A Theoretical Investigation of the Next Generation of MeV Ion Nanobeams

by

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This thesis investigates the design of quadrupole probe forming lens systems with resolution in the nanometre range. To achieve sub-micron resolution, big improvements must be made in focusing, lens aberration, and reduction of scattering processes. This thesis presents the results of a theoretical investigation into the performance of two-stage magnetic quadrupole lens systems with an intermediate focus. Such systems are capable of far greater demagnification than single-stage systems, but the challenge is to find a two-stage system with an acceptable ratio between demagnification and aberration. The results of a systematic survey of two-stage lens systems using the numerical raytracing technique to accurately calculate the lens aberrations of each system are presented.

This thesis also investigates the use of pre-lens electrostatic scanning with magnetic quadrupole lenses. It is shown that in spite of the large third order aberration of quadrupole systems, the use of dog-leg deflection systems in which the beam always crosses the optical axis at the entrance principal plane of the lens, can minimize distortion due to off-axis aberration.

An evaluation of the lens aberrations in microbeam and nanobeam systems caused by stray DC magnetic fields is also presented. The relative thickness of the beamline optical elements compared to the curvature of the beam in stray magnetic fields causes aberration where the beam axis differs from the optical axis of the lens system. Numerical raytracing is used to study the influence of stray DC magnetic fields on beam resolution at the sub-micron level.
Statement of Originality

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Chapter 1

Introduction

Improvement of the spatial resolution of nuclear microbeam systems has been a field of great interest since the development of the first collimated ion microbeam in 1953. The necessity for this improvement arises from the two fundamental applications of ion microbeams. Firstly a focused beam can be used as a sharp pencil to draw patterns on suitably sensitive materials. These can be processed to create complex structures which have very small lateral dimensions (tens of nanometres) but with straight sides for depths of tens of micrometres. Secondly, the beam can be used as a sensitive probe to allow us to do chemical analysis of objects on the nanometre scale.

These unique capabilities result from the physics of the interaction between high energy protons and the atoms of the samples, which is such that the particles penetrate for long distances (around 100 micrometres) without being deflected from a straight line path, yet at the same time they transfer enough energy to atoms in the locality of the ion tracks so that the solubility may change (to allow structures to be made) or radiation may be emitted which allows us to identify the chemical elements present.

The main disadvantage of using high energy protons is that they are difficult to focus to small dimensions and at the present stage of development the smallest spot with suitable current for analysis that we can achieve routinely is around 1 micrometre for analytical beam currents. This development took place in the UK over twenty years ago, and systems based on this work are widely used around the world. However, the expected progression to operation in the sub-micrometre region has not taken place.

The subject of this PhD is the design and creation of a “Nanobeam” capable of achieving resolutions in the order of nanometres, thus breaking this one micron barrier that has limited microbeam research in recent years.
1.1 Motivation

Focusing MeV ions to sub-micrometre dimensions is a major challenge both in fundamental physics and in high precision engineering. However, if the diameter of the ion beam can be reduced from the present level of 1 micrometre to 100 nanometres or below at analytical beam currents, then there are several compelling reasons for doing so: Firstly, a sub-micron beam will allow us to probe the chemical composition of samples with a far higher resolution (for example, to study the way that trace elements are distributed inside biological cells, or to characterise single environmental pollution particles). Secondly, the improvement in resolution from micron to sub-micron will give us the ability to use the beam as a ‘sharper’ ultrafine ‘scalpel’ to write patterns onto materials which can be processed to create the microscopic machines and structures which will form part of the nanotechnology revolution. This technique of lithography using MeV ions (also called proton beam writing - PBW) offers unique advantages of small feature size (<10nm) and long depth (>10μm), and 3-dimensional capability. Proton beam writing is set to become an important process for nanofabrication.

1.1.1 Ion Beam Analysis

One of the great strengths of nuclear microbeam analysis is the ability to carry out several forms of spectroscopy simultaneously. By scanning the beam across a sample and by having several radiation detectors in the chamber it is possible to carry out simultaneous PIXE (Particle Induced X-ray Emission) [34], RBS (Rutherford Back-Scattering analysis) [11], STIM (Scanning Transmission Ion Microscopy) [7], IBIC (Ion Beam Induced Charge) [8] and secondary electron imaging of the sample. The combination of these techniques together with the micron resolution mapping capability allows the measurement of the 2-D distribution of trace element concentration (detection limits of a few ppm for elements with atomic masses greater than magnesium), major element composition and elemental depth profiles.

Sub-micron probes will allow the extension of this capability to objects with length scales smaller than the present 1μm limit. Little is known about the distribution of trace elements on this scale, especially in biology, where sub-100nm spatial resolution will enable the exciting prospect of observing directly metal metabolism on the sub-cellular scale. It is outside the scope of this thesis to discuss each of these techniques in depth, but if more information is required then a number of detailed books exist on the subject [20], [5].

1.1.2 Proton Beam Writing

Proton Beam Writing (PBW) is a newly emerging advanced lithography technique using focused beams of MeV protons to expose sensitive materials and fabricate structures by direct writing [53]. PBW offers many advantages compared with conventional lithographies: the theoretical minimum lateral feature size may be as little as 5 nm, the sidewall angle can be very
close to 90 degrees for depths of tens of micrometres, it can be carried out in a wide range of materials and it is the only direct write lithography capable of forming three-dimensional structures at a scale of 1\,\mu m or less. This technique is so new that the potential of such high aspect ratio structures in micro- and nano-technology is still waiting to be explored. Obvious fields of application include integrated optics (waveguides, photonic bandgap devices), microfluidics and tissue engineering, but as with any novel capability it is likely that real niche applications are yet to be discovered.

1.1.3 Single Ions

An application that has not been mentioned thus far is the use of single ions. There is a growing interest in the use of aimed single ions as stimuli to probe objects or to fabricate very small structures. The energy deposited by single ions in a sample is confined to a track which may have a diameter of no more than a few nanometres. Thus by accurately targeting the ions, energy, damage, charge, or ions can be deposited in a very localised region, and the response of that region to single ions can be investigated.

The effect of cosmic radiation on electronic devices in satellites and spacecraft has been a problem in the past and is becoming more important with decreasing feature sizes. The radiation induces transient currents in devices, causing single event effects, which can eventually lead to the failure of the device. Single ions from a submicron nuclear microprobe can be used to target specific circuit elements of the device (transistors, capacitors, etc) and simulate single event effects [55].

Single ions can be generated in the nanobeam using a fast beam switch as part of the focusing system.

1.1.4 Cellular Irradiation

Charged particle beams consisting of light ions are an important development in radiotherapy. Conventional radiotherapy uses high energy photons (x-rays). Compared with conventional x-rays, charged particle beams can deposit their energy more selectively. As the particle passes through the tissue it loses energy due to inelastic scattering and finally comes to rest through nuclear interactions. For protons, the rate of energy loss in the tissue peaks immediately before the particle come to rest. This is called the ‘Bragg’ peak. By positioning the Bragg peak at the same depth as the tumour it is possible to maximise the dose to the tumour while minimising the dose to the surrounding healthy tissue.

During the 1990’s it became apparent [45] that the simple linear-quadratic relationship between cellular damage did not hold true at low doses. A group of effects, collectively termed the ‘non-targeted’ effects have begun to be discovered. These non-targeted effects include:

- The bystander effect, where cells other than those irradiated are damaged [49].
• Low dose hyper-sensitivity, where cell lines that are normally radio-resistant show extreme sensitivity at low doses of radiation [35].

Investigating the response of cells to single ions or precisely controlled numbers of ions will enable the mechanisms by which radiation damage occurs in living cells to be understood. For tumour cells, the information will feed directly into improved radiotherapy strategies. For healthy cells, it will provide information about how background radiation can initiate DNA damage and mutation that leads to cancer.

1.2 Microbeam Performance

To clarify the requirement for greater resolutions, we can quantify the performance of a microbeam for a given application or analytical technique.

The performance of a microbeam can be given in terms of the rate of counts, \( R \), detected:

\[
R = Y \Omega i
\]  
(1.1)

Where \( Y \) is yield of the ion beam analysis technique in use, \( \Omega \) is the detector solid angle, and \( i \) is the beam current delivered to the target.

The beam current transmitted to the target is dependent on the brightness of the beam, \( B \), and the acceptance of the beamline, \( A \):

\[
i = BA
\]  
(1.2)

Where the acceptance of the beamline is determined by the apertures in the system, as a combination of the initial beam diameter, determined by the object aperture diameters \( x_0, y_0 \) in the X and Y planes, and the beam divergence allowed by the collimator aperture. The object aperture is imaged onto the image plane by a lens with a short focal length.

![Schematic diagram of a microbeam system](image)

Figure 1.1: Schematic diagram of a microbeam system

The size of the apertures also determines the diameter of the focused image. The displacement of a ray in the image plane can be expressed by a polynomial related to the entrance co-ordinates \((x, y, \theta, \phi)\):

\[
x_i = \frac{x_0}{D_x} + x | \theta > \theta + \theta \delta + \ldots + \theta^3 + \ldots + f(x, y, \theta, \phi, \delta, \rho)
\]  
(1.3)
Where $x_o$ is the position of the particle in the object plane, and the $\langle \rho \rangle$ terms denote the aberration coefficients, determined by the geometry, magnetic field, and quality of the lens system. Beam divergence is denoted by $\theta, \phi$ in the X and Y planes respectively. The term $D_z$ denotes the demagnification coefficient in the x-z plane. In the first order approximation, the diameter of the beam spot in the image plane is given by the diameter of the object aperture multiplied by the demagnification of the beamline. This is referred to as the ‘geometric’ contribution to the image dimension. The dominant intrinsic microbeam aberrations are chromatic $< x | \theta \delta >$ and spherical aberration $< x | \theta^3 >$, where $\delta$ denotes a fractional momentum shift from the mean.

We can vary the proportions of the geometric contribution and the aberrated contribution to the final image by varying the dimensions of the object and collimator apertures, for a constant spot size in the image plane. Optimisation of aperture dimensions is complex, and is discussed in more detail in section 2.5. However if we consider a simple example, making the assumption that the only aberration terms to affect the image are chromatic, $< x | \theta \delta >$ and $< y | \phi \delta >$, then it can be shown that optimum transmission occurs when the geometric contribution is half the total image dimension. The optimum acceptance in this simple case is given by:

$$A_{opt} = \frac{1}{64} \frac{d^4}{\delta^2} \frac{D_x D_y}{< x | \theta \delta > < y | \phi \delta >}$$

Thus an acceptance dependence can be given as a function $f(C)$ of the aberration coefficients of the system:

$$A = xy\theta\phi = \frac{d^n}{f(C)}$$

Where $d$ is the desired spot size dimension in the image plane, and $n$ is dependent on the dominant aberration of the system:

- $n = 4$ for chromatic aberration, $< x | \theta \delta >$, $< y | \phi \delta >$.
- $n = \frac{8}{3}$ for spherical aberration, $< x | \theta^3 >$, $< y | \phi^3 >$.

So, it is clear that if we want improved spatial resolution without degradation of the count rate then we must investigate the following:

- The Ion source brightness which defines the minimum collimation that retains sufficient beam on the specimen.
- The probe forming lens system demagnification which provides the lower limits on the probe diameter.
- High yield reactions.
- The detector efficiency, in particular the solid angle, places a limit on the minimum usable beam current. The design of the data acquisition system is also important, since this limits the maximum rate at which data can be collected and hence the speed with which an image can be completed.
The first two points provide engineering limits on the spatial resolution of a nuclear microprobe system. The last two points constrain the time required to make a measurement with sufficient statistical accuracy and, importantly, convenience. They are particularly important with the advent of new technology detectors with high efficiency for the proton induced x-ray emission technique. However, investigation of these last two points does not fall into the field of beam optics, and is therefore considered outside of the scope of this thesis.

Several powerful analytic techniques are available for use with modern microbeams, the key four of these being:

- Proton (or particle) Induced X-ray Emission (PIXE).
- Elastic (or Rutherford) backscattering (RBS).
- Nuclear Reaction Analysis (NRA).
- Scanning Transmission Ion Microscopy (STIM).

However, as shown in equation 1.1, the performance of a microbeam lies in the yield of the applied technique, and as such we should note that the yield, $Y$, required for good PIXE, RBS, NRA analysis is in the order of $Y \sim 10^{-7}$ with modern detectors, roughly equivalent to $100\mu$A. Whereas, for ion microscopy and single ion techniques $Y = 1$, requiring currents in the order of femto-amps, allowing a much finer resolution.

1.3 Components of a Microbeam Facility

The important components of an nuclear microprobe facility are the ion source, the accelerator, an energy filter, such that a beam can be produced of a monochromatic energy, and a beam-transport system to deliver and focus the beam onto the target.

This thesis concentrates on the behaviour of the beam transport system between the object aperture and the image plane. However it is necessary to introduce the entire system of a nuclear microprobe before beam optics can be discussed.

Figure 1.2 shows a schematic diagram of the Surrey microprobe system up to the object slits, starting from the duoplasmatron ion source, to the 2MeV High Voltage Engineering Tandem accelerator, and ending at the switcher magnet.

1.3.1 The Ion Source

At the University of Surrey Ion Beam Centre, a duoplasmatron ion source is used. A schematic diagram of a duoplasmatron ion source can be seen in figure 1.3. The duoplasmatron source is a very efficient high-brightness source and is routinely used at the University of Surrey for the production of hydrogen, helium and oxygen ions.
The free electrons are produced by boiling them off a heated cathode. Atoms of the gas are injected into a chamber containing the cathode and a positively charged (20 kV) anode. There is a potential difference between the cathode, the heated filament, and the anode. As the electrons accelerate toward the anode, they collide with the molecules of the gas, producing ions. Negative ions are produced by dissociative electron attachment, whereas positive ions can be produced if the energy of the electron is greater than the ionisation energy.

The ions are then focused electrostatically and magnetically by the shape of the electric and magnetic fields into a dense plasma in the region just before the anode aperture. The plasma bulges slightly through the anode aperture forming an “expansion ball”. The negative ions are then selected by an extractor which is at ground potential. A sheath exists at the boundary of the plasma core containing negative ions, and they can be extracted by offsetting the anode aperture.[19]. The spatial resolution of a nuclear microprobe system is strongly related to the brightness of the ion source. The brightness of the beam injected into the accelerator is determined by the physical processes taking place in the ion source. For a given ion source the brightness cannot be increased by subsequent ion-optics system.

1.3.2 The Einzel Lenses

The Einzel lenses are used to focus low energy ions from the source before they enter the MPI (Multi-Purpose Injector) magnet. The Einzel lenses are the only focusing elements before the accelerator, and are therefore essential in order to achieve good transmission of the beam through the accelerator. A strong lens effect exists at the entrance to the acceleration tube, and the Einzel lens are crucial to overcome this, such that beam brightness is not lost during injection of the beam into the accelerator.

The Einzel lenses are electrostatic, and therefore their ability to focus ions is dependent on the energy of the ions.

![Figure 1.2: Schematic diagram of Tandem accelerator and ion source][51]
Figure 1.3: Duoplasmatron Source [9]

Figure 1.4: Einzel lens [59]
1.3.3 The Accelerator

The function of an ion accelerator in an ion microbeam is to accept the ions produced in the source, and accelerate them to a high energy and inject them into the energy filter, which in most microbeam cases is a switcher magnet, or a 90 degree bend magnet.

It will be shown later in this report that the key requirements of an accelerator for microbeam operation are low momentum spread and optimum transmission of beam brightness. All lens systems suffer from chromatic aberration, which will be discussed in chapter 2. Electromagnetic lenses tend to over-focus ions whose energy is less than that of the mean-beam energy, and under-focus ions whose energy is greater than that of the mean. Thus a beam with a large momentum spread will have a resultant beam focus degradation due to the halo caused by chromatic aberration. Recent improvements in the terminal voltage stability of modern accelerators have meant that the beam delivered from the accelerator is nearly monoenergetic, reducing the effect of chromatic aberration. However, historically, the larger energy spread in old accelerators meant that many early microbeams were affected by chromatic aberration.

A common debate in the microbeam field examines the relative benefits and disadvantages of using single-ended or tandem accelerators for microbeam applications. It is widely accepted that the single-ended accelerator generates a higher-beam brightness, and lower energy spread than that of tandem accelerators, which is favourable for the reasons discussed above. However, tandem accelerators offer a higher-beam energy at the same terminal voltage, combined with an external ion source, allowing easier and less time-consuming maintenance [54]. In single-ended systems, the ion source must be incorporated within the pressure vessel.

The Tandem Accelerator is a form of electrostatic generator that uses a two-stage principle to utilise the terminal voltage twice. These negative ions are accelerated up the accelerating tube to the positively charged terminal where they enter a stripping canal with a foil or gas stripper, which removes \( n + 1 \) electrons. Here they emerge as an ion with a charge of \( ne \) where they continue to be accelerated towards ground potential. Thus the final energy is \( (n + 1) \times \text{terminal potential} \), and the net result is an ion with the kinetic energy of \( (n + 1)eV \) [38]. The stripper, used to change negative ions into positive ions, degrades the brightness of the final accelerated beam due to scattering, and can increase the energy spread due to energy straggling, but studies of this effect on the Oxford microprobe system by Grime et al. [22] suggest that an optimum stripper pressure exists which represents a trade-off between stripping efficiency and brightness.

Grime states in [22] that significant factors in the loss of brightness in accelerators are from aberrations in the injector region of the first accelerating tube, and in the stripper of tandem accelerators. In the stripper, small angle scattering causes the beam to diverge, and thus degrades the brightness. The necessity and presence of a stripper in tandem accelerators separates their performance in terms of brightness from that of single-ended accelerators, where a stripper is not required to generate ions for a second accelerating stage.
Grime has used the beam optics program MULE to calculate the effect of stripper gas density on the normalised emittance of a beam passing through the stripper, and presents the results in [22]. His results show an increase in beam emittance as the stripper density increases, and consequently a fall in the brightness of the beam.

![Schematic of the University of Surrey Ion Beam Centre 2MV Tandetron Accelerator](image)

1. Cockcroft-Walton Stack
2. Q-snout electrode
3. L.E. Accel tube
4. Gas Stripper
5. Terminal
6. H.E. Accel Tube
7. E/S Quad. Triplet

Figure 1.5: Schematic of the University of Surrey Ion Beam Centre 2MV Tandetron Accelerator[51]

1.3.4 Terminal Voltage

In early microbeam systems chromatic aberration was the dominant aberration limiting the improvement of microbeam resolution. Chromatic aberration in the microbeam stems directly
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from the chromatic spread of the beam delivered from the accelerator. Therefore it is critical
that the voltage ripple at the terminal is minimized. Three methods of generating high stability
terminal voltages are discussed.

Van de Graaff
The Van de Graaff belt-charged electrostatic generator as a method for particle acceleration is
named after its inventor R.J. Van de Graaff. Van de Graaff described his first generator to the
American Physical Society in 1931 [13]. In the early years of focused ion beams, the simple
construction and the steady direct voltage made this method favourable as a voltage source for
positive-ion acceleration.

A schematic diagram of a Van de Graaff electrostatic generator is shown in figure 1.6. A rounded
high-voltage terminal is supported by an insulating column. A moving belt carries
charge to the terminal. The belt runs from a motor-driven pulley at ground potential to a pulley
within the terminal. Electric charge is sprayed on the belt at the grounded end from a fine wire
or from a row of corona points extended across the width of the belt. This charge is carried by
the belt into the terminal, and is removed by a corona-point collector, electrically connected
to the terminal. If the pulley within the terminal is well insulated, it will rise to a potential
sufficiently above that of the terminal to maintain the necessary corona discharge. The charge
appears on the outer surface of the terminal, so that the area inside of the terminal is field
free. Thus the charging process occurs within the grounded base, and the discharging process
occurs within the equipotential terminal. Both these operations are separately controllable,
and independent of terminal voltage.

Charge carried on the belt produces a steady current \( i = \frac{dQ}{dt} \), and this gives an electrostatic
potential on the terminal. If \( C \) is the capacitance of the terminal to ground, the terminal will
be raised to a potential \( V \) by a charge \( Q = CV \), and the rate of increase of potential with time
is given by:

\[
\frac{dV}{dt} = \frac{i}{C} \tag{1.6}
\]

The magnitude of the corona spray current is usually controlled by varying the primary ac
voltage, and in this way determining the potential to which the terminal will rise. It is also
possible to spray charge of the opposite sign on the descending belt within the terminal, and
collect it at the grounded terminal. In this manner, the charging current is doubled.

Current can return to ground from the high voltage terminal by many paths. The useful
current is the beam of accelerated ions down the accelerating tube. However, stray ions may
strike the tube walls and hence be accelerated up the column to produce X-rays on striking the
ion source. Frequently a resistive load is built in the insulating column, uniformly distributed
along the length of the accelerator tube to form a potential divider.
Figure 1.6: Van de Graaff Electrostatic Generator

Figure 1.7: A horizontal Van de Graaff accelerator for 4Mev protons[38]
CHAPTER 1. INTRODUCTION

Pelletron Charging Chain

The Pelletron charging chain is a trademark of National Electrostatics Corporation (NEC). The Pelletron charging chain is in essence similar in principle to that of the Van de Graaff charging belt. However, instead of a belt, a Pelletron chain is made of metal pellets connected by insulating nylon links. The metal pellets are charged by electrostatic induction from an electrode.

Positive charge is induced onto each up-going pellet by an inductor while they are in contact with the grounded drive pulley. Since the pellets are still inside the inductor field as they leave the pulley, they retain a net positive charge. The chain then transports this charge to the high-voltage terminal, where the reverse process occurs. When it reaches the terminal, the chain passes through a negatively-biased suppressor electrode which prevents arcing as the pellets make contact with the terminal pulley. As the pellets leave the suppressor, charge flows smoothly onto the terminal pulley, giving the terminal a net positive charge.[52][25].

A single-ended Pelletron accelerator located in a temperature-controlled environment can be voltage stabilized to within 75 to 100 V/h using a rotating vane generating voltmeter and a capacitor pickup to provide error signals and a corona probe to make corrections[17].

Cockcroft-Walton Voltage Multiplier

The first successful acceleration of particles using the voltage multiplier method was achieved by Cockcroft and Walton in 1932 [12]. Today the principle of accelerating particles using a voltage multiplier principle is commonly referred to as “a Cockcroft-Walton stack”.

The principle of a voltage multiplier is that capacitors are charged in parallel and discharged in series. It operates on alternating current, using one half cycles to charge the capacitors, and the other half-cycle to transfer the charge, as directed by the rectifiers, resulting in a steady direct voltage [38].

The output voltage multiplication factor N is equal to the total number of capacitors in the multiplication stage, assuming no current drain. With finite current drain, the output voltage is reduced below the optimum, and ripple is present in the output. Lorrain gives the results in the following form [41]:

\[ V = NV_i - \frac{I}{12fC} \left( N^3 + \frac{9}{4}N^2 + \frac{1}{2}N \right) \]  \hspace{1cm} (1.7)

Where V is the output voltage, \( V_i \) is the input voltage, frequency \( f \), capacitance \( C \) and load current \( I \).

The ripple voltage is given by equation 1.8

\[ \pm V = \frac{I}{16fC}N(N+2) \]  \hspace{1cm} (1.8)

Table 1.1 shows a comparison of manufacturers specifications for terminal voltage ripple for a Pelletron and Tandetron accelerator. Tandetron 2MV
Figure 1.8: A Cockcroft-Walton Voltage Multiplier Circuit

<table>
<thead>
<tr>
<th>Accelerator</th>
<th>Manufacturer</th>
<th>Terminal Voltage Ripple (± V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1MV Pelletron (Single ended)</td>
<td>NEC[17]</td>
<td>75</td>
</tr>
<tr>
<td>2MV Tandetron (Tandem)</td>
<td>HVEE[10]</td>
<td>30</td>
</tr>
</tbody>
</table>

Table 1.1: Manufacturers specifications for Terminal Voltage Ripple
1.3.5 The Switcher Magnet

The switcher magnet used in the Surrey Tandetron Accelerator facility serves two purposes. Firstly, it allows the beam from the accelerator to be directed into one of four beamlines. Secondly, it acts as a momentum filter for ions which enter the selected beamline. The magnetic field of the switcher magnet separates ions with respect to their momentum by deflection angle. As such, only ions with the desired momentum will pass through the object slits of the chosen beamline.

If the energy stability of the accelerator is insufficient to form a good focus with the lens system, then it is common to employ slit-stabilisation systems in which the charge collected when the beam strikes either the outer or inner jaw of the object slit with respect to bend angle can be fed back to the control system of the accelerator to adjust the accelerating potential appropriately. However, the terminal voltage stability of the Tandetron accelerator used at the University of Surrey Ion Beam Centre is of sufficiently high specification that this technique is unnecessary.

1.4 The History of Ion Microbeams

Zirkle and Bloom were the first to develop a collimated microbeam, in 1953, at the University of Chicago [62]. The system operated by passing a 2MeV proton beam from the vacuum of an accelerator, through a thin mica window, and then through a 2.5µm scratch on one of a pair of optically flat jaws, with which they targeted animal cells [20]. However, although the beam intensity in this design was ideal for their purpose, it was far too low for the analytical techniques discussed in chapter 1.1. Thus, a significant time period ensued before the first attempts to use collimated microbeams for positional analysis. These attempts appeared in the same issue of Nature in 1966, by two groups, Pierce, Peck and Cuff at Harwell, UK, and Mak, Bird and Sabine, at Lucas Heights, Australia [36]. The resolution of these collimated probes quickly improved to below 100µm, but it was realised that the brightness of the beam delivered from the ion source must be improved if collimated beams were to achieve better resolution. Ferguson suggested at this time that the beam from a moderate size collimator might be tightly focused by a quadrupole lens. This does not increase the brightness of the beam, but accepts a greater of volume of beam into a spot size on target of the same (or smaller) diameter. This suggestion really defines the starting point for focused ion microbeams, and this thesis will focus exclusively on microprobe systems using quadrupole lenses for beam focusing.

