure is to high, the ionization gauge or even the thermocouple gauge may be damaged [38]. Specifications and calibration techniques are listed and detailed in the Sentorr Gauge Controller Manual [37].

3.2 The Ion Trap Apparatus

The trapping system present in our laboratory was originally built by Mark Welling at the Max-Planck-Institut für Quantenoptik in Garching bei München, Germany [6]. It is a linear quadrupole trap composed of four stainless steel rods segmented into three electrically isolated sections. Each rod is separated by a distance of 2.0mm from each adjacent rod forming a rectangular box 2.0mm x 2.0mm x 150.2mm (please see figure 3.3).



Figure 3.3: Schematic diagram of the four rods comprising the ion trap. This figure was generated in Microsoft Powerpoint.

The ion trap apparatus is mounted on two 8" flanges. These flanges are mounted in a six-way cross (please see figure 3.4). All electrical connections (i.e. to ovens, trapping fields, electron guns, etc.) are made through ceramic insulated vacuum feedthroughs located in smaller $2\frac{3}{4}$ " flanges mounted on each 8" flange.



Figure 3.4: Artist's illustration of the ion trap located within the six way cross. This figure was generated in Microsoft Powerpoint.

Ions can be loaded into the trapping volume at four different locations as illustrated in figure 3.5. In each case, neutral atoms (or molecules) are first created by running a high current ($\approx 1.2 - 1.6A$) through a stainless steel wire wrapped around a small capillary tube made of tungsten (W). Each capillary tube is open at one end (where material can be loaded) and pinched off at the other. This is referred to as an "atomic oven". As the current in the wire heats the W tube, the material inside also becomes hot. Pressure builds inside the oven as the substance vaporizes and forms a gas. As a result of this increase in pressure, the newly formed gas is expelled from the tube into the trapping region.

This neutral atomic gas is then bombarded by electrons forming ions. The electrons are generated and collimated into a beam by an electron gun located at an



Figure 3.5: Diagram showing the four locations for ion generation, namely the atomic ovens and their corresponding electron gun assemblies. This figure was generated in Microsoft Powerpoint.

angle of 90 degrees to the atomic oven in each case (please see figure 3.6).

The electron gun is comprised of a tungsten-iridium filament mounted in a ceramic flange at one end of a stainless steel cylinder (known as a Wehnelt cylinder). The other end of the cylinder has a small hole located along the central axis. A high current is run through the filament ($\approx 1.6A$) to generate electrons. By biasing the filament with a negative dc voltage ($\approx 90 - 250V$) and grounding the outside cylinder, the electrons are driven down the central axis of the cylinder and out the opening at the opposite end. Once outside the Wehnelt cylinder, the fast-moving electrons are free to collide with neutral atoms thus forming ions!

In three of the four cases, the electron gun is mounted such that the electron beam collides with free floating atoms in the actual trapping volume thus forming



Figure 3.6: Schematic diagram of the atomic oven and electron gun assembly with an enlarged diagram of the electron gun assembly. This figure was generated in Microsoft Powerpoint.

ions within the trap itself. On the left hand side of the trap, the injection system is slightly different.

In this case both the atomic oven and electron gun are positioned outside the trapping volume. The atomic and electron beams crisscross outside of the trap, but along the trap axis (please see figure 3.7). Two electrodes, one curved and one circular/flat, focus and drive the newly formed ions into the trapping volume.

The curved electrode is mounted directly behind the atomic oven, between the electron gun and oven. Its vertex is aligned with the trap center (along the z-axis). Directly in front of the four rods (that comprise the trap), is a flat circular electrode which has at its center a small hole also aligned with the trap center. Ions are generated in the region between the curved electrode and the flat circular electrode.



Figure 3.7: Schematic diagram of the Mg ion injection system. This figure was generated in Microsoft Powerpoint.

By grounding the curved electrode (effectively biasing it positively) and biasing the flat circular electrode slightly negatively, any positive ions generated will be repelled away from the curved electrode and attracted towards the circular plate. These ions are then injected into the trap along its axis via the small hole in the circular plate.

This type of injection system helps to collimate the ion beam entering the trapping region. This is important for two reasons. Firstly this system injects ions with high efficiency and secondly, when doing collision experiments, it helps to eliminate velocity components in the x and y directions and control the z-component velocity spread.

3.2.1 Problems We Encountered

The ion trap system is extremely fragile. It is also divided into two distinct physical entities: the Mg^+ source injection system and the C_{60} source/ion trap (please see figure 3.8). This design makes the physical mounting of the ion trap and the removal



Figure 3.8: Diagram illustrating the two unconnected sides of the ion trap system. This figure was generated in Microsoft Powerpoint.

of the ion trap from the chamber precarious. We have found that:

a) filaments are easily broken (for example, when loading an atomic oven, repositioning the oven, etc.)

- b) wires easily shift creating electrical short circuits
- c) wires are easily broken (in particular on the flange with the Mg^+ source)

3.2.2 Solutions

These problems will always be encountered when working with this system. In order to minimize the amount of time your system is exposed to atmospheric gases⁶, it is important to check all connections with an ohm-meter to ensure that no short circuits have developed with movement of the apparatus.

It is also important to do a visual inspection of the system both after the ion trap has been removed from the chamber and before it is replaced in the six way cross. With regards to the visual inspection, check to see if any wires are touching (or are in danger of touching), broken, whether or not a joint is well attached (do any connections appear poor or in danger of breaking), is there enough material in either or both ovens, etc.

If wires did need to be repaired, we found that spot welding was most effectively done on low current settings with medium amplitude pulses. When repairing broken wires, we found that it was also easier in many cases to spot weld two wires to a small piece of flat metal (stainless steel shim grade 0.005") rather than trying to spot weld two rounded wires (cylinders) together. It is also easier to observe the quality of the connection made between the wire and the metal strip.

Thin pieces of ceramic tubing are also used extensively inside the vacuum chamber to isolate wires not only from each other, but from ground (the chamber itself is grounded). It is important to ensure that all ceramic insulators are correctly positioned. We found that in many cases it was a shifted ceramic insulator that had

⁶Atmospheric gases contaminate the chamber on the atomic scale, metals tend to act like sponges, absorbing gas at high pressures. At low pressures this gas is re-emitted. This results in a long pump down time, meaning that it takes much longer for the system to achieve ultra high vacuum. Ultra high vacuum is extremely important if one is to experiment on and observe changes that occur on the atomic scale.

caused a wire to short to ground, rendering parts of our system inoperable.

Also, it is extremely useful to have several extra parts available in case of an accident with either a flange or with a vacuum feedthrough connection. Vacuum feedthroughs are especially susceptible to damage because of the ceramic insulation (they can be easily cracked or broken!). Different companies have various shipping times which is strongly influenced by the availability of the part in question. If you need to replace one part in the system, it is an extremely good idea to order another immediately so that one is always on hand.

3.3 The Resonant Circuit

In order to trap an ion in the x-y plane (as described in Chapter 2.1) an angular frequency and a.c. voltage must be chosen in accordance with the equation:

$$q = \frac{2zeV}{mr_0^2\Omega^2}$$

where $q \leq 0.908$. The magnitude of the voltage applied to the quadrupole trap electrodes is normally on the order of 500 to 3000V with an angular frequency of 6 to 12 MHz. These values of course vary according to the mass and charge of the ionic species desired to be trapped, as well as the desired trap depth, Φ_o (from equation 2.10).

Along the z-axis, three separate d.c. voltages are applied to each of the three segments. These differences in potential allow the experimenter to control particle motion in the z direction. Typically, the left most segment (please see figure 3.3) is biased, relative to ground, with anywhere from -10 to -15 V, the center segment from -20 to -120 V, the right most segment from -15 to -110 V, and the C_{60} oven from

+60 to +200 V. We positively bias the C_{60} oven as well to ensure that high velocity ions cannot escape out of the trap at that end (by biasing it with a large positive d.c. potential relative to ground, we create a large potential barrier along the C_{60} end of the trapping volume). How does one apply these voltages to the trap? The



Figure 3.9: Circuit diagram of the resonant control circuit. This figure was generated in Microsoft Powerpoint.

resonant circuit (figure 3.9) allocates to each trap segment the appropriate a.c. and d.c. voltage required to confine an ion.

This circuit is a variation on the basic RLC circuit. The main inductor (12 turns) is an auto transformer which amplifies the input signal, from a function generator

coupled to a radio frequency amplifier, 36 times (ground to the input is $\approx \frac{1}{3}$ of a turn with the trap electrodes connected across the full 12 turns). This signal then travels to each branch.

Capacitors are placed in series with each of the three segments. Using a biological analogy, these capacitors serve as semi-transparent membranes. They allow a.c. current to travel through to each of the three segments, but do not allow the individual d.c. voltage applied across each trap component to bias the other two segments.

Capacitors are also used to help eliminate noise from ground and in the case of the center segment, help to protect power supplies from a.c feedback (low pass filters that eliminate signals with frequency larger than ≈ 7 MHz).

3.3.1 Problems We Encountered

I cannot begin to describe the problems we have encountered with this circuit. Fortunately, we have resolved many of these difficulties in the past month.

First, it is very important to understand that this circuit is **extremely** sensitive to noise, temperature change, input frequency, stray capacitance (for example in cables), etc. As such, it is very difficult to measure the actual input voltage to the trap electrodes or determine the resonant frequency of the system.

Due to the circuit's extreme sensitivity, one of the other challenges has been impedance matching. The commercial amplifier we purchased will only operate if it detects a fifty ohm load.

3.3.2 Solutions

The first thing we wanted to do was to supply low power, and therefore low voltage, to the ion trap. We hoped to better characterize the behaviour of the resonant circuit box and the ion trap safely in this manner. This meant that the amplifier and the resonant circuit/ion trap needed to be impedance matched.



look like 50 ohms)

Figure 3.10: Block diagram of the rf trapping field power supplies and set-up. This figure was generated in Microsoft Powerpoint.

Since the circuit is composed of inductors and capacitors, sources of complex impedance, we placed two variable capacitors and a variable inductor in a pi configuration in series with our resonant circuit [39] (please see figure 3.10). By varying the capacitance and inductance values we hoped to match or make our resonant circuit appear as though it were a 50 Ω load. We monitored and analyzed both its impedance and resonant frequency with the aid of a black box SWR analyzer. This seemed to work fairly well at low input voltages.

