



Calculation of the Spherical and Chromatic Aberrations for Electrostatic Lenses Using Genetic Algorithm

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ABSTRACT

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Optical aberrations degrade the detecting performance in electron spectrometers. It is very difficult to calculate optical aberration parameters for complex electrostatic lens systems. In order to overcome this difficulty, the genetic algorithm method as a solution is introduced in this study. GAs are an intuitive research method based on the principle of generating new sequences of chromosomes in order to solve complex ordered problems. These algorithms target the global optimization of mathematical functions. This study uses a genetic algorithm to demonstrate the results of optimum aberration coefficients as a function of magnification for three-element electrostatic cylinder lenses. This algorithm is used to search for high-performance values. Different mutation and crossover probability values and also different selection and crossover types are tested. The optimum solution is obtained with a mutation rate of 0.01 and uniform crossover with a rate of 0.7. The proposed approach ensures the optimal solution for the aberration problems of the electrostatic lenses.

1. INTRODUCTION

Rotationally symmetric lenses have emerged as indispensable components in experimental systems aimed at transporting and controlling charged particle beams [1]. Among the various configurations available, multi-element electrostatic lenses have become the preferred choice for experimental studies, primarily due to their ability to operate across a wide range of voltages [2, 3].

The key advantage of these lenses lies in their capability to achieve the desired magnification at the precise position of the image point (Q) by manipulating the applied voltages. This adjustability allows researchers to finely tune and optimize the behavior of charged particle beams within the lens region to meet specific experimental requirements [3-5].

Given the widespread utilization of these lenses, numerous methods have been developed to compute the trajectories of charged particles within their lens regions. These computational techniques play a crucial role in optimizing the lenses' performance and facilitating precise beam control. By solving the equations of motion for charged particles in the presence of the electric fields, these methods enable researchers to study and refine the behavior of charged particle beams within rotational symmetric lenses [6-8]. In these calculations, it is required to determine spherical and chromatic aberration coefficients. The accurate characterization and understanding of optical aberrations, particularly spherical and chromatic aberrations, are essential for the development and improvement of high-resolution experimental systems. These aberrations can significantly affect the quality and precision of imaging and measurement techniques, leading to distortions, and fringing in the observed results. To overcome these limitations and optimize the performance of optical systems, it is crucial to determine the aberration coefficients accurately.

The calculations of the spherical and chromatic aberrations in electrostatic lenses have a long history [8-11]. The effort to calculate these aberrations is motivated by the desire to achieve higher resolution and greater accuracy in various applications, such as microscopy, spectroscopy, and particle accelerators. By analyzing the obtained data and comparing it with theoretical models, researchers can estimate the aberration coefficients and gain insights into the performance limitations of electrostatic lenses. The calculation results of the aberration coefficients of charged particles in the lens region, considering the axial potential distributions, are available in the literature [9-18]. The aberration coefficients for two- and three-element lenses were studied by Szilagy [18] for different voltage ratios. Various correction methods have been developed to reduce the aberrations [19-24]. In addition to different methods such as differential algebraic methods, many computer programs have been developed to quickly calculate spherical and chromatic aberration coefficients with high accuracy. The main ones among these programs are LENSYS [15], SIMION [25] and CPO [26]. These programs use traditional methods such as the finite difference method and boundary element method to calculate these lens defects [27-29]. Calculation of these lens defects by using traditional methods involves multiple steps that can take a lot of time and have some limitations.

In recent years, artificial intelligence methods have shown high performance in prediction and classification studies for electron-optical devices. The most widely used artificial intelligence algorithms are artificial neural networks [30-33] and genetic algorithms [34-42] for these studies. Artificial neural networks mimic the biological brain to develop algorithms that can be used to model complex problems. Learning ability is a fundamental feature of an ANN. Similar to the biological brain's ability, artificial neural networks can learn relationships between data from input and output

datasets. Inspired by brain synaptic networks, artificial neural networks consist of a large number of interconnected simple processors. In contrast, the genetic algorithm method (GA) can be used to determine optimum data without the need for data sets [34]. The GA is an optimization algorithm that perform mutation, crossover, and selection operations to obtain optimum solutions. This algorithm, which can select operators and optimal parameters, is highly robust in searching for optimal solutions to complex problems.

