

Optimization of electron optics in a resonator cavity  
using Nelder-Mead simplex search for the quantum  
electron microscope

by

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B.S., Bilkent University (2013)

Submitted to the Department of Electrical Engineering and Computer  
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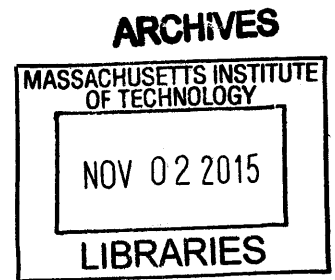
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**Abstract**

The Quantum Electron Microscope (QEM) is a proposed imaging modality that aims to reduce or eliminate the effects of radiation on living cells compared to traditional electron microscopy techniques. In recent years, an interaction free measurement scheme was proposed by Putnam and Yanik [1], and an implementation of this idea is being developed by an international collaboration. The current implementation foresees an electron cavity, which can be installed into a regular scanning electron microscope, to allow multiple passes of two electron wavefunctions over the specimen. In order to implement this idea, multiple different electron optical designs were proposed. Extensive simulation work is required to test and validate these designs.

This work outlines the simulation work done for QEM, and proposes a general framework for optimizing electron trajectory simulations using Nelder-Mead search. It also provides a library of MATLAB wrapper functions and optimization methods to be used with the Integrated Lorentz-2E software.

Thesis Supervisor: Mehmet Fatih Yanik

Title: Visiting Professor



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# Chapter 1

## Introduction

Electron microscopy (EM) is a well-established technique for imaging specimens well beyond the diffractive limit of visible light. However, imaging biological samples using EM remains a challenge to this day. A traditional EM system requires multiple physical conditions (e.g. vacuum, high intensity electron beam) that are inhospitable for many living cells. There has been significant effort to overcome these limitations, some of which are outlined in the following paragraphs. The newest of these efforts, however, is the Quantum Electron Microscope (QEM): a device that utilizes quantum mechanical concepts to achieve reduced-interaction or interaction-free measurement. Such a system can greatly reduce the damage on living cells, enabling new breakthroughs in biology and life sciences.

### 1.1 Electron imaging modalities and their limitations for biological specimens

Attempts to image living cells were made soon after first electron microscopes were available [2], with mixed success. However, one of the fundamental limitations of electron microscopy is that the incoming electron beam at TEM/SEM level of energies will necessarily alter the chemical structure of the specimen. This happens in many ways; most notably through irradiation, breaking atomic bonds, and heating.

Calculations suggest that a biological specimen under a high beam current may receive as much radiation as a 10 megaton hydrogen bomb explosion 30 yards away [3]. The effect is strong enough that high energy electron beams are used for sterilization purposes [4, 5].

In recent years, many imaging modalities have been proposed as potential solutions to the problems outlined above. These most notably include cryo-electron imaging [6, 7], which allows the specimen to be imaged without any staining. This is partly because the specimen does not need to be dehydrated before imaging; they remain in a “frozen hydrated” state, preserving the overall shape of the cells [8]. The lack of staining also prevents any conformational or chemical changes that can be inadvertently applied on the specimen during preparation. Cryo-EM imaging remains one of the popular ways of imaging biological specimens as of today.

One more issue with electron microscopy in living cells is that most traditional SEM/TEM systems require the specimen to be placed in a vacuum to operate. This means that the cells should be dried properly beforehand, otherwise they will go unexpected conformational changes when exposed to the vacuum. To solve these problems, an environmental scanning electron microscope (ESEM) was developed [9]. An ESEM, by definition, can handle water vapour pressure at 273 K, allowing water to remain in liquid phase.

## 1.2 Automated simulations and QEM design

The high costs and complicated physics involved in using and building electron microscopes mean that all possible designs of the QEM should be thoroughly tested and validated in theoretical grounds first. An “experimental playground”, while preferable to simulations, would be an engineering challenge in addition to being prohibitively expensive. Our choice of simulation environment is therefore critical to the project progress.

Designs analyzed in this work use Lorentz-2E as the simulation engine [10]. Most of the time, the graphical user interface is not used; instead the application is accessed

through a COM interface [11], using an array of MATLAB scripts developed by the author for automation of certain tasks (which we call Lorentz Controller Library<sup>1</sup>). The library implements MATLAB wrappers for the functions exposed by the software’s API, and builds on that foundation by automating certain tasks and adding specialized scripts for data input/output. Most importantly, the library implements a framework for electron trajectory optimization, a feature that is not included within Lorentz-2E. This enables us to not only validate our designs using the software, but also to actively *create* new designs using simulations.

### 1.3 Nelder-Mead simplex optimization of simulations

The Nelder-Mead simplex search [12] is a very popular unconstrained optimization method. It applies gradient-free optimization to a given function that may or may not be smooth. Due to this flexibility, it has been the method of choice for optimizing the results of industrial simulation software [13]. This makes Nelder-Mead simplex search a prime candidate for our simulation optimization purposes using Lorentz as well.

Previous work that applies Nelder-Mead optimization to various parameters in electrostatic optics exist in literature [14, 15], but these works focus on optimization of a single element. In general, many electrostatic optics elements exist together in a system; and it becomes crucial to optimize them in a way that does not destructively interfere with global optimization.

The gradient-free nature of this optimization technique is important; since our function calls are expensive, we would like to have as few evaluations as possible per iteration. Still, methods that utilize finite derivatives for gradients [13] can be a possible future direction for this work.

We use the built-in MATLAB function `fminsearch` for optimization purposes [16]. Combining this optimizer and the Lorentz-2E API provides a useful tool which can advance QEM research.

---

<sup>1</sup>Source code is available at [github.com/otceliker/](https://github.com/otceliker/)



# Chapter 2

## Design of the QEM electron cavity

In this chapter, we explain the basic electron optical elements of the QEM design, and show how these can be combined in various ways to create an electron resonator cavity.

Building a QEM resonator requires, at the very least, the following:

1. An input aperture where the beam enters the resonator.
2. Electron lenses to guide the beam to the sample.
3. Electron mirrors to keep the beam within the resonator.
4. Some time-dependent element to place the beam between (and out of) two reflecting surfaces.

The electron cavity design is not finalized yet; but possible candidates exist. In this work, we will eventually be investigating a specific design called QEM1. A representative image can be seen in Figure 2-1. This design makes use of electron mirrors and lenses, with a future addition of a “barn door”.

### 2.1 Electron mirrors

In its simplest fashion, an electron mirror is a surface that is being held at a negative potential compared to the ground. The absolute value of the potential should obvi-

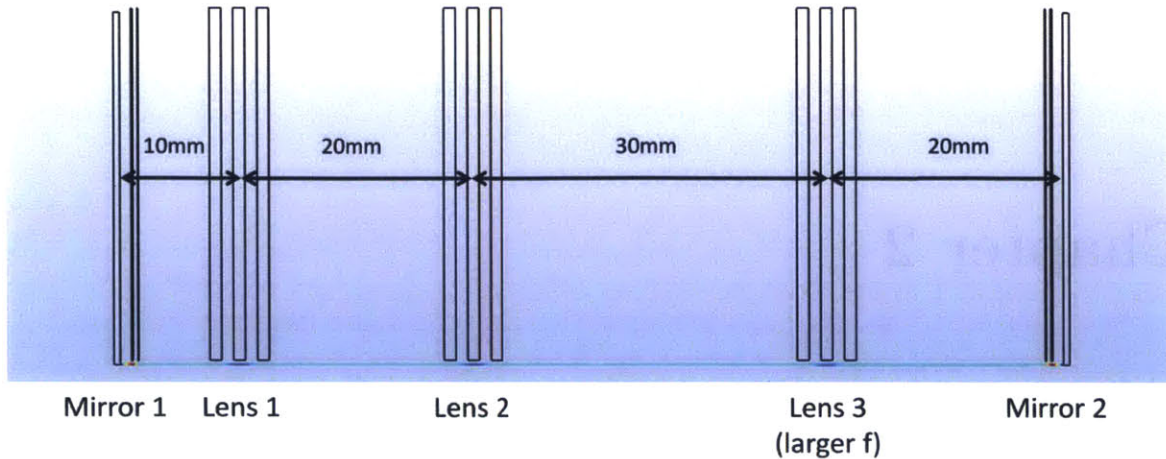


Figure 2-1: General mechanical design of QEM1: two mirrors and three unipolar lenses.

ously be more than the accelerator voltage used to couple electrons into the system; otherwise the electrons are absorbed by the surface, causing unpredictable results. In case of an insulating material where the absorbed electrons do not freely move, this phenomenon can be utilized to create an electron mirror in a scanning electron microscope [17]. The surface can then be used to view the interior of the SEM.

The designs used in QEM use a three-electrode mirror. This allows to keep the potential contours near the mirror surface flat (i.e. parallel to the surface), which is important in order to eliminate any nonuniformities in the mirror output. One other important consideration is the position of the contour with potential  $-V_e$ , the acceleration potential of the electrons. The position of that contour is the actual mirror "surface" for the incoming electrons, as they will reach zero energy there and subsequently be reflected. The position of this contour can *not* be on the surface of the electrode, nor can it be too close to it; any deformities will otherwise non-negligibly impact the mirror flatness. Moreover, choosing a surface location too far away from the electrode will affect the electron optics design as the mechanical placement resolution is expected to be on the order of millimeters.

The second electrode, with its high positive potential and proximity to the surface, creates a very strong electric field pointing away from the first electrode. However,

this creates a negative lens effect on the electrons. The third electrode, grounded, tries to eliminate this lens effect.

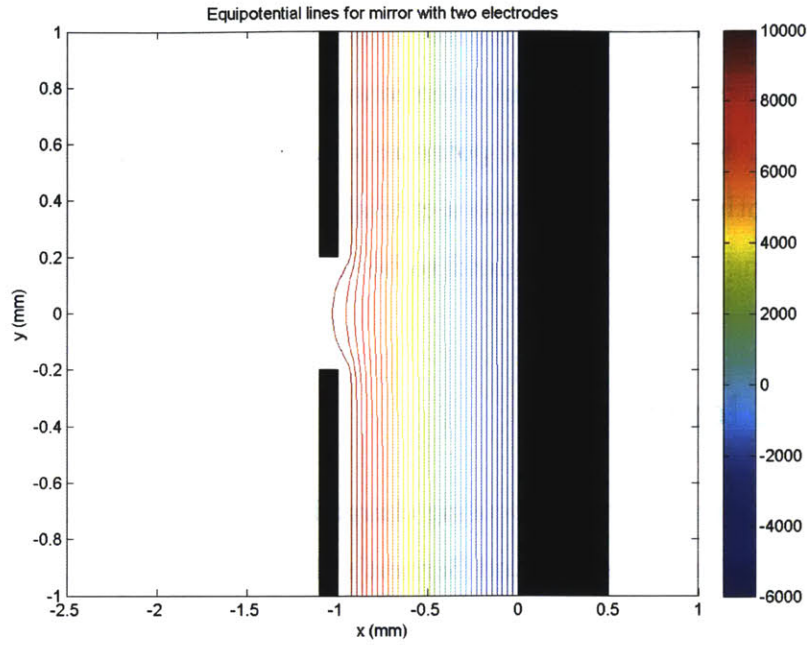
A special variant of the electron mirror would be the *grating mirror*. In this case, the equipotential lines are not flat, but intentionally curved like sinusoids – this creates a diffraction effect. See Figure 2-3 for potential contours of one such mirror. Splitting the beam into zeroth and first orders is a crucial part of the proposed QEM method; and as such, grating mirrors are planned to be used in the finalized implementation.