The voltage amplification across the primary inductor was determined roughly by placing two cladding wires (inner wire and insulator of a coax RG59 cable) a small fixed distance from either end of the inductor. At low voltage values, we used high voltage probes (\div 1000) to physically measure the voltage across the inductor (taking into account the probes de-rating curves (please see appendix E)) and compared this value to the voltage induced in the two wires.

With this system, we managed to determine the voltage across the inductor as being $\approx 2000V$ for an input voltage (V_{fnp-p}) to the amplifier of $\approx 0.17V$. While this was relatively successful, we experienced problems in maintaining the high voltage needed across the primary inductor (the autotransformer located in the driving tank circuit of the resonant circuit) in order to trap ions. One reason for this appeared to be a poor connection in a homebuilt capacitor (comprised of two parallel cylindrical capacitors made of copper with a polyvinyl chloride dielectric) located in parallel to the primary inductor. This capacitor was clearly shorting between its outer and inner plates (we could see visible arcing). We initially replaced this capacitor with ceramic capacitors rated at 5 kV.

After re-testing our circuit, we found we could achieve stable⁷ voltage values across the primary inductor on the order of $\approx 2500V$ for an input voltage to the

⁷By stable I mean we could sustain a constant rf trapping voltage of 2500 V for several minutes (five minutes or more).

amplifier (V_{fnp-p}) of 0.19 V. We decided to try to trap C_{60}^+ and then later Mg^+ alone.

We were very excited by the results we obtained (further detailed in chapter 4). However, when we tried to increase the voltage (increasing the trap depth) to $\approx 3000V (V_{fnp-p} = 0.21V)$ to see if we could capture more ions, something in the circuit changed. The standing wave ratio (SWR), the ratio of the maximum peak voltage to the minimum peak voltage (as measured anywhere along the line), was much greater than 1.0 (≈ 1.6)⁸.

Instabilities previously had been due to coax cable length, coax cable age, poor solder joints, etc. We began by replacing all of the coax cables in our system and checking all solder joints in the resonant circuit. We also removed the tuner from the system to help reduce the complexity of the problem. This, however, did not fix the problem.

Due to the age of the components present in the resonant circuit box (some capacitors dating back as far as 1995), we replaced all of the capacitors and checked once again all of the solder joints in the circuit box. We then tried several tests (beginning at very low voltage values) only to discover that our replacement primary (tank) capacitor, which was in parallel with the primary inductor, was darkened and damaged. It is not clear whether this damage was caused by high voltage (it is possible that the estimated voltage across the primary inductor was grossly underestimated due to the accuracy of our non-invasive probes), or higher current

⁸If the impedance is mismatched (i.e the resonant circuit does not appear as a 50 Ω load to the amplifier) then "RF energy reaching the end of a mismatched line will not be fully absorbed by the load impedance. Instead, part of the energy will be reflected back towards the source. The amount of reflected versus absorbed energy depends on the degree of mismatch between the characteristic impedance of the line and the load impedance connected to its end."p.19.4[39].

values than expected, or the capacitor's inability to dissipate the heat generated by such a high rf voltage (it is located in a closed box with little air circulation).

We had the Science Workshop, located here at the University of Calgary, duplicate the original home built capacitor created by Mark Welling (the dielectric used in the new capacitor was polypenco acetron, "delrin"). We removed the damaged



Figure 3.11: Graph of resonant frequency versus temperature of the tank capacitor. This figure was generated by data collected with Labview in Microsoft Excel.

capacitor, replaced it, and began to test our system again.

Interestingly enough, we discovered that as the circuit naturally heated up due to the rf voltage input, the resonant frequency of the system changed. This temperature dependence appeared to be caused primarily by the tank capacitor! We had not noticed this phenomena in any of our previous trials. Using a heat gun and a digital thermometer connected to the back of the tank capacitor with heat sync compound, I measured the relationship between temperature and frequency (shown in figure 3.11).

Figure 3.12 (located on page 59) shows the FWHM (full width half max) for our resonance point, f = 7.37 MHz (please see Appendix B and F). From this figure, it is clear that the FWHM is on the order of 1.5 MHz. As the temperature of the resonant circuit increases, the frequency changes by ≈ 0.08 MHz. This frequency drop is far less than the FWHM point for our resonance point which is extremely encouraging. This suggests that changes in the resonance point caused by temperature fluctuations are manageable.

Also of interest was the overall response of the system as we slowly increased the input voltage. As the voltage increased, the pressure inside the chamber began to rise. At first, Lanny Murdoch and myself attributed this change in pressure to outgassing⁹, however, we quickly revised our opinion when the pressure continued to rise sharply¹⁰.

At this point we decided to look into the chamber via a glass flange (located on the top of the six way cross). We both noticed a faint orange-red glow emanating from the lower corner of the side supporting the C_{60} source when V_{fnp-p} was 0.12 V.

We first thought that this faint glow was caused by perhaps a poor metal/metal

⁹Outgassing refers to the state inside the chamber when the pressure becomes so low that loose particles on the sides of the chamber, on wires, etc. come "free" (in an effort to equalize the pressure difference) and thus naturally causes a momentary rise in pressure.

¹⁰Normally with outgassing, the pressure levels off at some point and then begins to fall again.

welding joint, a short to the chamber (perhaps a wire had shifted), or a dirty spot weld joint. As such, we took apart the chamber, cleaned all joints (with high grade methanol), checked all joints (we re-welded several connections), and then sealed our system and re-established vacuum.

Still we noticed a faint orange glow emanating from the lower corner of the side supporting the C_{60} source when V_{fnp-p} was 0.12 V. We increased the input voltage, V_{fnp-p} , to 0.13 V. At this point the glow inside the chamber dramatically increased while externally the tank capacitor violently discharged.

The results of these trials clearly indicate that something, either the resonant circuit or the ion trap itself within the chamber, is drawing fairly high levels of current. The most likely cause was a faulty connection in either in the vacuum chamber or else externally in the resonant circuit. We felt that one possible solution might be to replace the flange which connects directly to the trap electrodes. It was possible that the vacuum feedthroughs on this flange were faulty. For example if they were dirty, too close to the chamber itself, were inadequate to carry this type of radio frequency voltage, etc. arcing could occur.

After replacing the flange and repairing the tank capacitor, we found that the resonant frequency of the system had changed from 7.37 MHz to 10.40 MHz and, more importantly, that while there was still a glow from wires inside the chamber, that the overall circuit/ion trap was far more stable. It was possible for us to reach voltage values of $V_{fnp-p} = 0.14$ V which corresponds to a trap electrode voltage of ≈ 1500 V. At this input voltage, there were no observed sparks or visible arcing in either the resonant circuit or in the vacuum chamber itself. We also localized the glow inside the chamber to two older braided wires. These wires connect the Mg

segment of the trap to the resonant circuit box.

Upon more careful inspection, we also discovered a short inside the chamber (one of the trap electrodes was being inadvertently grounded). We felt that this might be the source of the high levels of current we were detecting. We opened the chamber, and fixed this short. Since then we have established that our resonant frequency is once again 7.37 MHz and, even more importantly, that we can once again operate the trap at $V_{fnp-p} = 0.19$ V which corresponds to a trap electrode voltage of ≈ 2500 V with no glow! (hallelujah)

3.4 The Electron Multiplier Tube

Charged species are detected in the vacuum chamber by an EMT (an electron multiplier tube purchased from Isomass Scientific Inc.). An electron multiplier tube works much the same as a photomultiplier tube. The main difference is that a photomultiplier tube has a photosensitive front plate unlike an EMT. In an EMT, a charged particle colliding with the first dynode, in a chain of resistors and dynodes, causes the dynode to eject an electron. This electron is accelerated to each successive dynode from which additional electrons are ejected. In this way a single ion interaction with the surface of the front dynode causes a cascade of electrons which amplifies the original signal (please see figure 3.14 on page 61). This signal can then be detected (in our system via a pulse discriminator and high frequency counter) as an ion count!

The EMT (please see figure 3.15 on page 62) cathode is biased to -3500 V, its anode is grounded and the signal output is fed into an Ortek Discriminator. It produces pulses ≈ 10 ns wide, ≈ 100 mV high. We can observe its signal by an oscilloscope, a frequency counter, and/or a computer¹¹.

3.4.1 Problems We Encountered

The main difficulty we encountered was actually due to the company from which we purchased the EMT, Isomass Scientific Inc. They inadvertently sent us the incorrect Electron Multiplier Tube. We were unaware that it was the incorrect multiplier because the specification sheet, that was sent with the multiplier, matched the part number we had originally ordered. It took us many trials to realize that the EMT itself (and not another piece of equipment such as the pre-amplifier or discriminator) was malfunctioning.

3.4.2 Solutions

Do not work with Isomass Scientific Inc. unless absolutely necessary.

¹¹Our initial trials were performed only with a frequency counter and oscilloscope. This enabled us to not only observe the shape of the pulses being emitted by the EMT, but the rate at which counts were being registered. This in turn allowed us to determine the appropriate discriminator settings.



Figure 3.12: Diagram of the resonant frequency of the ion trap/resonant circuit system. This figure was generated by data collected through a Tie-pie 2 channel handyscope interface package in Microsoft Excel.



Figure 3.13: Diagram of the internal connections in an electron multiplier tube. This figure is a modified version of the figure on page 599 in [40].

,


Figure 3.14: Diagram of the external electron multiplier tube connections. This figure was made in Microsoft Powerpoint.

Chapter 4

Analysis and Results

Flashed all their sabres bare,
Flashed as they turned in air
Sabring the gunners there,
Charging an army, while
All the world wondered:
Plunged in the battery-smoke
Right through the line they broke;
Cossack and Russian
Reeled from the sabre-stroke
Shattered and sundered.
Then they rode back, but not
Not the six hundred

Alfred, Lord Tennyson $[32]^1$

4.1 Ultrahigh Vacuum Chamber Operation

To date we have a fully operational vacuum system. The lowest pressure we have achieved (with only a rotary and turbo molecular pump in operation) is 9.1×10^{-8}

¹from the "Charge of the Light Brigade"

Torr. Typically, it takes several days of operation to achieve such pressures. As such, I have plotted below pressure as a function of time for both the rotary and the turbo molecular pump.



Figure 4.1: Logarithmic plot of the amount of time it takes for the vacuum chamber to be evacuated by the rotary pump to pressures on the order of 10^{-2} Torr. The logarithmic data has been fitted with an exponential curve. This figure was made in Origin, Version 6.0.