Electrostatic lenses play a crucial role in various optical systems, ranging from spectroscopy to imaging devices. The accurate determination of aberration coefficients is essential for optimizing lens performance and achieving high-quality imaging. However, the existing limitations and time-consuming nature of traditional methods hinder the optimization process. The adoption of the GA as a computational tool holds great promise in overcoming these limitations. The GA's ability to simulate natural selection and evolution allows for an efficient search for optimal solutions within a vast parameter space. Furthermore, the utilization of the GA offers the advantage of automation, enabling the researchers to rapidly explore a wide range of parameter combinations. This approach not only saves time but also provides a more comprehensive analysis of lens defects, facilitating a deeper understanding of their impact on imaging systems.

By utilizing the GA, the efficiency, accuracy, and automation of this process is enhanced, ultimately contributing to the advancement of optical systems and improving the quality of imaging technologies.

In this study, the application of a Genetic Algorithm (GA) is investigated to determine the optimal values for both the spherical and chromatic aberration coefficients. The goal is to minimize these aberrations as lower values indicate improved optical performance. Employing a GA algorithm, it is intended to iteratively search for solutions that exhibit a decreasing trend in the fitness graph, or to maintain a constant level of fitness until better solutions are found. This study is organized into four sections. The Materials and Methods Section introduces the aberration coefficients and outlines the steps of the proposed GA method. Optimal set of parameters that minimize the spherical and chromatic aberrations are given in Results Section. The Conclusion Section provides detailed information about the methodology and findings of this study, shedding light on the potential benefits of using a GA for coefficient of deviation optimization.

2. MATERIALS AND METHODS

2.1 Aberration coefficients

Electrostatic lens systems are devices used to control and focus electrons with different energies and directions in atomic and molecular physics experiments. To design a lens with a fixed image position (Q), at least a three-element lens system should be used. However, magnification cannot be kept constant in three-element lens systems. Figure 1 shows three-element electrostatic lens system with equipotential surfaces due to different voltages applied to the lenses. The focused electron beam at image point Q (Figures 1(a) and 1(b)) shows the broad electron beam at image point due to the spherical aberration effect. The intersections of the rays in Figure 1 define the object and image distance, P and Q, respectively. For three-element lenses, the first lens voltage was placed at

the same potential ($V_1=1V$) relative to the primary energy of the incoming charged particles. The second lens voltage was placed at a high or low potential to accelerate or decelerate the charged particle beam. The third lens element was held at a specified voltage ratio to bring the charged particle beams to the desired energies. The most important parameter that indicates the focusing state of the electron beam is magnification (M). The lens parameters are related by the following equation where i is the number of lens elements [15].

$$M = -\frac{f_1}{P - F_1} = -\frac{Q - F_2}{f_2} \quad (1)$$

$$r_{object} \alpha_{object} V_1^{1/2} = r_{image} \alpha_{image} V_i^{1/2} \quad (2)$$

where, F_1 is the first mid-focal length, F_2 is the second mid-focal length of the lens, f_1 is the first focal length and f_2 is the second focal length is given by the relation $f_2 = \sqrt{\frac{V_i}{V_1}} f_1$. Eq.

(2) is the Liouville theorem where r_{image} is the diameter of the electron beam in image point, r_{object} is the diameter of the electron beam in object point, α_{image} and α_{object} are the pencil angles of electrons in the image and object point, respectively. The linear magnification M is determined by the ratio of the diameter of the final beam on the radial axis to the diameter of the first beam, r_{image} / r_{object} .