## 2.2 Einzel lenses

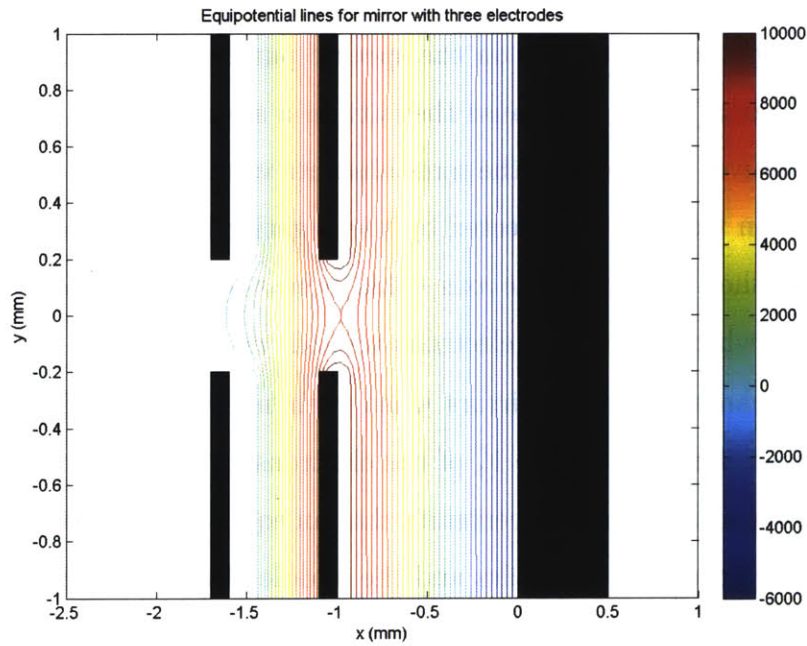
An einzel lens is a common way of focusing charged particles. A detailed introduction of them can be found in Klemperer and Barnett’s electron optics book [18]. The einzel lenses we use in our design and simulations are three-diaphragm unipotential lenses; i.e. they consist of three thin electrodes (cylinders with diameter much larger than height) and the outside two electrodes are kept in zero potential. The choice of the middle electrode potential depends on the specific purposes of the design; we use a decelerating (negative) voltage because they attain a stronger focus compared to an accelerating (positive) voltage with the same absolute value [18]. The downside of this is that the electron trajectories, affected by the negative lens effect of the grounded electrodes, are pushed away from the axis – this increases aberration compared to the accelerating lens, which pushes the electrons toward the axis.

Einzel lenses can also act as mirrors when their middle electrode voltage  $V_m$  is larger than the acceleration voltage  $V_e$  of the electrons. This happens because when  $V_m < -V_e$ , there is a mathematical certainty that an equipotential line of  $-V_e$  will fall between the outer grounded electrodes and the middle electrode. Incoming electrons will be completely stopped and reflected on this line. A fortunate consequence of this is that einzel lenses can deliberately be adjusted to behave as a mirror when necessary. This provides a convenient way of coupling electrons into a resonator (see Barn door – Section 2.3).

In the following chapters, we will demonstrate methods of attaining specified mir-



(a)  $V_s = -6000V$ ,  $V_{cap1} = 10000V$ ,  $V_{c2} = 0V$ .



(b)  $V_s = -6000V$ ,  $V_{cap1} = 10000V$ .

Figure 2-2: Equipotential lines for two and three electrode mirrors.

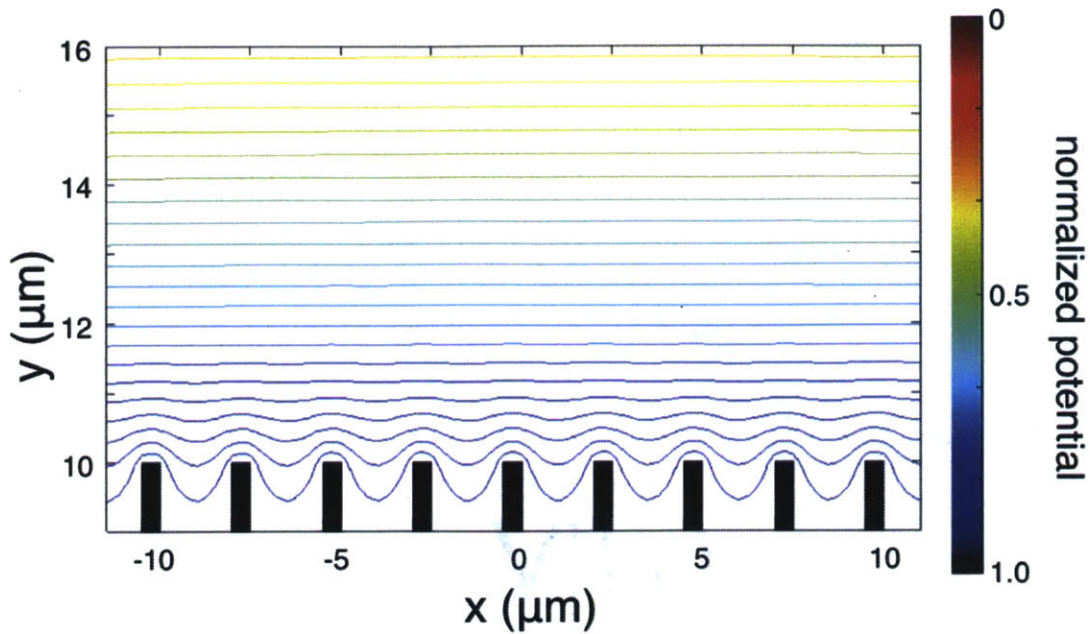


Figure 2-3: Equipotential lines for the grating mirror. Only the surface electrode is shown in this figure; there exists a grounded electrode in the positive  $y$  direction.

ror and lens behavior without analytical calculations.

## 2.3 Barn door

The *barn door* is a specific term to QEM. It refers to an electron optical system that can act as a reflector or an outcoupler, depending on the voltage applied to it.

In the current proposed QEM system, a resonator is added to a traditional QEM system. This calls for a consistent method of coupling the electron into this additional stage. A barn door, when “open”, acts as an ordinary einzel lens and allows the electron to enter the resonator.

While the electron is in the resonator, the barn door needs to be “closed”; i.e. the electron should be reflected from the middle electrode. We have mentioned that this can be accomplished in an einzel lens by decreasing the electrode voltage to appropriately negative levels – and this is the exact idea in a barn door application.

With a (preferably small) voltage swing, the electron can be outcoupled, allowing the detectors to process it.

The timing of a barn door system is important. Assuming an unrelativistic electron, we can estimate the speed in case of 500 eV of kinetic energy:

$$K_e = \frac{1}{2}m_e V_e^2 \tag{2.1}$$

$$V_e = 1.32 \times 10^7 \text{ m/s} \tag{2.2}$$

At such a speed, it would take

$$t_e = 20 \text{ mm}/V_e = 1.50 \times 10^{-9} \text{ s} \tag{2.3}$$

for the electron to traverse the length of the resonator cavity. We therefore need voltage supplies that are fast enough to switch within that time frame. This is another part of ongoing research for the QEM project.

# Chapter 3

## Simple electron optics using Lorentz and MATLAB

### 3.1 Introduction

The simulation engine of Lorentz exposes an API to Microsoft's COM interface, which can be accessed through MATLAB. This introduces scripting abilities to the simulator, which greatly increases of possible scenarios that can be simulated.

The possible uses of scripting in a simulation software will be briefly discussed below.

**Sweeping multiple parameters concurrently.** One of the most straightforward applications of using scripting is the ability to sweep multiple parameters, far beyond what Lorentz graphical user interface allows.

**Running optimization on the simulation.** This is the main starting point for this work. Using MATLAB's optimization toolboxes and Lorentz API for data input/output, simulation results can be used to optimize a certain parameter or satisfy a given constraint. The individual simulations for this work usually require less than 10 seconds to complete, which allows running many of them in a tightly constrained optimization loop. Results for such optimizations will be demonstrated in the upcoming sections and chapters.

**Implementing time-dependent simulations using electrostatics software.**

A time varying electric field produces a magnetic field as predicted by Maxwell's equations. However; it may be possible to run approximately correct simulations using electrostatics software, given that the electric field change is small and the magnetic field is therefore negligible. Such a simulation can be run on a pure electrostatics simulator as follows. Assuming that an electric field change occurs at  $t = t_0$ :

1. Compute the kinematics of the electron(s) up to time  $t_0$ .
2. Save the last position, velocity and other relevant properties of the electrons.
3. Recompute the new electric field using the new parameters.
4. Continue simulation, using the saved state as the initial state of the new run.

We have also discovered that researchers from the Stanford University team for QEM also independently considered using this approach, for COMSOL in their case [19]. As they also note, the simulated world becomes physically impossible due to instantaneous change of electric field, but this is not a problem for our engineering purposes.

While this approach is straightforward, it can generalize to arbitrary functions of voltage change. To avoid discontinuities in trajectory, electric field changes should be constrained to areas that are sufficiently far away from the electrons. A good rule of thumb may be to have one or more unchanged boundary condition between the modified area and the electrons.

## 3.2 Simulation of an electrostatic lens

An electrostatic lens is a fundamental component of electron optics. While there are multiple different types of electrostatic lenses, such as the two-electrode accelerators and decelerators, our work mostly focuses on einzel lenses, or unipolar lenses (Figure 3-1). These lenses consist of three electrodes. The two outside electrodes are grounded, while the middle electrode carries a positive or negative voltage. They are useful since

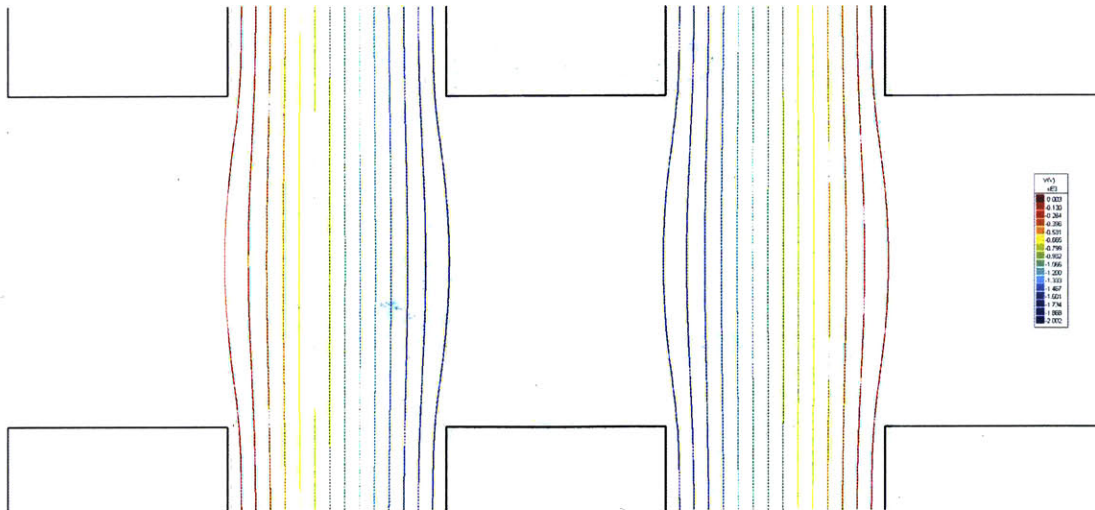


Figure 3-1: Voltage contours of a unipolar lens with mid-voltage of -2000 V. Image captured from Lorentz simulation software.

they preserve the energy of the charged particles, which is crucial for the quantum electron microscope.