Figures 4.1 and 4.2 illustrate the time it takes the rotary pump to achieve pressures on the order of 10^{-2} Torr. Figure 4.3 shows the time it takes the turbo molecular pump to achieve pressures on the order of 10^{-7} Torr. Please note that for this figure I have neglected to show the first 10 minutes of operation for the turbo molecular pump. During these 10 minutes, the pressure falls very rapidly from 1.0×10^{-2} Torr to 1.0×10^{-6} Torr.



Figure 4.2: An enlarged region of graph 4.1 for the amount of time it takes for the vacuum chamber to be evacuated by the rotary pump to pressures on the order of 10^{-2} Torr. The logarithmic data has been fitted with an exponential curve. This figure was made in Origin, Version 6.0.

It is quite amazing to see how long it takes the rotary pump in comparison to the turbo molecular pump to achieve various pressures. The rotary pump evacuates the chamber from atmospheric pressure, ≈ 720 Torr, to pressures less than 1 Torr in ≈ 10 minutes whereas it takes the turbo molecular pump ≈ 7.5 days to decrease the pressure only a fraction, from 4.5×10^{-7} Torr to 1.5×10^{-7} Torr!

There are many ways to minimize the chamber evacuation time. For example by ensuring that the chamber is exposed to atmospheric gases for only a short period of time, by keeping the chamber clean and free of dirt and other contaminants, etc. the pump down time for the vacuum chamber may be significantly reduced.



Figure 4.3: Graph of the amount of time it takes for the vacuum chamber to be evacuated by a turbo molecular pump to pressures on the order of 10^{-7} Torr. The data has been fitted with an exponential curve. This figure was made in Origin, Version 6.0.

Lower pressures can be achieved with our system (as mentioned in Chapter 3.1) with the combination of an ion getter pump and "baking"² the chamber. It takes ≈ 7 days to bake out a system. Since we are still in the testing phase of our apparatus, ultra high vacuum is not necessary and as such, we decided not to attempt to reach ultra high vacuum at this time.

²By wrapping electric heating cords around the outside of the chamber and then covering both the heating cords and chamber with tin-foil, we effectively "bake" the vacuum chamber. As the chamber gets hot, particles are released from the inner surface of the chamber (boiled off $(T \approx 210^{\circ}\text{C})$ so to speak), lowering the pressure of the chamber.

4.2 Ion Source and Detector Operation

In order to confirm the function of our ion sources (i.e. the atomic ovens and electron guns), we wanted to run several trials, analyzing the count rate determined by our detection system (composed of an EMT, discriminator and frequency counter), as a function of time for various sources. These sources were the Mg oven source, the Mg electron gun, the C_{60} oven source, and the C_{60} electron gun.

Each of the following figures shows the frequency of particle detection for several different stages in ion generation. The frequency of particle detection for each of these figures was time averaged over 10 second intervals. The EMT was operated at a bias of -3500 V so as a result, it only detects positively charged ions.

The first set of data, shown in figure 4.4, shows the frequency of particle detection as a function of time for when the Mg oven was initially enabled, secondly for the Mg ion source (i.e. the atomic oven and its corresponding electron gun), thirdly the results of when the Mg electron gun was turned off (the Mg oven was left on during this time) and finally the count rate detected when all sources were turned off (i.e. the background rate). The starting pressure for this trial was 1.4×10^{-7} Torr. The final pressure (after all data was taken) was 4.1×10^{-7} Torr. The Mg oven and the Mg electron gun's operating currents were 1.4 A and 1.6 A respectively.

From this figure, we can see that the frequency of particle detection increases slightly from when the Mg oven source is first turned on to when the Mg electron gun is enabled. This is because as the Mg oven source warms up, it begins to glow. Photons are emitted by the glowing wires. High energy photons (photons with energy in the far ultra-violet) can generate photo-electrons in the EMT registering



Figure 4.4: Semi-logarithmic plot showing the frequency of particle detection as a function of time for the Mg oven source alone, the Mg electron gun alone, and the when the Mg oven source and electron gun operate together (please note that the connecting line has been added to aid the eye only). This figure was made in Microsoft Excel.

false ion counts. Also, hot filament ionization may occur resulting in an increase in the count rate. The frequency then sharply rises and plateaus approximately 20 seconds after the electron gun is first enabled. This increase in frequency is a result of ion generation. (As detailed in Section 3.2, electrons collide with neutral atoms creating ions.)

We were pleased to see this trend as it implies that our ion source (the Mg oven and its associated electron gun) is functioning properly, generating large numbers of



Figure 4.5: Semi-logarithmic plot showing the frequency of particle detection as a function of time for the Mg oven source alone, the Mg electron gun alone, and the when the Mg oven source and electron gun operate together after having flushed the chamber with He gas (please note that the connecting line has been added to aid the eye only). This figure was made in Microsoft Excel.

charged particles. The rate then decreases sharply after the electron gun is turned off and continues to decrease steadily after all sources have been disabled.

Prior to our second trial, we flushed the chamber with helium in an attempt to clean the chamber of loose Mg atoms that, from our previous trial, had not become ions. Mg atoms can easily be deposited on the flat circular electrode, the trap electrodes, or even the vacuum chamber. After injecting He into the system, we allowed the pressure to re-equilibrate to 1.4×10^{-7} Torr.

Figure 4.5 shows the frequency of particle detection initially when everything was off (the background rate), with just the Mg electron gun alone, with just the Mg oven source alone, and finally the frequency of particle detection when both the Mg oven and its associated electron gun were turned on together (generating ions). The starting pressure as mentioned for this trial was 1.4×10^{-7} Torr. The final pressure (after all data was taken) was 2.7×10^{-7} Torr. The Mg oven and the Mg electron gun's operating currents were 1.4 A and 1.6 A respectively.

Again in figure 4.5 we see similar trends as those observed in figure 4.4. In this particular trial however, we wanted to observe and note the behaviour of the Mg electron gun alone. We can see from the data that for the Mg electron gun, the frequency of particle detection is quite high. It is unlikely that the effects of photoelectrons and hot filament ionization could cause such high frequency detection alone. We would have seen this in previous trails (in figure 4.4 the background count rate never exceeded 10 Hz!). It is more likely that this effect was caused by He or Mg not evacuated from the chamber. The electron gun could have ionized He, Mg and/or surface ionized deposited Mg, causing an increase in the number of detected counts.

The important thing to note however is that the frequency of particle detection for the electron gun source is not as high as the frequency of particle detection for the Mg oven and electron gun together. This confirms that our Mg ion source is functioning as an ion source.

We then turned our attention to the C_{60} ion source and attempted to measure in a similar manner the relationship between the frequency of particle detection and time for several different stages in ion generation.

Figure 4.6 displays the data we obtained from the C_{60} ion source after flushing

the system with helium. We again flushed the chamber with helium before this trial in an attempt to clean the chamber of loose atoms that, from our previous trial, had not become ions. After injecting He into the system, we allowed the pressure to re-equilibrate to 1.4×10^{-7} Torr.



Figure 4.6: Semi-logarithmic plot showing the frequency of particle detection as a function of time for the C_{60} oven (operated at 1.5 A) source alone, the C_{60} electron gun (operated at 1.6 A) alone, and the when the C_{60} oven source and electron gun operate together after having flushed the chamber with He gas (please note that the connecting line has been added to aid the eye only). This figure was made in Microsoft Excel.

Figure 4.6 shows the frequency of particle detection initially when everything was off (the background rate), with just the C_{60} electron gun alone, with just the C_{60} oven source alone, and finally the frequency of particle detection when both the C_{60} oven and its associated electron gun were turned on together (generating ions). The starting pressure as mentioned for this trial was 1.4×10^{-7} Torr. The final pressure (after all data was taken) was 3.1×10^{-7} Torr. The C_{60} oven and the C_{60} electron gun's operating currents were 1.5 A and 1.6 A respectively.

This figure does not follow the same trends as the previous two illustrating the Mg ion source operation. In fact, from this trial it appears as though the frequency of particle detection decreases when the C_{60} oven and its associated electron gun are in operation. However, in comparison, the frequency of particle detection for the Mg oven source is much much less than the frequency of particle detection for the C_{60} oven source. We thought that there might be some relation between the observed high count rate from the C_{60} oven and the lack of counts from the C_{60} ion source.

At this point, it is important to briefly discuss the detection system (further detailed in Section 3.4). The detection system is comprised of an EMT, a pulse discriminator, and a frequency counter (please see Appendix C). The EMT appears to function properly, however, it is unclear whether or not our discriminator/frequency counter, is capable of handling the rate at which pulses are being registered by the EMT.

For example, if too many charged particles collide virtually simultaneously with the front of the EMT, then the time difference between pulses may be undiscernible to the discriminator/frequency counter. As a result, the discriminator/frequency counter may view many counts as one continuous count. This, therefore, could explain the trends we observe.

From figure 4.6, we can see that when the C_{60} oven source is on alone that the frequency of particle detection increases to 100 kHz and then begins to decrease. This fact along with the reduced frequency of particle detection when the C_{60} ion source is enabled implies that the discriminator/frequency counter is not capable of handling the rate at which pulses are being registered by the EMT³.

To test this we reduced the currents in both the C_{60} oven and the C_{60} electron gun in order to reduce the total number of generated particles by both sources and in doing so decrease the rate at which pulses are being registered by the EMT. By reducing the total number of particles that the EMT could detect, we hoped to observe an increase in the frequency of particle generation when the C_{60} ion source was in operation.

The data we obtained from the C_{60} ion source after flushing the system with helium and lowering the currents through both the C_{60} oven and electron gun is shown in figure 4.7. We again flushed the chamber with helium before this trial in an attempt to clean the chamber of loose atoms that, from our previous trial, had not become ions. After injecting He into the system, we allowed the pressure to re-equilibrate to 1.5×10^{-7} Torr.

Figure 4.7 illustrates the frequency of particle detection initially when everything was off (the background rate), with just the C_{60} electron gun alone, with just the C_{60} oven source alone, and finally the frequency of particle detection when both the C_{60} oven and its associated electron gun were turned on together (generating ions). The

³One other possibility not discussed above is that it could be that our EMT is over saturated. The specification sheets are not clear in this regard.

starting pressure as mentioned for this trial was 1.5×10^{-7} Torr. The final pressure (after all data was taken) was 2.7×10^{-7} Torr. The C_{60} oven and the C_{60} electron gun's operating currents were 1.3 A and 1.4 A respectively.