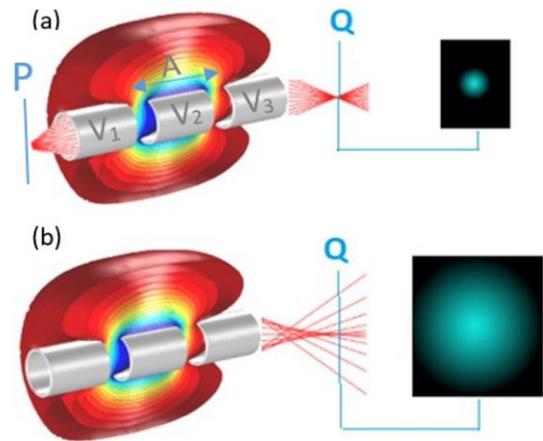


Figure 1. A three-element lens system which consist of three coaxial cylinders of same diameter D

Note: The voltage values applied to the lenses are shown as V_1 , V_2 and V_3 , respectively. 'A' stands for the length of the center electrodes including half the gap to each side. P: Object point, Q: Image point. (a) Focused electron beam at image point Q. (b) Broad electron beam at image point due to the spherical aberration effect.

It is important to determine the spherical and chromatic aberration coefficients in the development of charged-particle optical instruments designed using electrostatic lenses. The calculation results provide guidelines not only for determining particle trajectories in the study region, but also for redesigning particle optical instruments. In the simplest case, it is assumed that the charged particle beam emanates from a point source (P) and is focused on a point image point (Q). However, this was not the case in reality. One of the main aberrations that negatively affects the focusing properties of electrostatic lenses is spherical aberration. The charged particles focus on different points after passing through equipotential surfaces. This event causes deviations from point focus are observed. Equipotential surfaces formed between

lenses of different voltages deflect the charged particles with different maximum half angles (α_0). With this lens defect, the charged particle beams are not focused in the working region after being accelerated or decelerated from the electrostatic lens region. Therefore, the spherical aberration affects resolution of optical instruments. The coefficient of spherical aberration (C_s) is defined by Eq. (3) [15].

$$\Delta r = -MC_s\alpha_0^3 \quad (3)$$

where, Δr is the radius of the spherical aberration disc in the working region, and M is the linear magnification.

Chromatic aberration is a problem in optics where a lens cannot focus all electrons having different energies. One of the beams that crosses the image plane has an energy of E_0 and a slightly higher energy beam has an energy of $E_0 + \delta E$. The chromatic aberration coefficient C_c is given by Eq. (4).

$$\delta r = -MC_c\alpha_0 \frac{\delta E}{E_0} \quad (4)$$

where, δr is the radius of the chromatic aberration disc in the working region.

2.2 Basic principles of the GA method

Genetic algorithms (GAs) are search methods obtained by applying the principle of conservation of the best and natural selection to computers. The GA was developed by Goldberg, inspired by Darwin's theory of evolution [34]. Darwin's theory of evolution was later adapted into a computational algorithm to find a solution to a problem. GAs targets the global optimization of mathematical functions. The feature that distinguishes GAs from other research methods is that after starting with a solution set, a process based on natural evolution is used for development. In the GA process, the best solution is tried to be obtained.

In this study, the GA used to obtain the optimum aberration coefficients began by creating the population consisting of a combination of chromosomes. Figure 2 shows the designed chromosome of the GA, where M is the magnification, C_s/D is the ratio of the spherical aberration to the lens diameter, D . C_c/D is the ratio of the chromatic aberration to the lens diameter. α_0 is the maximum half-angle of the charged particles and $\delta E/E_0$ is the energy ratio of the electrons.

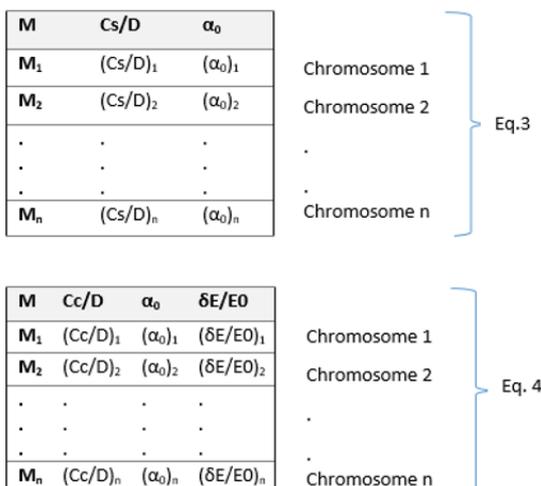


Figure 2. Designed chromosome form of the GA

The generated chromosomes were passed through a fitness function to measure the fitness of the solution. Some chromosomes produce new chromosomes via a crossover process. Some chromosomes also had mutations in their genes. Crossover and the number of chromosomes to mutate are controlled by the crossover rate and the mutation rate value. The chromosome with the higher fitness value is more likely to be selected again in the next generation. After a few generations, the chromosome value was determined by convergence to the best solution to the problem. Figure 3 shows the flowchart of the GA.