The first focused ion microprobe was constructed at Harwell in 1969, and achieved a spatial resolution of around 2.2µm with a beam current of 250pA [31]. The Harwell microprobe used Dymnikov’s Russian Quadruplet geometry, which included the ability to scan the beam [36]. Dymnikov’s design, which became known as the “Russian Quadruplet”, was first investigated as a replacement for round lenses in high energy electron microscopes. This system was
CHAPTER 1. INTRODUCTION

built at Harwell in 1969 [19]. The "Russian Quadruplet" configuration consists of two successive identical doublets, in which the polarity of the lenses in the second doublet is reversed from that of the first lens such that the fields in the identical lenses of the two doublets are rotated through 90 degrees relative to each other [15]. Figure 1.9 shows the beam envelope of the Harwell Microprobe with its Russian Quadruplet lens configuration. The beam envelope was traced using MULE, a matrix based optics code developed by G.W. Grime.

![Figure 1.9: Harwell Microprobe Beam Envelope](image)

The Harwell Russian Quadruplet was capable of achieving demagnifications of -5.6 in both the X and Y planes. [20]. Due to the low aberrations associated with this geometry, the image diameter was determined largely by the object aperture, which was an 18μm pinhole, thus forming an image of 4μm.

Variations of the Russian Quadruplet geometry were used by several other microbeam laboratories around the world, most notably the Melbourne system, which differs in that the outer two lenses are two-thirds the length of the outer lenses giving a demagnification of -20 in both planes [36]. Figure 1.10 shows the beam envelope for the Melbourne Microprobe geometry.

In the early 1980's Grime and Watt developed the high excitation coupled triplet lens, achieving the first microprobe with a resolution of 1 micron [57]. In beam optics this represented the next significant breakthrough, which came as a result of a survey of many different lens configurations. In the Oxford Triplet configuration, the first and second lens share a power supply, and thus have equal but opposite excitation. The demagnification of the Oxford Triplet configuration is far higher than the previous system, but the aberrations are also large. The effect of the large aberrations can be controlled by reducing the angular divergence of the beam [36] [20] [57]. The beam envelope for the Oxford High Excitation coupled triplet lens configuration is shown in Figure 1.11. The Oxford Triplet system has demagnifications of 68
and -15 in the x and y planes respectively. It is reported that the Oxford Scanning Microprobe could achieve 0.5\( \mu \)m resolution for beam currents of 25pA. [21]. Today, most of the existing quadrupole microprobe systems are similar in configuration to those we have discussed, employing a combination of between two and four lenses, ranging from the simple doublet to systems similar to the Oxford or Melbourne configuration.

It can be seen on figure 1.12\(^1\) that until recently few systems have been able to improve

---

\(^{1}\)Please Note: Figure 1.12 does not attempt to detail the resolution of all existing microbeams. The author has included only those microbeams capable of achieving resolutions near the leading edge of microprobe development for the age.

---

Figure 1.10: Melbourne Microprobe Beam Envelope

Figure 1.11: Oxford High Excitation Coupled Triplet Beam Envelope
Resolution of Microbeam Systems

Figure 1.12: Resolution of microbeam systems at analytical beam currents since 1953 [20]

significantly upon the 1\(\mu\)m resolution achieved at analytical beam currents by Grime and Watt in the 1980's [57]. Currently, the leading microbeam system in the world in terms of resolution is at the National University of Singapore. This beamline has achieved resolutions of 290 x 400nm with its high-excitation triplet of magnetic quadrupole lenses, at a beam current of 50pA [58], and smaller resolutions at much lower beam currents. However the new CENBG nanobeam line developed at the University of Bordeaux is expected to achieve resolutions of 300nm in high current mode, and below 100nm in STIM mode[2].
1.4.1 The One Micron Barrier

The fundamental limitations facing the improvement of spatial resolution in microbeam facilities can be divided into two groups: The limiting factors which are intrinsic to the physics of microbeam design, and those which arise due to the practical limitations for the construction of a microbeam facility.

Intrinsic resolution limitations belong mainly to scattering processes, in the form of slit scattering, and gas scattering, and the aberrations of the lens system.

Slit scattering occurs when slits are used to create an aperture through which the beam can pass. The problem is most significant at the object aperture due to the large volume of beam that falls on this aperture compared to the region of the slit where scattering occurs. In an ideal slit design, any beam striking the slits would be completely stopped, however, this is not the case. At the leading edges of the slit, an area exists that is 'transparent', i.e. this area has insufficient thickness to completely prevent an ion from traversing it. Thus some ions are allowed to pass through this transparent region of the slit, and suffer an energy loss combined with a random change of direction. These ions will be over-focused by the lens system, and will result in highly aberrated rays. This is possibly the most significant limitation facing microbeam design today.

This effect is shown in figure 1.13. If it is assumed that the slits are composed of identical slit jaws where the jaw has a circular edge, as shown in figure 1.13, then the area of transparent slit is defined by the range of the ions in the slit material, \( \rho \). The height of this region of slit presented to the beam is:

\[
R - \frac{1}{2} \sqrt{4R^2 - \rho^2}
\]  

(1.9)

Where \( R \) is the radius of the slit jaw.

\[
\frac{\text{Scattered flux}}{\text{unscattered flux}} = \frac{\rho^2}{2Rd}
\]

(1.10)
Therefore the ratio of scattered beam to unscattered beam is given by equation 1.10. If the design of the slit jaw is optimum, then the length of the transparent region is fixed. Thus the ratio of scattered to unscattered beam can only be improved if the separation of the jaws is increased, which requires beamlines with high demagnifications.

Gas scattering is a process that occurs over the whole length of the beamline whenever an ion collides with a residual particle due to incomplete vacuum. The result is a general beam broadening. Gas scattering can be significant in the bore aperture of a quadrupole lenses system, where the small bore diameter of the lens forms a restriction against good pumping. It is important to ensure that this region is well pumped.

The practical limits challenging the design of microbeams today are engineering issues encompassing the design and construction of not just the microbeam itself, but the infrastructure of the facility supporting the microbeam. This thesis covers many of the issues related to the design and beam optics of the microbeam system, but two engineering issues that are fundamental to achieving sub-micron resolution must be mentioned here:

- Quadrupole field purity
- Quadrupole power supply stability

Both of these issues have been solved in modern microbeam systems. Modern quadrupole lenses are cut to micron precision from a single stress-relieved billet of high quality magnet iron. Thus lens aberrations caused by deviation from perfect four-fold symmetry are now negligible. Quadrupole power supplies are available which have stability of one part in 100 thousand which is adequate for submicron precision.

The most important engineering limitations of the construction and facility are:

- Vibration
- Stray magnetic fields

Vibration of the microbeam can result in minute variations of the target with respect to the object aperture, or optical elements. If the target is moving in respect to the beam axis, the result will be that the positional accuracy of the beam on the target is degraded, and thus the effective ability to focus the beam to a given position on the target. Sources of these parasitic vibrations may originate from sources both internal and external to the laboratory. Some common sources of vibration in the Surrey experimental hall are:

- Vacuum pumps, especially rotary pumps, or other devices with moving parts.
- Foot-fall within the laboratory, especially upon the steel cable-trays integral to the laboratory floor surface.
- The passage of trains on the section of railway that runs closest to the Ion Beam Centre.
• The passage of motor vehicles over the speed-bumps located on the University perimeter road.

Another fundamental practical limitation of high resolution microbeam design is the presence of stray magnetic fields within the experimental hall. If a stray field is present near the beamline, then the magnitude of its influence at the target can be directly related to the strength of the field. The layout of electronic equipment in the experimental hall should be carefully considered to minimise sources of stray magnetic fields. The proximity of the source of the stray field to the object aperture is also critical, by virtue of the fact that this provides the stray field within the maximum lever arm over which to deflect the beam before it reaches the target. A more detailed investigation of stray fields will follow in chapter 8.

In summary, we have discussed a variety of factors, both intrinsic and practical, which will challenge the designer of a nanobeam. However, we have not thus far mentioned the fundamental beam optics as a limitation in the resolution of nanobeam design.

The pursuit of the optimal design with respect to beam optics is equivalent to the holy grail for microbeam designers, since it allows the designer not only to reduce the aberrations limiting the system, but also to reduce the influence of the intrinsic and practical limitations mentioned above. For this reason the study of beam optics forms a significant part of this thesis on nanobeam design.
Chapter 2

Beam Optics

2.1 Liouville's Theorem

The art of beam optics is matching emittance to acceptance. To understand the term *emittance*, we must first understand what a *beam* is. To completely specify a particle within a 3 dimensional Cartesian coordinate system, we need to know its three co-ordinates, \(x, y, z\), and the three momentum components, \(p_x, p_y, p_z\). All this information can be represented as a point within a 6 dimensional *phase space*. As the particle travels in the beam, it will move around within this phase space. Thus, a beam is represented by a group of points within phase space, one for each particle in the beam, and for a beam of finite dimensions, the representative points will lie within a 6 dimensional hypervolume.

Liouville's theorem states that:

*Under the action of forces which can be derived from a Hamiltonian, the motion of a group of particles is such that the local density of the representative points in the appropriate phase space remain constant.* [1]

For beam optics, Liouville's Theorem imposes restrictions on what can be done without loss of beam current, because of the need to conserve the 6 dimensional hypervolume. If we choose the \(z\) axis as the direction of propagation, then it is possible to make a conceptual simplification if we assume that the three components of motion are mutually independent in real space, and thus in phase space the motion is confined to three planes, \((x, p_x), (y, p_y)\) and \((z, p_z)\) which can all be treated separately, hence Liouville's Theorem can be simplified to mean that the areas of the regions containing the representative points in each plane remain invariant [1]. Another simplification is possible if we assume that the axial momentum of the beam remains constant and the magnitude of transverse momenta is far less than that of the axial momentum. This is true whenever the beam is not accelerated on the \(z\) axis, i.e in beamlines. In this case, the angular divergence of a beam relative to the beam axis is equal to the ratio of the transverse and axial momenta, and thus \(p_x\) is replaced by \(\theta\) and \(p_y\) is replaced by \(\phi\) and \(p_z\) can be dealt
with a fractional momentum spread. In simple terms the implication of Liouville’s theorem is:

\[
\text{If you confine the beam in space you make it more divergent and if you try to make the beam more parallel, the diameter has to be bigger.}
\]

If the 6 dimensional phase space of the beam is projected onto a two dimensional plane, then a beam can be characterised by the area it occupies, \(A\), in that phase-space, its emittance \(E\), defined by equation 2.1, where \(A\) is the acceptance defined in equation 1.2.

\[
E = \frac{A}{\pi}
\]

The \(\pi\) term in the equation comes from the elliptical nature of phase-space contours. Ellipses are used to describe beams in phase space due to the relation that a single particle travelling in an infinitely long converging quadrupole will trace an elliptical path in the phase space due to harmonic oscillation. A more detailed explanation of emittance and phase space contours can be found in [1]. The term acceptance refers to an phase space volume defined by the apertures or slits of the beamline.

It is clear that the emittance of a beam is invariant only when the axial momentum of the beam \(p_z\) is constant. This is an acceptable assumption when discussing the emittance of the beam within the beam-line. However, if we wish to compare emittances from the ion source and accelerator where the beam is within the accelerating field, then we must multiply the emittance by a factor proportional to the axial momentum to maintain its invariance. The resulting term is named normalised emittance, \(E_n\).

\[
E_n = E \left(KE\right)^{\frac{1}{2}}
\]

Where \(KE\) is the kinetic energy of the beam in units of MeV. The units of normalised emittance are \(\text{mm.mrad.MeV}^{\frac{1}{2}}\).

### 2.2 Emittance - Acceptance Matching

When the emittance of the beam exceeds the acceptance defined by the slits or apertures of the beamline system, then only a fraction of the injected beam can be transmitted. However, for optimum transmission the phase-space ellipse for the emittance of the system must be brought into coincidence with the phase-space ellipse for the acceptance of the beamline. The procedure for achieving this is known as ‘matching’.

The emittance of a beam is invariant due to Liouville’s theorem, but the shape and orientation can be modified. In field-free drift regions of the beamline, the displacement of a ray from the beam axis will change, but the divergence of the ray will remain constant. Over a drift of
length \( l \) the phase space ellipse will be transformed by the slant relation:

\[ (x, \theta) \rightarrow (x + l\theta, \theta) \]  

(2.3)

This effect is shown in figure 2.1. The location of a “waist” in the beam can be identified where the slant of the phase-space ellipse is zero.

The action of a thick lens on the phase-space ellipse of a beam in shown in figure 2.2. If a divergent ray entering the lens is focused sufficiently to become convergent then the phase-space ellipse is reflected across the displacement axis. The width of the phase-space ellipse may also be reduced depending on the length and excitation of the lens.

By means of an appropriate combination of drift spaces and lenses, any ellipse can be transformed into any other ellipse having the same area, and thus optimum transmission can be achieved.
Figure 2.2: Action of a thick converging lens on the emittance phase space ellipse
2.3 The Quadrupole Field

In order to understand the nature of a quadrupole focusing system, it is necessary to discuss the nature of the magnetic field associated with a quadrupole magnet. An ideal normal quadrupole magnet is a magnet, which, within its aperture, produces a two-dimensional magnetic flux density parallel to the plane and such that:

\[ B_x = G \cdot y \quad B_y = G \cdot x \quad (2.4) \]

where \( G \), the magnetic field gradient is defined by:

\[ G = \frac{B_p}{r_0} \approx \frac{2\mu_0 n I}{r_0^2} \quad (2.5) \]

where:
- \( B_p \) = the magnetic field at the pole tip
- \( r_0 \) = the quadrupole aperture radius
- \( nI \) = the total ampere turns per pole

The field lines within a quadrupole magnet are rectangular hyperbolae, asymptotic to axes inclined at 45 degrees to the x and y axes of the beam, as shown in figure 2.3. Hence the displacement from the origin gives rise to a linear defocusing or focusing action on the charged particle beam.

It is also possible to construct electrostatic quadrupole lenses, in which the force on a charged particle is parallel to the field lines. However, electrostatic quadrupoles are not widely used since the pole voltages required are proportional to the particle energy, which could be problematic for high energy ions.

To obtain a net focusing effect along both x- and y-axes, focusing and defocusing quadrupole magnets can be used alternately in series [19].
For matrix methods of calculation, discussed in section 3.1, a simple profile for the longitudinal field of a quadrupole lens will be used. Since the fringing fields of the quadrupole lens are challenging to model analytically, a simple rectangular field profile will be used, based on an effective length marginally greater than the mechanical length to provide some empirical correction for the effect of the fringing fields upon the field profile of the quadrupole magnet. Three dimensional quadrupole fields are described in more detail in section 3.2.2. Fringing fields will also be examined in section 3.2.3.

2.4 Aberrations

The position of a particle in the image plane can be expressed by equation 2.6.

\[ x_i = \frac{x_o}{D_x} + < x | \theta > + < x | \theta \delta > + ... + < x | \theta^3 > + ... + f(x, y, \theta, \phi, \delta, P) \]  

(2.6)

Where \( x_o \) is the position of the particle in the object plane, and the \(< | >\) terms denote the aberration coefficients. The dominant aberrations for microbeam systems are shown in table 2.1, and an explanation of the parasitic aberration is provided in figure 2.4.

Due to lens aberrations, the final position of a particle having passed through a lens system is not only dependent on the initial position of that particle in the object plane, but also on the path taken by that particle through the magnetic or electrostatic fields comprising the system, and the momentum shift from the mean.

Quadrupole lenses suffer from many different types of imaging aberration, and the final resolution of the microbeam is a trade-off between a high demagnification, or large system aberrations. In a perfect lens, the image would be a prefect reproduction of the object, demagnified by the demagnification coefficients \( D_x, D_y \). However, each ray enters the system with an initial position in the x and y planes, \( x, y \), and an initial divergence, \( \theta, \phi \). As such, each ray experiences slightly different forces upon it, due to a range of aberrations, and thus its final position will not only be determined by the demagnification, but also by the combined effect of the aberrations.

Wollnik illustrates the influences of lens aberrations excellently in [60], as shown in figure 2.5.

2.4.1 Astigmatism

We have already described the quadrupole lens, we know that a single quadrupole will form a line focus. The term astigmatism refers to the difference in line foci positions between the x and y planes for a quadrupole system. Hence for a focused system, the astigmatism terms should be zero.
<table>
<thead>
<tr>
<th>Order</th>
<th>Coefficient</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st Intrinsic</td>
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<td>x &gt;$</td>
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<tr>
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<tr>
<td></td>
<td>$&lt; x</td>
<td>\theta &gt;$</td>
</tr>
<tr>
<td></td>
<td>$&lt; y</td>
<td>\phi &gt;$</td>
</tr>
<tr>
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</tr>
<tr>
<td></td>
<td>$&lt; y</td>
<td>\phi^3 &gt;$</td>
</tr>
</tbody>
</table>

Table 2.1: Dominant Aberrations in Quadrupole Systems
2.4.2 Parasitic aberrations

The dominant parasitic aberrations listed in table 2.1 arise due to misalignment of optical elements from the beam axis. Since each element can be independently misaligned, the parasitic terms listed in table 2.1 carry a \( n \) subscript, where \( n \) denotes the number of the quadrupole to which the aberration relates. Translation is the transverse misalignment of a quadrupole from the optical axis. The terms \( <x|U_n> \) and \( <y|V_n> \) indicate translation in the \( xz \) and \( yz \) planes respectively. Tilt occurs in the \( xz \) plane when a quadrupole is rotated about its \( y \) axis, and in the \( yz \) plane when a quadrupole is rotated about its \( x \) axis. \( x \) tilt and \( y \) tilt are denoted by \( <x|\alpha_n> \) and \( <y|\beta_n> \) respectively. Translation and tilt aberration coefficients contain no dependence on the angular divergence of the beam, and are thus considered aberrations of the zeroth order. Hence the effect of translation and tilt is a simple transverse displacement of the image from the beam axis, as shown in figure 2.5. Both translation and tilt can be easily removed by quadrupole alignment procedures. Rotational misalignment occurs when a quadrupole is rotated about the beam axis, as shown in figure 2.4. Rotation misalignment terms are denoted by \( <x|\phi \rho_n> \) and \( <y|\theta \rho_n> \). Rotational misalignment is simple to remove since the rotation of one quadrupole lens within a system is sufficient to compensate for the rotational misalignment of the other lenses. It is easy to identify rotational misalignment since the cross-coupling nature of the misalignment gives an rhombus shaped beam-spot that appears to rotate as the aberration is minimised. A fourth parasitic aberration arises from excitation changes to a quadrupole, causing an aberration which is angle dependent to the first order. This aberration is denoted by \( <x|\theta \varepsilon_n> \) and \( <y|\phi \varepsilon_n> \) where \( \varepsilon \) denotes a percentage change in the excitation of a quadrupole.
CHAPTER 2. BEAM OPTICS

Figure 2.5: Intensity distributions in the image plane for systems causing aberrations of the zeroth, first, second or third order. [60]
2.4.3 Chromatic Aberration

Chromatic aberration is caused by the dependence of the focusing force in a quadrupole lens on the momentum of a particle. Thus for beams with large momentum spread, particles within the beam of different momenta will experience different axial forces resulting in a broadening of the beam spot. Energy or momentum change of a particle is usually expressed as a fractional shift in momentum from the mean:

\[ \delta = \frac{\Delta(mv)}{mv} \]  

(2.7)

2.4.4 Spherical Aberration

Spherical Aberration arises from the fact that particles travelling in the lens with a divergence from the beam axis experience a slightly different force from particles moving parallel to the axis, as assumed in the paraxial approximation. Thus it is not possible to make the assumption that the axial velocity remains constant or that the force is radial. The effect of spherical aberration is that rays of different initial divergence are focused to different positions on the z axis. This can be seen in figure 2.6. The cross-terms, \(< x | \theta \phi^2 >\) and \(< y | \theta^2 \phi >\) are responsible for drawing the beam spot out into the characteristic cross shape associated with spherical aberration in the Oxford Triplet lens geometry; This is illustrated by figure 2.7 which shows the beam spot due to a number of rays traced from a single point in the object plane, referred to as the "point-spread".

2.5 Optimisation

The recent discussion of aberration leads us to the conclusion that, apart from the simple demagnification term in equation 2.6, the dominant terms defining the beam diameter in the image plane are all dependent to some degree on the entrance divergence of the beam, and not the object size. It is therefore clear that the beam spot observed on target will be composed of the demagnified object, referred to as the geometrical component of the image due to its dependence on the object, and a halo of aberration, referred to as the aberrated contribution to the image, which is dependent on divergence. None of the present applications of microbeams require that the image is a quality reproduction of the object, but are merely concerned with focusing maximum beam current into the minimum beam spot diameter. Therefore, the best focus will be a combination of the geometrical and aberrational contributions, chosen to maximise the overall acceptance whilst ensuring that all rays pass within a certain diameter in the image plane.
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Figure 2.6: Simulation of rays of varying divergence in image plane for Bordeaux-Rossendorf Nanobeam; The difference in focal position is due to spherical aberration.

Figure 2.7: Simulation of a beam spot due to “point-spread” for the Surrey Microbeam
2.5.1 Jamieson and Ryan's Figure of Merit

The somewhat complex relationship between demagnification, aberration, and optimum beam current necessitates that a figure of merit is defined such that microbeam geometries can be compared easily by some figure that adequately explores the parameter space describing a microbeam geometry. Jamieson and Ryan define such a figure in [50], which they have used to explore the possibilities for the design of the CSIRO-GEMOC quintuplet microbeam system.

This figure of merit is designed to reflect the maximum beam current into a given spot size under the effects of spherical aberration, since it recognises the favourable effect of greater demagnification, and also the unfavourable increases in spherical aberration, often associated with greater demagnification.

It is easy to derive this figure of merit based on a few simple assumptions. If a uniform beam-brightness distribution is assumed, such that the beam-current is proportional to the phase-space accepted by the system, defined by the object and collimator apertures, then we can find a ratio of geometric and aberrational terms necessary for the optimum focusing of current into a given beam spot-size.

If we assume that spherical aberration is the dominant aberration of any microbeam system, and that chromatic aberration and the spherical aberration cross-terms are of negligible importance, then the position of a ray in the image plane can be defined by the contribution of geometric and aberrational terms in respect to the object co-ordinates of the ray.

This can be described by equation 2.8 where the image size is the sum of the geometric and aberration coefficients in quadrature.

\[ x_i^2 = \left( \frac{x_0}{D_x} \right)^2 + \left( \langle x | \theta^3 \theta^3 \rangle \right)^2 \]  

(2.8)

If we make the x coordinate at the object the subject of this equation, then we can derive the beam current through the system as a function of the accepted divergence for a set image size.

\[ x_0 = D_x \sqrt{x_i^2 - \langle x | \theta^3 \theta^3 \rangle^2} \]  

(2.9)

\[ I \propto x_0 \theta_0 \]  

(2.10)

\[ I \propto D_x \sqrt{x_i^2 - \langle x | \theta^3 \theta^3 \rangle^2} \theta_0 \]  

(2.11)

It is clear from figure 2.8 that this relationship has a maximum value, beyond which the aberration component has gained such significance that the current focused within the given image size cannot be maintained. Differentiating twice to prove that solution is a maximum shows that an ratio exists between the contribution from geometric and spherical aberration for the maximum beam current into a given spot-size. This ratio, when only the spherical aberration term is considered, gives a ratio shown in equation 2.12.
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Input divergence

Figure 2.8: Beam current as a function of input divergence for a given image size, from equation 2.11

\[ \frac{x_0}{D_x} : \langle x | \theta^3 \rangle \theta^3 = \sqrt{3} \]  \hspace{1cm} (2.12)

Jamieson states in his derivation of the figure of merit [50] that for a good focus the geometric term is about double that of the aberration term. We can see from equation 2.12 that this is an acceptable engineering approximation.

If equation 2.8 is rearranged to include this newly defined relationship, it gives:

\[ x^2 = \left( \frac{x_0}{D_x} \right)^2 + \left( 2 \langle x | \theta^3 \rangle \theta^3 \right)^2 \]  \hspace{1cm} (2.13)

Thus yielding expressions for \( x_0 \) and \( \theta_0 \) respectively.

\[ x_0 = 0.89D_x X_i \]  \hspace{1cm} (2.14)

\[ \theta_0 = 0.68 \left( \frac{X_i}{\langle x | \theta^3 \rangle} \right)^{\frac{1}{3}} \]  \hspace{1cm} (2.15)

Substituting back into equation 2.10, it is clear that maximum current corresponds to a maximum figure of merit given by 2.16.

\[ Q = \frac{D_x D_y}{\sqrt{\langle x | \theta^3 \rangle \langle y | \phi^3 \rangle}} \]  \hspace{1cm} (2.16)

The Q value provides an acceptable method to evaluate the optimisation of these parameters, since systems with a high figure of merit, or 'Q' value potentially offer a superior performance. The equation for this figure of merit is given in equation 2.16.

To recap on the assumptions made:

1. The assumption of a uniform beam brightness distribution, thus beam current is proportional to the total phase space accepted by the system
2. Chromatic aberration and spherical aberration cross-terms are of negligible importance.

3. The assumption that for a good focus the geometric term is approximately double that of the aberration terms.

The first assumption means that the flux-peaking phenomenon, discussed in [31] is ignored. This phenomenon reduces the sensitivity of the probe to angle dependent aberrations which means that a system is likely to have better performance than indicated by the figure of merit, but the optimisation via the figure of merit will still produce an optimised performance. Of more significance is the assumption that the spherical aberration cross-terms are of negligible importance. For a truly useful figure of merit, the spherical cross-terms must be included. Jamieson and Ryan state in the same paper [50] that reduction of the spherical cross-terms was their guiding philosophy in the design of the CSIRO-GEMOC nuclear microprobe.