Figure 4.7: Semi-logarithmic plot showing the frequency of particle detection as a function of time for the C_{60} oven (operated at 1.3 A) source alone, the C_{60} electron gun (operated at 1.4 A) alone, and the when the C_{60} oven source and electron gun operate together after having flushed the chamber with He gas (please note that the connecting line has been added to aid the eye only). This figure was made in Microsoft Excel.

Figure 4.7 displays more or less the trends we expected and hoped to see. The frequency of particle detection increased rapidly when the C_{60} oven was enabled to ≈ 10 kHz. We did not observe an increase in the number of particles generated when the C_{60} ion source was enabled. During this time however, we did observe a steady number of detected counts.

We believe that this steady count rate is a result of the physical location of the C_{60} ion source. Physically the C_{60} oven is more in the open than the Mg oven. The Mg oven, as you may recall from Section 3.2, is mounted in front of a curved electrode slightly behind a flat circular electrode (please see figure 3.7). The C_{60} oven in contrast is suspended by its connecting wires directly in front of the trap electrodes. This means that there is physically less "stuff" between the C_{60} oven and the EMT than for the Mg oven source. As a result, it is possible that more short wavelength photons and ions produced from hot filament ionization processes reach the EMT from the C_{60} oven source. Also, the C_{60} electron gun is farther away from the C_{60} atoms would be ionized. These two factors suggest that fewer ions are generated by the C_{60} ion source and therefore, that the signal to noise ratio is significantly reduced. More tests need to be done in this area to determine not only the capabilities of the detection system, but the ion generation capability of the C_{60} ion source.

4.3 **Results of Trials at Various He Pressures**

After we had established that the solid state ion sources were working reasonably well, we were curious to see what effect the He pressure in the chamber had on ion generation. In Section 4.2, I presented the data we had collected from ions formed of metal and powder neutral atoms. One of the motivations for He gas trials was to see how a gaseous atomic source would react with the electron guns to produce ions.

All of the trials we performed were quite similar. As such, I have chosen to display and discuss only two of these experiments here.

The results of our first trial are shown in figure 4.8. This experiment was performed using the Mg e-gun source operating at a current value of 1.6 A. The starting pressure in the chamber was 1.4×10^{-7} Torr. The final pressure in the chamber was 1.5×10^{-6} Torr.

In this figure, it is clear that the frequency of particle detection increases as the He pressure in the chamber increases. This is reasonable because there is more He to ionize as the pressure increases.

Figure 4.9 shows the results of a similar experiment conducted at even higher He pressures. For this trial, the starting pressure was 2.2×10^{-6} Torr. The intermediate pressure was determined to be 4.5×10^{-6} Torr. The final pressure of the system was 1.4×10^{-7} Torr. Again the Mg e-gun, operated at 1.6 A, was the electron generation source.

In Figure 4.9, the frequency of particle detection is very similar to that shown in figure 4.8 when He was injected into the chamber. The final equilibrium pressure of the data shown in figure 4.8 (1.5×10^{-6} Torr) is very close to the starting pressure



Figure 4.8: Semi-logarithmic plot showing the frequency of particle detection as a function of time for the Mg e-gun with He being injected into the chamber ≈ 60 s after the e-gun was first enabled. This figure was made in Microsoft Excel.

for the data shown in figure 4.9 $(2.2 \times 10^{-6} \text{ Torr})$. As the He pressure in the chamber increased to 4.5×10^{-6} Torr, there was a slight increase in the frequency of particle detection. This rate then decreases as He is evacuated from the chamber. These trials are all in accordance with our intuitive feeling about how the He pressure should affect the system. We expect that as the He pressure inside the chamber increases so should the frequency of particle detection. Figure 4.10 summarizes our results. As you can see from this figure, the frequency of particle detection increases linearly with He pressure in the chamber.



Figure 4.9: Semi-logarithmic plot showing the frequency of particle detection as a function of time for the Mg e-gun with He being injected into the chamber ≈ 60 s after the e-gun was first enabled and then evacuated from the chamber ≈ 60 s later (please note that the connecting line has been added to aid the eye only). This figure was made in Microsoft Excel.

It is thus possible to use a gaseous atom (or molecule) source in conjunction with the electron guns present in the chamber to produce ions!

4.4 Results of Preliminary Trapping Tests

As detailed in chapter 1, we hope to not only perform collision experiments, but to laser cool, at least initially, simple ionic species such as charged atoms or diatomic



Figure 4.10: Plot showing the frequency of particle detection as a function of He pressure for the Mg e-gun. A best fit line has been added. This figure was made in Microsoft Excel.

molecules.

Therefore, it is important at this junction to describe the differences between these two types of experiments:

First, the rf voltage amplitude required to trap heavy complexes (such as MgC_{60}^+) formed through collision processes is much larger than the rf voltage needed to trap ions (or diatomic molecules) injected into the system. This is because the rf trapping voltage is directly proportional to the mass of the desired trap species. You may recall from Chapter 2 that we determine the necessary trapping field parameters from the largest intersecting region in q-a space (please see figure 2.3). In this area, we choose

$$a = 0$$

and

$$0.908 \ge |q| = \frac{2zeV}{mr_o^2\Omega^2}$$

In order to maintain a specified q coefficient, if the charge and frequency of field oscillation do not change, the ratio of voltage to mass must remain constant. Therefore, as the mass of the charged species increases, so must the amplitude of the trapping voltage.

Since preliminary laser cooling experiments would be performed with single ions (such as Mg^+ which has an atomic mass of 24 amu) mixed with charged diatomic molecules, the mass of such species would likely be substantially less than a molecule like MgC_{60}^+ (which has an atomic mass of 744 amu). As a result, our trapping voltage does not need to be as large.

Secondly, the duration of a collision experiment is much shorter than one involving laser cooling. Our goal was to produce a system that could operate at high voltages $(V_{rf} = 2000V \text{ or more})$ for a couple of minutes and at low voltages $(V_{rf} = 1000V \text{ or})$ less) for an arbitrary time span.

4.4.1 High RF Voltage Trials and Results

The following outlines my results obtained at high rf voltage values:

On September 2, 2001, we attempted to observe trapped ions. Our experimental procedure was as follows:

1) We began by preheating the atomic oven to operating temperature (this took approximately 60 s).

2) After 60 s, we then simultaneously turned on the electron gun assembly and the trapping rf voltage for approximately 15 s in order to load the trap. Electrons from the electron gun hopefully would collide with the neutral atoms ejected from the oven forming ions during this time. These ions would then be caught in the trap.

3) We turned off the electron gun and atomic oven and waited approximately 25 - 75 s to allow the buffer gas (He) to cool the generated trapped ions

4) We then turned on the EMT noting how many counts we measured upon its initialization (i.e. are ions pulled instantaneously out of the trap?)

5) Approximately 5 to 10 s later, we slowly turned down the trapping rf amplitude (q-scanning - please see section 2.2) while watching for bursts in the number of counts which indicate ion detections.

Table 4.1 shows the voltage values used for these trials on the corresponding power supplies that supply d.c. voltages to each of the three segments (please see Appendix C for further detail on electrical connections):

> $U_{Mg_{segment}} = -U_{pull} + U_{filter}$ $U_{centre_{segment}} = -U_{centre} - U_{collision} - U_{pull} + U_{filter}$ $U_{C60_{segment}} = -U_{collision} + U_{filter} - U_{pull} + U_{centre}$

The data we obtained on September 2, 2001 is summarized in the tables that follow:

Power Supply Voltages					
Power Supply	Voltage				
	(V)				
U_{filter}	1.9				
U_{C60}	60.1				
U_{centre}	0.7				
$U_{collision}$	5.5				
U_{pull}	14.5				
U_{dump}	10.7				
Experimentally Measured Values					
$U_{Mg_{segment}}$	-12.4				
Ucentresegment	-18.6				
$U_{C60_{segment}}$	-18.0				

•

Table 4.1: Power Supply voltages used on September 2, 2001 to generate trapping fields in the vacuum chamber.

Results of Ion Trap Tests										
Trial Mg flange	I _{Mg}	$ I_{e-gun} $	$U_{wehnelt}$	P_{He}	$t_{oven preheat}$	$t_{e-gunon}$	V_{fnp-p}	t_{before}	Counts	Counts
	(A)	(A)	(V)	(Torr)	(s)	(s)	$(x10^{-1}V)$	EMT on(s)	EMT on	V_{fnp-p} off
1	1.10	1.5	90	$1.0 \mathrm{x} 10^{-5}$	60	15	1.7	25	8	107
2	1.10	1.5	90	$1.0 \mathrm{x} 10^{-5}$	60	15	1.7	25	10	29
3	1.10	1.5	90	1.0×10^{-5}	60	15	1.7	25	3	9
4	1.10	1.5	90	1.0×10^{-5}	60	15	1.7	25	3	12
5	1.10	1.5	90	$1.0 \mathrm{x} 10^{-5}$	60	15	1.8	25	5	18
Trial C_{60} flange										
6	1.40	1.6	90	9.0×10^{-6}	70	15	1.9	25	4	17
7	1.45	1.6	90	9.0×10^{-6}	90	15	1.9	25	7	30
8	1.45	1.6	90	9.0×10^{-6}	70	15	1.9	50	60	126
9	1.45	1.6	135	9.0×10^{-6}	70	15	1.9	75	8	31
10	1.50	1.6	135	9.0×10^{-6}	70	15	1.9	75	20	80
Note:prior to this point, the He source had been turned off when the e-gun was turned off - next 3 trials He source left on!										
11	1.50	1.6	135	9.0×10^{-6}	70	15	1.9	75	10	59
12	1.50	1.6	135	9.0×10^{-6}	70	15	2.1	75	0*	2^*
13	1.50	1.6	135	9.0×10^{-6}	70	15	1.9	75	0*	0*

*please note at this point we noticed that the reflected power was equal to the forward power

Table 4.2: Results of ion trap tests at high input rf voltage (please note that a $V_{fnp-p} = 0.17$ corresponds to a trap electrode voltage of $\approx 2000V$, $V_{fnp-p} = 0.19$ corresponds to a trap electrode voltage of $\approx 2500V$ and $V_{fnp-p} = 0.21$ corresponds to a trap electrode voltage of $\approx 3000V$)

82

•

EMT Background Count Tests				
Time	Counts registered			
(s)				
30	35			
30	34			
30	22			
30	17			
30	34			

Table 4.3: EMT background count tests

Table 4.3 indicates that the average background count rate as measured by the EMT was $\approx 1 \text{count/s}$. Table 4.2 shows the number of instantaneous counts registered initially when the EMT was enabled and finally when the trapping voltage was turned off (≈ 10 s after the EMT was first turned on). It is clear from the first 11 trials, that the number of counts registered when the trapping voltage was turned off, cannot be attributed to the background count rate. It is also interesting to note that we observed a large number of these counts while lowering the amplitude of the rf voltage (q-scanning, please see section 2.2) with, for example, most events for C_{60} studies occurring at a V_{fnp-p} of ≈ 0.17 V.