Designing an einzel lens is a well-defined engineering problem. The input parameters and output characteristics are straightforward, and the system is governed by well-known differential equations. However, computing the characteristics of an einzel lens is surprisingly challenging to be done analytically. Commercial simulation software is therefore widely used in designing such electron optics components.

### 3.2.1 Optimization framework for an einzel lens

To solve the optimization problem, we first need a set of inputs and a set of constraints.

We first define the optimization space. We assume and follow the rule that electrons approach the einzel lens from negative x-axis, and the lens itself is centered at  $x = 0$ . The lens is symmetric with respect to the point  $x = 0$ , as well as being axisymmetric. The outside electrodes are always grounded, but the middle electrode voltage can vary. Geometry is usually predefined in accordance with mechanical requirements, but can also be changed in certain cases.

Designing a lens usually involves optimization towards a required focal length,

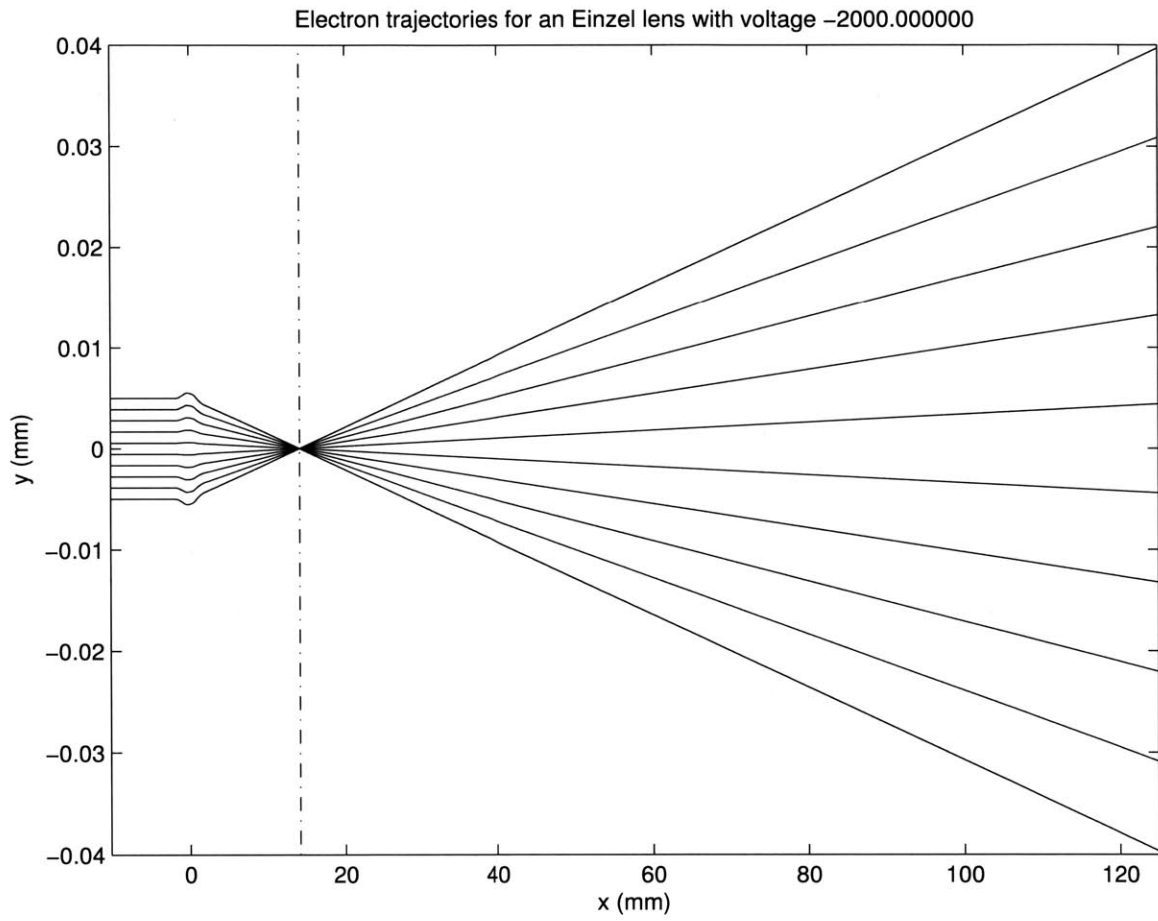


Figure 3-2: Trajectories of 5 keV electrons passing through a simple unipolar lens with middle electrode voltage  $V = -2000$  volts. The focal point of this lens is calculated as  $x = 14.05$  mm, which is marked with the dotted line in the plot.

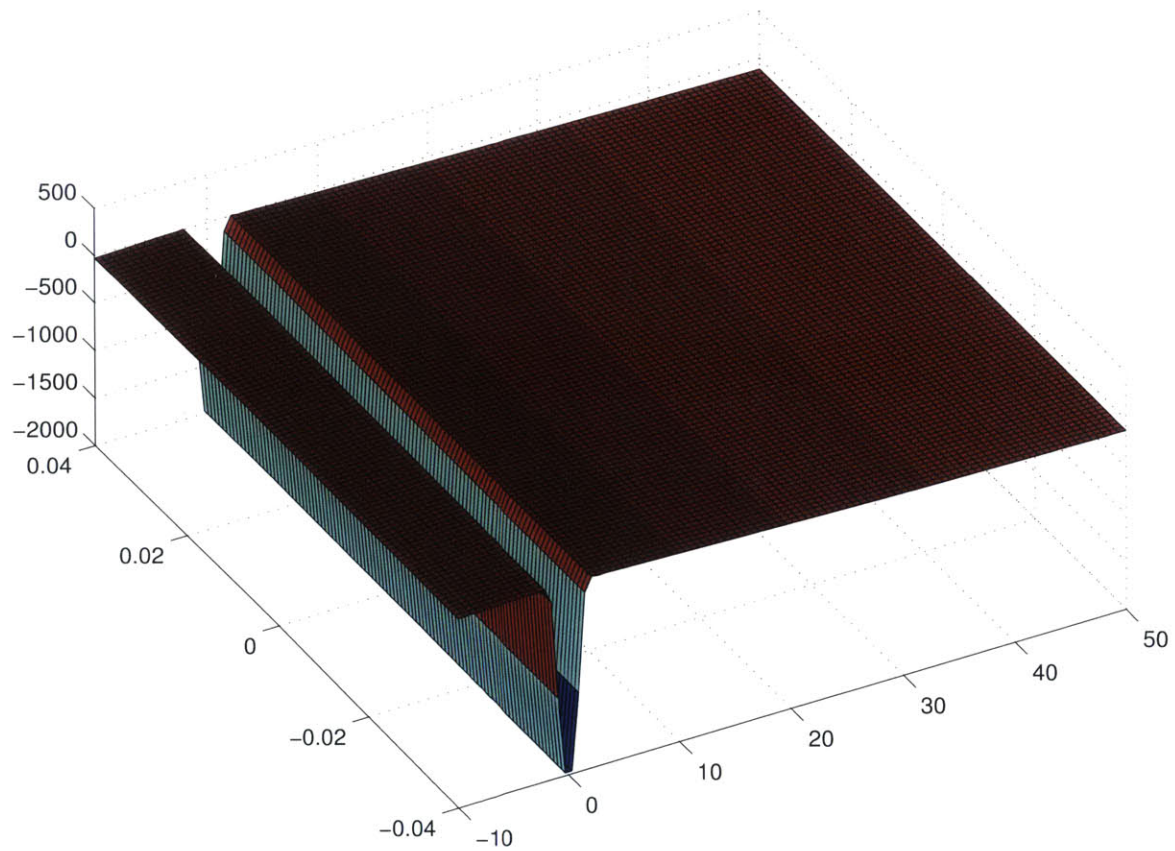


Figure 3-3: Voltage profile of the einzel lens shown in Figure 3-2. We see that the voltage profile is almost completely independent of the radial distance in the region where the electrons are located.

both in geometric and electron optics. Our einzel lens optimizer also follows this convention. Using the time-invariant features of optics, we can define the focal length  $f$  in two different ways:

1. An incoming parallel electron beam to the lens from negative  $x$  reaches smallest beam width (*spot size*) at  $x = f > 0$ .
2. Electrons emanating from a point source at  $x = -f$  produce a parallel beam on the other side of the lens. (Note that this requires a definition of how “parallel” a beam is.)

With this definition, we can tell the optimizer to minimize the simple absolute difference  $|f - f_0|$  where  $f_0$  is the desired focal length.

Let  $\theta_i$  be the angle of the  $i$ th electron with the optical axis at a given point  $x = x_0 \gg W$ , where  $W$  is the lens width. In this case, a parallel beam can be defined in terms of the sum of squares (SS) of these angles:

$$\sum_i \theta_i^2 \approx 0 \tag{3.1}$$

An interesting exercise would be to find other functions  $f(\theta_i)$  of these angles which can improve simulation time or accuracy. We will, however, be not considering such functions for this work.

### 3.2.2 Results of optimization for focal length of an einzel lens

Using the framework above, we can run our optimizer to get some initial results.

Assume we require a focal length of 10 mm for electrons with 5keV of energy. Using our definition of focal length and the MATLAB `fminsearch` function, we can estimate the required voltage to fine precision.

The optimization history is shown in Figure 3-6. The process takes about 80 seconds on a desktop computer; this can be adjusted in favor of more precision or higher speed. The optimizer calculates the focal length of the finalized design as

10.00001 mm, which has an error smaller than the accuracy we can expect from the simulator.

There are a few important details to note in Figure 3-6. First and foremost is that not all the initial values converge to the correct result – for higher voltages (near -100 V), the simulated trajectory terminates before the actual focal point is reached. Since the focal point is determined by the lowest spot size, it is assigned to the tip of the simulated trajectory. Therefore the focal point does *not* change between different trials, and the optimizer incorrectly concludes that it is exploring a constant function. The function similarly fails with initial values exceeding the maximum electron energy, as it behaves like a mirror in that case. The objective function is designed to return NaN in that case, to indicate there is no real focal point in the +x axis. The second important point is that there are *two* acceptable results within the  $[0, V_e]$  range – the second acceptable value is very close to the electron energy, and it causes the electrons to cross the optical axis twice: once inside the lens, and once in the actual focal point (see Figure 3-5).

This is an undesirable solution both because it causes crosstalk between electrons, and because it requires a higher voltage than the other acceptable solution.

The figure shows that it takes less than 10 iterations to get within 10% of the correct analytical value. This increases our confidence that Nelder-Mead simplex search is a viable way of optimizing electron optics simulations.

### 3.3 Simulation of an electric mirror

In this section, we will apply the previously discussed methods on the simulation and optimization of an electric mirror as used in the QEM project.