### 2.5.2 Acceptance Optimisation

The spherical aberration cross-terms can make a significant contribution to the point spread function. The author has developed a method for evaluating a system based on its spherical aberration coefficients including cross-terms. This is based on optimising the acceptance for a system with a given spot size in the image plane. If we assume that the final beam profile is a convolution of the various components, the position of a ray in the image plane as a function of geometric and spherical components can be expressed as:

\[
x_i = \sqrt{\left(\frac{x_o}{D_x}\right)^2 + (\langle x|\theta^3\rangle\theta^3)^2 + (\langle x|\theta^2\phi\rangle\theta^2\phi)^2}
\]

\[
y_i = \sqrt{\left(\frac{y_o}{D_y}\right)^2 + (\langle y|\phi^3\rangle\phi^3)^2 + (\langle x|\theta^2\phi\rangle\theta^2\phi)^2}
\]

(2.17)

This can be expressed in terms of object co-ordinates where \( r \) represents the radius of the spot-size in the image plane:

\[
x_o = \sqrt{D_x^2 (r^2 - \langle x|\theta^3\rangle^2\theta^3 - \langle x|\theta^2\phi\rangle^2\theta^2\phi^4)}
\]

\[
y_o = \sqrt{D_y^2 (r^2 - \langle y|\phi^3\rangle^2\phi^3 - \langle x|\theta^2\phi\rangle^2\theta^2\phi^4)}
\]

(2.18)

Therefore, the acceptance of the system, \( A = x_o y_o \omega \theta \phi \), is:

\[
A = \theta \phi \sqrt{D_x^2 (r^2 - \langle x|\theta^3\rangle^2\theta^3 - \langle x|\theta^2\phi\rangle^2\theta^2\phi^4)} \sqrt{D_y^2 (r^2 - \langle y|\phi^3\rangle^2\phi^3 - \langle x|\theta^2\phi\rangle^2\theta^2\phi^4)}
\]

(2.19)

The optimal value of acceptance can be found when the following conditions are satisfied:

\[
\frac{\partial A}{\partial \theta} = 0 \quad \text{and} \quad \frac{\partial A}{\partial \phi} = 0
\]
\[
\frac{\partial^2 A}{\partial \theta^2} < 0 \quad \text{and} \quad \frac{\partial^2 A}{\partial \phi^2} < 0
\]

A plot of the acceptance function for an Oxford Triplet geometry is shown in figure 2.9. However, the algebraic solution of these terms is not simple, and a numerical optimisation method has been used in the survey to find the optimal value of the acceptance function.
Figure 2.9: A plot of the acceptance function for two beamline geometries. The vertical scale is in units of $\mu m^2.mrad^2$. The horizontal scale is in units of mrad.
Chapter 3

Calculating The Motion of Particles in Magnetic and Electric Fields

3.1 Matrix Methods

3.1.1 Introduction

There are two main methods for analysing the theoretical behaviour of microbeam systems: matrix methods, and raytracing. Raytracing techniques are far more accurate than matrix methods, and will be discussed in the next chapter. However, matrix methods are computationally much faster than raytracing, and thus provide a quick way to compare the suitability of microbeam geometries for microbeam applications. This is useful because it can use many iterations of a minimizer routine to find the quadrupole excitations required to give the best focus, which would be time-consuming if each iteration was computed by the raytracing technique. Thus matrix methods can provide a good starting point for the raytracing technique.

3.1.2 The Matrix system

If a particle enters a microbeam system with the entry coordinates $x_i, y_i$ describing the particle’s transverse position in the object plane, and $\theta_i, \phi_i$, which describe the particle’s divergence from the axis of beam propagation in x-z and y-z planes respectively, then the coordinates of the particle after travelling through the system can be represented as a polynomial series where the coefficients express the aberration coefficients of the microbeam system, as shown in Equation 3.1.
\[ x_f = m_{11}x_i + m_{12}y_i + m_{13} \theta_i + m_{14}\phi_i + m_{15}\delta + \ldots \]

\[ y_f = m_{21}x_i + m_{22}y_i + m_{23}\theta_i + m_{24}\phi_i + m_{25}\delta + \ldots \]

\[ \theta_f = m_{31}x_i + m_{32}y_i + m_{33}\theta_i + m_{34}\phi_i + m_{35}\delta + \ldots \]

\[ \phi_f = m_{41}x_i + m_{42}y_i + m_{43}\theta_i + m_{44}\phi_i + m_{45}\delta + \ldots \]

(3.1)

Where the \( m_{nn} \) terms represent the first order aberration coefficients described in table 2.1. These equations may be written in matrix notation:

\[
\begin{pmatrix}
  x_f \\
  y_f \\
  \theta_f \\
  \phi_f
\end{pmatrix}
= 
\begin{pmatrix}
  m_{11} & m_{12} & m_{13} & m_{14} & m_{15} & \ldots & \ldots \\
  m_{21} & m_{22} & m_{23} & m_{24} & m_{25} & \ldots & \ldots \\
  m_{31} & m_{32} & m_{33} & m_{34} & m_{35} & \ldots & \ldots \\
  m_{41} & m_{42} & m_{43} & m_{44} & m_{45} & \ldots & \ldots \\
\end{pmatrix}
\begin{pmatrix}
  x_i \\
  y_i \\
  \theta_i \\
  \phi_i
\end{pmatrix}
\]

(3.2)

Equation 3.2 gives the exit coordinates for a particle leaving a system, but it does not express the higher order aberration coefficients directly, which is useful in the comparison of probe forming systems. This can be achieved by formulating a new matrix:

\[
\begin{pmatrix}
  x_f \\
  y_f \\
  \theta_f \\
  \phi_f \\
  x_f^2 \\
  x_f y_f \\
  x_f \theta_f \\
  \vdots \\
  \vdots \\
  \vdots \\
  \vdots \\
  P_{NN}
\end{pmatrix}
= 
\begin{pmatrix}
  p_{11} & p_{12} & p_{13} & p_{14} & p_{15} & \ldots & \ldots \\
  p_{21} & p_{22} & p_{23} & p_{24} & p_{25} & \ldots & \ldots \\
  \vdots & \vdots & \vdots & \vdots & \vdots & \ldots & \ldots \\
  \vdots & \vdots & \vdots & \vdots & \vdots & \ldots & \ldots \\
  \vdots & \vdots & \vdots & \vdots & \vdots & \ldots & \ldots \\
  p_{ij}
\end{pmatrix}
\begin{pmatrix}
  x_i \\
  y_i \\
  \theta_i \\
  \phi_i \\
  x_i^2 \\
  x_i y_i \\
  x_i \theta_i \\
  \vdots \\
  \vdots \\
  \vdots \\
  \vdots \\
  \vdots \\
  P_{NN}
\end{pmatrix}
\]

(3.3)

The \( p \) matrix elements shown in equation 3.3 can be derived by simple algebra from the elements of the \( m \) matrix shown in equation 3.2. Equation 3.4 shows the \( x_f^2 \) term.

\[ x_f^2 = (m_{11}x_i + m_{12}y_i + m_{13}\theta_i + m_{14}\phi_i + m_{15}\delta_i)^2 \]

(3.4)

The second order transfer matrix will be a 20 x 20 matrix, and the third order matrix will be 55 x 55.
3.1.3 First Order Matrices

The system matrix for a microbeam system can be built up from the transfer matrices for each element within a system. Simple microbeam systems are composed of both drift spaces and quadrupole lenses. The transfer matrix for a drift space is shown in equation 3.5.

\[
\begin{pmatrix}
x_f \
y_f \\
th_f \
\phi_f
\end{pmatrix}
= \begin{pmatrix}
1 & 0 & L & 0 \\
0 & 1 & 0 & L \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
x_i \
y_i \\
th_i \
\phi_i
\end{pmatrix}
\] (3.5)

Where \( L \) is the length of the drift.

The field profile of a quadrupole lens is described in equation 2.4. From this an expression can be obtained for the equation of motion of the particle in the lens:

\[
\begin{align*}
\frac{dv_x}{dt} &= -\frac{e}{m} x (G_m v_z) \\
\frac{dv_y}{dt} &= \frac{e}{m} y (G_m v_z)
\end{align*}
\] (3.6)

Using equation 3.6 an equation for \( x \) and \( y \) positions as a function of the axial position \( z \) can be derived, assuming that the force applied to the particle is always normal to the axis of propagation. This is known as the paraxial approximation and is the reason why first order matrices cannot calculate spherical aberration.

\[
\begin{align*}
\frac{d^2 x}{dz^2} &= -k^2 x \\
\frac{d^2 y}{dz^2} &= k^2 y \\
k^2 &= \frac{e}{m v_z^2} (G_m v_z)
\end{align*}
\] (3.7)

A uniform quadrupole lens with length \( l \) is represented by the following matrix:

\[
\begin{pmatrix}
x_f \
y_f \\
\theta_f \
\phi_f
\end{pmatrix}
= \begin{pmatrix}
\cos kl & 0 & \frac{1}{k} \sin kl & 0 \\
0 & \cosh kl & 0 & \frac{1}{k} \sinh kl \\
-\frac{k}{l} \sin kl & 0 & \cos kl & 0 \\
0 & \frac{k}{l} \sinh kl & 0 & \cosh kl
\end{pmatrix}
\begin{pmatrix}
x_i \
y_i \\
\theta_i \
\phi_i
\end{pmatrix}
\] (3.8)

One of the fundamental inaccuracies of using matrix methods to calculate microbeam systems is the inability to accurately model the fringing field of the quadrupole lens, i.e. the field which extends beyond the geometric length of the quadrupole lens. Banford states in [1] that the following expression for effective length is a reasonable approximation that agrees well with empirical measurements.
\[ l_x = l_o + 1.1a_0 \]  

Where \( l_o \) is the geometric length, and \( a_0 \) is the bore radius of the lens.

### 3.1.4 Focused Systems

For a focused microbeam system, all rays from a single point in the object aperture should ideally arrive at a single point in the image plane. The image distance must be calculated such that the image plane is in the same position in both the xz and yz-planes, otherwise the system is astigmatic.

The image distance can be calculated by considering the microprobe system in two sections:

1. The system from the object aperture up to the end of the effective length of the final quadrupole lens.

2. The drift length from the final lens to the image plane.

Thus:

\[
\begin{bmatrix}
    x_f \\
    y_f \\
    \theta_f \\
    \phi_f
\end{bmatrix} = \begin{bmatrix}
    1 & 0 & l_x & 0 \\
    0 & 1 & 0 & l_y \\
    0 & 0 & 1 & 0 \\
    0 & 0 & 0 & 1
\end{bmatrix} \begin{bmatrix}
    m_{11} & 0 & m_{13} & 0 \\
    0 & m_{22} & 0 & m_{24} \\
    m_{31} & 0 & m_{33} & 0 \\
    0 & m_{24} & 0 & m_{44}
\end{bmatrix} \begin{bmatrix}
    x_i \\
    y_i \\
    \theta_i \\
    \phi_i
\end{bmatrix}
\]  

(3.10)

For a simple first order system, the motion in the xz and yz planes in a pure quadrupole field is independent, hence all the cross terms in 3.10 are zero.

Since the condition for a focused system is that the x and y positions in the image plane are not dependent on the divergences \( \theta \) and \( \phi \), the system is focused when \( \langle x/\theta \rangle = 0 \) and \( \langle y/\phi \rangle = 0 \), thus, the image distances can be calculated:

\[
\begin{aligned}
  l_x &= \frac{-m_{13}}{m_{33}} \\
  l_y &= \frac{-m_{24}}{m_{44}}
\end{aligned}
\]  

(3.11)

Hence, the demagnifications are given by:

\[
\begin{aligned}
  D_x &= \frac{1}{m_{11} + l_x m_{31}} \\
  D_y &= \frac{1}{m_{22} + l_y m_{42}}
\end{aligned}
\]  

(3.12)
3.1.5 Principal Planes

If an optical system has an object perpendicular to the axis at the object plane, then it could be said to give a geometrically similar image, perpendicular to the axis at the image plane. The geometrical similarity will be in the form of a transverse magnification, \( m \), i.e. the object will be magnified at the image. The principal planes are the points where \( m = +1 \). These planes intersect the axis at the principal points, \( P \) and \( P' \), as shown in figure 3.1. \( H \) and \( H' \) are the conjugate points in the principal planes, such that \( H'P' = HP \) by definition. [40]

The principal planes have the property that a ray crossing the axis at \( P \) leaves the lens at \( P' \) with the same angle with respect to the beam axis. This is important for beam scanning since it allows the deflection sensitivity in the image plane to be calculated if the principal planes of the system are known.

The position of the principal planes can be found simply using matrix methods if one considers the system as 3 matrices; the object drift matrix, the system matrix, and the image drift matrix, and then solves for the magnification term in the drift matrices.

The principal planes of the Surrey Microbeam are marked in figure 3.2. \( H \) and \( H' \) denote the entrance and exit principal planes respectively, and the subscripts refer to the plane of motion. The Surrey Microbeam has an Oxford Triplet lens geometry, and thus the principal planes occur as described by Grime, Watt and Takacs in [23]. The axial crossing of the beam profile in the x-z plane within the first quadrupole lens causes the exit principal plane \( H'_{x} \) to occur beyond the image plane. The proximity of \( H'_{x} \) to the image plane compared to \( H'_{y} \) in the Oxford Triplet geometry means that beam scanning in the X-Z direction requires a greater entry angle to the entrance principal plane in comparison to beam scanning in the Y-Z plane to achieve similar beam deflection in the image plane.

The concept of principal planes is important in the design of beam scanning systems, particular pre-lens scanning where the beam may enter the lens off-axis. Calculations by Grime using the OXRAY software [23] show that for the Oxford proton microprobe the major aberrations introduced by pre-lens scanning are second order terms \( < x | \theta^2 > \) and \( < y | \phi^2 > \).
Using a dog-leg configuration magnetic scanning system he observed that the $\langle y | \phi^2 \rangle$ term passes through zero as the axial crossing point is moved through the entrance principal plane in the Y-Z plane. The implication of this is that if the beam were to enter the entrance principal plane off-axis, then aberrations would be introduced into the systems, and the beam-spot would degrade as the system was scanned away from the axis. There are no measurements of this effect in the literature.

3.1.6 Calculation of Aberration Coefficients using Matrices

We have seen that calculation of the first order properties of a microbeam system using matrices is a relatively straightforward process. Calculation of the second order properties is somewhat more complex, although expressions for chromatic aberration are easy to derive from the first order properties by variation of the $k$-value to incorporate spread of energy within the beam.

The effect of a momentum spread $\delta$ on the $k$-values for $\delta << 1$ can be expressed as:

$$k'_m = k_m \left(1 - \frac{\delta}{2}\right)$$

(3.13)

$$k'_e = k_e (1 - \delta)$$

(3.14)

Where $k'$ denotes the effective $k$ value, and the m and e subscripts denote the magnetic and electrostatic cases respectively. Substituting the above equations into the matrices for each

![Figure 3.2: Beam profile of the Surrey Microbeam, with principal planes marked, calculated using the matrix based beam optics software PRAM [30]](image)
active element in a system, the following second order aberration coefficients may be extracted:

\[ \langle x | x\delta \rangle = f k \text{sinkl} \]  
(3.15)

\[ \langle x | \theta\delta \rangle = f \left[ \frac{\text{sinkl}}{k} - \coskl \right] \]  
(3.16)

\[ \langle y | y\delta \rangle = -f k \text{sinkl} \]  
(3.17)

\[ \langle y | \phi\delta \rangle = f \left[ \frac{\text{sinkl}}{k} - \coskhkl \right] \]  
(3.18)

\[ \langle \theta | x\delta \rangle = f [k \coskl + \text{sinkl}] \]  
(3.19)

\[ \langle \theta | \theta\delta \rangle = f k \text{sinkl} \]  
(3.20)

\[ \langle \phi | y\delta \rangle = -f k [k \coskhkl + \text{sinkhkl}] \]  
(3.21)

\[ \langle \phi | \phi\delta \rangle = -f k \text{sinkhkl} \]  
(3.22)

where \( f = 0.5 \) for magnetic quadrupoles, and \( f = 1 \) for electrostatic quadrupoles.

Heck [24] has derived a method for calculating second order aberrations due to misalignment of optical elements. The process adopted by this method is the formation of transformation matrices such that the co-ordinate frame can be manipulated to suit the misaligned element. This method is not straightforward, and the reader is referred to Heck's article on this subject for further information.

Calculation of the third order aberrations using matrix methods requires complex algebra. The potential distribution in a quadrupole lens is symmetric about the centre of the lens, and so the potential must be an even function of radius, i.e:

\[ \phi(x, y) = -\phi(-x, -y) \]  
(3.24)

Since the force on the particle is proportional to \( \nabla \phi \), the force must be an odd-function of radius [19]. Thus it is clear that after the first order focusing, the next imaging aberration to appear will be of third-order, of which spherical aberration is the most important. The nature of spherical aberration was discussed in section 2.4.4. To model the effect of spherical aberration, one must model the change in axial velocity as a particle departs from the axis, thus abandoning the para-axial approximation upon which we based the first-order equations. To further complicate the process, the fringing fields of each element must be fully modelled, since these regions include higher-order harmonics which may affect the third order aberrations.

### 3.1.7 The Dymnikov method

Dymnikov, Fishkova, and Yavor [14] have derived a set of approximations for spherical aberrations in individual quadrupole lenses based on a short lens approximation, and an expression for the spherical aberration of a system as the compound effect of the individual spherical aberration for each lens, which is reviewed in the book by Breese, Jamieson and King [5]. A brief review of the method is provided here.
The displacement of a ray in the image plane due to spherical aberration is:

\[ x_i = \langle x | \theta^3 \rangle + \langle x | \theta \phi^2 \rangle \]

\[ y_i = \langle y | \phi^3 \rangle + \langle y | \theta^2 \phi \rangle \]

(3.25) (3.26)

However, in stigmatic quadrupole lens systems the cross terms are related, as shown in equation 3.27.

\[ \langle x | \theta \phi^2 \rangle = M_y \langle y | \theta^2 \phi \rangle \]

(3.27)

Where \( M_x \) and \( M_y \) are the horizontal and vertical magnifications of the system respectively. Thus only three independent spherical terms exist.

The spherical aberration coefficients of a thin quadrupole lens have been derived by Dymnikov et al. [32].

\[ C_p = \frac{1}{3} \frac{\psi}{L} \frac{a_x^2}{f_x^2} \]

(3.28)

\[ C_s = -\frac{1}{\psi} \frac{a_x^2 a_y^2}{L f_x f_y} \]

(3.29)

\[ D_p = \frac{1}{3} \frac{\psi}{L} \frac{a_y^2}{f_y^2} \]

(3.30)

\[ D_s = C_s \]

(3.31)

Where:

- \( a_x \) and \( a_y \) are the lens object distances in the respective planes.
- \( f_x \) and \( f_y \) are the lens focal lengths in the respective planes.
- \( L \) is the lens effective length, described in chapter 3.1.
- \( \psi \) is a correction factor for the the shape of quadrupole fringe fields. A full explanation of this can be found in the work by Jamieson in [32]. For rectangular lens field profiles it is acceptable to approximate \( \psi = 1 \).
- \( C_p \) and \( C_s \) represent a component of the spherical aberration coefficient of the lens for the pure, and cross-term respectively in the \( x-z \) plane.
- \( D_p \) and \( D_s \) represent a component of the spherical aberration coefficient of the lens for the pure, and cross-term respectively in the \( y-z \) plane.

Dymnikov's coefficients can be related to equations 3.25 by the following relations:

\[ \langle x | \theta^3 \rangle = M_x C_p \]

\[ \langle x | \theta \phi^2 \rangle = M_x C_s \]

\[ \langle y | \theta^2 \phi \rangle = M_y C_s \]

\[ \langle y | \phi^3 \rangle = M_y D_p \]

(3.32)
Yavor et al. also defined a formula for the summation of the spherical aberration coefficients for a system of such lenses [32].

\[
C_p(k) = \sum_{n=1}^{k} n C_p / M_x^{4(n-1)}
\]

(3.33)

\[
C_s(k) = \sum_{n=1}^{k} n C_s / M_x^{2(n-1)} M_y^{2(n-1)}
\]

(3.34)

\[
D_p(k) = \sum_{n=1}^{k} n D_p / M_y(n-1)
\]

(3.35)

\[
D_s(k) = C_s(k)
\]

(3.36)

Where the n-sub-prefix denotes the nth lens and \(M_x(n-1)\) and \(M_y(n-1)\) are the combined magnifications of the first \((n - 1)\) lens in the system, as given by equation 3.37.

\[
M_x(n-1) = \prod_{i=1}^{n-1} M_x
\]

(3.37)

\[
M_y(n-1) = \prod_{i=1}^{n-1} M_y
\]

(3.38)

Where \(iM_x\) and \(iM_y\) are the magnifications of the \(i\)th lens.

The author has developed a software package called ELUM for calculation of particle trajectories using first order matrices, and calculation of the spherical aberration coefficients for a beamline using the Dymnikov method. A comparison of aberration coefficients calculated by ELUM using the Dymnikov coefficients, and calculations using numerical raytracing for a single quadrupole lens are presented in section 3.2.3. It has been found that the Dymnikov coefficients significantly underestimate the spherical aberration of a quadrupole lens when a high lens excitation is used.

### 3.2 Raytracing

#### 3.2.1 Introduction

Numerical raytracing provides a method to calculate the higher order aberrations of a microbeam system based on numerical methods instead of the analytical algebraic method discussed in the previous section. There are few software packages available for numerical raytracing suitable for microprobes, a comparison of raytracing softwares will be presented in chapter 4.

Raytracing involves tracing the path of a single particle through a mathematical representation of the real fields step by step through the system, allowing the calculation of the effects of complex field distributions. This is achieved by solving the differential equations of motion for a representative set of particles within a numerical model of the fields in the system.
Chapter 3. Calculating the Motion of Particles

It is necessary to specify a series of simultaneous first-order differential equations, representing the equations of motion for a particle in magnetic and electrostatic fields, where the axis of the beam is the independent variable.

The motion of a particle in a electrostatic or magnetic field is given by the equation of motion:

\[
\frac{d(m\dot{u})}{dt} = e(\vec{E} + \nu \times \vec{B})
\]  

(3.39)

Where \( m\nu \) is the relativistic momentum of the particle given as

\[
m\nu = m_0\nu \left(1 - \frac{|\nu|^2}{c^2}\right)^{-\frac{1}{2}}
\]  

(3.40)

with \( m_0 \) the rest mass of the particle (kg), \( \nu \) the velocity of the particle (m/s), \( c \) the velocity of light (m/s), \( B \) the magnetic field (T) and \( E \) the electrostatic field (V/m).

The axial distance, \( z \), can be made the independent variable by substitution, thus the expansion of equation 3.39 gives:

\[
\begin{align*}
\frac{dv_x}{dz} &= \frac{e}{mv_x} (v_y B_z - v_z B_y + E_z) \\
\frac{dv_y}{dz} &= \frac{e}{mv_x} (v_z B_x - v_x B_z + E_y) \\
\frac{dv_z}{dz} &= \frac{e}{mv_x} (v_x B_y - v_y B_x + E_z) \\
\frac{dx}{dz} &= \frac{v_x}{v_z} \\
\frac{dy}{dz} &= \frac{v_y}{v_z}
\end{align*}
\]  

(3.41)

The initial conditions are simply the positions and velocities of the ray at the object. The velocities can be found from the energy and divergence of a ray at the object:

\[
|\nu| = c \left(1 - \frac{1}{\left(1 + \frac{e\nu}{m_0c^2}\right)^2}\right)
\]  

(3.42)

\[
\theta = \frac{v_x}{v_z} \\
\phi = \frac{v_y}{v_z}
\]  

(3.43)

These equations must be solved numerically to determine the position and velocity of the particle at the desired point along the beam axis. Usually this point corresponds with field free region in the image space of the beamline system. For a full solution, initial conditions for the position and velocity vectors are necessary.
Most strategies for the solution of the equations 3.2.1 operate by stepping in discrete values along the beam axis using a Taylor series expansion to extrapolate the next value of the solution to each equation from the preceding values.

\[ y_N = y_{N-1} + h y'_{N-1} + \frac{h^2}{2!} y''_{N-1} + \ldots \]  

(3.44)

where \( y_n \) represents the value of each of the components after the \( n^{th} \) step in \( z \), and \( h \) is the size of the increment in \( z \).

Significant computation effort can be saved in numerical raytracing with no loss of accuracy if an adaptive stepsize routine is used.

The stepsize adjustment procedure begins by calculating the desired error level for each component of the solution, and then comparing this to the observed error at each step. The desired error is given by:

\[ D_i = \epsilon_{\text{abs}} s_i + \epsilon_{\text{rel}} | y_i | \]  

(3.45)

Where \( \epsilon_{\text{abs}} \) is the absolute error, and \( \epsilon_{\text{rel}} \) is the fractional error. \( D_i \) is actually a vector of the desired accuracies for the solution of each differential equation, and \( s_i \) is a vector of scaling factors for the absolute error allowed in each component.