This lead us to the exciting hypothesis that what we were actually measuring was ion counts from particles stored in our trap for 25 to 75 seconds!

In order to confirm these encouraging results, we decided to turn up the trapping field amplitude (increasing the trap depth) in the hopes that we would trap more ions and therefore register an even higher count rate. Unfortunately, due to instabilities in our resonant circuit, this resulted in two null trials (trials 12 and 13 in table 4.2).

As detailed in section 3.3, these resonant circuit instabilities have persisted, how-

ever, our recent results at high rf voltage suggest that these difficulties may finally be resolved. As such, future work will hopefully corroborate the results we obtained on September 2, 2001.

4.4.2 Results of Diagnostic tests

In an effort to first try to determine the effects of temperature on the trapping voltage, I performed several experiments on the resonant circuit and ion trap system at low input voltage values. As mentioned at the beginning of this chapter and in Section 1.4, if laser cooling is to become a viable option for this system, it is important to determine how this apparatus behaves when operated for fairly long time spans (≈ 15 min) at low voltage values.

In order to characterize its general behaviour, two diagnostic outputs located on the rf amplifier (please see Appendix D) were used. These outputs allow one to observe both the reflected and forward voltage being supplied to the resonant circuit box in real time. If the impedance is mismatched (i.e the resonant circuit does not appear as a 50 Ω load to the amplifier as detailed in Section 3.3) then "RF energy reaching the end of a mismatched line will not be fully absorbed by the load impedance. Instead, part of the energy will be reflected back towards the source. The amount of reflected versus absorbed energy depends on the degree of mismatch between the characteristic impedance of the line and the load impedance connected to its end."p.19.4 [39]. These two diagnostic outputs allow us to measure qualitatively this degree of mismatch.

At this point you may be wondering why this mismatch in impedance between the load (our resonant circuit and ion trap) and the amplifier output terminal matters. As explained in Section 3.3, the rf amplifier (please see Appendix B) has a built in SWR meter. The standing wave ratio (SWR) is a measure of the ratio of the maximum peak voltage to the minimum peak voltage (as measured anywhere along the line). If this ratio is larger than 1.5^4 the amplifier automatically switches itself off.

We had already established that as the resonant circuit's temperature increased, the resonant frequency of the entire trapping system decreased (please see figure 3.11) and, as a result, we were concerned that the system's characteristic impedance might drastically change with temperature. A change in the characteristic impedance of the resonant circuit could render our system inoperable.

To reiterate then, we not only wanted to establish the stability of our system at low voltage values, but to try and understand how our circuit/ion trap was behaving in general. We hoped that these trials might provide us with some insight into the problems we had been observing at high voltage values.

The data presented below was taken in real time with Labview (please see appendix D) via the rf amplifier diagnostic outputs:

Figure 4.11 shows the reflected voltage and forward voltage as functions of time for an input voltage of $V_{fnp-p} = 0.06V$ which corresponds to a trap electrode voltage of $\approx 700V$. The duration of each trial was ten minutes. I waited fifteen minutes between trials to allow the system to cool back to its initial state. This graph illustrates how our resonant circuit/ion trap behaved over the first ten minutes of

⁴Please note that the technical manual associated with the rf amplifier does not give the threshold SWR value for which the amplifier will operate. I am basing the figure quoted here on direct measurements made from the tuner assembly that was located in series with the amplifier for the trials shown in Table 4.1.



Figure 4.11: Reflected voltage and forward voltage as functions of time for $V_{fnp-p} = 0.06V$. This figure was made in Microsoft Excel.

operation. As we can see from the graph, the amplitude of reflected voltage rapidly increases during the first five minutes of operation. It then appears to plateau and stabilize. During this time, we can also see from the graph, that the amplitude of the forward voltage did not vary. We did not expect the forward voltage to vary since the job of the rf amplifier is to act as a constant power source.

This graph is however a bit misleading. From this data you may think that the reflected voltage, as measured by the amplifier, is greater in amplitude than the forward voltage. It turns out that this is not the case. Internally, in order to generate a measurable signal, the amplifier scales the actual value of both the reflected and forward voltage by some factor. Unfortunately, the technical manual associated with this device does not give the scaling factor. In fact no information is given in regards to the outputs except that one is a measure of the reflected voltage and the other of the forward voltage. Regardless of the fact that we cannot quantify either the reflected or forward voltage, we can obtain important qualitative information on the overall behaviour of the system.

Having said this, I then became curious to see whether or not the relationship between reflected voltage and time was dependent upon the input voltage. Perhaps at a higher input voltage, the reflected power would not approach some constant value, but rather exponentially grow with time. As such, I performed two trials, each for ten minutes, at each of three different input voltage values, $V_{fnp-p} = 0.06V$ (which corresponds to a trap electrode voltage of $\approx 700V$), $V_{fnp-p} = 0.07V$ (which corresponds to a trap electrode voltage of $\approx 850V$), and $V_{fnp-p} = 0.08V$ (which corresponds to a trap electrode voltage of $\approx 950V$). I again waited fifteen minutes between trials to allow the system to cool back to its initial state. These results are shown in figure 4.12.

These results reaffirm those shown in figure 4.11. Again, the amplitude of the reflected voltage rapidly increased during the first five minutes of operation and then appeared to plateau and stabilize for each of the different V_{fnp-p} values.

Next I wanted to reassure myself that the reflected voltage was not just reaching a plateau or constant value, but staying at that value. As such, I decided to record the reflected voltage as a function time after the system had been in operation for fifteen minutes. These results are shown in figure 4.13.



Figure 4.12: Reflected voltage as a function of time for various low input amplifier rf voltages. This figure was made in Microsoft Excel.

From figure 4.13, it is clear that the reflected voltage did not increase, but rather decreased slightly over the ten minute trial. The reasons for this decrease in the reflected voltage are unclear, however, the important thing to remember here is that the reflected voltage did not increase.

While these results fail to shed light on the resonant circuit/ion trap instabilities that occur at high rf voltage values, they are nonetheless extremely encouraging. It is important to note that the amplifier, during all of these trials, never turned itself off. Also, the reflected voltage did not steadily increase. These two facts imply that



Figure 4.13: Reflected voltage as a function of time after having been in operation for 15 minutes at $V_{fnp-p} = 0.06V$. This figure was made in Microsoft Excel.

the ion trap system can operate and be stable at low trapping amplitude for long periods of time!

Chapter 5

Conclusion

I have climbed to the snows of Age, and I gaze at a field in the Past,Where I sank with the body at times in the sloughs of a low desire,But I hear no yelp of the beast, and the Man is quiet at lastAs he stands on the heights of his life with a glimpse of a height that is higher.

Alfred, Lord Tennyson $[32]^1$

We have accomplished many things this past year. We have established a working vacuum system capable of achieving pressures on the order 10^{-8} Torr (please see Section 4.1). We have determined that our atomic ovens and electron gun assemblies are functioning properly (please see Section 4.2).

Also, the diagnostic tests performed on October 23, 2001 were extremely encouraging. The fact that the reflected voltage did not steadily increase implies that the ion trap system can operate and be stable at low trapping amplitude for long periods of time (please see Section 4.4). This is extremely important if laser cooling experiments are to become a viable research tool for further exploration into the nature of both charged atoms and molecules.

The results we obtained on September 2, 2001 were also encouraging. It appears as though we were successful in trapping ions although further work is needed to corroborate these results.

¹from "By an Evolutionist (Old Age Part II)"

There are still many issues left to be resolved with respect to this system. First, one extremely important factor, which must be dealt with in my opinion if this system is to ever be operational, is technical support. We did not have adequate knowledge of the type of electronics and radio frequency circuits we would have to deal with. While I feel that we have gained a lot of knowledge with respect to ion trap systems, it has been very frustrating not knowing how to proceed or where to find technical assistance.

Secondly, the resonant circuit's general behaviour must be explained and electrical stability achieved. One modification that may need to be made to the resonant circuit box is some sort of temperature control unit. It was clear in our trials that as the tank capacitor's temperature increased, the resonant frequency of the entire apparatus decreased. This decrease in resonant frequency may not cause a problem with the actual operation of the overall system, but may influence the accuracy at which one can perform mass spectrometry during the shorter time span collision experiments. As such, further study and analysis should be done with respect to the relationship between temperature and resonant frequency once electrical stability has been achieved.

Future work should also be done to improve detection consistency. While it appears as though our EMT is functioning properly, there have been inconsistencies in some of the measurements we have made (please see Section 4.2).

In conclusion, I feel that this project has great potential. There are many interesting experiments which can be performed with this system once it is fully operational. I believe this apparatus can produce research that will contribute to our understanding of the chemical nature of atoms and molecules.

Bibliography

- W. Paul. Electromagnetic traps for charged and neutral particles. In
 E. Arimondo et al, editor, Proceedings from the International School of Physics Enrico Fermi, Laser Manipulation of Atoms and Ions, pages 497-517, 1992.
- [2] http://www.nobel.se/physics/laureates/1989/press.html.
- [3] Robert I. Thompson et al. Gas Phase Ion Studies of Collisionally formed MgC⁺₆₀ Complexes . Manuscript - to be published, 2001.
- [4] Yousef Basir and Scott Anderson. Interaction of Mn⁺ and Mn⁺₂ with C₆₀.
 Exohedral and Endohedral metal-fullerene bonding . Chemical Physics Letters, 25:45-48, 1995.
- [5] Mark Welling et al. Ion/molecule reactions, mass spectrometry and optical spectroscopy in a linear ion trap. International Journal of Mass Spectrometry and Ion Processes, 172:95-114, 1998.
- [6] Mark Welling. Erzeung und Untersuchung von MgC⁺₆₀ Fulleren-Komplexen in einer linearen Ionenfalle. PhD thesis, Ludwig-Maximilians-Universität, München, 1995.
- [7] Francais A. Carey. Organic Chemistry. The McGraw-Hill Companies, Inc., 1996.
- [8] H. Kroto et al. C₆₀:Buckministerfullerene . *Nature*, 318:162–163, 1985.
- [9] http://cnst.rice.edu/nobel.html.