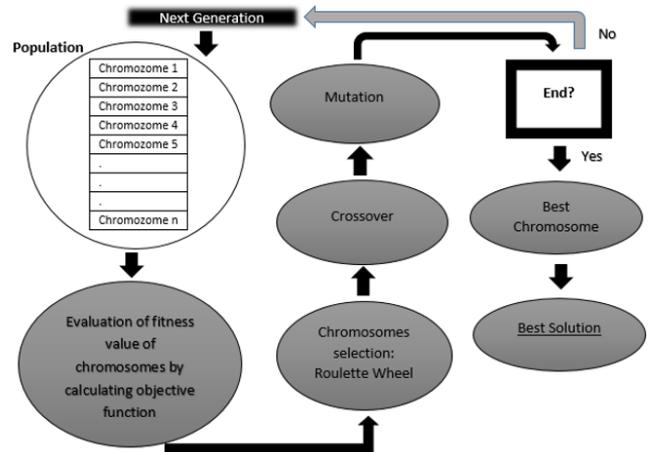


Figure 3. Schematic representation of GA flowchart

In this study, the spherical and chromatic aberration coefficients were calculated using the GA method. In this study, the GA results were obtained using MATLAB R2012b. The proposed GA was used to find the optimal results using Eqs. (3) and (4). The fitness function to be minimized for spherical and chromatic aberration coefficients can be determined using Eq. (5) and Eq. (6) respectively.

The proposed GA was used to optimize Eq. (3) which aims to minimize for spherical aberration coefficients. The fitness function in Eq. (3) is given by

$$F(x) = -\Delta r - MC_s\alpha_0^3 \quad (5)$$

The proposed GA was also run to optimize Eq. (4) which aims to minimize for chromatic aberration coefficients. The fitness function in Eq. (4) is given by:

$$F(x) = -\delta r - MC_c\alpha_0 \frac{\delta E}{E_0} \quad (6)$$

The boundaries of the constraint variables are selected as $0 \leq M \leq 2$, $0 \leq \alpha_0 \leq 0.2$, $0 \leq C_s/D \leq 500$, $0 \leq C_c/D \leq 500$, $0 < \delta E/E_0 \leq 500$. The steps of the proposed GA are as follows.

Step 1. Initialization

The number of chromosomes in the population is n ($n=100$). The random values of genes M , α_0 , C_s/D , C_c/D , and $\delta E/E_0$ for n chromosomes were also determined based on the parameters of Eqs (5) and (6), respectively.

In this study, chromosomes were expressed using real numerical values within solution space boundaries. Real-coded GA is more useful in solving the aberration problem, using the real values of the genes. In addition, the fact that the solutions are defined with real values considerably increases the computational efficiency.

Step 2. Evaluation

In this step, the objective function value for each chromosome produced in initialization step is computed.

Step 3. Selection

In selection step, the most suitable parents were selected by the roulette wheel selection method.

Step 4. Crossover

In the crossover step, the parent chromosome of the mate was selected. In this process, the mate chromosome number was checked using the crossover rate. A high crossover rate results in rapid exploration of the search space. Therefore, better individuals deteriorate quickly. A low crossover rate will cause very few new and different individuals to enter the new generation as a result of reproduction, and the research space will not be adequately scanned. Therefore, an appropriate crossover ratio must be determined based on this problem. In this study, the crossover rate was set as 0.7.