If the observed error \( E_i \) exceeds the desired error level \( D_i \) by more than 10% the then stepsize is reduced by the expression given in equation 3.46:

\[ h_{\text{new}} = h_{\text{old}} * S * \left( \frac{E_i}{D_i} \right)^{-\frac{1}{q}} \]  

(3.46)

Where \( S \) is a safety factor of 0.9, and \( q \) is the consistence order of the method to used to solve the ordinary differential equations. Alternatively, if the observed error level is less than 50% of the desired error level, the stepsize can be increased:

\[ h_{\text{new}} = h_{\text{old}} * S * \left( \frac{E_i}{D_i} \right)^{\frac{1}{q-1}} \]  

(3.47)

Careful choice of the maximum allowed error for a single step determines both the overall accuracy, and the speed of computation, however it is in the nature of this approach that errors propagate through the system with each step taken. This is especially critical if we consider quadrupole fields and deviations from the axis in error conditions.
CHAPTER 3. CALCULATING THE MOTION OF PARTICLES

3.2.2 Field Distributions of Cylindrical Harmonics

The common magnetic and electrostatic elements of a microbeam can be described easily using cylindrical field harmonics, i.e. dipole, quadrupole, octupole.

The magnetic scalar potential derived from a two dimensional Laplace equation for a multipole with perfect fourfold symmetry and no variation of field with length takes the form

$$\phi(r, \theta) = \sum_{n=2, 6, 10...} k_{2n}(\sin 2\theta) r^n$$ (3.48)

Where \(n\) is the multipole index such that \(n = 2\) represents a quadrupole, \(n = 3\) represents a sextupole, \(n = 4\) represents an octupole etc. However, for accurate modelling of a quadrupole field, the model must be extended to 3 dimensions to account for the cylindrical harmonics and variation of the field with respect to the optical axis of the beam. Using a cylindrical polar co-ordinate system, where the origin is the centre of the element being modelled, and the \(z\)-axis is the optical axis of the element, an equation for the magnetic fields of an element with cylindrical harmonics of order \(n\) can be formed.

In this region a magnetic scalar potential may be defined by

$$B = -\nabla \psi$$ (3.49)

with

$$\nabla B = -\nabla^2 \psi = 0$$ (3.50)

Lobb [39] shows the solution of Laplace’s equation in two dimensions to be the Fourier series given in equation 3.52.

$$\psi(r, \theta) = \sum_{n=1}^{\infty} \frac{p_n}{n} (\frac{r}{a})^n \sin(n\theta - \chi_n)$$ (3.52)

where \(p_n\) and \(\chi_n\) are constants, and the scaling parameter \(a\) has been inserted for convenience.

$$\psi = \sum_{n=1}^{\infty} \cos(n\theta + \chi_n) \sum_{i=0}^{\infty} a_{n+2i}(z)r^{n+2i}$$ (3.53)

$$B_r = \sum_{n=1}^{\infty} \cos(n\theta + \gamma_n) \sum_{i=0}^{\infty} (n + 2i)a_{n+2i}(z)r^{n+2i-1}$$

$$B_{\theta} = -\sum_{n=1}^{\infty} \sin(n\theta + \gamma_n) \sum_{i=0}^{\infty} n a_{n+2i}(z)r^{n+2i-1}$$

$$B_z = \sum_{n=1}^{\infty} \cos(n\theta + \gamma_n) \sum_{i=0}^{\infty} a'_{n+2i}(z)r^{n+2i}$$ (3.54)
The left-hand side sum terms of equation 3.54 can be replaced by an excitation parameter \( C_n \).

\[
B_r = C_n \cos(n\theta + \gamma_n) \sum_{i=0}^{\infty} (n + 2i) a_{n+2i}(z) r^{n+2i-1}
\]

\[
B_\theta = -C_n \sin(n\theta + \gamma_n) \sum_{i=0}^{\infty} i a_{n+2i}(z) r^{n+2i-1}
\]

\[
B_z = C_n \cos(n\theta + \gamma_n) \sum_{i=0}^{\infty} a'_{n+2i}(z) r^{n+2i}
\]

(3.55)

The excitation parameter \( C_n \) can then be related to the pole-tip field of the quadrupole:

\[
C_n = B_r \frac{k_n}{n} a_0^{n-1}
\]

(3.56)

Where \( k_n \) is the relative strength of the harmonic of order \( n \), which may be obtained either by calculation[3], finite element modelling, or by spectrum analysis of rotating coil measurements [18].

The coefficients \( a_n \) in equation 3.54 are derived from the axial field gradient distribution \( f_n(z) \) given by:

\[
a_{n+2i} = \frac{(-1)^i a'_n n!}{4^i i!(n + i)!}
\]

\[
a^m_n = \frac{d^m}{dz^m} (f_n(z))
\]

\[
a'_{n+2i} = \frac{d}{dz} (a_{n+2i})
\]

(3.57)

The phase term \( \gamma_n \) accounts for the relative alignment of the components.

### 3.2.3 Fringing Fields

The function \( f_n(z) \) controls the shape of the fringing field. This function is based on the function used by Enge [16] for modelling dipole fringing fields. Grime and Watt suggest in [19] the modification of the numerator to match the uniform field region at \( s = 0 \)

\[
f_n(z) = \frac{1 + e^{\alpha}}{1 + e^{P_n(s)}}
\]

(3.58)

Where:

\[
P_n(s) = c_0 + c_1 s + c_2 s^2 + c_3 s^3 + c_4 s^4 + c_5 s^5
\]

\[
s = \frac{|z - z_1|}{a_0}
\]

(3.59)
CHAPTER 3. CALCULATING THE MOTION OF PARTICLES

Where $z_1$ is the beginning of the fringing field on the $z$ axis of the element, and $a_0$ is the bore radius of the element.

The coefficients $c_0$ to $c_5$ can be chosen to fit the shape of the fringing field.

The effect of the fringe field length parameter, $z_1$, is merely to truncate the fringing field, resulting in a sharp-cutoff. This has the effect of saving calculations, but does not accurately represent a quadrupole fringing field. Therefore, this parameter should be chosen such that the fringing field has sufficient length to avoid any significant discontinuities in the field profile.

The OM50 and OM52 quadrupole lenses are two precision quadrupole lenses produced by Oxford Microbeams Ltd. The physical properties of these lenses is given in Table 3.1.

<table>
<thead>
<tr>
<th>Profile</th>
<th>Bore diameter (mm)</th>
<th>Geometric Length (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>OM50</td>
<td>15.0</td>
<td>100.0</td>
</tr>
<tr>
<td>OM52</td>
<td>7.5</td>
<td>55.0</td>
</tr>
</tbody>
</table>

Table 3.1: Physical properties of the OM50 and OM52 quadrupole lens

Figure 3.3: Measured longitudinal field profile away from the centre of an OM52 lens at a radius of ~3 mm away from the lens axis [6]

Table 3.2 shows the Enge fringe field coefficients for the five fringe field profiles shown in figure 3.6. Profile 1 is a rectangular field profile for an OM50 quadrupole lens. Profile 5 is the measured fringe field profile for a OM50 quadrupole lens.

All the aberration coefficients in table 3.2 were calculated for a OM50 quadrupole lens with a pole tip field of 0.1 Tesla, an object distance of 1 metre, and a image distance of 0.1 metres, measured from the centre of the lens.
Figure 3.4: Measured longitudinal entry field profile away from the centre of an OM52 lens at a radius of \(~3\, \text{mm}\) away from the lens axis, compared to fitted profile calculated using Enge coefficients. \[6\]

Figure 3.5: Measured longitudinal field profile away from the centre of an OM50 lens at a radius of \(~3\, \text{mm}\) away from the lens axis \[26\]
Figure 3.6: Quadrupole fringe field profiles. Fringe field profiles numbered in the legend correspond with fringe field profiles from table 3.2.

Figure 3.7: Quadrupole fringe field profiles
Table 3.2: Spherical aberration coefficients for a variety of quadrupole fringe field profiles, as shown in figure 3.7.

| Profile | z0 (mm) | c0 | c1 | \( < x | \theta^3 > \) | \( < x | \theta^2 \phi > \) | \( < y | \theta^2 \phi > \) | \( < y | \phi^3 > \) |
|---------|---------|----|----|-----------------|-----------------|-----------------|-----------------|
| 1       | 50      | 0  | 0  | -0.00169        | -0.0064         | 0.00343         | 0.0126          |
| 2       | 40.2    | -6 | 3.5| -0.00441        | -0.0438         | -0.0001         | 0.0128          |
| 3       | 30.7    | -6 | 2.0| -0.00458        | -0.0454         | 0.00113         | 0.0142          |
| 4       | 3.11    | -6 | 0.9| -0.00418        | -0.0462         | 0.00103         | 0.0158          |
| 5       | 28.8    | -10| 3.09| -0.0051        | -0.0467         | 0.00273         | 0.0143          |

Table 3.3: Aberrational effect of fringe fields on Oxford Triplet

<table>
<thead>
<tr>
<th>Aberration Coefficient</th>
<th>Rectangular Fields</th>
<th>Measured Fringe Fields</th>
</tr>
</thead>
<tbody>
<tr>
<td>( &lt; \theta</td>
<td>\theta &gt; )</td>
<td>80.088</td>
</tr>
<tr>
<td>( &lt; \phi</td>
<td>\phi &gt; )</td>
<td>-23.908</td>
</tr>
<tr>
<td>( &lt; x</td>
<td>\theta^3 &gt; )</td>
<td>108.89</td>
</tr>
<tr>
<td>( &lt; x</td>
<td>\theta^2 \phi &gt; )</td>
<td>70.217</td>
</tr>
<tr>
<td>( &lt; y</td>
<td>\theta^2 \phi &gt; )</td>
<td>-234.05</td>
</tr>
<tr>
<td>( &lt; y</td>
<td>\phi^3 &gt; )</td>
<td>-288.34</td>
</tr>
<tr>
<td>Figure of Merit Q</td>
<td>-60.695</td>
<td>-24.089</td>
</tr>
</tbody>
</table>

Table 3.3: Aberrational effect of fringe fields on Oxford Triplet
Aberration coefficients published in the literature for the Oxford Triplet lens system and other beamline geometries are likely to have been made using the Enge coefficients suggested in [19] of \( c_0 = -6, c_1 = 3.5, c_{2-4} = 0 \) to model the fringe field region of an Oxford style quadrupole. However recent unpublished finite element analysis calculations by Sebastien Incerti [26] suggests that a better fit for an Oxford OM50 lens is given by the Enge coefficients of profile five in table 3.2. Calculations made using incorrect fringe field profiles, or worse, a rectangular fringe field profile are likely to greatly underestimate the spherical aberration coefficients of beamline.

The aberration coefficients calculated by the software packages ELUM, TRAX, and XART for a single OM50 quadrupole lens shown in figure 3.8 are particularly significant with respect to assessing the accuracy of the Dymnikov coefficients. The software package ELUM, discussed in section 3.1.7 uses Dymnikov coefficients to calculate the spherical aberration of the quadrupole lens. TRAX and XART both use numerical raytracing to calculate the path of particles through the magnetic field of the quadrupole lens, and calculate the spherical aberration coefficients from the position of the particles in the image plane. TRAX and XART are examined in more detail in chapter 4. It is clear that for the OM50 quadrupole lens the Dymnikov coefficients significantly underestimate the spherical aberration when the pole-tip field of the lens exceeds 0.3 Tesla. Below 0.3T, the Dymnikov coefficients can be at best considered an approximation. In this range, the Dymnikov coefficients overestimate the spherical aberration, particularly for the pure spherical aberration terms \( \langle x | \phi^3 \rangle, \langle y | \phi^3 \rangle \) by up to a factor of two. For most microbeam systems using 3MeV protons, the pole-tip fields required to find a focus at common working distances (\( > 100\text{mm} \)) rarely exceed 0.3T. For example, the Surrey Microbeam uses an Oxford Triplet lens geometry which requires OM50 quadrupole pole-tip fields of 0.219T and 0.1959T to give an focus after an working distance of 160mm for a 3MeV proton beam.

### 3.2.4 Locating the Image Plane

An important aspect of numerical raytracing is the ability of the focusing algorithm to find the best focus of the beam in the image plane. A numerical minimiser is used to find the set of lens excitations that give the minimum value of a function representing the focus conditions.

The image plane can be located using numerical raytracing simply by tracing an axial ray and a paraxial ray from a point at the object, and determining the point in the x-z and y-z planes respectively where these rays intersect. A focus can be achieved at a given position on the beam axis by using a numerical minimiser to find the set of lens excitations that minimise the separation of the image points in both planes from the specified position on the beam axis. This technique may be referred to as "image" focusing, since it finds the first-order location of the image plane.

However, every ray that traverses the beamline model will suffer aberration. If the "image" focusing technique is repeated for many paraxial rays of differing divergences, the location
Figure 3.8
Figure 3.8: Aberration coefficients for a single quadrupole lens, for a 3MeV proton, calculated by different methods. ELUM, TRAX, XART denote calculations by the named software packages for a rectangular field profile. "Fringe" denotes calculation using XART, and the fitted OM50 lens profile. Units (\(\mu m, \mu rad\)).
of the image plane will be spread due to the aberrations of the system. The implication is that the point where a ray crosses the beam axis is dependent on the divergence of the beam. Therefore, for highly aberrated systems (such as two-stage systems), a first-order technique such as "image" focusing may not be sufficient to find a good focus. To locate the image plane with accuracy, "radius" focusing must be used. If many rays are traced through the system over a range of equal and opposite divergences then a waist is formed in the region of image space where all rays intersect. If the radius of displacement from the axial ray of all traced rays is measured as a function of distance along the path of the axial ray, a minima will be found. This is known as the "curve of least confusion". A curve of least confusion for an Oxford Triplet system is shown in figure 3.9. The minimum radius of this curve of least confusion will give the optimum focal position for the set of rays traced. XART traces 7 rays over a divergence range of 3 orders of magnitude; if the maximum divergence is chosen such that the displacement of this ray from the axial ray at the desired position on the beam axis is approximately equal to the desired beam spot radius, then this technique is satisfactory.

![Figure 3.9: Curve of least confusion in the image space of an Oxford Triplet system](image)

### 3.2.5 Calculation of Aberration Coefficients

Coefficients for any aberration term to any order can be calculated using numerical ray tracing. If the desired variables are used to set the conditions of the system or ray, then sufficient rays of different values must be traced such that a polynomial of the variables can be fitted to the image plane displacement and divergence of each ray.

An equation can be given in general terms for the polynomial formed by the variables for
which aberration coefficients will be fitted:

\[ x = c_{000} + c_{100}v_1 + c_{010}v_2 + c_{001}v_3 + c_{200}v_1^2 + \ldots + c_{i_1i_2\ldots i_T}v_1^{i_1}v_2^{i_2}v_3^{i_3} \ldots v_T^{i_T} + \ldots \]  

(3.60)

where

\[
\begin{align*}
0 \leq i_1 & \leq n_1 \\
0 \leq i_2 & \leq n_2 \\
& \vdots \\
0 \leq i_T & \leq n_T 
\end{align*}
\]  

(3.61)

(3.62)

where \( n \) is the maximum order to which each variable is fitted and \( c_{i_1i_2\ldots i_T} \) is the coefficient \( \langle x|v_1^{i_1}v_2^{i_2} \ldots v_T^{i_T} \rangle \), and \( T \) is the total number of variables.

\( N \) simultaneous equations are required to fit a solution for all the unknown aberration coefficients in equation 3.60. These equations are obtained by tracing \( N \) rays each with a unique set of values for each variable. The total number of rays, \( N \), required to fit a solution is:

\[ N = \prod_{k=1}^{T} (n_k + 1) \]  

(3.63)

The \( N \) rays are chosen by stepping each variable \( v_k \) through \( n_k + 1 \) values forming a grid of values for all variables. Recording the displacement of each ray, \( x_m \) in the image plane, for each value of each variable \( m v_k \) forms a results matrix of the form:

\[ X = \begin{bmatrix} x_1 & x_2 & x_3 & \ldots & x_m & \ldots & x_N \end{bmatrix}^T \]  

(3.64)

The \( N \) simultaneous equations may also be written in matrix form:

\[ X = V \cdot C_x \]  

(3.65)

Where \( V \) is a matrix containing the polynomial functions of each variable:

\[
V = \begin{bmatrix} 
1 & v_1 & v_2 & v_3 & \ldots \\
1 & v_2 & v_3 & v_4 & \ldots \\
1 & v_3 & v_4 & v_5 & \ldots \\
& \vdots & & & \\
1 & m v_1 & m v_2 & m v_3 & \ldots \\
& & & & \\
1 & N v_1 & & & \\
\end{bmatrix}
\]  

(3.66)

and \( C_x \) is a matrix of the aberration coefficients:

\[
C_x = \begin{bmatrix} 
c_{000} & c_{100} & c_{010} & c_{001} & c_{200} & \ldots & c_{i_1i_2\ldots i_T} 
\end{bmatrix}^T
\]  

(3.67)
The solution of equation 3.65 for $C_x$ is obtained by multiplying both sides of the equation by the inverse of $V$. Thus:

$$C_x = V^{-1} \cdot X$$  \hspace{1cm} (3.68)

Similarly, a solution can be obtained for the aberration coefficients $< y | v_1^i v_2^i \ldots v_T^i >$, $< \theta | v_1^i v_2^i \ldots v_T^i >$, $< \phi | v_1^i v_2^i \ldots v_T^i >$ by recording the image co-ordinates for each ray traced in the matrices $Y, \Theta, \Phi$, and applying the inversion matrix $V^{-1}$ to give $C_y, C_\theta, C_\phi$. 
Chapter 4

Comparison of Beam Optics Software Packages

4.1 Introduction

An number of software packages exist capable of raytracing MeV ions through quadrupole fields with sub-micron accuracy. Two popular choices for this purpose are GEANT4, and TRAX. The comparison between these two packages really represents a comparison between the old, well tested software, and the new relatively untested software GEANT4.

4.2 TRAX

TRAX arose as a development of OXRAY, which was developed in Oxford by G.W. Grime in the 1980’s. It was written in the Fortran programming language, and utilises a number of algorithms from the Nuclear Algorithms Group to solve the differential equations of motion, and fit the aberration coefficients, as described in the previous chapter. The capabilities of TRAX include the accurate modelling of magnetic and electrostatic dipoles, quadrupoles, and octupoles. Trax also includes a simplistic model of slit scattering, although the author has no experience with this part of the code. The advantages of TRAX are the ease of use of the software, and its advanced optimisation engine, allowing the user to specify a wide-range of parameters related to the geometry of the simulation, and excitation of elements, and optimise these parameters as a function of beamsize or position in the image plane.

However a number of factors are expediting the approach of the end of the TRAX software life-cycle. The hardware required to execute TRAX has become obsolete, and it is now only with the kind permission of Richard Bryan at the Molecular Biophysics Lab at the University of Oxford, that the author is able to access the necessary hardware to execute TRAX. Also the inability to modify and recompile the source code for TRAX has meant that it is not possible to update the software to incorporate new features.
CHAPTER 4. COMPARISON OF BEAM OPTICS SOFTWARE PACKAGES

4.3 GEANT4

GEANT4 is the latest version of the CERN simulation program GEANT. GEANT4 exists as a set of C++ libraries and classes for the modelling of particle interaction and transport designed for the high energy physics community. The GEANT4 community is a vibrant and active community and the uses of GEANT4 have quickly expanded into many fields stretching from medical physics to astrophysics. The classes for modelling of magnetic and electrostatic fields included in GEANT4 make it ideal for raytracing applications such as beam optics. GEANT4 is a comparably young software, and no literature has been published as yet to verify its results for the raytracing of MeV ions through quadrupole fields with experimentally collected results.

In order to use GEANT4 for microbeam simulation, Sebastien Incerti of Centre d’Etudes Nucléaires de Bordeaux-Gradignan (CENBG) developed and implemented new Quadrupole field modules. A comparison of these raytracing codes was carried out as a collaboration between the University of Surrey, and CENBG [28]. The results of this paper will be summarised in this chapter.

4.4 XART

XART is a raytracing software written by the author specifically for the survey of two-stage systems described in chapter 5. The vast parameter space requiring investigation in the survey of two-stage systems demanded a fast but accurate solution, with enough flexibility to adjust the simulations to the needs of the survey. GEANT4 and TRAX both provide the required accuracy, but what GEANT4 lacks in speed, TRAX lacks in flexibility. XART aims to fill that gap. XART was inspired by TRAX, and takes it name from TRAX, but similarly to GEANT4, has been designed as a C++ library. This gives the user great flexibility to build simulations of novel beamline designs without the constrictions of limited set of commands.

4.5 Comparison

To compare the ray-tracing techniques, a geometry for simulation was chosen. This geometry was chosen because it was a system under study in Bordeaux for implementation for a sub-micron resolution beamline at the time of the study. This geometry is referred to as the Bordeaux-Rossendorf geometry, and utilises an intermediate image, forming a two-stage system. This system uses a quadrupole doublet to form an intermediate focus and crossover which is then further demagnified by a quadrupole triplet chosen for its low spherical aberration. The geometry of the system is shown in figure 4.1. This system has demagnifications of 65 in the X-Z plane and 100 in the y-z plane, with a 250 mm working distance. The study [28] found that pole-tip fields calculated with both raytracing softwares to form an image at the specified
distance were in good agreement, with agreement to 4 decimal places between TRAX and GEANT4 for pole-tip fields specified in kilogauss.

No fringing fields were modelled for the quadrupole fields, and thus the two dimensional field profile for each length was rectangular. This was done so that a direct comparison of the ray-tracing abilities of each program could be compared, avoiding any differences in the procedure for specifying fringing fields in the two programs.

![Bordeaux-Rossendorf setup](image)

**Figure 4.1:** Beam Geometry for Bordeaux-Rossendorf Nanobeam: Labels indicate position on the beam axis of the centre of an optical element

![Beam Envelope for Bordeaux-Rossendorf Nanobeam Geometry](image)

**Figure 4.2:** Beam Envelope for Bordeaux-Rossendorf Nanobeam Geometry

Beam-spot profiles were also compared for TRAX and GEANT4. For this simulation, two different object and collimator aperture geometries were chosen to reflect different applications of the nanoprobe. For STIM applications, a maximum beam divergence before the first lens of 0.001 mrad was chosen, and for PIXE applications an maximum divergence of 0.1 mrad was chosen. A set of rays for simulation was chosen with a Gaussian distribution in $\theta$ and $\phi$ was chosen with a zero mean. The standard deviations of beam divergence were calculated
from FWHM’s for STIM of $2 \times 0.001 \text{mrad} = 2.354\sigma$ and for PIXE, $2 \times 0.1 \text{mrad} = 2.354\sigma$, with a Gaussian momentum spread distribution chosen to match the new Singleton facility at CENBG, assuming $\delta = 10^{-3}\%$.

The resultant beam-spot for STIM and PIXE simulations is shown in figure 4.3.

Figure 4.3: beam spots for the Bordeaux-Rossendorf Nanobeam Simulation (units in $\mu$m)
### Table 4.1: Comparison of quadrupole pole tip fields in the Bordeaux-Rossendorf system for TRAX, GEANT4 and XART

<table>
<thead>
<tr>
<th>Simulation Code</th>
<th>Quadrupole Pole Tip Field (T), Quadrupole number</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>TRAX</td>
<td>0.089839699</td>
</tr>
<tr>
<td>GEANT4</td>
<td>0.089839725</td>
</tr>
<tr>
<td>XART</td>
<td>0.089839699</td>
</tr>
</tbody>
</table>

### Table 4.2: Comparison of dominant intrinsic aberration coefficients in Bordeaux-Rossendorf system for TRAX, GEANT4 and XART

<table>
<thead>
<tr>
<th></th>
<th>Aberration Coefficient μm.mrad</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TRAX</td>
</tr>
<tr>
<td>$D_x$</td>
<td>63.557</td>
</tr>
<tr>
<td>$D_y$</td>
<td>99.409</td>
</tr>
<tr>
<td>$\langle x</td>
<td>3.0893E+3</td>
</tr>
<tr>
<td>$\theta^3 \rangle$</td>
<td>3.5789E+2</td>
</tr>
<tr>
<td>$\langle y</td>
<td>2.2920E+2</td>
</tr>
<tr>
<td>$\theta^2 \phi \rangle$</td>
<td>1.4896 E+2</td>
</tr>
</tbody>
</table>
TRAX, GEANT4 and XART are capable of calculating the intrinsic aberrations to any order. TRAX uses a Householder transformation to calculate the aberration, using the now obsolete Fortran NAG routine F04AMF. As in input to this routine TRAX traces an number of rays from a point source with varying divergences, such that the routine has enough equations for all the unknown coefficients. For this comparison, we traced the 32 rays as chosen by TRAX for a fifth order fit. A fifth order fit was chosen to give a reasonable degree of accuracy to third order for comparison of the spherical aberration coefficients. These rays were traced by both TRAX and GEANT4, and a comparison made of their positions in the image plane, and the coefficients were fitted with using a simple polynomial fitting routine.

In conclusion, the agreement with TRAX, GEANT4 and XART was found to be acceptable. TRAX is the benchmark standard in ray-tracing softwares, but it needs to be verified at nanometre precision. GEANT4 will be capable of this detailed simulation to include effects not implemented in TRAX or XART, such as slit-scattering and gas scattering. The author hopes that XART will prove a suitable replacement for TRAX for simulation of nanobeam optics. Full details of the comparison between TRAX and GEANT4 can be found in the paper by Incerti et al [28].
Chapter 5

Two Stage Systems

It has been shown that to achieve a higher resolution, one can limit the emittance of the system, thus reducing the angle dependent aberrations, or the geometric image, or both, but this will result in a loss of beam current transmitted through the system, thus degrading the analytical capabilities of the microbeam. To improve the resolution of the microbeam without loss of current, either the beam delivered from the accelerator must be improved, or the performance of the lens system must be improved.

Systems of 4 or more lenses with an intermediate image may provide the high demagnification to low aberration ratio required for the nanobeam generation of lens systems. The reason that few papers have been published on the concept of two-stage optics for microbeam systems may be simply because until the recent improvements in accelerators and construction of quadrupole lenses, other factors may have been considered more urgent, such as investigation into techniques for reduction of chromatic, spherical and sextupole aberration (introduced by pole misalignment in poorly constructed quadrupoles).