- [10] http://buckminister.phsyics.sunysb.edu/images.
- [11] H. Aldersey-Williams. The Most Beautiful Molecule, The Discovery of the Buckyball. John Wiley Sons, Inc., 1995.
- [12] S.D. Taylor and W.W. Duley. The formation of long carbon chains in diffuse clouds . Royal Astronomical Society, 286:344-348, 1997.
- [13] G.H. Herbig. The diffuse interstellar bands IV, the region 4400-6850Å
 . The Astrophysical Journal, 196:129-160, 1975.
- [14] G.H. Herbig. The diffuse interstellar bands VIII new features between
 6000 and 8650Å. The Astrophysical Journal, 382:193-203, 1991.
- [15] Patrick Hale, editor. The Collins English Dictionary. Collins, 2 edition, 1986.
- [16] Z. Wan et al. Collision of alkali ions with C₆₀/C₇₀: Insertion, thermionic emission, and fragmentation. Journal of Chemical Physics, 99:5858, 1993.
- [17] Y. Chai et al. Fullerenes with metals inside . Journal of Physical Chemistry, 95:7564, 1991.
- [18] T. Weiske et al. Injection of He atoms into doubly and tribly charged c_{60} cations . Journal of Physical Chemistry, 95:8451, 1991.
- [19] Robert Thompson Mark Welling and Herbert Walther. Photodissociation of MgC⁺₆₀ complexes generated and stored in a linear ion trap. Chemical Physics Letters, 253, 1996.

- [20] Mark Welling Robert I. Thompson and Herbert Walther. Studies of Photodissociation of MgC⁺₆₀ in a linear ion trap. Recent Advances in the Chemistry and Physics of Fullerenes, 4:70–81, 1997.
- [21] Clement Moses Raymond Serway and Curt Moyer. Modern Physics . Saunders College Publishing, 2 edition, 1997.
- [22] Gerhard Herzberg. Molecular Spectra and Molecular Structure I. Spectra of Diatomic Molecules. D. Van Nostrand Company, Inc., 2 edition, 1950.
- [23] Allon Bartana and Ronnie Kosloff. Laser cooling of molecular internal degrees of freedom by a series of shaped pulses. Journal of Chemical Physics, 99:196-210, 1993.
- [24] David Appell. Laser cooling traps: the Nobel prize . Laser Focus World, pages 103-109, 1998.
- [25] Phillip Gould. Laser cooling of atoms to the Doppler Limit . American Journal of Physics, 65:1120–1123, 1997.
- [26] C.N. Cohen-Tannoudji and W. D. Phillips. New Mechanisms for Laser Cooling . Physics Today, pages 33–40, 1990.
- [27] http://entropy.davidson.edu/Projects/SuFischer/node10.htm.
- [28] Peter H. Dawson, editor. Quadrupole Mass Spectrometry and its applictions. Elsevier Scientific Publishing Company, 1976.

- [29] D.A. Church. Storage-ring ion trap derived from the linear quadrupole radio-frequency mass filter. Journal of Applied Physics, 40:3127–3133, 1969.
- [30] Ethan R. Badman and R. Graham Cooks. Cylindrical ion trap array with mass selection by variation in trap dimensions. Analytical Chemistry, 72:5079-5086, 2000.
- [31] P. Forck et al. Molecular physics in storage ring: Dissociative recombination of cold hd+ . Nuclear Instrumentation and Methods, 79:273-275, 1993.
- [32] W.H. New and W.E. Messenger, editors. *Literature in English*. Prentice-Hall Canada, 1993.
- [33] Charles A. McDowell, editor. Mass Spectrometry . McGraw-Hill Book Company, Inc., 1963.
- [34] http://www.webabout.com/jokes/index.html.
- [35] Varian Vacuum Technologies. High/Ultra-High Vacuum Seminar.
- [36] Varian Vacuum Technologies. Thermocouple gauge.
- [37] Varian Vacuum Technologies. SenTorr Gauge Controller.
- [38] Varian Vacuum Technologies. Ionization gauge.
- [39] Bruce S. Hale, editor. The 1989 ARRL Handbook for the Radio Amateur. The American Radio Relay League, 66 edition, 1989.

[40] Paul Horowitz and Winfield Hill. The Art of Electronics. Cambridge University Press, 1983.

.

-

[41] Inc. Tektronix. Tektronix High Voltage (1000:1) Oscilloscope Probes P6013.

,
Appendix A

The wave-mechanical nature of the Franck-Condon Principle

integral *adj*(*in*t*i*grel,in*iɛ*grel) **1.** (often followed by *to*) being an essential part (of); intrinsic (to). **2.** intact; entire. **3.** formed constituent parts; united. **4.** *Maths.* **a.** of or involving an integral... **5.** *Maths.* the sum of a large number of infinitesimally small quantities, summed either between stated limits or in the absence of limits **6.** a complete thing, whole.

Dictionary definition ¹

The Franck-Condon Principle is: "the electron jump in a molecule takes place so rapidly in comparison to the vibrational motion that immediately afterwards the nuclei still have very nearly the same relative position and velocity as before the 'jump'." (p.194 [22]) For example, if in a diatomic molecule a given transition from one state, $\nu'' = 0$, to a second excited state, $\nu' = 1$, results in a substantial increase in the bond length between two atoms, then the transition is less likely to happen (a substantial increase in bond length could result in large amplitude vibrational oscillations or even break the molecule apart). A transition that preserves the relative distance between the two nuclei would be most probable.

¹from Collins English Dictionary p. 791

This idea is mathematically as follows:

The probability of a transition occurring between two states ψ_1 and ψ_2 is proportional to the square of R, the electric dipole moment (also called the transition moment [22]) of the system:

$$R = \int \psi_1^* M \psi_2 d\tau$$

where R, a probability amplitude, is the off-diagonal matrix element corresponding to the dipole coupling of the states ψ_1 and ψ_2 , $d\tau$ is a volume infinitesimal, and M, the electric dipole moment. M is composed of two quantities: \vec{E} , the electric field associated with the incoming photon (the photon couples the two states together in the transition process) and μ , the dipole moment of the molecule $(M = \vec{E} \cdot \vec{\mu})$.

This system can be further resolved into two parts; one dependent upon the nuclei and one dependent upon the electrons:

$$M = M_e + M_n$$

where M_e is the electronic contribution to the electric dipole moment and M_n , the nuclear contribution. Similarly we can express the wavefunction as a superposition of the electronic and vibrational states² present within the system ψ .

$$\psi = \psi_e \psi_{\nu(e)}$$

therefore,

$$\psi_1 = \psi_{e1} \psi_{\nu 1(e)}$$

²While the vibrational wavefunction is different from the electronic wavefunction, vibrational states are different for each electronic state. They are coupled (for example changes in electron position relative to the nucleus can change the overall vibrational motion of the molecule). Henceforth, I have expressed this dependence by labelling ψ_{ν} as a function of the electronic eigenstates, e.

$$\psi_2 = \psi_{e2} \psi_{\nu 2(e)}$$

Substituting into the expression for R, (the probability amplitude):

$$R = \int \psi_{e1}^* \psi_{\nu 1(e)}^* M_e \psi_{e2} \psi_{\nu 2(e)} d\tau + \int \psi_{e1}^* \psi_{\nu 1(e)}^* M_n \psi_{e2} \psi_{\nu 2(e)} d\tau$$

and remembering that since the vibrational wavefunctions are real, $\psi_{\nu}^* = \psi_{\nu}$ [22] and that M_n is not electron coordinate dependent:

$$R = \int \psi_{e1}^* \psi_{\nu 1(e)} M_e \psi_{e2} \psi_{\nu 2(e)} d\tau_n + \int \psi_{\nu 1(e)} M_n \psi_{\nu 2(e)} d\tau_\nu \int \psi_{e1}^* \psi_{e2} d\tau_e$$

where $d\tau_e$ represents an infinitesimal volume space element of the electron coordinate system and $d\tau_n$ respectively an infinitesimal volume space element of the nuclei coordinate system. Furthermore, each electronic eigenfunction is orthogonal to each other electronic state. Thus,

$$\int \psi_{e1}^* \psi_{e2} = 0$$

eliminating the second term in the sum. After a bit of re-arranging, the expression for the probability amplitude becomes:

$$R = \int \psi_{\nu 1(e)} \psi_{\nu 2(e)} dr \int \psi_{e1}^* M_e \psi_{e2} d\tau_e$$

where dr has been substituted for $d\tau_n$. This change in notation is due to the fact that the vibrational eigenfunctions depend on the internuclear distance, r, alone.

The second integral in the expression for R:

$$R_e = \int \psi_{e1}^* M_e \psi_{e2} d\tau_e$$

is referred to as the electronic transition moment. "The wave-mechanical formulation of the Franck-Condon Principle rests on the assumption that this variation of R_e with r is slow and that R_e may be replaced by an average value $\overline{R_e}$ (p.200[22]). Therefore,

$$R = \overline{R_e} \int \psi_{\nu 1(e)} \psi_{\nu 2(e)} dr$$

and thus, the probability of a transition occurring is:

٢

.

$$P_{probability} = |R|^2 = \overline{R_e^2} [\int [\psi_{\nu 1(e)} \psi_{\nu 2(e)}] dr]^2$$

It is proportional to the square of the overlap integral of the vibrational wavefunctions.

Appendix B

Secular Frequency Determination

This appendix describes in more detail how the frequency of the secular motion of the particle is determined. This is an approximation technique that has been demonstrated to be accurate over normal ranges of the operating parameters. This derivation is based on that shown on pages 211-212 in [28].

The Mathieu differential equations are:

$$\frac{\partial^2 x}{\partial \tau^2} + (a_x + 2q_x \cos[2\tau])x = 0 \tag{B.1}$$

$$\frac{\partial^2 y}{\partial \tau^2} - (a_y + 2q_y \cos[2\tau])y = 0 \tag{B.2}$$

where

,

$$-a_x = a_y = \frac{4zeU}{mr_o^2\Omega^2}$$
$$-q_x = q_y = \frac{2zeV}{mr_o^2\Omega^2}$$
$$\tau = \frac{\Omega t}{2}$$

Analyzing the particle's acceleration in the x-direction alone (the y-direction analysis is equivalent and independent):

$$\frac{\partial^2 x}{\partial \tau^2} = -(a_x + 2q_x \cos[2\tau])x \tag{B.3}$$

The total distance the particle moves, x, in a given amount of time can be represented by:

$$x = \delta + \chi \tag{B.4}$$

where δ represents the micromotion of the particle (the high frequency oscillations) and χ represents the macromotion of the particle (the much lower frequency secular oscillation).