Step 5. Mutation

In this step, the mutation operator scans different regions of the solution space by inserting new information into an existing population. In this way, it helps overcome the problem of early convergence. In this study, the mutation rate was determined as 0.01. When the mutation process is completed, one iteration or generation of the GA is obtained. The objective function is evaluated after one generation. This process was repeated until a predetermined number of generations was generated. To ensure the success of the algorithm, it is extremely important to properly determine the control parameters of the GA operators. The GA parameters for the aberration problem are listed in Table 1.

Table 1. Parameters of the GA

Genetic Algorithm Parameters	
Algorithm	Real-Coded Genetic Algorithm
Population Size	100
Selection Rule	Roulette Wheel Selection
Crossover Operator	Uniform Crossover
Crossover Rate	0.7
Mutation Operator	Multi-Point Mutation Operator
Mutation Rate	0.01
Maximum Iteration Number	3000

3. RESULTS

In this study, it was determined as the stopping criterion that the maximum number of iterations is exceeded or that the absolute value of the function value is less than $E=10^{-5}$. The optimization process ends when the obtained function value is less than 10^{-5} value. Otherwise, the search process continues for 3000 iterations.

In a genetic algorithm, the objective function values vs. the iteration number graph provide insight into the progress and convergence of the algorithm as it searches for an optimal solution. Figures 4(a) 4(b) show the convergences of the GA for spherical and chromatic aberration problems, respectively. The objective function represents the criteria that the genetic algorithm aims to optimize. It quantifies the fitness or quality of a candidate solution within the population. The goal of the genetic algorithm is to find the best possible solution that maximizes or minimizes the objective function, depending on the problem's nature. In Figure 4, the x-axis of the graph represents the iteration number, indicating how many iterations the genetic algorithm has gone through. In Figure 4,

the y-axis represents the objective function values corresponding to the candidate solutions in each iteration. The Figure 4 reveals the behavior of the genetic algorithm over time. Initially, the objective function values may vary significantly from one iteration to another as the algorithm explores different candidate solutions. As the algorithm progresses, it aims to improve the objective function values by selecting the most promising individuals, applying genetic operators (crossover and mutation) to generate new offspring, and evaluating their fitness.

The difference in iteration numbers in subgraphs (a) and (b) of Figure 4 required to reach convergence for the spherical aberration and chromatic aberration problems can be attributed to several factors. The two aberrations, spherical and chromatic, are caused by different factors and have distinct characteristics. The complexity of the mathematical formulation for each aberration may vary, resulting in different convergence rates. It's possible that the chromatic aberration problem involves more intricate calculations or a higher-dimensional search space, requiring more iterations to converge. Some optimization problems are highly sensitive to initial conditions. The initial guess or starting point can significantly affect the convergence behavior. If the chromatic aberration problem is more sensitive to initial conditions compared to the spherical aberration problem, it may require additional iterations to converge to the desired solution.

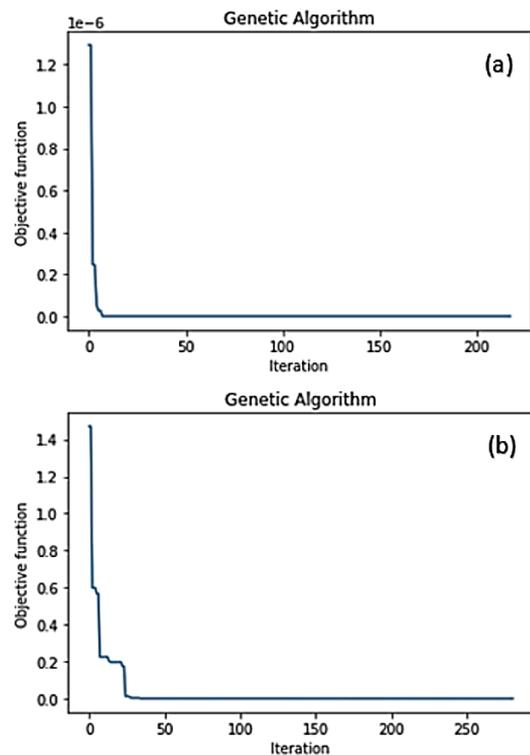


Figure 4. Objective function values vs. the iteration number.