Chapter 2 describes the history of microbeam geometries so far. The work of Grime and Watt in [19] on calculated properties of systems of up to 4 lenses indicates that the opportunities for improvement of lens systems containing no more than 4 lenses and two coupled power supplies have been well explored. The work of Grime and Watt was not exhaustive, nor based upon a figure of merit, which makes comparison between geometries difficult. However it should be noted that there are no other publications within the last 25 years that have investigated the whole range of single-stage geometries with such accuracy.

This chapter presents the results of a systematic survey of two-stage lenses for nanobeam design. The scope of the survey is bound by a number of practical limitations for nanobeam design. The survey encompasses systems of up to 8 quadrupole lenses and 4 independent power supplies arranged as two groups of up to four lenses constrained to form an intermediate image. The parameter space for this survey is vast, and even restricting the quadrupole lengths to those commercially available and to the 7.2m beam length available in the University of Surrey Ion Beam Centre laboratory, several million system geometries have been considered. A matrix based beam optics software has been developed which surveys the parameter space to deter-
mine the optimum value of a figure of merit based on the ratio of demagnification to spherical aberration. This uses the analytical approximations for spherical aberration in quadrupole lenses derived by Dymnikov, Fishkova, and Yavor [14]. Matrix calculations for beam optics are straightforward, and are explained in section 3.1. Calculation of the Dymnikov coefficients is explained in section 3.1.7. The performance of selected systems with good figures of merits have been further investigated using numerical raytracing software and the results are presented.

5.1 Characteristics of Two Stage Focusing Systems

The key characteristic of two-stage focusing systems is the intermediate image formed by the first stage of the lens system. This intermediate image acts as a virtual object, from which the final image is formed by the second stage lens system.

The position of a ray in the image plane given the object coordinates for a system consisting of a single stage can be expressed as:

\[
x_i = \frac{x_0}{D_x} + < x \mid \theta > + < x \mid \theta \delta > \theta \delta + ... + < x \mid \theta \phi \delta > \theta \phi \delta + < x \mid \theta, \phi \delta > \theta \phi \delta ...
\]  

(5.1)

Where \(x_0\) is the position of the ray in the object plane. \(D_x\) is the system demagnification in the x-z plane. \(< x \mid \theta > \theta \delta\) and \(< x \mid \theta \delta > \theta \phi \delta\) represent the astigmatism and chromatic aberration terms respectively. \(< x \mid \theta \phi \delta > \theta \phi \delta\) and \(< x \mid \theta \phi > \theta \phi^2\) are the spherical aberration term and the spherical aberration cross term respectively.

Spherical aberration is the dominant aberration under microbeam conditions, therefore it is convenient to simplify the equation by assuming that chromatic aberration and spherical aberration cross-terms are negligible:

\[
x_2 = \frac{x_0}{D_1 D_2} + \theta^3 (\frac{S_1}{D_2} + \frac{S_2}{D_1^3})
\]  

(5.2)

where \(S_{1,2}\) represents the \((x \mid \theta^3)\theta^3\) spherical aberration term, in the first or second-stage as denoted by the subscript. A similar expression exists for the Y-Z plane. Using this expression to form the entrance coordinate to the second stage of the focusing system, an expression for transport through both stages is obtained.

The equation describes the effective spot size for two-stage systems which form an intermediate image. It can be seen that the resolution of a two-stage system is crippled by the spherical aberration in the second stage since this term is multiplied by the cube of the first stage demagnification.

Spherical aberration is the dominant intrinsic aberration limiting the reduction of microbeam resolution today. Optimisation of nanobeam performance with regard to spherical
aberration, including the spherical aberration cross-terms $< x \mid \theta \phi^2 >, < y \mid \theta^2 \phi >$, is the major aim of this survey. All other aberration terms are assumed to be negligible in this survey.

### 5.2 Procedure

It is clear that optimisation of a microbeam design involves the exploration of a wide parameter space to find the optimum set of system attributes to give the smallest focus. If we wish to evaluate the performance of all systems within this wide parameter space then an organised approach to this exploration becomes crucial.

Grime and Watt [19] identified 10 unique systems employing between 2 and 4 lenses, with no more or less than two power supplies, as shown in figure 5.1.

Thus there are ten possibilities of lens configurations for each stage of the two-stage system, yielding 100 possible lens configurations.

The survey examines a number of parameters for each of these lens configurations (figure 5.2):

1. The working distance of the first stage. The intermediate image distance is arbitrarily fixed at the mid-point of the beam-line and the object distance of the first stage is varied to suit.

2. The drift space between the first and second quadrupoles of the first stage.

3. The drift space between the second and third quadrupoles of the first stage (if the first stage is a triplet or quadruplet geometry).

4. The drift space between the third and fourth quadrupoles of the first stage (if the first stage is a quadruplet geometry).

5. The drift space between the first and second quadrupoles of the second stage.
6. The drift space between the second and third quadrupoles of the second stage (if the second stage is a triplet or quadruplet geometry).

7. The drift space between the third and fourth quadrupoles of the second stage (if the second stage is quadruplet geometry).

8. The system balance. The demagnification and spherical x and y terms of the second stage can be swapped if the excitations of the second stage are inverted.

9. The excitation mode of each stage. For each quadrupole geometry, the possibility for beam cross-overs means that a number of excitation modes exist. Quadrupole excitations are chosen up to the specified maximum pole-tip field such that for each geometry all excitation modes are explored.

The survey is confined by a number of practical limitations:

1. The space requirements of the Surrey Ion Beam Centre laboratory dictate that the object to image distance of the beamline cannot exceed 7.2 metres.

2. The working distance of the beamline must be long enough to support a practical end-stage and detector geometry for all planned applications of the nanobeam. Therefore the working distance of the final lens should not be less than 0.1 metres.
CHAPTER 5. TWO STAGE SYSTEMS

3. Four independent quadrupole power supplies are available.

4. Six precision quadrupole lenses are available, and thus the survey is limited to systems of no more than 8 quadrupole lenses.

A system of recursive loops is used to iterate through each survey parameter. As each unique geometry is selected, a numerical minimiser attempts to focus the system by reducing the astigmatism terms $< x \mid \theta > \theta, < y \mid \phi > \phi$. At each stage the system is evaluated by the figure of merit and system acceptance. When the recursive loop is exhausted, the next geometry from the list of possible stages is loaded.

A significant number of steps is required in each parameter, such that an optimum system can be identified. If each parameter is varied in 10 increments, this will yield in excess of 10 million possible system configurations. Accurate modelling of each geometry using numerical raytracing techniques is far too slow to explore the vast parameter space for two-stage systems. For this reason, it is preferable to use the matrix approximations to the third order aberrations derived by Dymnikov et al [14], as described in section 3.1.7, which provide a fast and easy method for approximating the spherical aberration coefficients of each geometry. However, the inaccuracies of the Dymnikov method for calculating spherical aberration, examined in section 3.2.3, mean that this method is likely to overestimate the spherical aberration of the two-stage system depending on the excitation mode of each stage. This overestimation will cause a bias towards low demagnification, low aberration systems. To verify the results a further survey using numerical raytracing with XART on the highest performance systems identified in section 5.3 is presented in section 5.4.

5.3 Results, Using Dymnikov coefficients
Figure 5.3: Procedure for survey of two-stage systems.
Table 5.1: 100 two-stage systems found using Dymnikov coefficients to calculate spherical aberration. Units of \( \mu m \) and mrad. System geometry numbers are shown in figure 5.1

| System Geometry          | \( <\theta|\theta> \) | \( <\phi|\phi> \) | \( <x|\theta^2> \) | \( <x|\theta^2\phi> \) | \( <y|\theta^2\phi> \) | \( <y|\phi^3> \) | Figure of Merit Q |
|--------------------------|------------------------|-----------------|-----------------|--------------------|-------------------|-----------------|------------------|
| Doublet then Doublet     | 25.158718              | 1275.2502       | 220.88845       | 54942.77           | 1083.936          | 370356.87       | 73.907091       |
| Doublet then Doublet     | 203.52603              | 157.63911       | 1505.5918       | 6791.7093          | 8768.6977         | 54246.854       | 73.947473       |
| Doublet then Triplet 1   | 66.584216              | -1746.4943      | 25348.3299      | 313411.76          | -11948.666        | -1315494.94     | 36.12925        |
| Doublet then Triplet 2   | 49.701524              | 311.09711       | 76.251912       | 24476.523          | 3910.4205         | 450419.62       | 47.567427       |
| Doublet then Triplet 3   | 49.559547              | 311.90833       | 1821.1768       | 24546.643          | 3899.25           | 18818.523       | 47.601407       |
| Doublet then Triplet 3   | 27.543046              | 405.88774       | 122.92623       | 36478.438          | 2475.3823         | 370808.76       | 31.295824       |
| Doublet then Triplet 3   | 64.6060234             | 172.89428       | 1499.2771       | 15538.566          | 5811.2234         | 30329.371       | 31.321037       |
| Doublet then Quadruplet 1| 16.894831              | 336.79895       | 110.3325        | 23498.784          | 1178.7684         | 100191.19       | 25.54349        |
| Doublet then Quadruplet 1| 53.551478              | 106.25591       | 402.89058       | 7413.5763          | 3736.3377         | 27333.776       | 25.575786       |
| Doublet then Quadruplet 2| 15.273142              | 343.52882       | 129.08401       | 27923.645          | 1241.4732         | 98325.45        | 22.492899       |
| Doublet then Quadruplet 2| 54.621479              | 96.056801       | 393.38665       | 7807.9504          | 4439.8918         | 31986.623       | 22.51964        |
| Doublet then Quadruplet 3| 15.278476              | 371.42712       | 116.52311       | 24043.89           | 989.03381         | 91884.688       | 25.74751        |
| Doublet then Quadruplet 3| 59.0574                | 96.09025        | 369.48675       | 6220.2871          | 3823.01           | 28861.799       | 25.781779       |
| Doublet then Quadruplet 4| 35.73827               | 224.76715       | 864.23862       | 29398.491          | 4674.3984         | 45096.43        | 23.692328       |
| Triplet 1 then Doublet   | -201.74648             | 503.13082       | -114181.19      | -68649.361         | 27527.169         | 22767.231       | 73.821914       |
| Triplet 1 then Doublet   | -1634.8163             | 62.092364       | -78084.471      | -8472.5321         | 223071.44         | 3375.3724       | 73.487199       |
| Triplet 1 then Doublet   | 2223.9132              | 164.3771        | 271603.87       | 92730.107          | 1254576.9         | 381542.09       | 36.12258        |
| Triplet 1 then Triplet 1 | -533.13092             | -685.68599      | -13016728       | -38616.23          | -300755.3         | -79625.756      | 36.122185       |
| Triplet 1 then Triplet 2 | -398.26774             | 122.43209       | -3912.76        | -30388.651         | 98853.322         | 27571.958       | 47.543024       |
| Triplet 1 then Triplet 2 | -397.09776             | 122.79579       | -90015.39       | -30479.646         | 98565.259         | 1168.2849       | 47.262825       |
| Triplet 1 then Triplet 3 | -220.58385             | 159.72228       | -63072.333      | -45299.879         | 62561.223         | 22707.312       | 31.256308       |
| Triplet 1 then Triplet 3 | -518.04488             | 68.012495       | -774204.92      | -19290.209         | 146931.74         | 1887.4668       | 31.048766       |
| Triplet 1 then Quadruplet 1| -134.97555             | 132.30407       | -56211.944      | -29021.823         | 29607.83          | 6116.3674       | 25.49104        |
| Triplet 1 then Quadruplet 1| -428.30335             | 41.694386       | -206886         | -9145.9343         | 93951.122         | 1714.213        | 25.228829       |
# Table 5.1: 100 two-stage systems found using Dymnikov coefficients to calculate spherical aberration. Units of μm and mrad. System geometry numbers are shown in figure 5.1

| System Geometry | $<\theta|$ | $>\phi|$ | $<x|$ | $\theta^2 >$ | $<y|$ | $y^2 >$ | Figure of Merit \(Q\) |
|-----------------|---------|---------|-------|---------|-------|---------|----------------|
| Triplet 1 then Quadruplet 2 | -121.83927 | 134.98339 | -65916.611 | -34567.515 | 31201.475 | 6002.6698 | 22.402055 |
| Triplet 1 then Quadruplet 2 | -436.97423 | 37.637868 | -203042.85 | -9638.8653 | 111906.86 | 2006.6632 | 22.185035 |
| Triplet 1 then Quadruplet 3 | -121.88063 | 146.12155 | -58407.299 | -29708.679 | 24780.139 | 6650.5279 | 25.693909 |
| Triplet 1 then Quadruplet 3 | -473.03126 | 37.650301 | -189615.49 | -7655.0922 | 96176.341 | 1814.7071 | 25.415471 |
| Triplet 1 then Quadruplet 4 | -285.84719 | 88.299188 | -92974.975 | -36313.54 | 117556.27 | 13087.826 | 23.64174 |
| Triplet 1 then Quadruplet 4 | -285.54718 | 88.299191 | -443097.9 | -36313.54 | 117556.29 | 2767.6027 | 23.580671 |
| Triplet 1 then Quadruplet 6 | -105.49503 | 192.48231 | -86762.592 | -63485.454 | 34794.886 | 8056.6113 | 22.851944 |
| Triplet 1 then Quadruplet 6 | -623.11464 | 32.587694 | -273924.31 | -10748.267 | 205519.37 | 26307.689 | 22.649076 |
| Triplet 2 then Doublet | -341.67375 | 669.09187 | -554641.14 | -205613.75 | 104997.27 | 5354.659 | 73.821891 |
| Triplet 2 then Doublet | -2768.7093 | 82.56954 | -379304.48 | -25373.854 | 850832.23 | 7939.0059 | 73.481699 |
| Triplet 2 then Triplet 1 | -722.90615 | 109.76496 | -93304.498 | -13441.023 | 88521.856 | 11360.5 | 36.122597 |
| Triplet 2 then Triplet 1 | 173.29954 | -457.87638 | -170409.83 | 56068.228 | -21221.008 | -23708.593 | 36.122582 |
| Triplet 2 then Triplet 2 | 129.46017 | 87.750793 | 1343.8811 | 4405.0758 | 6975.3196 | 47553.166 | 47.496032 |
| Triplet 2 then Triplet 2 | 129.08041 | 81.997635 | -32826.567 | 4418.036 | 6954.8577 | 342.76078 | 47.496032 |
| Triplet 2 then Triplet 3 | -373.7088 | 212.36509 | -306701.4 | -135672.78 | 238749.75 | 53373.216 | 31.25624 |
| Triplet 2 then Triplet 3 | -877.66449 | 90.424874 | -3764778.6 | -57769.356 | 506709.79 | 4437.2696 | 31.045454 |
| Triplet 2 then Quadruplet 1 | -228.7578 | 175.87352 | -273646.59 | -8615.52 | 113050.58 | 14367.567 | 25.490906 |
| Triplet 2 then Quadruplet 1 | -725.89661 | 55.424476 | -100716.78 | -27390.406 | 358733.25 | 4028.6716 | 25.224456 |
| Triplet 2 then Quadruplet 2 | 39.751851 | 90.185045 | 2289.2759 | 5035.0693 | 2219.3683 | 1786.0218 | 22.41798 |
| Triplet 2 then Quadruplet 2 | 142.56983 | 25.145794 | 7051.8947 | 1403.9004 | 7959.7339 | 583.29068 | 22.374982 |
| Triplet 2 then Quadruplet 3 | 39.765269 | 97.626106 | 2063.2 | 4237.4409 | 1762.6622 | 1667.8901 | 25.713842 |
| Triplet 2 then Quadruplet 3 | 154.33317 | 25.154264 | 6585.5331 | 1115.0011 | 6841.0521 | 526.0541 | 25.656298 |
| Triplet 2 then Quadruplet 4 | 93.262867 | 59.003587 | 15389.505 | 5290.6675 | 8362.5902 | 819.33999 | 23.642365 |
| Triplet 2 then Quadruplet 6 | -178.79391 | 255.86714 | -422368.97 | -190126.9 | 132856.18 | 18995.369 | 22.851813 |
Table 5.1: 100 two-stage systems found using Dymnikov coefficients to calculate spherical aberration. Units of $\mu m$ and mrad. System geometry numbers are shown in figure 5.1

| System Geometry | $<\theta | \theta>$ | $<\phi | \phi>$ | $<x | \theta^2>$ | $<x | \theta^2 >$ | $<y | \phi^2 >$ | $<y | \phi^3 >$ | Figure of Merit Q |
|----------------|------------------|----------------|----------------|----------------|----------------|----------------|------------------|
| Triplet 2 then Quadruplet 6 | -1056.0602 | 43.319015 | -133394.87 | -32189.007 | 784725.38 | 6182.0931 | 22.645985 |
| Triplet 3 then Doublet | -233.50037 | 538.83696 | -177040.71 | -91137.799 | 39493.783 | 27967.148 | 73.819513 |
| Triplet 3 then Doublet | -1892.1564 | 66.494839 | -1210703.5 | -11246.803 | 320035.51 | 4145.6389 | 73.485537 |
| Triplet 3 then Triplet 1 | 2572.0875 | 175.89649 | -420561.5 | 122806.37 | 1795764.7 | 467510.27 | 36.122226 |
| Triplet 3 then Triplet 1 | -616.60078 | -736.6691 | -2037693 | -512456.82 | -430570.27 | -97617.985 | 36.122226 |
| Triplet 3 then Triplet 2 | -461.01626 | 131.1162 | -60688.423 | -40343.572 | 141851.61 | 33864.864 | 47.543103 |
| Triplet 3 then -Triplet 2 | -459.66339 | 131.50209 | -1458016 | -40462.31 | 141435.34 | 1434.7444 | 47.263614 |
| Triplet 3 then Triplet 3 | -255.37676 | 171.06156 | -97827.656 | -60139.694 | 89773.687 | 27890.065 | 31.25635 |
| Triplet 3 then -Triplet 3 | -599.66692 | 72.83361 | -1200837.3 | -25607.43 | 210835.75 | 2317.8483 | 31.049327 |
| Triplet 3 then Quadruplet 1 | 20.310737 | 122.07766 | 191.78023 | 3719.5775 | 618.84671 | 4791.6194 | 25.503504 |
| Triplet 3 then Quadruplet 1 | 64.460291 | 38.473141 | 705.01676 | 1172.1803 | 1963.7323 | 1304.9921 | 25.493034 |
| Triplet 3 then Quadruplet 2 | 18.334052 | 124.54863 | 224.87337 | 4430.199 | 652.14285 | 4702.5941 | 22.413287 |
| Triplet 3 then Quadruplet 2 | 65.754825 | 34.7272 | 691.91811 | 1235.2477 | 2338.9014 | 1530.0675 | 22.404863 |
| Triplet 3 then Quadruplet 4 | 43.01351 | 81.473466 | 316.91305 | 4652.9228 | 2456.4874 | 10261.587 | 23.653906 |
| Triplet 3 then Quadruplet 4 | 23.63507 | 81.473472 | 1509.8934 | 4652.9232 | 2456.4872 | 2154.4535 | 23.651568 |
| Triplet 3 then Quadruplet 6 | 15.874608 | 177.60303 | 295.9449 | 8135.2005 | 727.1483 | 6343.4877 | 22.854606 |
| Triplet 3 then Quadruplet 6 | 93.764627 | 30.068679 | 933.40199 | 1377.3117 | 2494.9383 | 2013.3419 | 22.846761 |
| Quadruplet 1 then Doublet | 19.355742 | 397.05742 | 101.47722 | 4107.0528 | 200.21047 | 11195.831 | 73.652615 |
| Quadruplet 1 then Doublet | 157.12455 | 48.912414 | 693.81027 | 505.93657 | 1625.2531 | 1634.9988 | 73.695835 |
| Quadruplet 1 then Triplet 1 | 2624.298 | -172.67276 | 4.46E+09 | 1207524.9 | -1.84E+08 | -42535.41 | 36.113124 |
| Quadruplet 1 then Triplet 2 | 38.309124 | 96.578839 | 34.901919 | 1820.091 | 721.96035 | 1357.34 | 47.46005 |
| Quadruplet 1 then -Triplet 2 | 38.194103 | 96.869199 | 839.65281 | 1825.5545 | 719.78934 | 563.10831 | 47.491745 |
| Quadruplet 1 then Triplet 3 | -307.56457 | 157.57801 | -7029.7821 | -12164.619 | 23743.199 | 341499.64 | 36.195498 |
| Quadruplet 1 then -Triplet 3 | 62.317968 | -777.71171 | 2122.446 | 60037.356 | -4810.7878 | -113654.93 | 36.195488 |
Table 5.1: 100 two-stage systems found using Dymnikov coefficients to calculate spherical aberration. Units of \( \mu \text{m} \) and mrad. System geometry numbers are shown in figure 5.11

| System Geometry | \( \langle \theta | \theta \rangle \) | \( \langle \phi | \phi \rangle \) | \( \langle x | \theta^2 \rangle \) | \( \langle x | \theta \phi \rangle \) | \( \langle y | \theta^2 \phi \rangle \) | \( \langle y | \phi^3 \rangle \) | Figure of Merit Q |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|------------------|
| Quadruplet 1 then Quadruplet 1 | -483.50407 | 141.01379 | -2258.692 | -1089.081 | 37370.459 | 89343.934 | 53.944304 |
| Quadruplet 1 then -Quadruplet 1 | 55.731061 | -1223.3885 | 5515.3848 | 94556.789 | -4307.5032 | -366080.03 | 53.94416 |
| Quadruplet 1 then Quadruplet 2 | 117.06389 | 106.54939 | 59.350641 | 2081.6107 | 228.70297 | 2954.2201 | 22.285282 |
| Quadruplet 1 then -Quadruplet 2 | 42.110136 | 29.620172 | 182.420876 | 578.67687 | 822.68805 | 957.92251 | 22.310005 |
| Quadruplet 1 then Quadruplet 3 | 117.10259 | 115.48892 | 53.452068 | 1785.6586 | 181.06087 | 2756.9307 | 25.604132 |
| Quadruplet 1 then -Quadruplet 3 | 45.643124 | 29.629989 | 170.24435 | 458.13086 | 705.72161 | 862.3755 | 25.636013 |
| Quadruplet 1 then Quadruplet 4 | 27.540337 | 69.684075 | 83.477092 | 2181.0243 | 861.97808 | 6434.6067 | 23.608385 |
| Quadruplet 1 then -Quadruplet 4 | 27.540337 | 69.684075 | 397.32881 | 2181.0243 | 861.97808 | 1350.7663 | 23.615246 |
| Quadruplet 1 then Quadruplet 6 | -59.345864 | -1085.6264 | -2420.4539 | -10655.345 | -582.39345 | -3727.698 | 30.947461 |
| Quadruplet 1 then -Quadruplet 6 | -429.05811 | -150.16017 | -2301.665 | -14742.261 | -4212.598 | -39029.86 | 30.947476 |
| Quadruplet 2 then Doublet | 16.645469 | 414.54374 | 62.486717 | 3806.2045 | 151.08137 | 12741.069 | 73.59722 |
| Quadruplet 2 then Doublet | 133.57475 | 51.06638 | 426.28414 | 468.87485 | 1226.4398 | 1860.5077 | 73.691245 |
| Quadruplet 2 then Triple 1 | -181.00592 | 135.33992 | -1464.9207 | -5116.7797 | 6843.2688 | 21304.695 | 36.115105 |
| Quadruplet 2 then -Triple 1 | 43.469501 | -563.55205 | 7059.2203 | 21306.144 | -1643.4461 | -4421.157 | 36.115127 |
| Quadruplet 2 then Triple 2 | 32.499772 | 100.88232 | 2137.4654 | 1684.8706 | 5427.8994 | 15469.874 | 47.413291 |
| Quadruplet 2 then -Triple 2 | 32.402144 | 101.18628 | 512.69415 | 1689.4971 | 541.15943 | 641.70162 | 47.493212 |
| Quadruplet 2 then Triple 3 | 17.989662 | 131.59607 | 34.458645 | 2512.3636 | 343.45534 | 12746.755 | 31.135835 |
| Quadruplet 2 then -Triple 3 | 42.267025 | 56.017065 | 422.43972 | 1069.3295 | 806.94086 | 1034.659 | 31.195062 |
| Quadruplet 2 then Quadruplet 1 | 10.994607 | 109.1202 | 30.817086 | 1612.4227 | 162.48263 | 3456.6149 | 25.36021 |
| Quadruplet 2 then -Quadruplet 1 | 34.928598 | 34.346892 | 112.78909 | 507.54317 | 516.13903 | 930.28557 | 25.435531 |
| Quadruplet 2 then Quadruplet 2 | 9.9091836 | 111.3541 | 36.193667 | 1925.1003 | 171.31092 | 3372.1017 | 22.244968 |
| Quadruplet 2 then -Quadruplet 2 | 35.645202 | 30.955868 | 110.70101 | 535.16803 | 616.23769 | 1093.2131 | 22.307896 |
| Quadruplet 2 then Quadruplet 3 | 9.9124979 | 120.69622 | 32.616766 | 1651.4742 | 135.63171 | 3146.8617 | 25.552728 |
| Quadruplet 2 then -Quadruplet 3 | 38.635591 | 30.965996 | 103.30505 | 423.70097 | 528.64237 | 984.13799 | 25.633826 |
Table 5.1: 100 two-stage systems found using Dymnikov coefficients to calculate spherical aberration. Units of \( \mu m \) and mrad. System geometry numbers are shown in figure 5.1