If the trapping force on the particle is small then $\delta \ll \chi$ while, due to the different frequency scales of the two motions, $\frac{\partial^2 \delta}{\partial \tau^2} \gg \frac{\partial^2 \chi}{\partial \tau^2}$. As such, if we substitute equation B.4 into equation B.3, eliminate the small terms and choose $a_x \ll q_x$:

$$\frac{\partial^2 \delta}{\partial \tau^2} = -(2q_x \cos 2\tau)\chi \tag{B.5}$$

Integrating this function twice gives:

$$\delta = +0.5q_x \chi \cos 2\tau$$

This approximate expression for δ may now be placed back into our expression for x:

$$x = \chi + 0.5q_x \chi \cos 2\tau$$

and our Mathieu equation now becomes:

$$\frac{\partial^2 x}{\partial \tau^2} = -(2q_x \cos[2\tau])\chi - q_x^2 \chi^2 \cos^2[2\tau]) \tag{B.6}$$

Substituting into:

$$\frac{\partial^2 x}{\partial \tau^2} = \frac{\partial^2 \delta}{\partial \tau^2} + \frac{\partial^2 \chi}{\partial \tau^2} \tag{B.7}$$

we are left with

$$\frac{\partial^2 \delta}{\partial \tau^2} + \frac{\partial^2 \chi}{\partial \tau^2} = -(2q_x \cos[2\tau])\chi - q_x^2 \chi^2 \cos^2[2\tau]) \tag{B.8}$$

If we consider the mean trapping force by averaging over one period of trap oscillation ($\tau = 0$ to $\tau = \pi$),

$$\frac{\partial^2 \delta}{\partial \tau^2} = 0$$

because δ has a period of $\frac{2\pi}{\Omega}$ leaving:

$$\left[\frac{\partial^2 \chi}{\partial \tau^2}\right]_{average} = -\frac{1}{\pi} \int_0^{\pi} \frac{\partial^2 x}{\partial \tau^2} d\tau$$
(B.9)

or

•

$$\left[\frac{\partial^2 \chi}{\partial \tau^2}\right]_{average} = \frac{1}{\pi} \int_0^\pi -(2q_x \cos[2\tau])\chi d\tau + q_x^2 \chi^2 \cos^2[2\tau] d\tau \tag{B.10}$$

Assuming that χ varies little over one trap period, it can be viewed as a constant and the integral of this equation is simply:

$$[rac{\partial^2 \chi}{\partial au^2}]_{average} = -rac{q_x^2}{2}\chi$$

which re-expressed in terms of time is:

$$[\frac{\partial^2 \chi}{\partial \tau^2}]_{average} = -\frac{q_x^2}{2} \frac{\Omega^2}{4} \chi$$

This equation represents the simple harmonic motion of the secular motion χ . We can re-write this as:

$$\omega_{sec} = \frac{1}{\sqrt{8}} q_x \Omega$$

where

$$\left[\frac{\partial^2 \chi}{\partial \tau^2}\right]_{average} = \omega_{sec}^2 \chi \tag{B.11}$$

Appendix C

Experimental Apparatus Components

They [the arts and sciences] compete with, and occupy the place of those mischievous and dangerous passions and employments, to which want of occupation and ennui give birth. They are excellent substitutes for drunkenness, slander, and the love of gaming.

Jeremy Benthan $[32]^1$

The following pages comprise a comprehensive list of the equipment used in conjunction with the ion trap system. Included in this list are all power supplies (both a.c. and d.c. sources), diagnostic equipment (such as the SWR analyzer and spectrum analyzer), all vacuum equipment and accessories, amplifiers, the detector and its accessories, as well as the model number for each piece of equipment, its usage and key characteristics (i.e. voltages, currents, etc) and its associated supplier.

The first page lists the dc power supplies required to operate the system. The second page lists the ion detection system components, the rf trapping field electronics, and the diagnostic electronics used in conjunction with our system (completed on the third page). Also on the third page is a list of all the vacuum components with the fourth page containing a list of important general accessory supplies.

¹from The Rationale of Reward, Book III: Reward Applied to Art and Science, from Chapter 1: Art and Science - Divisions

List of Equipment					
Equipment	Supplier	Model Number	Remarks	Description of Use	
Power Supply (Voltage)	Hewlett Packard	E3612A	0-60V,0-5A/0-120V,0-	U_{Mg^+} $pprox$	
			0.25A	0 - (-100)V	
Power Supply (Voltage)	Hewlett Packard	E3612A	0-60V,0-5A/0-120V,0-	$^{*}U_{C_{60}} \approx 60V(60 - 1)$	
			0.25A	200V)	
Power Supply (Voltage)	Hewlett Packard	E3612A	0-60V,0-5A/0-120V,0-	$U_{Center} \approx$	
		700101	0.25A	0.07V(0-32V)	
Power Supply (Voltage)	Hewlett Packard	E3612A	0-60V, 0-5A/0-120V, 0-	$U_{Wehnelt} \approx 90 -$	
		700104	0.25A	250V	
Power Supply (Voltage)	Hewlett Packard	E3612A	0-60V, 0-5A/0-120V, 0-	$^{*}U_{filter} \approx 2V(0 -)$	
Derrow Group In (Malta as)	TIlott Do al-and	T72619 A	0.20A	00 <i>V</i>)	
rower Supply (voltage)	newlett Packard	E301ZA	0.000, 0.000,	10V(0-60V)	
Power Supply (Voltage)	Howlett Packard	E3612A	0.20 A 0.60 V 0.5 A /0.120 V 0.	$*U_{\rm v} \approx 15V(0-$	
Tower Suppry (Voltage)	ILEWIEUU I ACRAIU	1501211	0 25A	20V	
Power Supply (Voltage)	Hewlett Packard	E3612A	0-60V.0-5A/0-120V.0-	$*U_{dumn} \approx$	
2 opp-5 (0.25A	10.5V(0-40V)	
Power Supply (Current)	Hewlett Packard	E3610A	0-8V,0-3A/0-15V,0-2A	$I_{Mge-gun} \approx 1.6 A$	
Power Supply (Current)	Hewlett Packard	E3610A	0-8V,0-3A/0-15V,0-2A	$I_{C_{60}e-gun} \approx 1.4A$	
Power Supply (Current)	Hewlett Packard	E3610A	0-8V,0-3A/0-15V,0-2A	$I_{Mgoven} \approx 1.1A$	
* the first number indicates our operating voltage value, the range of possible voltages appears in brackets					

List of Equipment cont.					
Equipment	Supplier	Model Number	Remarks	Description of Use	
Electron Multiplier	Isomass Scientific Inc.	AF140	replacement for SEV 217	used for mass selec-	
Tube			Balzers EMT	tion and q-scanning	
High Voltage Power Supply	SRS	PS350	0-5000V/0-25W	power supply for EMT ($\approx 3500V$)	
Amplifier Discrimina-	Ortec	9302	set screw adjustment, set	on loan from Senior	
tor			at 20dB gain	Physics Laboratory	
				(Patrick Irwin)	
Frequency Counter	Hioki	3601		on loan from Senior	
				Physics Laboratory	
				(Patrick Irwin)	
Function Generator	SRS	0S345	0-30MHz function gener-	supplies AC trap-	
			ator	ping potential (fre-	
				quency $\approx 7.0 -$	
DE Amplifon	2	MIKOOM	high frequency amplifier	9.0MHZ	
RF Ampliner	-		$2.30 MH_{\sigma}/0.200 W/0_{\odot}$	notential	
			1000W	potentiai	
High Voltage DC	Hewlett Packard	6268B	0-40V/0-30A	power supply for	
Power Supply				amplifier (requires	
I Olloz Sappij				220V/25A line)	
Spectrum Analyzer	Hewlett Packard	3585A	20Hz-40MHz	on loan from the	
				Space Physics	
				group (Peter King)	
SWR Analyzer	MFJ Enterprises	MFJ259B	HF/VHF	measures	
				impedance, res-	
				onant frequency	
				and SWR	

List of Equipment cont.					
Equipment	Supplier	Model Number	Remarks	Description of Use	
Versa Tuner V	MFJ Enterprises	MFJ989C	two capacitors and an	used to impedance	
			inductor in pi circuit	match resonant cir-	
			(all variable)	cuit to 50 Ω	
pH/MV/TEMP	Markson Science Inc.	95	digital	used to measure	
meter				temperature of	
				tank capacitor	
Two Stage Rotary	Edwards Scientific Inc.	E2M42	12L/s two stage gas	pressure range	
Pump			compression pump	$10^{-1} - 10^{-3}$	
			with oil lubricated		
TV 141 Newignston	Varian Vacuum Tachnologies	0600384	1201./s (for He) turbo	Dressure range	
1 V 141 Wavigator	Varian Vacuum recimologies	2022004	molecular nump with	$10^{-5} - 10^{-8}$	
			air bearings	10 10	
Vacion Plus 300 Star-	Varian Vacuum Technologies	9490746	$340 L/s$ (for N_2)Ion	pressure range	
cell			getter pump with a ti-	$10^{-8} - 10^{-11}$	
			tanium cathode		
Thermocouple Gauge	Varian Vacuum Technologies	BA2	pressure range 10 -	used to determine	
			10^{-3} Torr	pressure in cham-	
				ber	
Ionization Gauge	Varian Vacuum Technologies	BA2C	pressure range 10^{-4} –	used to determine	
			10^{-10} Torr	pressure in cham-	
		D 4 a		ber	
Vacuum Gauge Con-	Varian Vacuum Technologies	BA2	Sen forr Vacuum	controls all pres-	
troller			Gauge, digital display	sure gauges in	
				chainder	

Table C.1: List of Equipment and a description of its usage

Meridian Scientific Inc. supplied additional copper gaskets, valves, o-rings, and fittings for our system.

VWR Canlab supplied gloves, tacky mats (to clean shoes), tubing, chemicals (such as Mg and C_{60}) and other delicate equipment (such as tweezers, scalpels, etc.)

•

Appendix D

Black box circuit diagrams illustrating all external connections to the ion trap

This appendix illustrates, in a block diagram format, all power supplies and external connections made to the ion trap via the vacuum feedthrough flanges (located on both the Mg flange and the C_{60} flange) and those connections made through the resonant circuit control box (located on the C_{60} flange). Also included in these diagrams are the connections made from the rf amplifier (which amplifies an rf voltage from a function generator) to the resonant circuit control box.