#### 3.3.1 Optimization framework for an electric mirror

We begin by making some definitions and assumptions. Our mirror to be optimized consists of one "mirror electrode" and two "cap electrodes" with pre-determined dimensions, as in Figure 3-7. We place the center point of the mirror electrode cylinder

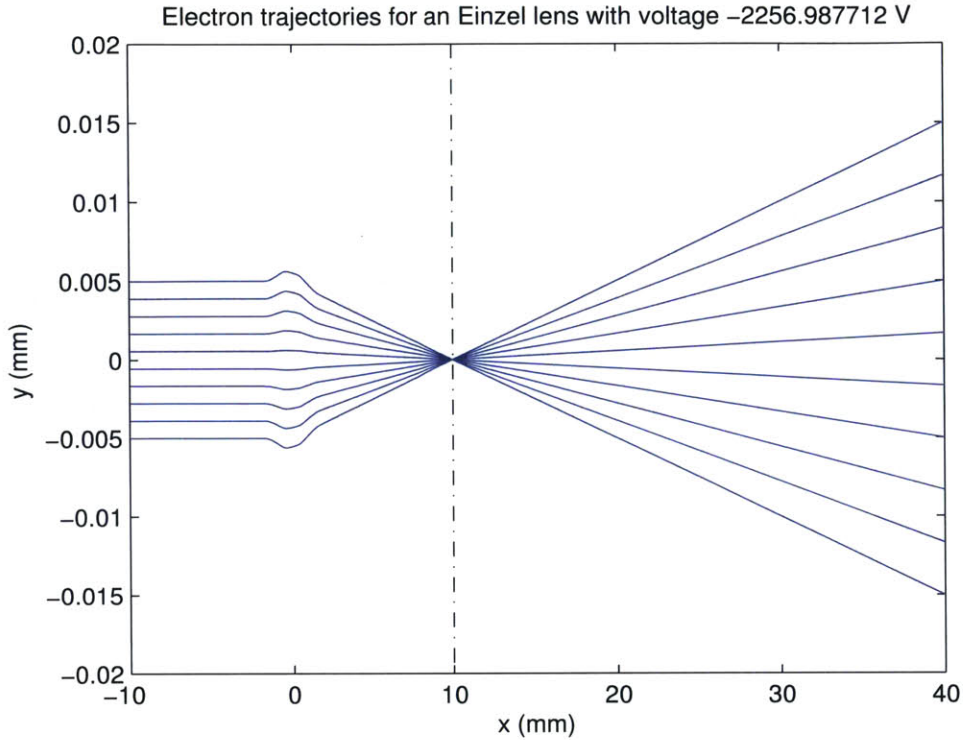


Figure 3-4: Electron trajectories for the optimized lens (primary solution).

on  $x = 0\text{mm}$ , and again work with an axisymmetric model.

We once again need to specify an objective function. We define our optimization goal as creating a system such that when it receives an incoming parallel beam in the positive  $x$  direction, it outputs an outgoing parallel beam in the negative  $x$  direction. (We will again need to define what makes a beam “parallel”.) In a sense, this can be thought of as an electric lens with infinite focal length. Indeed, the two cap electrodes can be thought of as a lens; specifically, a two-aperture decelerating lens. Given this context, we believe that the sum of squared errors (SSE) of the angles is again a reliable candidate for evaluating mirror performance.

There is one aspect of the SSE approach that needs to be modified. We found through experience that the electrons that are leaving the system do *not* follow a linear trajectory; instead, they follow a curved path that eventually crosses the optical axis. (See Figure 3-9 for an example.) Since the angle with the axis is now a function of the  $x$ -position in the trajectory, we also need to specify the argument to this function;

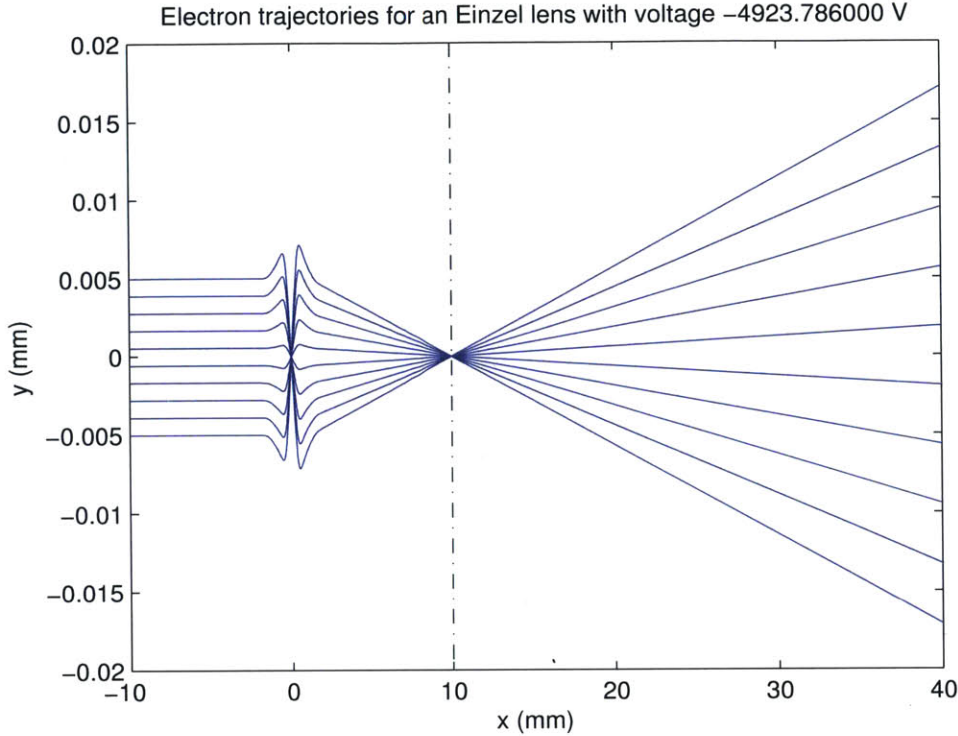


Figure 3-5: Electron trajectories for the optimized lens (secondary solution).

i.e. we need to specify the  $x$  value(s) for which we calculate the angle. To eliminate spurious results, we choose a 2 mm range close to the mirror axis. This also has the benefit of ensuring the optimization result does not suffer from the aforementioned curve problem too early in its trajectory.

We find that Equation 3.1 also applies here for the parallel beam definition. We place our electrons at  $x = -10\text{mm}$ , each with 5 keV of initial energy, spread over  $40\mu\text{m}$  in the  $y$  dimension.

### 3.3.2 Results of optimization for the electron mirror

The simulation is initiated with the values  $V_{c1} = 0\text{ V}$ ,  $V_{c2} = 1 \times 10^4\text{ V}$ ,  $V_s = -6 \times 10^3\text{ V}$ . Only the cap 1 voltage is modified for optimization, as we expect it to have the highest influence on the lens effect.

The optimization history for various initial voltages and the resulting sample elec-

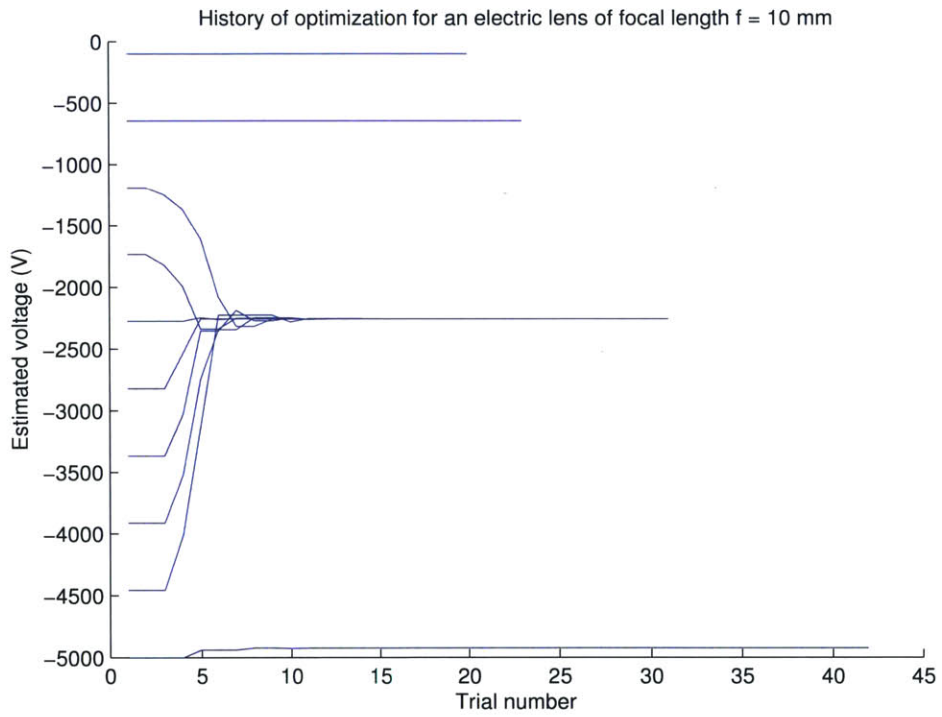


Figure 3-6: History of optimization for a simple einzel lens for focal length  $f = 10$  mm, starting from different initial voltages.

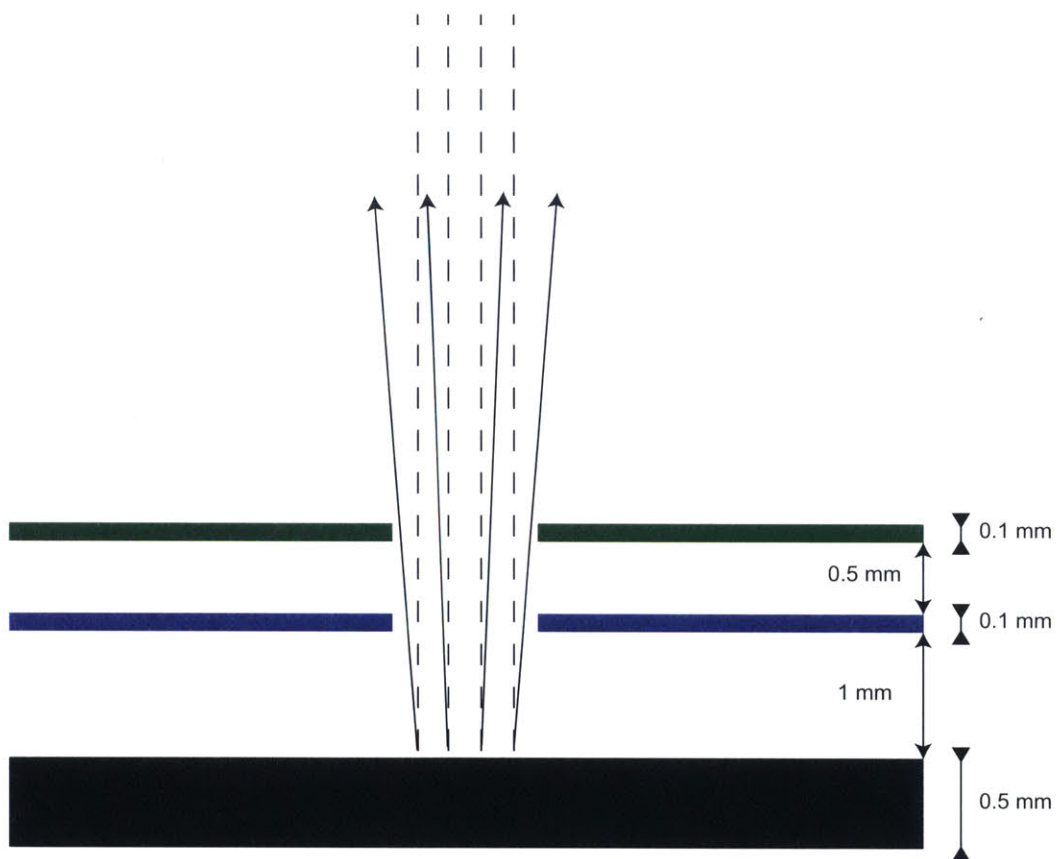


Figure 3-7: Simple diagram of an electron mirror (to scale, except for the ray traces, which are for demonstration only). The objective function makes use of the angles between incoming rays (dashed) and outgoing rays (solid). Outside cap (green) is always set to ground voltage, and the dimensions are assumed to be fixed.