| System Geometry         | <\( \theta | \theta >\) | <\( \phi | \phi >\) | <\( x | \theta^2 >\) | <\( x | \theta \phi >\) | <\( y | \theta^2 >\) | <\( y | \theta \phi >\) | Figure of Merit \( Q \) |
|-------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Quadruplet 2 then Quadruplet 4 | 23.313394 | 72.816084 | 50.729128 | 2016.3735 | 645.57867 | 7342.2256 | 23.594156 |
| Quadruplet 2 then -Quadruplet 4 | 23.311706 | 72.818409 | 241.05885 | 2016.3698 | 645.51014 | 1541.5281 | 23.611509 |
| Quadruplet 2 then Quadruplet 6 | 8.5897834 | 158.90237 | 47.479928 | 3528.1666 | 190.72201 | 4543.3463 | 22.758866 |
| Quadruplet 2 then Quadruplet 6 | 50.865596 | 28.83419 | 149.08971 | 595.80897 | 1129.3867 | 1435.7278 | 22.817744 |
| Quadruplet 3 then Doublet | 16.518796 | 453.00863 | 63.182499 | 4562.5309 | 166.37104 | 1662.9996 | 73.611985 |
| Quadruplet 3 then Doublet | 134.09601 | 55.804476 | 431.28927 | 562.04147 | 1350.564 | 2427.635 | 73.694351 |
| Quadruplet 3 then Triplet 1 | -181.7154 | 148.08031 | -1482.207 | -6149.2802 | 7546.0332 | 27904.374 | 36.11564 |
| Quadruplet 3 then -Triplet 1 | 43.640249 | -616.59757 | 7142.439 | 25605.236 | -1812.2337 | -57907.373 | 36.11566 |
| Quadruplet 3 then Triplet 2 | 32.627063 | 110.377 | 21.606842 | 2024.5786 | 598.45349 | 2024.5676 | 47.426719 |
| Quadruplet 3 then -Triplet 2 | 32.529064 | 110.70956 | 518.7228 | 2030.6782 | 596.6089 | 840.31781 | 47.496729 |
| Quadruplet 3 then Triplet 3 | 18.060435 | 143.98261 | 34.89761 | 3018.8903 | 378.67402 | 1669.444 | 31.145656 |
| Quadruplet 3 then -Triplet 3 | 42.4326 | 61.282801 | 427.40982 | 1284.9195 | 889.68638 | 1354.907 | 31.197533 |
| Quadruplet 3 then Quadruplet 1 | 11.037907 | 119.54015 | 31.132747 | 1942.1038 | 179.32687 | 4517.4464 | 25.372525 |
| Quadruplet 3 then -Quadruplet 1 | 36.065936 | 37.628342 | 114.11128 | 611.32723 | 569.69722 | 1222.7957 | 25.439371 |
| Quadruplet 3 then Quadruplet 2 | 9.9451297 | 121.9926 | 36.567888 | 2318.8037 | 189.09147 | 4433.7337 | 22.256239 |
| Quadruplet 3 then -Quadruplet 2 | 35.755313 | 33.913307 | 111.99631 | 644.6153 | 680.1979 | 1436.9634 | 22.311314 |
| Quadruplet 3 then Quadruplet 3 | 9.9518485 | 132.22875 | 32.952049 | 1989.2905 | 149.71419 | 4137.7317 | 25.567095 |
| Quadruplet 3 then -Quadruplet 3 | 38.759301 | 33.924747 | 104.52861 | 510.36158 | 583.54361 | 1293.592 | 25.638016 |
| Quadruplet 3 then Quadruplet 4 | 23.404064 | 79.784504 | 51.292662 | 2429.6069 | 712.70323 | 9567.669 | 23.599332 |
| Quadruplet 3 then -Quadruplet 4 | 23.403987 | 79.784766 | 243.89954 | 2429.6148 | 712.70089 | 2027.0832 | 23.614693 |
| Quadruplet 3 then Quadruplet 6 | -48.230657 | 402.41461 | -4207.1885 | -47526.993 | 5696.2598 | 95976.683 | 26.258979 |
| Quadruplet 3 then -Quadruplet 6 | -118.04428 | -164.41898 | 2422.6122 | 19418.629 | -13941.566 | -166675.58 | 26.259007 |
| Quadruplet 4 then Doublet | 35.778169 | 290.43725 | 640.03802 | 4062.5303 | 500.45198 | 4381.9696 | 73.684954 |
| Quadruplet 4 then Doublet | 290.43725 | 35.77817 | 4381.8247 | 500.45198 | 4062.5303 | 641.1924 | 73.641505 |
Table 5.1: 100 two-stage systems found using Dymnikov coefficients to calculate spherical aberration. Units of \( \mu m \) and mrad. System geometry numbers are shown in figure 5.1.

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<th>System Geometry</th>
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<th>( x \psi \phi )</th>
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</table>
Table 5.1: 100 two-stage systems found using Dymnikov coefficients to calculate spherical aberration. Units of μm and mrad. System geometry numbers are shown in figure 5.1.

| System Geometry   | $<\theta|\theta>$ | $<\phi|\phi>$ | $<x|\theta^3>$ | $<x|\theta^2\phi>$ | $<y|\theta^2\phi>$ | $<y|\phi^3>$ | Figure of Merit Q |
|-------------------|-------------------|----------------|-----------------|-------------------|-------------------|-----------------|------------------|
| Quadruplet 5 then Quadruplet 1 | -65.203778 | -1065.8647 | -6692.0952 | -911564.51 | -557653.432 | -3202409.2 | 25.021393 |
| Quadruplet 5 then -Quadruplet 1 | -207.14468 | -335.50657 | -23609.044 | -2869.117 | -177153.8 | -866260.58 | 25.413578 |
| Quadruplet 5 then Quadruplet 2 | -58.769111 | -1087.6656 | -7843.6004 | -108383.38 | -58805.214 | -3142209.9 | 21.96482 |
| Quadruplet 5 then -Quadruplet 2 | -211.40337 | -302.36554 | -23174.785 | -302551.66 | -211533.5 | -1017851.5 | 22.288328 |
| Quadruplet 5 then Quadruplet 3 | -58.788593 | -1178.9225 | -7097.1834 | -933508.75 | -46550.699 | -2932363 | 25.196704 |
| Quadruplet 5 then -Quadruplet 3 | -229.14044 | -302.46581 | -21626.004 | -239502.48 | -181441.01 | -916212.15 | 25.612615 |
| Quadruplet 5 then Quadruplet 4 | -138.25294 | -711.38174 | -10702.533 | -1140776.5 | -221703.34 | -6847521.5 | 23.504001 |
| Quadruplet 5 then -Quadruplet 4 | -138.25295 | -711.38168 | -50407.084 | -1140776.3 | -221703.33 | -1436620.2 | 23.595683 |
| Quadruplet 5 then Quadruplet 6 | 297.87015 | 11079.805 | 3066685.8 | 55722382 | 1498043.9 | 3.96E+08 | 30.947202 |
| Quadruplet 5 then -Quadruplet 6 | 2153.5476 | 15325151 | 2909799 | 7707300.6 | 10380588 | 4.17E+08 | 30.947419 |
| Quadruplet 6 then Doublet | 13.437512 | 675.77937 | 34249403 | 82506843 | 16423941 | 55196.02 | 73.440696 |
| Quadruplet 6 then Doublet | 109.052 | 83247405 | 23218585 | 10174787 | 1333.25 | 8057.166 | 73.697218 |
| Quadruplet 6 then Triplet | -148.00334 | 220.83681 | -8008632 | -11139.158 | 7465.3885 | 925532.89 | 36.115433 |
| Quadruplet 6 then -Triplet 1 | 35.544102 | -919.55024 | 3859.1716 | 46382.733 | -1792.8684 | -192067.65 | 36.115495 |
| Quadruplet 6 then Triplet 2 | 26.572429 | 164.6097 | 11783025 | 3667503 | 59203353 | 67204.545 | 47.278989 |
| Quadruplet 6 then -Triplet 2 | 26.494053 | 165.10525 | 2803739 | 36787386 | 59031858 | 2786.4247 | 47.49498 |
| Quadruplet 6 then Triplet 3 | -213.35377 | 265.58435 | -2346.4713 | -24513006 | 19472253 | 1690867.3 | 36.197016 |
| Quadruplet 6 then -Triplet 3 | 43.2291 | -1325.5766 | 70502143 | 120981.99 | -39454093 | -562762.21 | 36.196948 |
| Quadruplet 6 then Quadruplet 1 | 9.0018484 | 178.21903 | 1718181 | 35211283 | 17785499 | 14968.796 | 25.227473 |
| Quadruplet 6 then -Quadruplet 1 | 28.508242 | 56.098727 | 61991447 | 11083999 | 5650243 | 40498473 | 25.431318 |
| Quadruplet 6 then Quadruplet 2 | 28.113278 | 181.87432 | 20162434 | 42040994 | 18753902 | 14691.45 | 22.135859 |
| Quadruplet 6 then -Quadruplet 2 | 29.184855 | 50.560113 | 60842992 | 11687067 | 67461348 | 4759.3006 | 22.30391 |
| Quadruplet 6 then Quadruplet 3 | 8.1159103 | 197.13369 | 1819591 | 36064128 | 14847448 | 13710311 | 25.413808 |
| Quadruplet 6 then -Quadruplet 3 | 31.633419 | 50.576872 | 56.77907 | 92526588 | 5787063 | 4284.0869 | 25.630213 |
Table 5.1: 100 two-stage systems found using Dymnikov coefficients to calculate spherical aberration. Units of \( \mu m \) and mrad. System geometry numbers are shown in figure 5.11.

| System Geometry                  | \(< \theta | \theta >\) | \(< \phi | \phi >\) | \(< x | \theta^2 >\) | \(< x | \theta \phi^2 >\) | \(< y | \theta^2 \phi >\) | \(< y | \phi^3 >\) | Figure of Merit Q |
|----------------------------------|--------------------------|----------------------|----------------------|----------------------|----------------------|----------------------|------------------|
| Quadruplet 6 then Quadruplet 4   | -87.8183                 | 350.87536            | -2719.2726           | -176300.83          | 44125.183            | 821429.67           | 23.572023        |
| Quadruplet 6 then -Quadruplet 4  | -87.818301               | 350.87535            | -12895.153           | -176300.8           | 44125.176            | 172383.81           | 23.61005         |
| Quadruplet 6 then Quadruplet 6   | 7.0329422                | 259.5341             | 26.402332            | 7705.2614           | 208.79976            | 19794.806           | 22.660368        |
| Quadruplet 6 then -Quadruplet 6  | 41.64661                 | 43.828015            | 81.888109            | 1301.2021           | 1236.4388            | 6251.0068           | 22.817839        |

1 The minus sign in the system geometry column indicates a polarity inversion in the excitement of second stage.
Results from this survey using the Dymnikov coefficients indicate that a low demagnification second stage is common in systems which achieve a high figure of merit. The results also indicate that there is little to be gained from using a quadruplet stage. In both the high excitation and low excitation modes the quadruplet systems produce an unfavourable ratio of demagnification to aberration, doing nothing to justify the cost of an extra lens. Table 5.1 shows each two-stage geometry from figure 5.1 in the most compact form. The ‘minus’ sign shown before the second stage system in column 1 of table 5.1 indicates that the polarity of the second stage has been inverted. In some cases this inversion can provide a closer balance for the demagnifications of the system. Aberration coefficients and performance can vary depending on the lens spacing of the system. This is presented in detail in section 5.4, where raytracing has been used to survey each system.

5.4 Results, using Raytracing
Table 5.2: Survey of highest performance two-stage systems using numerical raytracing

| System Geometry     | $< \theta | \theta >$ | $< \phi | \phi >$ | $< x | \theta \phi >$ | $< x | \theta \phi^2 >$ | $< y | \theta^2 \phi >$ | $< y | \phi^3 >$ | Figure of Merit Q |
|---------------------|-----------------|-----------------|---------------------|---------------------|---------------------|---------------------|------------------|
| Doublet then Doublet | 361.1           | 141             | 6580                | 14600              | 37120              | 40090              | 79.37            |
| Doublet then Triplet 1 | -390            | 417.5           | -10770              | -257100            | 241000             | 5065000            | 42.99            |
| Doublet then Triplet 2 | 67.2            | 312             | 198.8               | 39070              | 8286               | 384500             | 49.52            |
| Doublet then Triplet 3 | 37.32           | 407.7           | 303.5               | 5.9830             | 5518               | 313100             | 33.35            |
| Triplet 1 then Doublet | -201.2          | 665.7           | -115100             | -179500            | 54350              | 41170              | 79.74            |
| Triplet 1 then Triplet 1 | -541.3          | -873.7          | -11070000           | -15650000         | -9705000           | -12060000          | 42.96            |
| Triplet 1 then Triplet 2 | -393.5          | 157.3           | -38590              | -57830             | 144700             | 49020              | 50.05            |
| Triplet 1 then Triplet 3 | -218.6          | 204.9           | -51190              | -88540             | 94510              | 39920              | 33.26            |
| Triplet 2 then Doublet | 102.6           | 396.1           | 15230               | 32360              | 8406               | 8685               | 79.73            |
| Triplet 2 then Triplet 1 | -1167           | 124.6           | -287400             | -68850             | 644100             | 135700             | 42.88            |
| Triplet 2 then Triplet 2 | 200.6           | 93.59           | 5110                | 10440              | 22370              | 10300              | 50.09            |
| Triplet 2 then Triplet 3 | -1695           | 153             | -859700             | -144700            | 1603000            | 253800             | 43.09            |
| Triplet 3 then Doublet | 385.2           | 67.87           | 7967                | 3574               | 20270              | 44200              | 79.76            |
| Triplet 3 then Triplet 1 | -512.7          | 182.9           | -24350              | -64970             | 182100             | 427200             | 42.96            |
| Triplet 3 then Triplet 2 | 88.09           | 137.2           | 438.5               | 9859               | 6297               | 32390              | 49.91            |
| Triplet 3 then Triplet 3 | -618.8          | -1247           | -16810000           | -3510000          | -1743000           | -3424000           | 43.06            |
Table 5.2 shows the aberration coefficients and performance of the highest performance systems identified in the survey of two-stage systems, which have been re-evaluated using numerical raytracing such that the aberration coefficients can be calculated with a greater accuracy. Each system is shown in the most compact lens spacing geometry. The performance response of the four highest performance systems identified in table 5.2 to changes in the spacing of the quadrupole lenses in each stage are presented in the following sections of this chapter. The performance response of the remaining systems are presented in appendix A. In the survey using the Dymnikov coefficients methods, the intermediate image position was a variable considered for optimisation, nominally the halfway point between the object aperture and the final image plane. For the re-evaluation, a fixed intermediate image position of 4.274 metres from the object aperture was chosen such that a Wien filter positioned between the object and collimating aperture could have sufficient free drift space to discriminate between scattered and unscattered particles from the object aperture. This Wien filter will be described in more detail in chapter 7.

In the following sections, the axis legends denote the variable that has been changed in the relevant simulation. Table 5.3 shows which legend corresponds to which variable. Beam profiles shown in the following section always show 6 quadrupole lenses contained in the simulation. For systems containing less than 6 lenses, the excitation of the unused lens is zero.

<table>
<thead>
<tr>
<th>Legend</th>
<th>Variable or Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>CEN 2</td>
<td>Centre of first quadrupole lens in first stage</td>
</tr>
<tr>
<td>CEN 3</td>
<td>Centre of second quadrupole lens in first stage</td>
</tr>
<tr>
<td>CEN 4</td>
<td>Centre of third quadrupole lens in first stage</td>
</tr>
<tr>
<td>CEN 5</td>
<td>Centre of first quadrupole lens in second stage</td>
</tr>
<tr>
<td>CEN 6</td>
<td>Centre of second quadrupole lens in second stage</td>
</tr>
<tr>
<td>CEN 7</td>
<td>Centre of third quadrupole lens in second stage</td>
</tr>
<tr>
<td>Dx</td>
<td>Aberration Coefficient ( \langle \theta</td>
</tr>
<tr>
<td>Dy</td>
<td>Aberration Coefficient ( \langle \phi</td>
</tr>
<tr>
<td>Sx</td>
<td>Aberration Coefficient ( \langle x</td>
</tr>
<tr>
<td>Ty</td>
<td>Aberration Coefficient ( \langle y</td>
</tr>
<tr>
<td>Ux</td>
<td>Aberration Coefficient ( \langle x</td>
</tr>
<tr>
<td>Vy</td>
<td>Aberration Coefficient ( \langle y</td>
</tr>
<tr>
<td>Q</td>
<td>Figure of Merit, ( Q )</td>
</tr>
<tr>
<td>A</td>
<td>Calculated system acceptance for 100nm beam spot diameter</td>
</tr>
</tbody>
</table>

Table 5.3: Explanation of legends for survey results using raytracing
5.4.1 Doublet - Doublet Geometry

Figure 5.5: A Doublet-Doublet system.
Figure 5.6: System aberration and performance as a function of quadrupole positions in the first stage lens of a Doublet - Doublet system.
Figure 5.7: System aberration and performance as a function of quadrupole positions in the second stage lens of a Doublet - Doublet system.
5.4.2 Triplet 1 - Doublet Geometry

Figure 5.8: A Triplet 1 - Doublet system.
Figure 5.9: System aberration and performance as a function of quadrupole positions in the first stage lens of Triplet 1 - Doublet.
Figure 5.10: System aberration and performance as a function of quadrupole positions in the second stage lens of Triplet 1 - Doublet.
5.4.3 Triplet 2 - Doublet Geometry

Figure 5.11: A Triplet 2 - Doublet system.
Figure 5.12: System aberration and performance as a function of quadrupole positions in the first stage lens of Triplet 2 - Doublet.
Figure 5.13: System aberration and performance as a function of quadrupole positions in the first stage lens of Triplet 2 - Doublet.
Figure 5.14: System aberration and performance as a function of quadrupole positions in the second stage lens of Triplet 2 - Doublet.
5.4.4 Triplet 3 - Doublet Geometry

Figure 5.15: A Triplet 3 - Doublet system.
Figure 5.16: System aberration and performance as a function of quadrupole positions in the first stage lens of Triplet 3 - Doublet.
Figure 5.17: System aberration and performance as a function of quadrupole positions in the first stage lens of Triplet 3 - Doublet.
Figure 5.18: System aberration and performance as a function of quadrupole positions in the second stage lens of Triplet 3 - Doublet.
5.5 Why not a Three Stage System?

It is obvious from examination of equation 5.2 that expansion to incorporate a third stage will result in demagnifications and aberrations far higher than those achieved by two-stage systems. It may be possible to create a three stage system that will satisfy the compromise relationship of demagnification and aberration in such a way that the performance will exceed those achievable by two-stage systems. However the practicalities of constructing a device make this unrealisable at the present time. Firstly, the high-demagnifications will require a large drift length between the object aperture and the collimating aperture to allow any reasonable angular definition of the beam. Any such beamline with this blend of extremely high demagnification is likely to require an extremely parallel beam to make any use of its high demagnification qualities. Thus the problem lies in the significant additional length required by a further stage. Not only will this increase the overall length of the beam path, thus broadening the beam spot due to increased gas scattering, but the added length will make the beamline increasingly vulnerable to stray magnetic fields due to the increasing lever arm effect. Similarly, the three stage system will have an increased response to parasitic aberrations in the first stage, since these will be amplified by a further two stages, with increased length. If the implications of these parasitic effects are insufficient to discourage the reader, then one must bear in mind a third critical constraint; The divergence of the beam at the exit of the second stage will be great, and unless the final two stages are particularly short - somewhat negating their performance improvements, then the diameter of the beam as it enters the the magnetic lens of the final stage will be great. Acceptance of this beam in the final stage will require magnetic lenses with a vast bore diameter. The practicalities of constructing such a lens to the required accuracy to prevent aberrations due to pole imperfection must be questioned.

5.6 The need for high quality resolution standards

Measuring beam resolution at the nanoscale requires the fabrication of high quality resolution standards. The standard procedure for measuring beam resolution for a microprobe involves the scanning of a 2000 grade copper grid, with bar spacings of 12.5μm.

The beam spot diameter is measured by sweeping the beam across a bar of the grid. Standard edge-convolution shows that if the beam is gaussian in profile, and the bar of the grid is sharp, then the full width, half maximum value will be given by the distance between 10% and 90% of the convolution height. The convolution height is measured experimentally in counts of backscattered particles of the beam which strike the copper grid, by the RBS technique.

However, the reality is not so simple. Firstly, the beam profile is not strictly gaussian. The beam profile is determined by the nature of the beam delivered by the accelerator and the aberration coefficients of the lens system. Secondly, the copper grid bars are not ‘sharp’, and this will produce inaccurate results when measuring beam profiles at the sub-micron level.
CHAPTER 5. TWO STAGE SYSTEMS

Micro-machined resolution standards measure the quality of their standards in terms of 'sidewall verticality', where 90° represents the perfect 'sharp' cut-off.

5.7 Selection of design candidate for the Surrey Horizontal Nanobeam

The purpose of this survey of two-stage systems was to identify the optimum lens geometry of a two-stage system for the design of a high performance nanobeam at the University of Surrey Ion Beam Centre. A number of practical design considerations for this nanobeam have set limitations for this survey:

- An image distance of 7.142 metres is a constraint fixed by the limit of the space available in the Surrey Ion Beam Centre Tandetron Accelerator laboratory.
- Three small bore OM52 quadrupole lenses, and three large bore OM50 quadrupole lenses are available for this project. The physical properties and fringe field profiles for these lenses are detailed in section 3.2.3. The larger beam envelope in the second stage of any two-stage system suggests that the larger bore OM50 quadrupole is used in the second stage to maximise the acceptance of the system over a range of beam spot diameters in the image plane.
- The intermediate image distance is fixed at 4.274m from the object aperture to satisfy two design specifications. Firstly, the first-stage must have sufficient drift length after a Wien filter situated between the object and collimator apertures. The energy discrimination performance of this Wien filter is directly a function of post-filter drift length. The design of this Wien filter will be described in Chapter 7. Secondly, the second stage must have sufficient space to incorporate an electrostatic dog-leg scanning system, and an "anti-halo" aperture before the entrance of this scanning system. The dog-leg scanning system minimises aberration incurred when the beam is deflected away from the beam axis at the entrance to the second-stage lens. The principle and design of this scanning system is described in chapter 9. The choice of drift length between the intermediate image and the entrance to the second-stage lens is a trade-off between mimitising the width of the beam envelope in the second stage lens, and optimising the halo-discrimination performance of the anti-halo aperture.
- A custom designed end-chamber for Proton Beam Writing applications allows a short working distance in the final stage of 100mm.

It is clear from the results of this survey that the second stage of the nanobeam design must be a low aberration stage, specifically a doublet configuration. The high demagnification Triplet 1 - Doublet geometry presented in section 5.4.2 consisting of a Oxford Triplet first stage
and a doublet second stage has several key advantages to recommend it as the design candidate for the Surrey Horizontal Nanobeam:

- A high demagnification system allows a larger object aperture to be used under optimum acceptance conditions for the beamline. Slit scattering is a fundamental limitation to nanobeam resolution. The opportunity to increase object aperture dimensions reduces the ratio of scattered flux to unscattered flux accepted into the beamline by the object aperture.

- A high demagnification system requires a more parallel beam under its optimum acceptance condition since it allows a large object aperture. Such a system will receive enhanced performance from the flux-peaking phenomenon described by Jamieson[31]. This phenomenon reduces the sensitivity of the probe to angle dependent aberrations which means that a system is likely to have better performance than indicated by the figure of merit.

- The high-demagnification Oxford Triplet first stage will act as a superior energy filter device than that of the lower demagnification systems. The benefits of this are twofold: firstly, and particles scattered from the collimator aperture will be over-focused by the first stage of the lens system, and will form a halo around the unscattered beam. This halo can then be prevented from entering the second stage of the lens system by an “anti-halo” aperture situated just before the entry to the second stage lens system. The performance of this anti-halo aperture is improved by the high-demagnification of the first stage. Secondly, although chromatic aberration is nearly negligible due to terminal voltage stability of the Surrey Tandetron accelerator, the energy selection qualities of the first stage lens system and anti-halo aperture are also enhanced by the use of a high demagnification first stage.

- Working distance can be extended to allow for larger detector geometries from the end chamber at the expense of system demagnification. With this high-demagnification choice, overall demagnification at extended working distance of up to 200mm is still higher than the other high performance geometries presented in this section at the nominal 100mm working distance. The beam profile and specification of the long working distance adaptation of this geometry is presented in figure 5.19.

The results of the survey of this system show that there is nothing to be gained from increasing the spacing of the lenses in either the first or second stages. The acceptance of the system is not sensitive to changes in the spacing of the first stage, including the working distance of the first stage. It is reasonable to conclude from this that the response of the system will not be strongly sensitive to changes in the position of the intermediate image within the practical constraints of intermediate image location. However, the system performance is
Figure 5.19: A Triplet 1 - Doublet system with a long working distance of 200mm

strongly related to the final working distance of the second stage, as all microbeam systems are since this determines the final demagnifications of the system. The minimum working distance achievable is limited by the end chamber design.

There are many practical advantages to be gained from using a compact lens geometry for both stages:

- Since the overall length of the system is limited to 7.142 metres, the additional length saved in a compact lenses design can be used to improve the performance of apertures in the object - collimator length of each stage. Not only will this improve the energy selection resolution of the Wien Filter by allowing extra drift length after the filter for unselected particles be dispersed, but it will also provide a similar enhancement to the anti-halo aperture after energy selection in the first stage lens.

- The narrow bore OM52 lenses used in the first stage of the design are susceptible to greater gas scattering within the lens since this small bore diameter creates a restriction to effective pumping. This effect will be reduced in a compact first-stage lens.

- Beam scanning in a compact lens can achieve greater displacements from the beam axis in the image plane before scanning is confined by the width of the beam envelope within the lens bore since there is a shorter drift length between lenses over which a divergent ray can stray from the beam axis.