Figure C.1 is an overview of the components that make up the ion trap. Figure C.2 describes all of the symbols to be used in the following block diagrams. Figures C.3 through C.7 deal with the various subsections of the electrical set-up of the system. Figure C.3 illustrates the dc bias voltage wiring used to manipulate ions into and within the trap. Figure C.4 illustrates how the rf trapping voltage is fed into the resonant circuit. Figure C.5 shows the electron gun connections. Figures C.6 and C.7 show the electrical connections made to the Mg and C_{60} flanges respectively (atomic ovens, electron guns, and bias voltages).



Figure D.1: This figure shows the ion trap in block format along with the various electrical connections made to it. This figure was made in Microsoft Powerpoint.

Legend:



Figure D.2: This figure shows the legend for all of the following diagrams. This figure was made in Microsoft Powerpoint.



Figure D.3: Block diagram of the dc power supplies used to bias the three trap segments. This figure was made in Microsoft Powerpoint.



Figure D.4: Block diagram of the rf trapping field power supplies. This figure was made in Microsoft Powerpoint.

r



,

Figure D.5: Block diagram of the dc power supplies used to bias the wehnelt cylinders in the electron gun assemblies. This figure was made in Microsoft Powerpoint.

,



Figure D.6: Diagram of the electrical connections made to the Mg flange. This figure was made in Microsoft Powerpoint.

;



Figure D.7: Diagram of the electrical connections made to the C_{60} flange. This figure was made in Microsoft Powerpoint.

Appendix E

Lab View Programming

Analysis on how the reflected power (measured by the amplifier unit in our resonant circuit) varied as a function of time was done with LabView, an interactive, graphical interface programming language designed to allow the user to interface with and control devices external to a computer. This language is extremely powerful and allows the user automate all external devices with a GPIB (General Purpose Interface Bus).

Below is a diagram of my program. This program was used to interface with a HP54600B digital oscilloscope, take measurements of the peak to peak voltage of the reflected power wavefunction, to then graph this data, and export the data to a spreadsheet called "data.xls".

Figure D.1 depicts the interface screen as seen by the user, as generated by the labview code outlined in figure D.2. Figure D.3 and D.4 summarize the interface controls and commands utilized in the programming.



Figure E.1: This is a reproduction of the graphical interface window as seen by the user. This figure was generated by the National Instruments software, LabView.



Figure E.2: This is a reproduction of the labview code which interfaces and operates the HP54600B digital oscilloscope. This figure was generated by the National Instruments software, LabView.

Controls and Indicators



VISA session

slope (T:pos)

Selects the slope of the edge trigger.

T - positive slope F - negative slope

EXT trigger level

Selects the level voltage of the active trigger.



bandwidth limit (F:off)

The switch selects the internal low-pass filter.

T - on F - off

U16 coupling (AC:0)

This selects the input coupling for the specified channel.

- 0 AC 1 - DC
- 2 ground
- **EXT** range(volts)

This defines the full-scale vertical axis of the selected channel. It can be set to any value from 16mV to 40V when using 1:1 probe. If the probe value is changed, the range is multipliedby the attenuation

U16 probe (1X:0)

This specifies the probe attenuation factor for the selected channel.

- 0 1X probe
- 1 10X probe
- 2 100X probe

EXT position

This value sets the voltage that is represented at the center screen for the selected channel. The range of the possible values varies with the RANGE command. If the position value is set outside of the Range, then it is automatically set to the nearest legal value.

EXT range(time)

Sets the full-scale horizontal time in seconds. It is ten times the time per division. When the delay timebase is selected, the RANGE command will set the full-scale horizontal time of the delayed

EXT delay

TF

This is the internal time between the trigger event and the onscreen delay reference point.

set up (T:auto)

The set up selector selects the autoscale or normal set up mode.

T - autoscale; Controls in box ignored

F - normal; Controls in box necessary

TF on/off

Figure E.3: A list of all of the interface controls used in the program and their function. This figure was generated by the National Instruments software, LabView.



HP546XXB Timebase Config.vi

E:\Program Files\National Instruments\LabVIEW 6\instr.lib\hp546xxx\HP546XXX.LLB\HP546XXB Timebase Config.vi

HPS460177
CHANNEL
24
L.,

HP54601A/602B Channel Config.vi

E:\Program Files\National Instruments\LabVIEW 6\instr.lib\hp546xxx\HP546XXX.LLB\HP54601A/602B Channel Config.vi



HP54601A/602B Edge Trigger.vi

E:\Program Files\National Instruments\LabVIEW 6\instr.lib\hp546xxx\HP546XXX.LLB\HP54601A/602B Edge Trigger.vi

HP546XXX Config Acquisition.vi

E:\Program Files\National Instruments\LabVIEW 6\instr.lib\hp546xxx\HP546XXX.LLB\HP546XXX Config Acquisition.vi

DIGITIZE HP54601A/602B Digitize.vi

E:\Program Files\National Instruments\LabVIEW 6\instr.lib\hp546xxx\HP546XXX.LLB\HP54601A/602B Digitize.vi



HP546XXX Autoscale.vi

E:\Program Files\National Instruments\LabVIEW 6\instr.lib\hp546xxx\HP546XXX.LLB\HP546XXX Autoscale.vi



HP54601A/602B Measurements.vi

E:\Program Files\National Instruments\LabVIEW 6\instr.lib\hp546xxx\HP546XXX.LLB\HP54601A/602B Measurements.vi



HP54601A/602B Read Waveform.vi

E:\Program Files\National Instruments\LabVIEW 6\instr.lib\hp546xxx\HP546XXX.LLB\HP54601A/602B Read Waveform.vi



Open/Create/Replace File.vi

E:\Program Files\National Instruments\LabVIEW 6\vi.lib\Utility\file.llb\Open/Create/Replace File.vi

Figure E.4: A list of the interface commands used that are specific to the HP54600B digital oscilloscope. This figure was generated by the National Instruments software, LabView.

Appendix F

Probe Derating Curves

This appendix provides technical information as well as a graph of voltage versus frequency for the high voltage tektronix oscilloscope probe [41]. These probes were used to help determine the peak to peak voltage across the primary inductor located in the resonant circuit control box.



Figure F.1: Figure showing the high voltage probe derating curves. This figure was taken directly from [41].

General

The Type P6013A Probe was developed to provide a means of observing waveforms of high amplitude on a conventional oscilloscope. The 1000:1 attenuation factor incorporated into the ?6013A enables the user to observe waveforms or pulses with a peak amplitude of as much as 12 kV up to 100 kHz¹ (kilohertz) in frequency, or DC voltages up to 12 kV without damage to the probe or the oscilloscope.

The P6013A Probe is designed for electrical and mechanical protection of its internal components, and is covered with thermoplastic offering high impact strength. Weight of the probe alone is ten ounces. The cable has a resistive center conductor, with the value of the resistance chosen to previde optimum performance of the probe. The cable assembly may be removed and replaced. The P6013A may be ordered either with a BNC connector (shown at left) or a UHF connector.

Electrical Characteristics

Attenuation-1000:1

Input Impedance-100 mag, 3 pF

XRisetime (with 7704A Oscilloscope and ZA13 Plug-In)—80 MHz

Moximum Voltage Rating (below 100 kHz)-

Max · DC-12 kV

Max Peak Pulse—12 kV

Max Peak AC—12 kV

COMPENSATING THE PROBE

The electrical components in the compensating box of the Type P6013A Probe includes four variable trimmer capacitors and two potentiometers. The RC networks in the box are arranged to affect the observed shape of the waveform at different but overlapping points during the first 300 μ s of the pulse.

Five of these adjustments compensate for variations in input capacitance from one instrument to another. For accuracy in pulse and transient

'Hz == hertz (cycles per second).

measurements, the probe should be checked frequently.

To check the probe, connect it to the Input connector of the oscilloscope. Set the Culibrator control for an output signal of suitable amplitude. Touch the probe tip to the Cal Out connector and cajust the oscilloscope controls for a display of several cycles. Optimum response is indicated by a flat-top square wave.

Attenuation Adjustment

Before compensating the probe, the attenuation must be checked. To do this, set the Volts/ Div of the oscilloscope or plug-in to 0.01 V/Div and the Calibraior control to 40 volts. Touch the probe tip to the Cal Out connector and check for four major graticule divisions of deflection the CRT screen. If the deflection is more or less than four major divisions, readjust R117 until exactly four major divisions are obtained.

NOTE

40-volt calibrator signal may be internal wired option. See 7704A manual.

Compensation

To compensate the proba, start by first adjusting C113. This setting affects the front corner and general level of that portion of the waveshape that can be compensated—in other words, the first 300 μ s of the waveform. After positioning the front corner, adjust C114, C115 and C116. Adjusting C114 affects the waveshape from 0.5 to 100 μ s. C115 affects the waveshape from 2 μ s to 120 μ s, and C116 affects the waveshape from 5 μ s to 150 μ s. Since there is interaction between the adjustments of the trimmer capacitors, it will be necessary to repeat the sequence.

A variable peaking-resistor (R112) is provided to compensate the first 0.3 μ s of the waveshape. Adjustment of this resistance requires the use of a Tektronix Type 106 Square-Wave Generator, or another square-wave generator capable of producing a pulse with a risetime of 15 ns or less.

If the compensation has been properly adjusted for an oscilloscope of 20-pF input capacitance, adjustment for another input capacitance can generally be achieved by readjusting C113 only.

Figure F.2: Technical information on the tektronix oscilloscope probe used in our experiments as obtained from the P6013 User Manual. This figure was taken directly from [7].

Appendix G

Determination of the Ion Trap Resonant Frequency

Each of the following two figures represents the resonant frequency of the ion trap system as determined by a Spectrum Analyzer. Each of the following diagrams was plotted with an xy plotter at two different frequency resolutions. Figure F.1 shows the resonant frequency of the ion trap system at a scale of 1 cm : 0.405 MHz. Figure F.2 shows the resonant frequency of the ion trap system at a scale of 1 cm : 1.61 MHz.



Figure G.1: Diagram of the resonant frequency of the ion trap/resonant circuit system. The scale of this figure is 1 cm : 0.405 MHz. This figure was created by the x-y plot function on the spectrum analyzer.



Figure G.2: Diagram of the resonant frequency of the ion trap/resonant circuit system. The scale of this figure is 1 cm : 1.61 MHz. This figure was created by the x-y plot function on the spectrum analyzer.