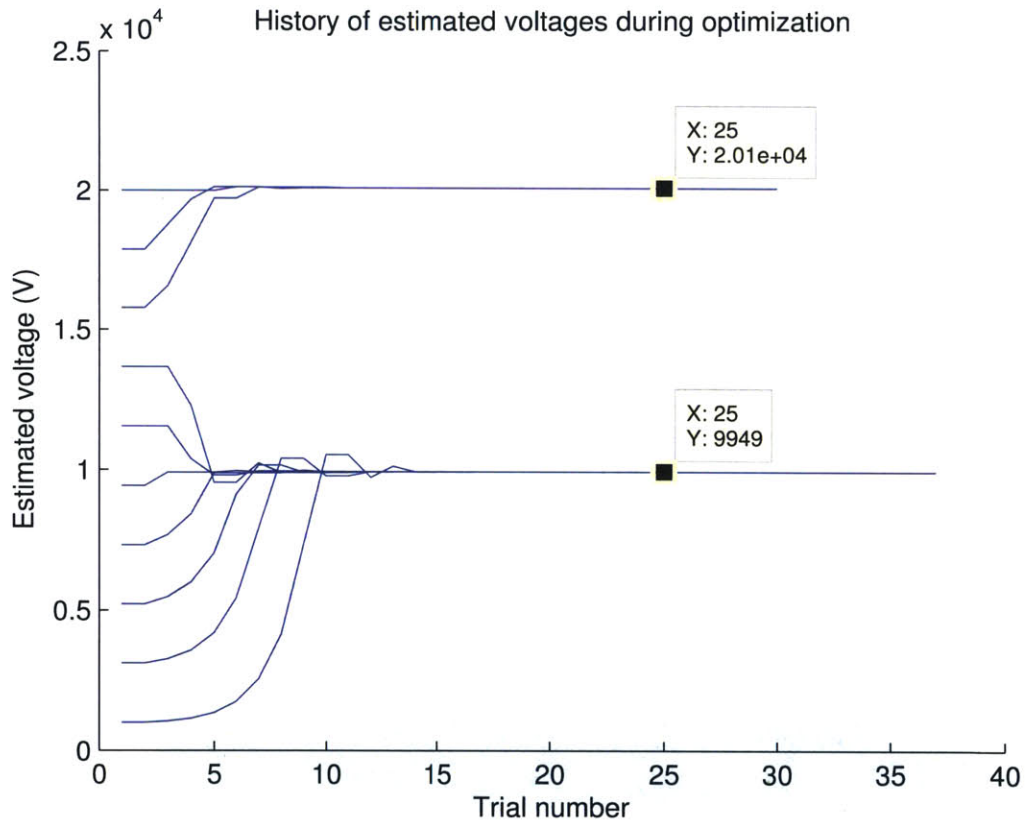


Figure 3-8: History of optimization for an electric mirror with surface voltage  $V_s = -6 \times 10^3$  V, for 10 different initial voltages ranging from 1000 V to 20000 V. The values for trial 25 is given for reference.

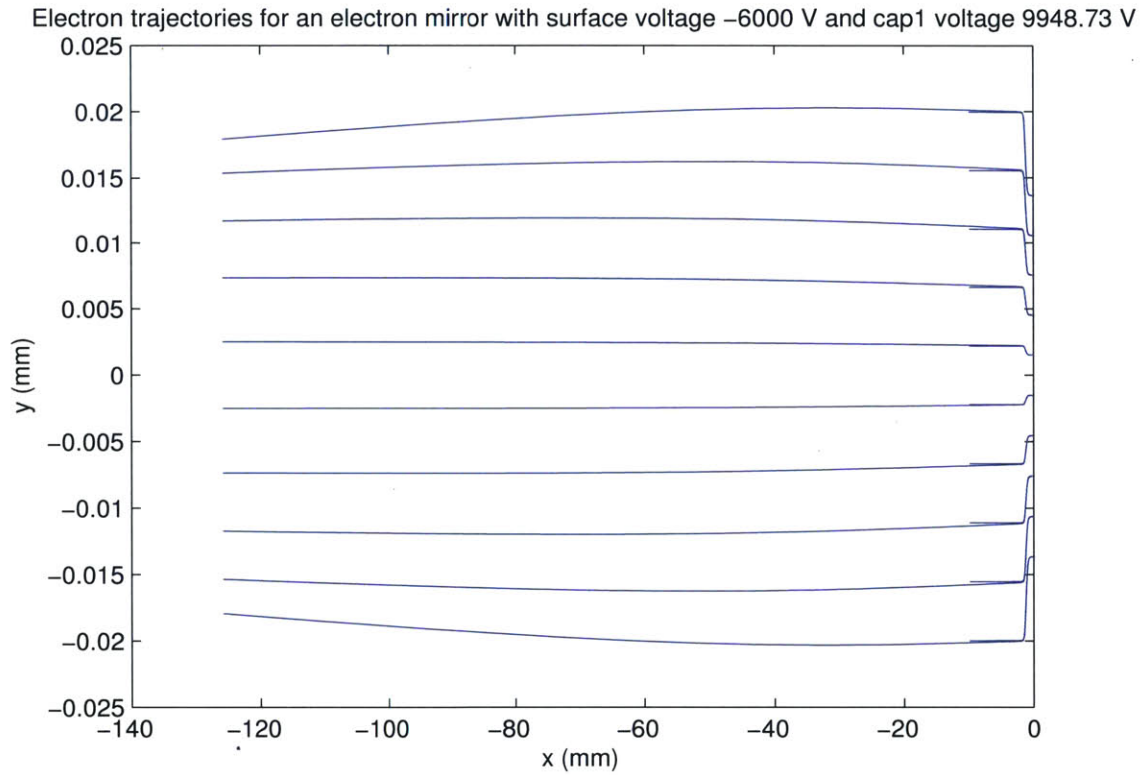


Figure 3-9: Trajectories of the optimized electron mirror with specified voltages. The curve toward the optical axis becomes prominent, especially for rays that have a higher  $y$ -offset, as the distance from the mirror surface at  $x = 0$ mm increases.

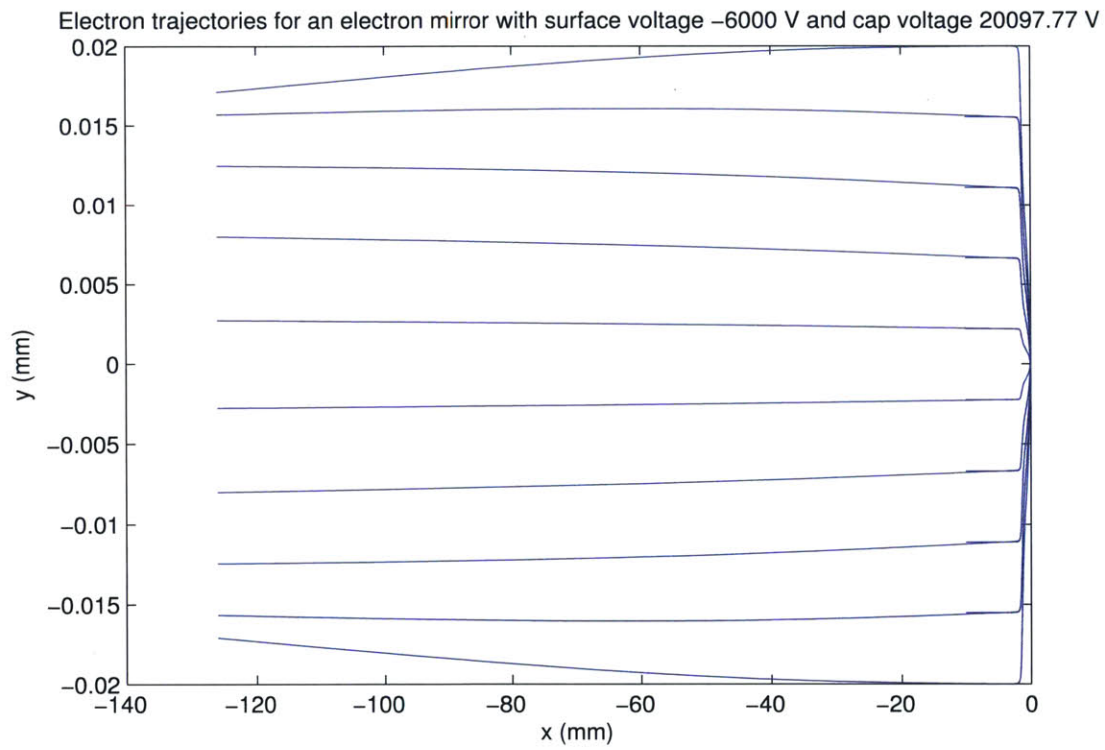


Figure 3-10: Trajectories of the optimized electron mirror with specified voltages for the minimum near  $20000$  V.

tron trajectory from one of the optimizations can be seen in Figures 3-8 and 3-9 respectively. (Resulting trajectory for the second, less desirable, minimum can be seen in Figure 3-10.) The optimization history shows that the optimizer can reliably converge on the desired minimum value in a reasonable range of initial voltages, and does it quickly (within 20 trials). The time to converge near (within 0.1V of) the optimized voltage is proportional to the distance from the nearest local minimum, which is also expected. This again increases our confidence that the optimizer works well and can be used in real life electron optics design.

### 3.4 Optimization of an einzel lens to augment working distance of a scanning electron microscope

In this section, we show that the Lorentz + MATLAB system and the optimization scheme can actually solve a real world problem. This also serves as a sanity check for our methods.

The diagram and dimensions of an SEM setup is shown in Figure 3-11. The purpose of the einzel lens in this system is to refocus electrons coming out of the electron gun to the surface of the sample. In this case, we are not interested in the focal length of the electric lens itself; we are interested in the effective working distance of the system when the lens is added. Therefore, we optimize the system as a whole instead of trying to analytically calculate the required focal length of the lens alone. We will see similar approaches in the following chapters.

The dimensions were acquired from the actual system being modeled. The electrons were modeled as 10 negatively charged particles that converge on the working distance, with an initial energy of 3 keV. The "angular spread" of the electrons were defined as  $\max_{ij} |\theta_i - \theta_j|$ , where  $\theta_i$  is the angle between the *initial* velocity of the electron  $i$  with the optical axis, and was given as 5 milliradians.

The results of the simulation is shown in Figure 3-12. It is clear that the simulation results agree well with measurements, especially on voltages that are less than

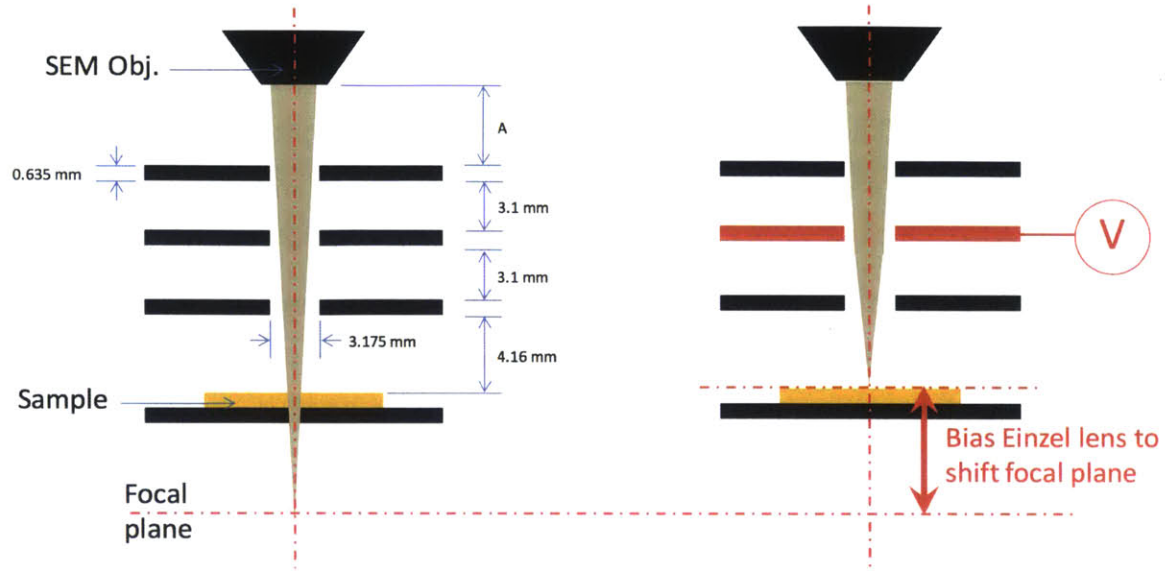


Figure 3-11: Diagram of the electron gun/einzel lens setup [20].

about -800 V. We expected to have better performance in that region as both the measurement errors and the simulation errors are reduced for voltages with higher bias away from ground. The mean error for the 16 different measurement/simulation pairs is 45.3 volts.