5.8 Conclusion

The results presented in this chapter show that the system performance of the surveyed two-stage systems is not greatly dependent on the quadrupole spacing of the first lens. By changing
the lens spacing of the first stage it is possible to decrease aberration and demagnification in one plane, but this causes a comparable increase in aberration and demagnification in the other plane. Thus the system performance measured in the image plane is not sensitive to changes in lens spacing in the first stage, although a greater balance between the overall demagnifications of the system can be achieved if this is desired by the beamline designer.

The performance response of two-stage systems has a greater dependence on the lens spacing in the second stage. As with single-stage systems, all the surveyed two-stage systems exhibit higher performance with a shorter working distance in the final stage, due to the increased demagnifications achievable with short working distances. The response of two-stage systems to the lens spacing of the first two lenses in the final stage varies depending on the particular geometry used. However systems which exhibit greater performance with a compact second stage may be preferable due to the decreased response of compact lenses to parasitic aberrations. A compact lens is advantageous in reduction of parasitic aberration and gas scattering within the lens bore. These effects are reduced due to the shorter path over which particle trajectory deviations caused can stray from the beam axis. Compact lens geometries also benefit from the minimum beam displacement within the lens bore when scanning the beam, resulting in greater scanning areas being achievable.
Chapter 6
Backward Raytracing and Aperture Shaping

6.1 Introduction

The collimating or "beam-defining" aperture in MeV microbeam systems is used to control the angular divergence of the beam leaving the object and accepted into the lens system. High demagnification lens systems suffer from strong angular aberration. Such apertures have traditionally been elliptical or square geometry in Microbeam systems. This chapter studies the use of backward raytracing to realise the optimum aperture shape to minimise these angular aberrations. A shaped aperture may be able to prevent the most aberrated rays from being accepted into the lens, thereby improving the relation between beam current and beam spot diameter in the image plane. It has been shown in section 2.5 that a relationship exists between probe size on target and transmitted beam current through the acceptance volume defined by the object and collimator apertures. The beam current is directly proportional to the acceptance volume, whereas the beam dimension at the target is defined by:

1. The geometrical contribution, defined by the diameter of the object aperture, and the system demagnification.

2. The aberrated contribution, dominantly the spherical aberration terms, limited by the diameter of the collimator aperture.

An improved aperture shape can be found using numerical ray-tracing techniques. The distribution of rays traced backwards from within the image beam spot diameter to object plane will determine the unique aperture shape for the system due to the contributions of all of its aberration coefficients. This method can be used to determine the shape of the object and collimator apertures to give the optimum balance between the geometric contribution and aberrated contribution to beam spot size.
6.1.1 Terminology

When forward raytracing, rays enter from the object plane of the system and arrive at the image plane, and thus the image plane shows an "image" of the object aperture shaped by the various aberration and geometric terms. In this chapter the concept of "backward" raytracing is introduced, whereby rays are traced using numerical raytracing through the simulation of the beamline from the image plane towards the object plane, and in this manner the object plane is the image plane. To avoid confusion the use of the terms "object" and "image" will remain consistent with the forward system in this chapter.

6.2 Simulation

6.2.1 Backward Raytracing

When rays are traced backwards through the beamline optical system, the result is a distribution of rays in the object plane which fall inside the desired beam spot diameter when traced forward. However, the angular and spatial distribution of this set of rays in the object plane may form a phase-space ellipse that is not realisable as a combination of two apertures. The phase-space ellipse contains all rays traced backwards to the object plane, but may be warped such that it is no longer elliptical. If an outer boundary is drawn around the limits of the phase-space ellipse this region may enclose undesirable rays that will not fall within the desired beam spot diameter when traced forwards. Therefore the boundary of the phase-space ellipse must be chosen carefully by setting the limits of the object aperture.

6.2.2 Process

- Reverse beamline.
- Generate rayset from within the desired beam spot size at the image plane.
- Trace rays backwards using raytracing to the object plane, with any apertures or restrictions in the beamline.
- Record and examine all rays which pass through the object plane, and determine maximum possible size of object aperture.
- Remove rays from rayset which fall outside of object aperture in object plane.
- Trace remaining rays in the forward direction to the collimator plane, and determine limits of collimating aperture appropriate to the rayset in this plane.

When converting the reverse ray hit locations in the object plane to the rayset for forward tracing from the object plane to the collimator plane it is necessary to reverse the sign of the angular component of the ray.
CHAPTER 6. BACKWARD RAYTRACING AND APERTURE SHAPING

6.3 Results

6.3.1 Designing apertures for the Surrey Vertical Nanobeam, 1µm spot diameter

The Surrey Vertical Nanobeam is a single stage beamline system with a triplet of OM52 lenses in the popular Oxford Triplet geometry. The beam profile from object to image of this beamline is presented in figure 6.1.

![Figure 6.1: Beam Profile of the Surrey Vertical Nanobeam](image)

![Figure 6.2: Input Rayset in Image plane (reverse)](image)

Figure 6.3 shows the distribution of rays in the object plane in the forward direction. The reversal process from a rayset in the backwards direction to a rayset in the forwards direction requires that the sign of the divergence of each ray in both planes is reversed. The \( y - \theta \) phase space ellipse in the object plane shown in figure 6.3.1 is strongly warped due to the strong spherical aberration in this plane.
Figure 6.3: Ray distribution in the object plane (forward)

Figure 6.4: Forward traced ray distribution in the collimator plane.
Figure 6.5: Forward traced ray distribution in the image plane.

Figure 6.6: Rays accepted between object and collimator apertures.
The “tails” of this phase shape ellipse belong to a subset of rays which exist beyond the limits of the object aperture. These rays have sufficient divergence in the opposite direction to their axial offset that when traced forwards they pass through the collimator aperture and enter the lens such that they are focused into the beam spot diameter. The range of accepted divergences for this subset of rays decreases with increasing displacement from the beam axis in the object plane. The dimensions of the object aperture cannot be increased to accept these rays without also accepting undesirable rays from outside the range of accepted divergences, shown as rays 5 & 6 in figure 6.6.

Figure 6.3.1 shows that these regions do not exist in the $x - \theta$ phase-space ellipse of rays in the object plane, due to the decreased spherical aberration in this plane.

The maximum region that can be accepted is limited by the extents of the central linear region of the phase space ellipse. Therefore the appropriate object aperture dimensions for a 1\(\mu\)m beam spot diameter at the target are 80\(\mu\)m, 15\(\mu\)m in the x and y planes respectively. This is closely related to the demagnifications of the Oxford Triplet system, indicating that the optimum ratio between the geometric and aberrated components of the beam spot strongly favours the geometric component for this beamline geometry and beam spot diameter.

Figure 6.4 shows the distribution of rays in the collimator plane when the rayset has been traced forwards through the new object aperture dimensions, removing the warped regions of the phase-space ellipse shown in figure 6.3. The shape of the collimating aperture can then be chosen such that these rays are accepted into the lens. In this case an elliptical aperture is appropriate, with a diameter of 150\(\mu\)m in the horizontal direction and 400\(\mu\)m in the vertical direction. The oval shape of the collimator aperture is important in the limitation and removal of the spherical aberration cross-terms $< x|\theta\phi^2 >$, $< y|\theta^2\phi >$, which are of greatest influence at the diagonal extents of rayset in the collimator plane.

Figure 6.5 shows the distribution of rays in the image plane after forward raytracing through both the object and collimator aperture. The rayset distribution is entirely confined to the desired beam spot diameter.
6.3.2 Designing apertures for the Surrey Horizontal Nanobeam, 10nm beam spot diameter

Compared to the majority of two-stage systems, the Oxford Triplet geometry examined in the previous section does not suffer from particularly strong aberration. The following figures show a repeat of the backward raytracing process for the high-demagnification two-stage system using a triplet 1 - doublet geometry described in chapter 5. The requirement is a 10nm beam spot diameter in the image plane. The beam profile of the Surrey Horizontal Nanobeam two-stage system is shown in figure 6.7. A design feature of the Horizontal Nanobeam is the presence of an “anti-halo” aperture in the pre-lens drift space of the second stage. The purpose of this aperture is to remove the halo of particles scattered from the collimator aperture of the system, and over focused by the first stage lens. The backward raytracing technique can be used to completely specify this aperture in the same manner that the collimating aperture of the Vertical Nanobeam is specified in the previous section. The positions of all apertures for this beamline are indicated on figure 6.7.

![Figure 6.7: Beam Profile of the Surrey Horizontal Nanobeam Design Candidate](image)

The high demagnifications of the two-stage system require a very parallel rayset for optimum performance, hence there is little difference in diameter between the collimator and object apertures. This requirement for a parallel beam rotates the phase space ellipse in the object plane in the counter-clockwise direction, as shown in figure 6.3.2. The process of backward raytracing has been repeated, but with the aim of achieving a 10nm beam spot diameter.
Figure 6.8: Input Rayset (reverse) in image plane for a 10nm beam spot with a two-stage system

Figure 6.9: Ray distribution in the object plane (forward)

Figure 6.10: Forward traced ray distribution in the collimator plane.
Figure 6.11: Forward traced ray distribution in the plane of the anti-halo aperture.

Figure 6.12: Forward traced ray distribution in the image plane.
6.4 Conclusion

This chapter has proven the use of the backward raytracing technique in the optimisation of object and collimating aperture dimensions to find the optimum acceptance of a beamline. It is a simple and effective method, although it does require human interaction to determine the width of the undistorted phase-space ellipse in the object plane. In terms of processor time, the requirements of this method are greater than those of the numerical optimisation of acceptance discussed in section 2.5.2. Indeed, to trace a ray in two directions consecutively is a good test of accuracy for any raytracing software.

The advantage of the backward raytracing method over the numerical optimisation is that it provides extra information into the precise shape of collimating aperture required to limit all the aberrations of the system, whereas the numerical optimisation method is limited to spherical aberration coefficients. Furthermore, the numerical optimisation method is limited to the assumption of a rectangular beam spot shape in the image plane. The backward raytracing method also has the ability to calculate the optimum aperture dimension at any point along the beam axis, which is particularly useful for designing beam “halo” removal apertures for two-stage systems.

The shaped aperture technique offers the interesting possibility of lithographic aperture fabrication in thin foils. If used in conjunction with an Wien filter in the object drift space, such apertures would only require sufficient thickness to provide an energy loss greater than the resolution of the Wien filter.
Chapter 7

The Use of the Wien Filter to Eliminate Object Slit Scattering

7.1 Introduction

A fundamental issue in the construction of proton microbeam focusing systems with sub micrometre resolution is the design of the initial object aperture. This defines the spatial extent of the beam which the lens subsequently transforms with reduced size onto the image plane, and depending on the demagnification of the lens may have dimensions less than 10 micrometres. However, the long range of MeV protons in matter (e.g. 25\(\mu\)m for 3MeV protons in Ta) means that such slits are (a) very difficult to fabricate, and (b) seriously affected by penetration of the ions. Figure 7.1a shows SRIM2008\[61\] simulations of the paths of 3MeV protons in 50\(\mu\)m tantalum foil. Figure 7.1 shows a scale drawing of a 5\(\mu\)m hole in 50\(\mu\)m tantalum foil, with the regions marked where particle penetration will cause slit scattering. The range of the protons within the tantalum foil allows particles penetrating the rim of the hole to be scattered into the lumen of the slit, and similarly particles penetrating the edge of the aperture to be transmitted through the foil with reduced energy. The problem is most significant for the first object aperture, since the current and diameter of the beam falling on the aperture at this point are usually orders of magnitude greater than the transmitted beam.

Microbeam designers have been aware of this problem since the earliest designs. Slit jaw profiles to minimise scattering were investigated by Nobiling et al. in the 1970s \[47\] as part of the design of the Heidelberg microbeam. Slit assemblies for microbeam systems often made from high density alloys which can be polished to a fine finish, for example, in the University of Surrey Microbeam system \[51\] tungsten carbide cylinders are used to form the slit jaws. However, it is clear that whatever the detailed profile of the occluding metal edge, slit scattering becomes increasingly important as the aperture is reduced.

Incerti et al. \[27\] have modelled the effects of collimator and gas scattering using the GEANT4 simulation package and reported that if no further measures are taken, scattering
Figure 7.1: A scaled drawing of a 5\(\mu\)m diameter hole in 50\(\mu\)m tantalum foil. Simulation of the paths of 3MeV protons in tantalum are shown to indicate the magnitude of the problem of scattering from slit edges.

from the edge of a 5\(\mu\)m circular aperture contributes about 5\% of the total beam flux reaching the image plane and this is spread into a halo of several mm diameter. In the Bordeaux design, this is largely removed by the careful positioning of an additional collimator following the object aperture. This chapter contains an investigation into the use of an energy selective Wien filter [37] to effectively remove all scattered particles before they enter the lens system.

The problems of fabricating very small apertures has led nanobeam designers to seek systems with very high demagnification (in order to maximise the object diameter). However, the Wien filter also offers the interesting possibility of using sharp-edged object apertures of arbitrary shape fabricated lithographically in thin foils, which only require sufficient thickness to provide an energy loss greater than the resolution of the Wien filter. The transparency zone be much smaller than what could be made using conventional methods, which will provide additional flexibility in the design of nanobeam systems for both continuous beam and single ion modes.

### 7.2 Wien Filter Design

In the Wien filter, crossed magnetic and electrostatic fields are arranged normal to the path of a charged particle so that at all points along the path of the particle, the resultant forces cancel out at a certain velocity \(v\), where \(E\) is the electrostatic field strength (\(V m^{-1}\)), \(B\) is the magnetic field strength (T) and \(q\) is the charge (C).

\[
F = Eq - Bqv = 0
\]

In the non-relativistic approximation this means that a singly charged particle of energy \(T\) MeV is transmitted with no deflection when:

\[
\frac{B}{E} = \sqrt{\frac{Am_p}{2eT \times 10^6}}
\]
$Am_p$ denotes the mass of the particle (kg) and $e$ is the electron charge (C).

In order to derive the energy dispersion of the Wien filter, consider the geometry shown in figure 7.2, in which a Wien filter of length $L$ is illuminated with a beam diverging from the object slit with full angle $\Theta$, and the deflected beam is intercepted by the collimator slit of width $d$, a distance $L_s$ downstream of the exit of the filter. Note that the collimator slit can be the divergence limiting slit of the microbeam lens, and that an additional collimator at the entrance to the Wien filter will be required to define $\Theta$ (assumed to be larger than the divergence angle defined by the lens collimator).

Now replace $T$ with $T + \Delta$, and if $E_0$ is the electrostatic field for zero deflection at energy $T$, then it can be shown that the deflection, $X$ of an axial ray in the plane of the Lens Collimator, is given by equation 7.3.

$$X = \frac{E_0 L}{4 \times 10^{12}} (L/2 + L_s) \cdot \frac{Q}{T^2} \Delta \quad (7.3)$$

Note that this does not depend on the ion mass.

In order to completely remove particles with energy shift $\Delta$, the extreme ray in the beam must be moved at least as far as the opposite edge of the lens collimator, and so we can derive an inequality which defines the smallest electrostatic field required to remove ions of a energy displacement $\Delta_{\text{Min}}$:

$$E_0 L > \frac{1}{2} (L_c \Theta + d_c) \cdot \frac{4 \times 10^{12} T^2}{\Delta_{\text{Min}} Q (L/2 + L_s)} \quad (7.4)$$

Table 7.1 shows how this inequality translates into practical values in a typical geometry:

This shows that assuming a maximum practical potential difference of 40kV, an energy loss of 15keV (~ 0.5%) for 3MeV protons can be discriminated, corresponding to approximately 200nm thickness of gold foil.

### 7.3 Raytracing investigations

In order to investigate whether the Wien filter has any adverse influence on the performance of a microbeam system, a system with the geometry specified in caption to Table 7.1 was placed
CHAPTER 7. THE USE OF THE WIEN FILTER TO ELIMINATE OBJECT SLIT SCATTERING

into a model of the well known Oxford Triplet system [57], and the performance was simulated using raytracing. The potential difference on the Wien Filter was set to 40kV and the magnetic field was optimised to give no deviation for 3MeV protons (a value of 0.084T).

Figure 7.3 shows the point spread function of the system with and without the Wien filter. This shows the expected result that the additional broadening of the spot for ions of the correct energy is negligible. The Wien filter relies on an exact balance between the magnetic and electrostatic force components over the entire length of the device. If the forces are unbalanced, for example in the fringing field regions, the filter will still provide energy discrimination, but the beam will emerge with either an angular or lateral displacement of the axis. This will be dependent on beam energy and is undesirable. This effect is shown in figure 7.4, which indicates the path of the central ray in a system in which a mismatch of fringing field has been modelled by symmetrically increasing the length of the magnetic field by 1 mm relative to the electrostatic field and retuning the filter to give an emerging beam parallel to the axis. The diagram indicates that the beam is displaced by 120 μm. Similar effects are observed for small geometric misalignments between the electrostatic and magnetic field.

In practice, small differences in effective lengths of the two fields will be corrected empirically, by using adjustable iron shims at the end of the magnet pole pieces. Figure 7.4 shows a simulation of beam axis displacement due to mismatched fields.

<table>
<thead>
<tr>
<th>Δ_{\text{min}} (keV)</th>
<th>Equivalent thickness of gold (μm)</th>
<th>Plate potential difference (kV)</th>
<th>B (T)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.014</td>
<td>558</td>
<td>1.17</td>
</tr>
<tr>
<td>2</td>
<td>0.029</td>
<td>279</td>
<td>0.58</td>
</tr>
<tr>
<td>5</td>
<td>0.071</td>
<td>111</td>
<td>0.23</td>
</tr>
<tr>
<td>10</td>
<td>0.143</td>
<td>55</td>
<td>0.11</td>
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<tr>
<td>20</td>
<td>0.286</td>
<td>27</td>
<td>0.058</td>
</tr>
<tr>
<td>50</td>
<td>0.714</td>
<td>11</td>
<td>0.02</td>
</tr>
<tr>
<td>100</td>
<td>1.429</td>
<td>5.5</td>
<td>0.012</td>
</tr>
<tr>
<td>200</td>
<td>2.857</td>
<td>2.79</td>
<td>0.006</td>
</tr>
</tbody>
</table>

Table 7.1: Plate voltage and magnetic fields required to achieve the energy discrimination shown in the first column for 3MeV protons in a practical Wien filter geometry with $L_c = 3m$, $L_s = 1m$, $L = 0.75m$, $d = 100 \mu m$ and $\Theta = 0.5$mr. The field is assumed to be generated by plates separated by 20mm. The second column shows the approximate thickness of gold required to cause this energy shift (assuming a stopping power of 70keV/μm).
Figure 7.3: Point spread function, with and without the Wien filter.

(a) PSF : Wien Filter Inactive

(b) PSF : Wien Filter Active

Figure 7.4: Transverse displacement of the beam axis by 120μm due to 1mm field mismatch within the Wien filter.
7.4 Conclusion

This chapter has shown that the use of a Wien filter in the object space of a nuclear microbeam focusing system can eliminate halo due to object slit scattering and allows the use of micrometre sized object apertures of arbitrary shape formed in thin metal foils. This introduces new flexibility into the design of sub-micron MeV ion focusing systems.
Chapter 8

The Influence of Stray Magnetic Fields

8.1 Introduction

Stray DC fields in the microbeam laboratory environment are unavoidable. To achieve good beam-spot resolution the optical elements of the beamline must be aligned to the path taken by the beam in the presence of such stray DC fields, otherwise the particles will enter the lens system off-axis, causing large parasitic aberrations. A study by Jamieson has shown that stray DC fields arising from misalignment of the stainless steel beamtube passing through the bore of the magnetic quadrupole lenses of the Melbourne microprobe leads to significant sextupole aberration[31]. Such a field may be cancelled by correct alignment of the beam-tube and lenses. However, the beam may be influenced by other stray DC fields in the laboratory causing curvature of the beam path, making alignment of such a relatively long beam-tube impossible.

The Earth generates a magnetic field in the order of 50 μT, and with common microbeam lengths greater than 5 metres this results in a deflection in the order of millimetres. The established experimental technique of dipole minimisation, as described by Grime and Watt[19], is to align the optical elements of the focused system to the true path of the ions through any stray fields, thus ensuring that the ions pass through the optical centre of each element, minimizing aberrations caused by misalignment of the beam and focusing system. However, in the presence of a stray field, the alignment procedure is only valid for the magnetic rigidity of ions for which the beamline was aligned.

The influence of stray AC magnetic fields is far more serious than that of DC magnetic fields, but this has been well addressed by Jamieson [31]. Watt states in [56] that studies of stray magnetic fields on the resolution of the National University of Singapore nuclear microprobe indicate that the presence of a NIM crate within 3.5 meters of the collimator slits can degrade beam resolution by around 100nm when the beam was focused to sub-micron spot sizes. Naturally, the influence of stray fields in the object space is attenuated by the demagnification of the system, in the same way that the strength of field required for electrostatic scanning in the high-demagnification plane is greater than in the low demagnification plane.
for non-symmetric systems. It is clear though that stray magnetic fields of this magnitude must be eliminated when considering nanobeam design. Jamieson states in [33] that for the new CSIRO-MARC novel quintuplet lens design stray magnetic fields have been the limiting factor in achieving greater spatial resolution. Jamieson also notes that the influence of stray magnetic fields scales as a square of the total length of the system, and Jamieson found this to be an influential factor when choosing between long and short geometries for the design of the quintuplet system. Parasitic aberration due to stray fields was measured in Melbourne by the beam rocking method, as detailed in [31]. It was found that the stainless steel beam-pipe caused such troublesome stray DC fields, introducing sextupole aberration, that the Melbourne group replaced the offending beam-tube with an aluminium counterpart. Stray AC fields have the effect of bending the beam axis, which is seen in the image plane as a displacement of the object. Jamieson gives equation 8.1 for this effect in [31] where the position of a ray in the image plane is changed by the external stray field.

\[ \Delta \alpha_i = \frac{M q B_{\text{stray}} L^2}{2 \sqrt{2 E m}} \]  

Where \( q \) is the beam particle charge, \( B_{\text{stray}} \) is the strength of the stray field which is assumed to fill the entire laboratory and be directed transverse to the beam direction, \( L \) is the length of the beamline upstream of the probe forming lens system, \( E \) is the beam energy, and \( m \) is the particle mass.

The Melbourne group have taken the preventative measure against stray fields of shielding the beamline by two layers of mu-metal wrapped on the beam-tube, with an outer shield of iron pipe with 1 cm wall thickness. Jamieson reports that the shielding yielded a factor of 10 improvement on stray fields experienced by the beam [31].

So we are presented with an interesting balance between systems which have high demagnification, and the associated high spherical aberration, which will be more tolerant to stray fields, in contrast with systems with low demagnification, and low aberration, but must be shorter to retain the same tolerance to stray fields.

8.2 The magnetic field of the Earth

The National Geophysical Data Centre, U.S.A [46] provides values for the strength of the Earth's magnetic field in London, UK. These values are the closest available to the University of Surrey Ion Beam Centre, and as such should be a good approximations to field strengths in Surrey, UK.

The microbeam system used for simulation here uses three magnetic quadrupole lenses in an Oxford Triplet geometry [57]. The beamline is 6.367 metres in total length from object to image planes.

For this simulation, the beamline is orientated directly from east to west, and a 2.5 MeV
beam of protons will receive deflections of -3.96 mm and 1.7 mm in the x-z and y-z axis respectively due to the Earth’s magnetic field.

To model the Earth’s magnetic field, a magnetic dipole with a pole tip field of 48,578 nT has been inserted into the simulation of the Oxford Triplet, and rotated by 1.6 radians about the y axis, and 0.41 radians about the x axis giving field strengths equal to those shown in table 8.2.

• The first concern is aberration arising from the imperfection in the alignment when relatively thick optical elements are aligned to the curved path taken by the beam in the presence of stray DC magnetic fields.

• The second concern is whether chromatic aberration increases due to the changing path of a chromatically spread beam in a DC magnetic field.

• The third concern is the degradation of focusing quality of the microprobe when ions of a different magnetic rigidity are used to that for which the optical elements of the beamline were aligned to.

The third concern is of particular significance, since beam alignment is an arduous process, which can take up to 30 minutes in duration for beam spot dimensions in \(1\mu\text{m}\) range [19], and considerably longer to achieve sub-micron performance. Such a delay may be detrimental to experiments requiring an change of ion rigidities between experimental runs. This is very relevant to the proton beam writing technique which often requires a range of ion rigidities to make multiple depth three dimensional structures.
8.3 Simulation

Simulation of the influence of stray DC magnetic fields using numerical raytracing is achieved by replicating experimental practice for aligning the centre of optical elements to the new beam axis. This can be achieved in the following steps.

1. Excitation of all active elements in the simulation are set to zero.
2. A magnetic dipole representing the stray field is added to the simulation, and excited.
3. A para-axial ray is traced, and the ray coordinates are recorded as the ray passes through the centre of each optical element, including object and collimator apertures, and the final position at the image plane is recorded.
4. The pre-object path of the particle is adjusted such that the particle passes through both object and collimating apertures despite the influence of the stray field.
5. The centre and tilt of all optical elements in the simulation are adjusted to the recorded positions of the paraxial ray.
6. The excitations of active elements in the simulation are optimised to give a focus at the new image position.

8.3.1 Aberration due to imperfect alignment in presence of stray DC field

Typical magnetic quadrupole lenses used in sub-micron microprobe systems are between 50 mm and 100 mm in length [6]. The curved path of the ions in the magnetic field mean that it is impossible for the microbeam operator to align a lens to the path of the ions over the whole length of the lens, although the deviation from perfect alignment is small, aberrations are introduced into the final image. The sensitivity of various systems to misalignment of individual lenses has been thoroughly addressed by Grime and Watt [19]. However, no study has been made of the cumulative misalignment of several lenses which may be found in the presence of a stray DC field.

Grime and Watt [19] recommend the method of "dipole minimisation" for alignment of optical elements in the presence of stray fields. This process requires the microbeam operator to form line foci in each plane consecutively with each magnetic quadrupole lens, at each stage adjusting the alignment of the lens to minimize any steering of the beam spot away from the observed beam axis. However, it is impossible for the microbeam operator to distinguish between tilt and translation misalignment since both are first order aberrations, causing a displacement of the image. The final alignment therefore may be some imperfect combination of tilt and translation that happens to give a beam spot that appears to coincide with the beam axis.
The dipole minimisation method only provides for the correction of translation misalignment, with any tilt corrected using a straight-edge across all lenses prior to the procedure. Therefore, the tilt-alignment shown in this section is presented as a best-possible case. However this tilt-alignment is unlikely to be necessary to reach the required tolerances for sub-micron beam-spots in most microbeam lens configurations.

The procedure for simulation detailed above aligns the tilt and translation of each optical element in the simulation exactly to the beam axis at the geometric centre of each element. Therefore any aberrations arising from misalignment are due to the curved path of the beam in the stray DC magnetic field. Figure 8.1 shows a comparison between point spread functions of the beamline with and without the presence of the Earth’s magnetic field.

The first order effect of such misalignment is evident in the slight offset of the centre of the point spread function shown in figure 8.1b.

Figures 8.1c and 8.1d show difference point spread functions for beamline aligned in translation, and translation-tilt respectively. The difference point spread function is generated by subtracting the aberration coefficients calculated in the absence of stray fields from those calculated with the aligned matrix, leaving a polynomial of difference terms. This is shown in table 8.3.

The degradation in focus quality due to imperfect alignment is characterised by an increase in 2nd and 4th order aberration terms in both planes, \( \langle x \mid \theta^2 \rangle \), \( \langle x \mid \phi^2 \rangle \), \( \langle y \mid \phi^2 \rangle \), \( \langle y \mid \theta^2 \rangle \), particularly the cross-coupling terms, \( \langle y \mid \theta \phi \rangle \), \( \langle y \mid \theta^3 \phi \rangle \), \( \langle y \mid \theta^5 \phi \rangle \).

The aberration \( \langle y \mid \theta \phi \rangle \) is by far the most dominant from the set of misalignment and chromatic aberrations introduced by the stray field, and can be reduced by a factor of two by correctly aligning each element in tilt as well as translation. Figures 8.1c and 8.1d show that the total contribution to the point spread function of the Oxford Triplet system due to stray field misalignment, for 2.5 MeV protons with angular divergence of 0.05 mrad is less than 5% of the point spread function in the absence of stray DC fields.

---

1 Aberration coefficients of magnitude less than \( 1 \times 10^{-3} \mu m/mrad/\% \) have not been shown due to their negligible influence on the ray coordinate in the image plane.
Aberration matrix: units: $\mu m / mrads.$

<table>
<thead>
<tr>
<th></th>
<th>$x$</th>
<th>$y$</th>
<th>$\theta$</th>
<th>$\phi$</th>
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</thead>
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<td></td>
</tr>
<tr>
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<td></td>
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</tr>
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<th>Mean</th>
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<td>$\phi$</td>
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<tr>
<td>$\delta$</td>
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<td>0.002</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 8.2: Matrix of aberration coefficients for Oxford Triplet without stray DC field.\(^1\)
### Aberration matrix: units: μm / mrads / %.

<table>
<thead>
<tr>
<th></th>
<th>(x)</th>
<th>(y)</th>
<th>(\theta)</th>
<th>(\phi)</th>
</tr>
</thead>
<tbody>
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<td>-0.0233</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\phi)</td>
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<td>0.0789</td>
<td>-0.238</td>
<td>-0.146</td>
</tr>
<tr>
<td>(\delta)</td>
<td>-2.44</td>
<td>-2.44</td>
<td>-2.44</td>
<td>-2.29</td>
</tr>
<tr>
<td>(\theta^2)</td>
<td>2.24</td>
<td>3.2</td>
<td>0.0365</td>
<td>0.0119</td>
</tr>
<tr>
<td>(\theta\phi)</td>
<td>-2.44</td>
<td>-20.5</td>
<td>-0.0115</td>
<td>-0.1</td>
</tr>
<tr>
<td>(\theta\delta)</td>
<td>0.0212</td>
<td>0.0979</td>
<td>0.0517</td>
<td>0.0183</td>
</tr>
<tr>
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</tr>
<tr>
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<td>-2.21</td>
<td>-0.0278</td>
<td>-0.0118</td>
</tr>
</tbody>
</table>

**Table 8.3:** Difference Matrix of aberration coefficients for comparison of beamline with and without stray DC field, when optical elements have been aligned in translation to the path of the 2.5 MeV H\(^+\) beam in the stray DC field.\(^1\)
Aberration matrix: units: $\mu$m / mrads / %.

<table>
<thead>
<tr>
<th></th>
<th>$x$</th>
<th>$y$</th>
<th>$\theta$</th>
<th>$\phi$</th>
</tr>
</thead>
<tbody>
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<td>0.0134</td>
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</tr>
<tr>
<td>$\phi$</td>
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<td>-0.0222</td>
<td></td>
<td></td>
</tr>
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<td>-0.0483</td>
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<td>0.0898</td>
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<td></td>
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<tr>
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<td>1.96</td>
<td>6.35</td>
<td>0.0259</td>
<td>0.027</td>
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<td>$\phi\delta$</td>
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<td>-0.0693</td>
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<tr>
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<td>-2.2</td>
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<td>-0.0117</td>
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<td>-0.0349</td>
<td></td>
<td></td>
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Table 8.4: Difference Matrix of aberration coefficients for comparison of beamline in stray DC field with translation and translation-tilt alignment.\(^1\)
Figure 8.1: Point spread functions ($\theta, \phi = 0.1\text{mrad}$, $\delta = 2 \times 10^{-3}\%$) for alignment procedures to stray DC field.
8.3.2 Increased chromatic aberration

Table 8.3 shows that chromatic aberration of the beamline is increased beyond the values given in the absence of stray fields not only due to over-focusing of the lens elements, but an aberration introduced by the angular spread arising from dispersion of the beam in the Earth's magnetic field. This leads to a beam that is spatially spread within the lenses, causing slight misalignments for particles not of the mean energy. However this effect is a negligible concern for microbeams.

The terminal voltage in 2MV Tandetron accelerator at the University of Surrey Ion Beam Centre is specified to be stable to better than 50 volts [51]. For the Oxford Triplet lens geometry, and a 2.5 MeV $H^+$ beam from the Surrey 2MV Tandetron, the increase in chromatic aberration when aligned to the Earth's magnetic field is five orders of magnitude less than the total magnitude of chromatic aberration in the absence of stray fields.

8.3.3 Focusing performance degradation when changing beam energy

In practice, when changing beam energy the microbeam operator will experimentally optimise beam current at the new beam energy by using any steering elements available before the object aperture such that the beam direction is matched to the acceptance defined by object and collimator apertures. This corrects for the transverse influence of the stray field before the collimating aperture, however this pre-object alignment can only correct the transverse offset of the beam to the beam geometric axis such that it arrives at the correct location in the collimating plane. The stray field will cause the beam to travel in a curved path, causing an angular deviation from the geometric axis leaving the collimating aperture.

Thus, the direction and radius of curvature of the beam leaving the collimating plane changes with magnetic rigidity of the beam, causing an effective misalignment of post-collimator elements. In two-stage systems this may cause considerable misalignment due to the "early" position of the collimating aperture in the first stage - causing a large distance from collimating aperture to image plane.

There is strong third order aberration associated with path changes due to variation of magnetic rigidity, as would be expected from high third order angular response of the Oxford Triplet lens system. The aberration terms $\langle x|\theta\phi\chi\rangle, \langle y|\theta\phi\chi\rangle$ cause a strong parasitic broadening effect on the focused image, where $\chi$ is used to denote the magnetic rigidity of the ions.

Displacement effects may be solved relatively easily by the use of fiducial marks on the sample holder, to provide accurate positions (requiring a recalibration for each change of rigidity). Beam broadening effects are more severe, and can only be corrected by the arduous process of re-alignment, or by reduction of the angular divergence of the beam, causing a significant reduction in beam current transmitted to the target. However, the magnitude of these beam broadening effects only becomes significant when the desired beam spot dimension is less than
Table 8.5: Displacement and Broadening of the image due to change in magnetic rigidity of ion from alignment rigidity (0.228 Tm).

Table 8.5 shows the magnitude of broadening and displacement effects for the Oxford Triplet lens geometry due to the stray DC field for a range of ion rigidities for the Oxford Triplet beamline aligned for a beam of 2.5 MeV protons.

Figure 8.2 shows the point spread functions for a range of $H^+$ beam energies from 1.0 MeV to 3.5 MeV for a system aligned at 2.5 MeV.
Figure 8.2: Point spread function ($\theta, \phi = 0.1$ mrad, $\delta = 2 \times 10^{-3}$%) when beamline is refocused but not re-aligned.
8.4 Conclusion

It is clear that stray DC fields in a microbeam environment do produce intrinsic and chromatic beam aberrations, but that the magnitude of these is relatively small in comparison to spherical aberration when optical elements are correctly aligned to the true path of the beam. A more concerning effect is focus degradation when changing ion rigidity. This degradation is important to the proton beam writing community who commonly use multiple ion energies to "write" three dimensional structures. A point of note is that higher ion rigidities particles will receive less deflection from the Earth's magnetic field, and thus aberrations introduced from lens misalignment will be reduced. An interesting point is that changes of beam energy can be made without changing the beam path in the presence of stray fields, or the focus condition of the magnetic quadrupole lenses if a beam of identical magnetic rigidity, but different ion species is delivered from the accelerator.

A further consideration relating to beamline construction is that mono-block lens assemblies will never achieve perfect alignment due to the inability to align lenses separately, and this may make them unsuitable for nanobeam performance systems, depending on the lens geometry used, although a possible advantage is that the re-alignment process of the entire assembly is far simpler and quicker than that of separated lenses.

Problems with stray DC and AC magnetic fields can be greatly alleviated by using mu-metal to shield the beamline from such fields. To shield a beamline effectively any long drift lengths should be shielded particularly between the object and collimator apertures. The influence of stray fields are most damaging in the vicinity of the object aperture due to the lever effect of any deflections introduced to the beam. Mu-metal shielding may prove critical to achieving beam spot dimensions in the nanometre range, depending on the geometry of the lens system used.
Chapter 9

Dog-Leg Electrostatic Scanning

9.1 Introduction

Scanning the beam in a nuclear microbeam system has been a problem from the inception of the technique. The combination of the short space between the lens and the sample (working distance) and the large electrostatic and magnetic rigidity means that post lens deflection over areas larger than a few tens of microns is impractical. Pre-lens magnetic scanning is commonly used, but has disadvantages: The beam diameter increases rapidly at large deflections due to the off-axis path of the beam through a lens with strong spherical aberration. Magnetic scanning is relatively slow and subject to hysteresis. Until recently this was not a serious problem; for ion beam analysis with pixel counts of 256 x 256 or less, the off-axis diameter in the popular Oxford Triplet was comparable with the pixel size in the data acquisition system.

The development of proton beam writing requiring high pixel counts and cell irradiation requiring fast targeting means that these are now significant limitations. Pre-Lens electrostatic scanning solves the problem of speed, high voltage amplifiers can operate at very high slew rates. However, the relatively high electrostatic rigidity of MeV ions means that large electric field strength and long deflectors are required. In addition, it is very difficult to overlap orthogonal deflectors in the same region without introducing serious unwanted multipole field contamination, so X and Y deflectors must be installed sequentially in the beamline. This means that the deflectors may be located a significant distance in front of the lens, which increases the problems of distortion and beam broadening. “Dog-leg” scanning uses two sets of plates in each plane which are connected in such a way that the beam always crosses the axis at the entrance principal plane of the lens. In the geometrical approximation, this means that the beam emerges from the lens at the exit principal plane and follows a path of minimum displacement through the lens. Using the raytracing program XART sufficient rays were traced through the system to enable aberration coefficients relating the applied voltage and the ratio of first and second plate excitations to be calculated. The ratio of excitations between the first and second plates of the dog-leg scanning system is referred to as the ‘coupling constant’. The coupling constant between the plates determines the position at which the deflected ray
intersects the beam axis. Aberration coefficients have been calculated for both the X-Z and Y-Z planes over a range of coupling constants around the geometric optimum (crossing at the principal plane).

### 9.2 Simulation

![Figure 9.1: Schematic diagram of microbeam system with a linear approximation of dog-leg scanning system. H and H' denote the entrance and exit principal planes respectively.](image)

Figure 9.1: Schematic diagram of microbeam system with a linear approximation of dog-leg scanning system. H and H' denote the entrance and exit principal planes respectively.

![Figure 9.2: Beam Envelope for the University of Surrey Vertical Nanobeam, undeflected, showing principal planes.](image)

Figure 9.2: Beam Envelope for the University of Surrey Vertical Nanobeam, undeflected, showing principal planes.

\[
\frac{E_2}{E_1} = \frac{L_1}{L_2} \left(1 + \frac{Z_1}{Z_2}\right) \tag{9.1}
\]

The linear deflection sensitivity was found to be 200\(\mu\)m per kV in the X-Z plane, and 600\(\mu\)m per kV in the Y-Z plane for a 3MeV \(H^+\) beam. However, the maximum scannable area
Figure 9.3: Beam Envelope for a fully scanned beam line in the University of Surrey Vertical Nanobeam. Beam divergence is 0.05mrad. Maximum deflection is 600μm in the X-Z plane and 260μm in the Y-Z plane.

Figure 9.4: Scanning aberrations as a function of cross-over distance in the X-Z plane.
is confined by the limits of the beam tube passing through the bore of the quadrupole lens. This allows a maximum scanned area of $550\mu m \times 1.2mm$. The most significant imaging aberrations induced by the deflection were found to be $\langle x|v^2\theta \rangle$, $\langle x|v\theta^2 \rangle$. These represent beam broadening with increasing deflection distance. $\langle x|v^3 \rangle$ is the geometrical distortion term (causing barrel or pin-cushion effects depending on the sign of the cross terms. These are plotted as a function of the axial crossing point in the figures below. It can be seen that there is a dramatic fall in the magnitude of these terms when the beam crosses the axis at the theoretical geometrical entrance principal plane, which is at 6.686m in the X-Z plane and 6.97 in the Y-Z plane. Section 3.1.5 describes the calculation of the principal plane to the first order. However due to the strong third order dependence of the Oxford Triplet system, a first order calculation cannot accurately determine the position of the principal plane, and therefore numerical raytracing must be used to identify the axial crossing location that corresponds with minimum aberration. This point is clearly shown in figures 9.4 and 9.5. Equation 9.1 gives the ratio of voltage required between the first and second set of plates comprising the dog-leg system to achieve a axial crossing point corresponding with the principal plane.

Figure 9.2 shows the undeflected beam profile on the University of Surrey Vertical Nanobeam, with the positions of the principal planes marked. $H_x, H_y$ denotes the axial position of the entry principal plane for scanning in the horizontal and vertical directions respectively. The Vertical Nanobeam has an Oxford Triplet lens geometry, and as such has a much stronger demagnification in the horizontal plane, due to the cross-over of the beam profile within the first lens.
This causes the principal planes to be situated beyond the geometrical length of the lens in the X-Z plane. The difference in demagnifications is responsible for the difference in deflection sensitivity.

The ray plot shown in figure 9.3 shows the path of the beam through the scanning system and lens. An important advantage of the dog-leg scanning technique is the confinement of the beam envelope with the bore of the quadrupole lenses during beam scanning. This is particularly important with small bore lenses such as the OM-52 lens system used in the University of Surrey Vertical Nanobeam. Indeed, dog-leg scanning is the only possible way to achieve beam deflection over a reasonable distance (≥ 500μm) with such a lens system, other than post-lens deflection. Using single stage scanning the off-axis displacement of the beam as it entered the first lens would cause the beam to be deflected into the beam-tube by the greater axial force experienced off-axis in a quadrupole lens. The displacement of the beam envelope even when the beam enters the lens on axis is clearly shown in figure 9.3.

Figure 9.6 shows point spread functions for the unscanned and fully scanned beams in the Surrey Vertical Nanobeam. It can be seen that even when the deflected beam crosses the axis at the position corresponding to minimum aberration, significant aberration still exists as a direct result of beam deflection. Comparison between figure 9.6 and the point spread functions shown in figure 7.3 in chapter 8 show a similarity in the aberration caused by beam paths that are not symmetric about the geometrical centre of the quadrupole lens.
Chapter 10

Conclusion

During this PhD, the author has developed a specialised raytracing program (XART), which has been extensively verified against existing raytracing softwares TRAX and GEANT4 and measurements carried out on our existing beamlines at the University of Surrey Ion Beam Centre. Using this precise simulation tool, the theoretical barriers to reaching nanometre beam size resolution have been investigated. The main achievement is a systematic survey of the "figure of merit" (an index expressing the focusing quality of a lens) of two-stage focusing systems using two sequential lens groups. It has been shown that two-stage systems can achieve a far greater ratio of demagnification to aberration than today's single-stage systems. Other aspects of nanobeam performance have been investigated such as the reduction of slit scattering by energy filtering, the effects of stray DC magnetic fields, and the minimisation of scanning aberrations. The method of designing shaped apertures by backward raytracing has been developed, and has been proven to be effective in calculating the precise optimum shape of object, collimator, and halo-removal apertures for microbeam and nanobeam systems. A thorough examination of the two different methods of calculating the spherical aberration coefficients that are so important to achieving nanometre beam spot dimensions has been undertaken. The limitations of the popular analytical method developed by Dyominikov, Fishkova, and Yavor [14] has been discussed. Furthermore, the critical importance of correctly modelling the fringing fields of magnetic quadrupole lenses has been identified.

It is hoped that the investigations presented in this thesis will become an integral part of beamline design for the next generation of focused MeV ion beam systems.

Great care has been taken in the composition of this thesis not only to report the results of the investigations into nanobeam performance, but to present the principles of beam optics in a logical sequence, such that a reader new to the topic of beam optics should receive a suitable introduction to all the principles that are relevant to modern beamline design. To this end, the popular Oxford Triplet lens geometry is used as a case study wherever possible, in the hope that the results presented may have relevance to a reader who may have used this popular system.
Chapter 11

Future Research

There is a great deal of work left to be done in this field. Of particular importance there are two topics which I believe may be greatly beneficial to this topic of nanobeam design.

11.1 Octupole Correction

Octupole lenses can be used to reduce spherical aberration. The principle effect of an octupole lens is identical in effect to spherical aberration of a quadrupole lens. Early work in electron optics, and work in ion optics by Dymnikov, Fishkova and Yavor in the mid 60's defined the equations for spherical aberration correction using octupole lenses [4]. Jamieson and Legge also conducted a study of octupole correction for Russian quadruplet systems and presented the results in [32]. A brief review of Dymnikov, Fishkova and Yavor's calculation is provided here. Referring back to equation 3.25 it can be seen that only three independent spherical aberration coefficients exist for a system, implying that complete spherical correction is theoretically possible with three octupole lens [32].

If octupole lenses are present in the lens system, then the spherical aberration coefficients may be rewritten as:

\[
\begin{align*}
\langle x | \theta^3 \rangle &= \langle x | \theta^3 \rangle^q + \langle x | \theta^3 \rangle^o \\
\langle x | \theta \phi^2 \rangle &= \langle x | \theta \phi^2 \rangle^q + \langle x | \theta \phi^2 \rangle^o \\
\langle y | \theta^2 \phi \rangle &= \langle y | \theta^2 \phi \rangle^q + \langle y | \theta^2 \phi \rangle^o \\
\langle y | \phi^3 \rangle &= \langle y | \phi^3 \rangle^q + \langle y | \phi^3 \rangle^o 
\end{align*}
\]  

where superscripts q and o denote spherical aberration contributions from quadrupoles and octupoles respectively.

Using a similar method to equation 3.28, the spherical aberration coefficients for an octupole
CHAPTER 11. FUTURE RESEARCH

pole lens are defined:

\[ C_p = -\frac{\psi \gamma}{5} \left[ (L + a_x)^5 - a_x^5 \right] \]  
\[ C_s = 3\psi \gamma \left[ a_x^2 a_y^2 L + a_x a_y (a_x + a_y) L^2 + \frac{1}{3} (a_x^2 + 4a_x a_y + a_y^2) L^3 + \frac{1}{2} (a_x + a_y) L^4 + \frac{1}{5} L^5 \right] \]  

Where:

\( \gamma \) is the octupole strength parameter, defined by equation 11.6.

\[ \gamma = \frac{B_0 e}{r_0 \rho} \]  

\( B_0 \) is the pole-tip field, \( \rho \) is the relativistic beam momentum, and \( r_0 \) is the octupole bore radius.

Equations 3.28,11.5 and 3.33 reduce to 3 simultaneous equations which can then be used to solve three independent octupole strengths to correct the three independent spherical aberration coefficients of the system.

The solution of the simultaneous equations presented above relies on the correct spherical aberration coefficients to be calculated. Previous calculations on this topic have used the Dymnikov coefficients to calculate the spherical aberration. I have shown in section 3.2.3 that the Dymnikov coefficients do not yield accurate results for the spherical aberration coefficients, particularly for high demagnification systems. Using the raytracing technique, the question of Octupole correction may be investigated with a much greater accuracy. It is possible that the higher order aberrations introduced by the octupole lenses nullify any advantage gained.

11.2 Pole-tip Shaping for Fringe Field Reduction

In the 1970’s Parzen investigated thoroughly the precise shape of the quadrupole pole-tip to reduce the duodecapole, 20-pole and higher order harmonic components of the quadrupole field [48]. However, Parzen’s study did not address the shaping of the entry and exit faces of the quadrupole pole-tip. Shaping of the pole entry and exit faces may reduce the strength of the fringing field of the quadrupole lens. Pole face shaping is frequently used in single plane bend magnets to provide imaging qualities, but it is unheard of for magnetic quadrupole lenses for MeV ions, perhaps because there were greater issues to address. Major advances have been made in the design of magnetic quadrupole lenses in the last two decades, and now defects in quadrupole symmetry which cause sextupole, octupole, decapole and higher order contamination are no longer an issue. Advances in accelerator technology mean that terminal voltages now suffer so little voltage ripple that chromatic aberration is no longer a dominant aberration in MeV ion microprobe systems. The correction of spherical aberration in quadrupole lenses will be the major challenge of the next generation of MeV nanobeam systems. Reduction of the strength of the fringing field in quadrupole lenses may prove critical to the reduction of the spherical aberration cross-terms. Figure 3.6 shows the magnetic field...
component $B_z$ which exists solely in the fringe field region of the lens. This field component is responsible for coupling ions in the X-Z plane into the Y-Z plane and vice-versa, causing the spherical aberration cross terms. To demonstrate the extreme case, the field component $B_z$ has been completely removed from the simulation of an Oxford Triplet geometry beamline. The point spread function for this simulation is shown in figure 11.1b, and the associated aberration coefficients displayed in table 11.2. For comparison, the normal case, where $B_z$ is correctly modelled is presented alongside, in figure 11.1a, and the aberration coefficients displayed in table 11.1. It is clear that the spherical aberration cross terms $<x|\theta\phi^2>, <y|\theta^2\phi>$ are greatly reduced when $B_z$ is removed from the simulation, but in reality it is unlikely that any pole face shaping will cause the $B_z$ term to vanish completely.

<table>
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<td>0.1</td>
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Table 11.1: Intrinsic aberration coefficients of Oxford Triplet
Figure 11.1: A comparison of the point spread functions of the Oxford Triplet beamline with and without the $B_z$ component of the quadrupole lenses.
Aberration matrix: units: $\mu m / mrad$.

<table>
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<tr>
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<td>$\phi^3$</td>
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</table>

Table 11.2: Intrinsic aberration coefficients of Oxford Triplet with quadrupole field component $B_2$ removed from simulation
Chapter 12

Acknowledgements

I would like to thank all the people who have helped me with this thesis. My supervisor, Dr. Geoffrey Grime has displayed great patience and understanding during the writing of this thesis, and his knowledge and wisdom in the field of beam optics and many other topics is endless. My parents, grandparents and sister have all provided moral support and encouragement. I'm very grateful to my team of proof-readers, Peter Merchant, Dr Vivian Merchant, who have provided moral support, scientific and linguistic improvements. I'd also like to thank all the staff at the University of Surrey Ion Beam Centre, in particular Professor Karen Kirkby for her support, Mark Browton and Adrian Cansell. Adrian taught me how to run a 2MV Tandetron accelerator, and Mark fixed almost everything I broke during the course of my PhD. Thanks are due to Richard Bryan of the Molecular Biophysics Lab at the University of Oxford, who kindly provided access to the necessary hardware to execute the raytracing software TRAX. This PhD was supported by the UK Engineering and Physical Sciences Research Council.
Chapter 13

Publications

The following papers have been published as a result of work undertaken during this PhD.


- M.J. Merchant and G.W. Grime. The influence of stray DC magnetic fields in MeV ion nanobeam systems. *Submitted to Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*


Bibliography


...
Appendices
Appendix A

Survey of Two Stage Systems using Numerical Raytracing

A.0.1 Doublet - Triplet 1 Geometry

Figure A.1: A Doublet - Triplet 1 system.
Figure A.2: System aberration and performance as a function of quadrupole positions in the first stage lens of Doublet - Triplet 1.
Figure A.3: System aberration and performance as a function of quadrupole positions in the second stage lens of Doublet - Triplet 1.
Figure A.4: System aberration and performance as a function of quadrupole positions in the second stage lens of Doublet - Triplet 1.
A.0.2 Doublet - Triplet 2 Geometry

![Diagram of a Doublet - Triplet 2 system with parameters and calculations.]

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