We showed in this chapter that simulation using Lorentz+MATLAB is a viable solution to the common engineering problems that arise during electron optical design. In the next chapter, we start focusing specifically on QEM and walk through some of the proposed designs over the course of the project.

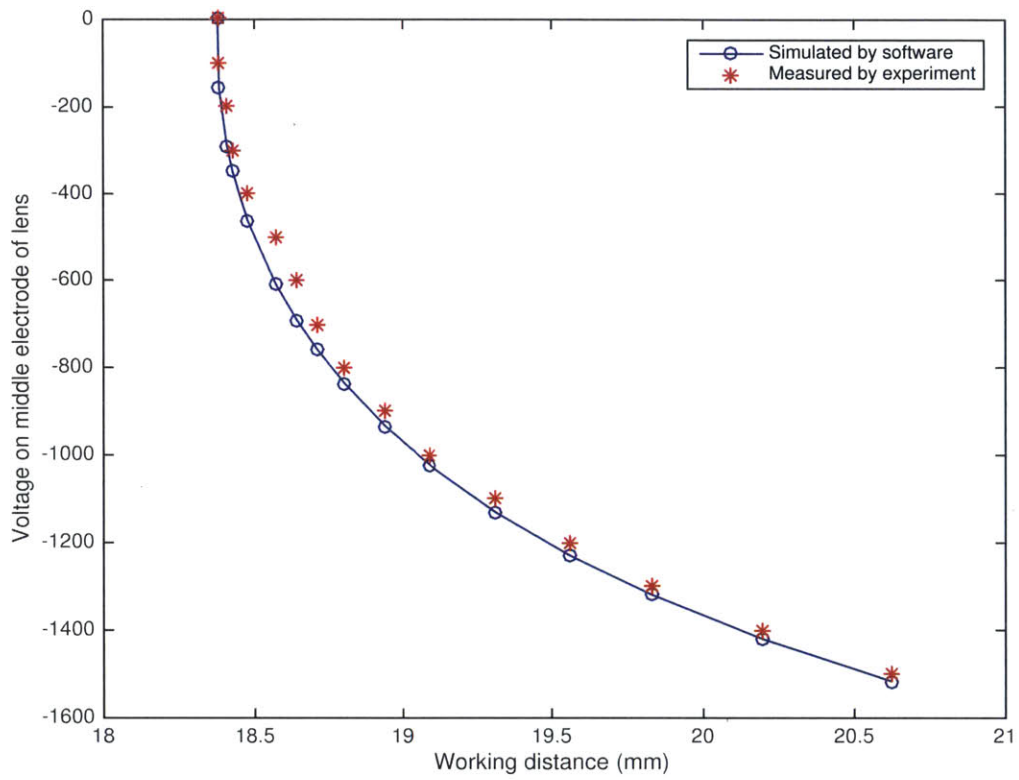


Figure 3-12: Results of the SEM working distance correction simulation, compared to the experimental data.



# Chapter 4

## Electron optical designs for the QEM

### 4.1 Introduction

In the previous chapters, we presented an introduction to the simulation software and showed basic examples of optimization for electron optics design. We now take this effort further by starting work on actual proposed designs for the QEM. The design that we investigate will be one of the first that was used in our simulations; it uses 3 unipolar electron lenses and 2 mirrors, allowing 9 degrees of freedom in electrostatics design. We will refer to this design as **QEM1**. Sample images from the Lorentz implementation of this design can be seen in Figures 2-1 and 4-1.

### 4.2 QEM cavity design and optimization

As noted above, there are 9 degrees of freedom in QEM1 electrostatic design. These are three electrode voltages for each mirrors, and one middle electrode potential for each of the three unipolar lenses (the outside electrodes of the lenses are always set to ground voltage).

The large number of variables poses an important problem: because of long execution times and possible discontinuities in data, it is hard to run a 9-dimensional simplex search on simulation results. Moreover, there is the risk of “overfitting”, in the sense that a solution to the design problem may not be stable (i.e. very sen-

sitive to small changes in voltage). It is also possible that the solution will fit all the constraints, but follow an unexpected path in the regions where no constraints are set. Such a solution, while still being technically valid, would subtract from our understanding of the system and make maintenance harder or impossible.

We therefore follow the modular approach outlined in the previous chapters. Every functional element of the design (mirrors and lenses) are treated as "black boxes" with expected outputs, and the inputs (electrode voltages) are optimized using MATLAB's `fminsearch` function.

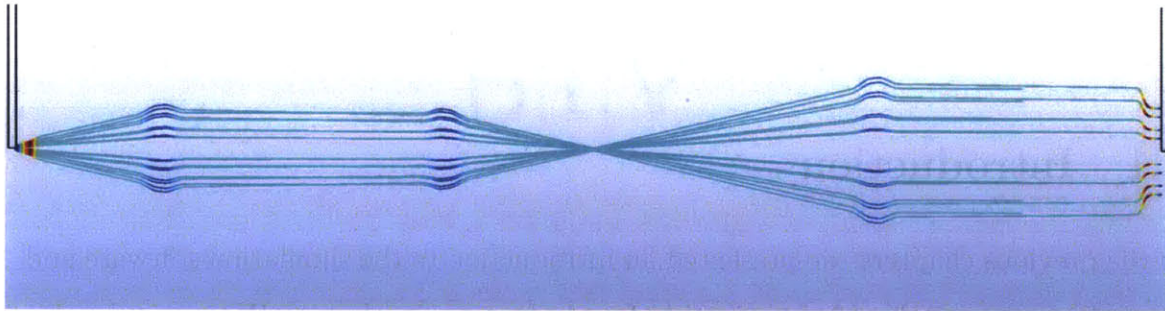


Figure 4-1: Expected electron trajectory of QEM1 design.

For this design, the electrons are placed in the midpoint of lens 1 and 2 ( $x = 20$  mm). At this point, we expect a parallel electron beam, and expect the electrons to be at their source energy. They are therefore initialized with an energy of 5 keV toward the positive  $x$  direction.

From the initial point, we wish to complete a full single roundtrip. For this, four optimizations are required:

1. Spot size of lens 2 at its expected focal point ( $x = 40$  mm). This will use the previously mentioned einzel lens optimization framework.
2. SSE of angles of ray traces after lens 3. This will again use the einzel lens optimization framework, but in reverse.
3. SSE of angles of ray traces being reflected from the right hand mirror. This will use the electron mirror optimization framework.

4. SSE of angles of ray traces leaving the left hand mirror + lens system. A parallel input beam to this system requires a parallel output beam – this can only happen if the lens focuses the beam on the mirror surface, therefore these two elements can be considered in a single optimization loop.

We also will need some initial voltages to begin our search. Suitable candidates for initial voltages of electron lenses can be found from individual optimizations of electric lenses, similar to ones explained in the previous chapter. For electron mirrors, we can start off with a large positive cap voltage and a large negative surface voltage (more negative than the accelerator voltage of the electron source).

### 4.2.1 Optimization of lens 2 voltage

We begin with optimizing lens 2 focal length to 10 mm. This helps to focus the electron beam onto the sample plane, which is at  $x = 40$  mm. The objective function is the spot size at  $x = 40$  mm, which is slightly different from previous practice: instead of finding the focal length by finding the minimum spot size in the positive  $x$  direction, we instead fix our spot size calculations to only  $x = 40$  mm and try to minimize it.

The initial value can be the optimization result from the previous chapter; although this does not have a significant effect on optimization success – see Figure 3-6. We run the optimizer with a search parameter tolerance of  $1 \times 10^{-4}$ , and plot the resulting trajectories in every iteration of the optimization.

The result after this phase is shown in Figure 4-2. The trajectories are not nearly close to what is expected yet; but this will change as we proceed in the optimization stages.

### 4.2.2 Optimization of lens 3 voltage

We now focus our effort on lens 3 and ensure it can produce a parallel beam from the output of lens 2. By our dimensions, this corresponds to a focal length of 20 mm, which we expect to emerge naturally with our optimization.

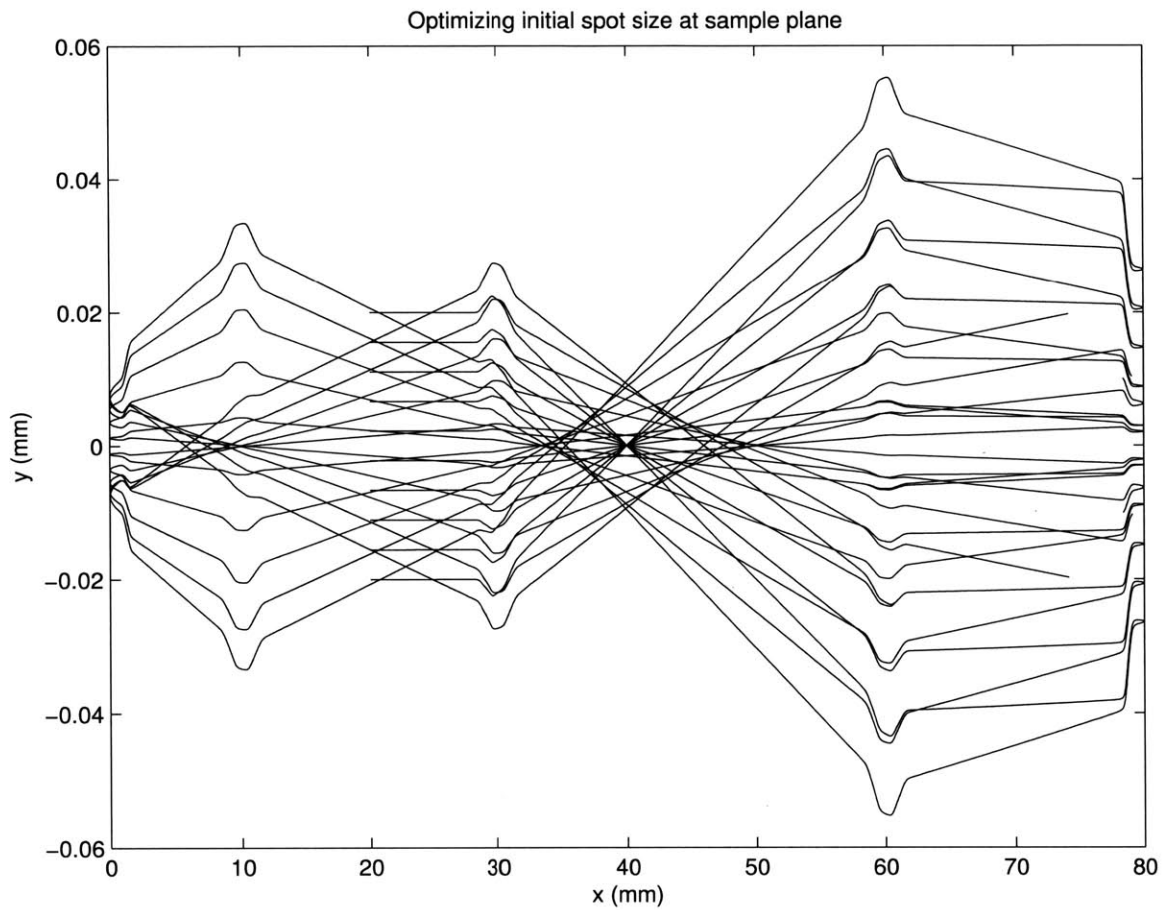


Figure 4-2: Resulting trajectories after optimization of spot size at the sample plane. The beam is clearly focused at  $x = 40$  mm.

The simulation parameters are similar, with the only change being that the lens 2 voltage is set to its calculated value now. The result of this phase, which took about 30 minutes, is shown in Figure 4-3.

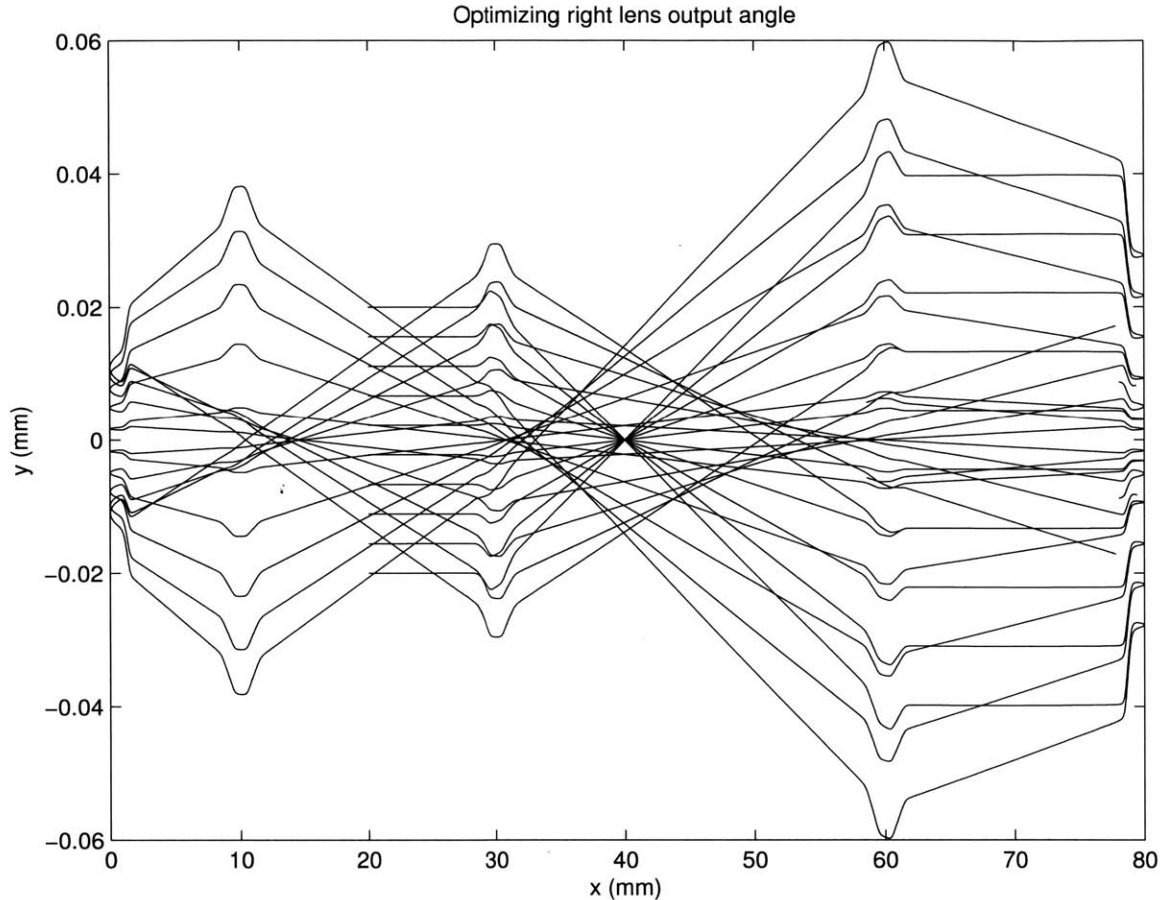


Figure 4-3: Resulting trajectories after optimization of output angles of lens 3.

### 4.2.3 Optimization of right mirror voltage

We now move on to optimizing the right side mirror. We choose to keep the surface potential at a fixed  $-5.35 \times 10^3$  V to simplify the process, and only change the positive potential on cap 1. Cap 2 is always at ground potential.

Optimization takes 44 minutes in our cluster. The results of this phase is shown in Figure 4-4. We can see that this phase has had a profound effect on trajectory correctness, because the previous two elements have already been implicitly optimized

for the output of the right side mirror.

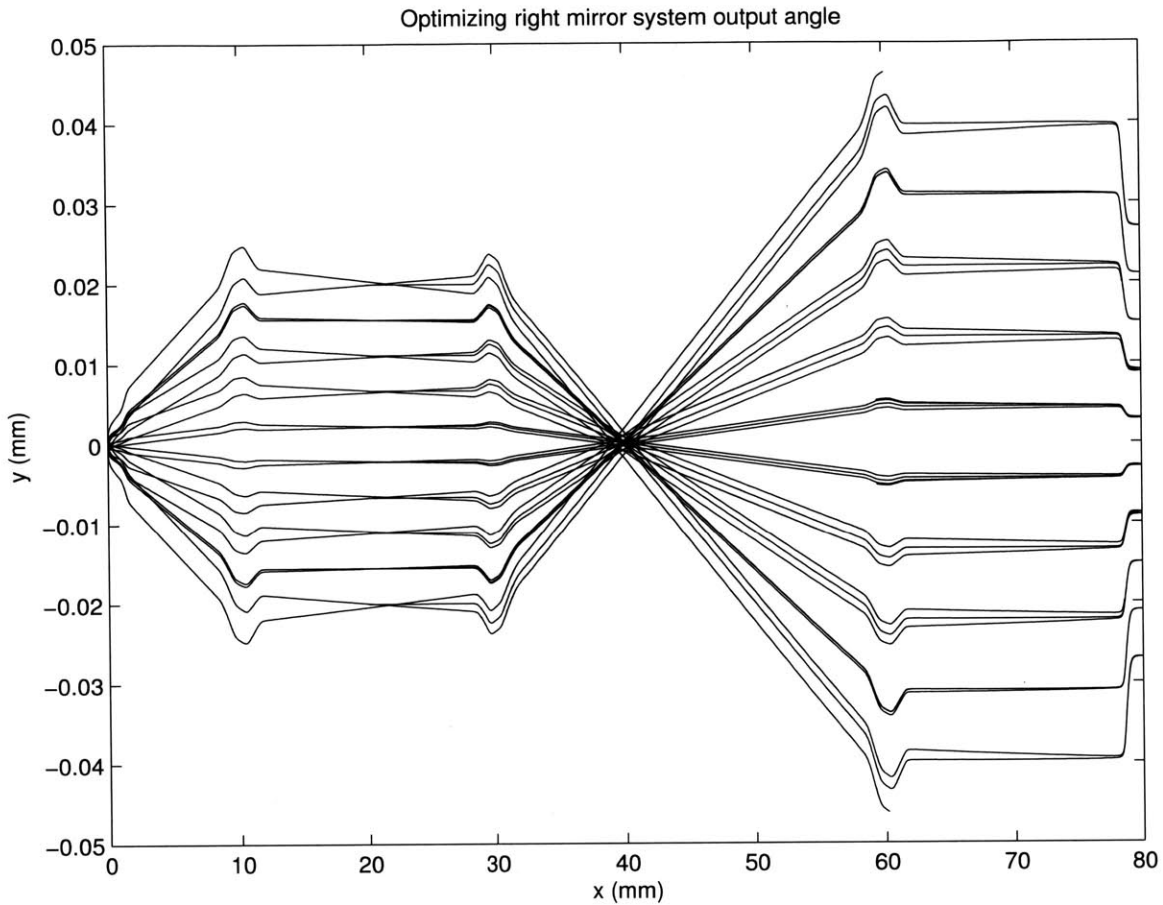


Figure 4-4: Resulting trajectories after optimization of output angles of the right side mirror.

#### 4.2.4 Optimization of left mirror and lens voltages

At the final stage of the process, we consider the left side mirror and lens together as a system that takes a parallel beam as input and returns a parallel beam as output. Simulation parameters remain as usual.

The results of this phase is shown in Figure 4-5. This phase, being a 2-dimensional search, takes longer than the previous phases: about 84 minutes. There seems to be slight (but important) improvement over the previous phase. The spot size on the sample plane after 1.5 roundtrips is about  $3 \mu m$ .

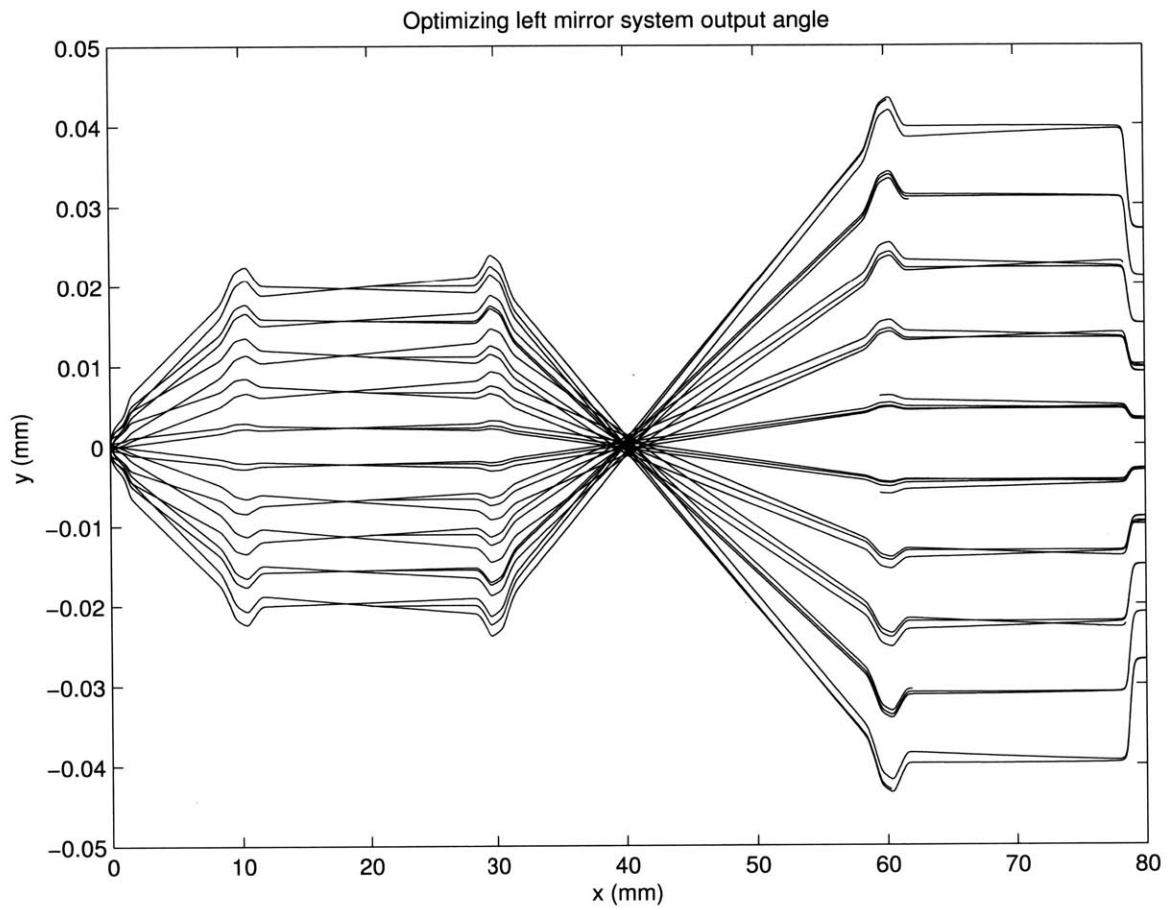


Figure 4-5: Resulting trajectories after optimization of output angles of the left side system.

### 4.2.5 Discussion and comments

We can immediately see that the trajectories build up errors over time. The aberrations contribute to the enlargement of the spot size in the sample plane, making it impossible to have more than a few roundtrips even at the optimized version. Looking at our knowledge from the previous chapter, the culprit seems to be the electric mirrors: we may need to find a better mechanical design, or yet, add mechanical parameters into the optimization loop. Fortunately, time is not a constraint for our optimization – we need to find a working design only once. Future steps on this effort should focus on the mirrors more than the lenses.

One other issue is that this design does not have a barn door. It is assumed that the electron will be coupled into the resonator perfectly at  $x = 20$  mm, which is rather unphysical. Iterations on this design has to include a barn door to this system, and start running time dependent simulations.

# Appendix A

## Future work and challenges

In the previous chapters, we have presented a simulation framework that can be used in context of the QEM. However, there still remains work to be done – most importantly, incorporating quantum mechanics effects into the simulation. In this chapter, we take a look at future challenges for QEM simulations.

### A.1 Extension of simulations into the quantum mechanical realm

The initial paper on QEM by Putnam and Yanik [1] shows that it is theoretically possible to have non-interfering measurements.

The Lorentz-2E software, by itself, does not allow adding any quantum mechanical effects into the simulation. However, coupled with MATLAB, we are free to attach any form of data to the electron trajectories, and this grants us infinite flexibility in implementing a quantum mechanical simulation.

## A.2 Analyzing the effect of aberrations and electron timing

In electric lenses, particles that are off-axis will necessarily suffer from spherical aberration (due to variation in voltage profile in the radial axis). In addition to this, imperfect electron energy spread is inevitable in a real life system (see Section A.3), resulting in chromatic aberration. All this makes it important to characterize these errors in trajectory, and finding out ways to correct them. Such characterizations are done in literature, and tools that do so are sometimes included with electron optics software. We were unable to use Lorentz-2E's aberrations analyzer, but implementing such a tool in-house can be possible.

## A.3 Physical limitations of real-life implementation

Most of the simulations in this work are created using an optimizer that searches for values over all of real numbers (i.e. there is no set precision limit). This can hardly be the case in a real life situation; almost all of the parameters of the electron cavity is limited in precision. For instance, we cannot expect a step size of less than 0.1 V for our high voltage supplies. Similarly, the electrode placement – with a hopeful estimate – will be limited in the order of hundreds of microns. Moreover, the electron gun in the SEM will not emit a monochromatic beam, causing chromatic aberration in the lenses. Yet we do not incorporate these issues in our simulations. We do this because assuming the optimizer outputs are theoretical best values we can use, the best real-life implementation is simply the one that uses those values to their respective maximum allowed precisions. This implies that there cannot be an infinite number of roundtrips in the electron cavity; there necessarily will come a moment where the small errors will build up to cause the system to catastrophically fail. Even in an infinite precision case, the chromatic and spherical aberrations will lead to the same result. The issue is further exacerbated by an issue of *accuracy*, i.e. voltage supplies with nonzero ripple voltage. All these issues can be simulated and will be

considered when the QEM design is close to being finalized.

## A.4 Visualization of simulation results

Industrial simulation software, like Lorentz-2E, need to be flexible in order to tackle the myriad of engineering problems in their field. Such software therefore have a great number of features; however, a very small number of them are actually useful to the researcher. Researchers that want to build in-house specialized software for their specific needs are put off by the large effort that needs to be put in for the numerical solver engine. A scriptable simulator, in this case, proves to be very useful: it allows us to take the solver engine and write our own GUI that wraps it. This is exactly what we have done for QEM9 simulation in the previous chapter. Using MATLAB, we created a tool *specific* to QEM9 simulation, with useful tools that help visualize the relevant and important details of the model in consideration. We believe that this is more useful than the stock GUI of Lorentz-2E.



# Appendix B

## Sample code

```
function [segNumber, iErr] = CreateLine(IEShandle, x1, y1, x2, y2)
% Low-level wrapper for Lorentz's Geometry2D_CreateLine function.
% Allocates output variables, calls the appropriate function and checks for errors.
% Orhan Celiker, MIT

    segNumber = int32(1);
    iErr = int32(1);

    [segNumber, iErr] = Geometry2D_CreateLine(IEShandle, x1, y1, x2, y2, segNumber, iErr);

    InterpretErrorCode(iErr);
end
```

Listing 1: Simple MATLAB function that wraps Lorentz's low-level API call.

```

function lens = CreateElectricLens(IEShandle, position, width, ...
                                height, electrodeWidth, voltage, name)

    % Lorentz wrapper function to create an electric lens.
    % oceliker@mit.edu

    % position is the vector [x,y] pointing to
    % [midpoint of middle electrode, aperture]

    % figure out electrode spacing
    spacing = (width - 3*electrodeWidth) / 2 + electrodeWidth;

    % electrodes
    electrode1 = DrawRectangle(IEShandle,...
        position - [spacing + electrodeWidth / 2, 0],...
        electrodeWidth, height);
    electrode2 = DrawRectangle(IEShandle,...
        position - [electrodeWidth / 2, 0],...
        electrodeWidth, height);
    electrode3 = DrawRectangle(IEShandle,...
        position + [spacing - electrodeWidth / 2, 0],...
        electrodeWidth, height);

    % begin building struct
    lens.E1 = electrode1;
    lens.E2 = electrode2;
    lens.E3 = electrode3;
    lens.objID = CreateObjectFromArray(IEShandle, name, 'segment', [lens.E1 lens.E2 lens.E3]);
    lens.E1obj = CreateObjectFromArray(IEShandle, [name '-electrode1'], 'segment', lens.E1);
    lens.E2obj = CreateObjectFromArray(IEShandle, [name '-electrode2'], 'segment', lens.E2);
    lens.E3obj = CreateObjectFromArray(IEShandle, [name '-electrode3'], 'segment', lens.E3);

    for i = 1:4
        SetVoltageBySegment(IEShandle, lens.E1(i), 0);
    end
    for i = 1:4
        SetVoltageBySegment(IEShandle, lens.E2(i), voltage);
    end
    for i = 1:4
        SetVoltageBySegment(IEShandle, lens.E3(i), 0);
    end
end

```

Listing 2: MATLAB function to create and set voltages of a three-electrode Einzel lens.

```

voltages = [-10, 4550, 150, 500, 500, 150, 5, -5, 5] ;
Geometry_Delete_All(IES);
Setup(IES);
% Place first mirror surface
rect = DrawRectangle(IES, [-0.8 0], 0.8, 50);

for i=1:length(rect)
    SetVoltageBySegment(IES, rect(i), voltages(1));
end

number_of_points = 4;
y_positions = linspace(-0.001,0.001,number_of_points);
x_position = 10;

energy = 300;
for n = 1:length(y_positions)
    EditEmissionPoint(IES, 'Points', n, x_position, y_positions(n),...
        0, 1, 0, 0, energy); % 0-0
end

Solve(IES);

data = cell(GetNumberOfRays(IES, 1, 1),1);
for i = 1:GetNumberOfRays(IES, 1, 1)
    data{i} = [GetRayPoints(IES, 1, 1, i) GetKinematics(IES,1,1,i)];
end

for i = 1:4
    if min(data{i}(:,1)) < 0 || max(data{i}(:,1)) > 25
        disp('Error -- particle out of bounds. Returning nan.')
```

Listing 3: MATLAB function to build and simulate Kruit's QEM9 design.



# Bibliography

- [1] W. P. Putnam and M. F. Yanik. Noninvasive electron microscopy with interaction-free quantum measurements. *Physical Review A*, 80(4):040902, 2009.
- [2] V. K. Zworykin, G. A. Morton, E. G. Ramberg, J. Hillier, and A. W. Vance. *Electron optics and the electron microscope*. Wiley New York, 1945.
- [3] D.T. Grubb. Radiation damage and electron microscopy of organic polymers. *Journal of Materials Science*, 9(10):1715–1736, 1974.
- [4] Juha-Pekka Nuutinen, Claude Clerc, Tuija Virta, and Pertti Törmälä. Effect of gamma, ethylene oxide, electron beam, and plasma sterilization on the behaviour of sr-plla fibres in vitro. *Journal of Biomaterials Science, Polymer Edition*, 13(12):1325–1336, 2002.
- [5] J.J. Skujins, L. Braal, and A.D. McLaren. Characterization of phosphatase in a terrestrial soil sterilized with an electron beam. *Enzymologia (Netherlands) Superseded by Mol. Cell. Biochem.*, Vol: 25, Nov 1962.
- [6] R. M. Glaeser and K. A. Taylor. Radiation damage relative to transmission electron microscopy of biological specimens at low temperature: a review. *Journal of Microscopy*, 1978.
- [7] M Adrian, J Dubochet, J Lepault, and A. W. McDowell. Cryo-electron microscopy of viruses. *Nature*, 308(5954):32–36, 03 1984.
- [8] G.C. Howard, W.E. Brown, and M. Auer. *Imaging Life: Biological Systems from Atoms to Tissues*. Oxford University Press, 2014.
- [9] G. D. Danilatos. Review and outline of environmental sem at present. *Journal of Microscopy*, 162(3):391–402, 1991.
- [10] Integrated Engineering Software. Lorentz-2E two dimensional/rotational-symmetric particle trajectory solver (electric).
- [11] Microsoft Corporation. COM objects and interfaces.
- [12] J. A. Nelder and R. Mead. A simplex method for function minimization. *The Computer Journal*, 7(4):308–313, 1965.

- [13] A. R. Conn, K. Scheinberg, and P. L. Toint. Recent progress in unconstrained nonlinear optimization without derivatives. *Mathematical programming*, 79(1-3):397–414, 1997.
- [14] A. Vertes, P. Juhasz, L. Balazs, M. De Wolf, and R. Gijbels. Non-linear optimization of cylindrical electrostatic lenses. *International Journal of Mass Spectrometry and Ion Processes*, 84(3):255 – 269, 1988.
- [15] M Kato and K Tsuno. Optimization of electron lens shape giving minimum spherical aberration coefficient. *Magnetics, IEEE Transactions on*, 26(2):1023–1026, 1990.
- [16] MATLAB R2015a documentation. fminsearch: Find minimum of unconstrained multivariable function using derivative-free method, April 2015.
- [17] F Croccolo and C Riccardi. Observation of the ion-mirror effect during microscopy of insulating materials. *Journal of microscopy*, 229(1):39–43, 2008.
- [18] Otto Klemperer and Michael Edwin Barnett. *Electron optics*. Cambridge University Press, 1971.
- [19] Brannon Klopfer. Stanford’s Delft report. Report prepared by the Stanford team of QEM project, unpublished, June 2014.
- [20] C. S. Kim. Working distance augmentation figure. QEM biannual conference in MIT, Cambridge, MA, March 2015.