(a) The convergence for spherical aberration problem has been reached after 230 iterations by satisfying condition; (b) The convergence for chromatic aberration problem has been reached after 280 iterations by satisfying condition

An elitist approach was also used in the algorithm to maintain the best chromosomes. In this approach, the selection pressure is prevented by keeping the elite selection rate low. In addition, the mutation operator of the GA allows the formation of new chromosomes, even if successful chromosomes are dominant in the next generation.

The GA explores the solution space and converges towards optical system configurations that exhibit reduced spherical and chromatic aberrations. The process involves continuously evaluating the fitness of the solutions, selecting promising ones, applying genetic operators to create new solutions, and repeating until a satisfactory solution is found or the termination condition is met. The obtained GAs values of the spherical (C_s/D) and chromatic aberration coefficients (C_c/D) in the image plane as a function of magnification for $\alpha_0 = 0.1$ are presented in subgraphs (a) and (b) of Figure 5, respectively. The aberration coefficients are highly dependent on magnification. Therefore, it is important to know the dependence of the spherical and chromatic aberration quantities on the magnification.

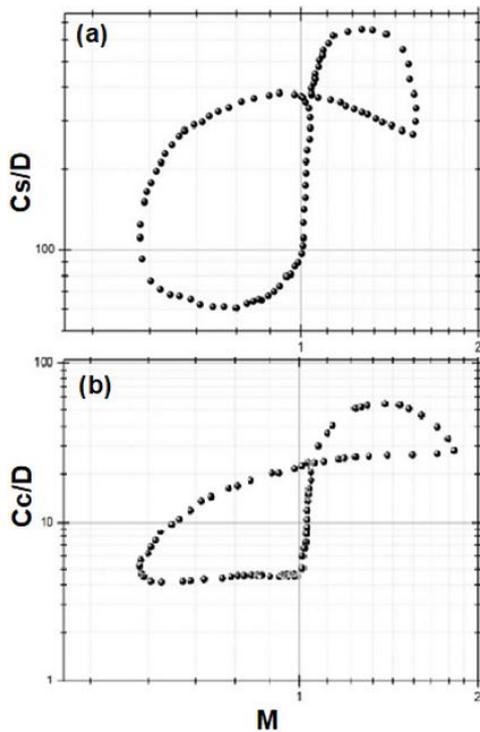


Figure 5. (a) Values of the spherical aberration coefficients (C_s/D) in the image plane as a function of the magnification ($A/D=1$ and $P/D=Q/D=3$). (b) Values of the chromatic aberration coefficients (C_c/D) in the image plane as a function of the magnification

4. CONCLUSION

Electron collision studies address the structure of atoms, their mutual interactions, and their dynamics. The goal of the experimental and theoretical efforts in these studies is a full understanding of atoms or molecules and their interaction results by electron impact. Therefore, the first step in increasing the resolution of the optical devices used in these experiments was to determine aberration coefficients. Lens systems with aberration correction are often designed using numerical ray tracing. Although the parameters that minimize spherical and chromatic aberrations can be calculated analytically for simple designs, these calculations are quite difficult for complex designs.

Numerical analysis is a computer-aided technique used for solving mathematical problems. In numerical analysis methods, the main goal is to obtain the correct result with a

small number of iterations and minimum errors. Therefore, GAs are especially useful in solving large problems where many local optima are generated, and they are less likely to become stuck in a local minimum than classical gradient-based search algorithms. Many classical methods require complex mathematical operations such as determining the appropriate initial conditions, many iterations and derivative calculations in each iteration to reach the optimal solution. GA is an intuitive search method that learns and decides by itself using random search techniques. The study highlights that the GA method provides more stable results compared to other artificial intelligence algorithms when applied to the optimization problem. This is valuable in lens design, as stability and reliability are crucial for achieving accurate and consistent results in electron collision studies. By offering stable solutions, the GA method enhances the reliability of the lens design process and the subsequent experimental outcomes.

While analytical calculations for minimizing spherical and chromatic aberrations exist for simple lens designs, complex designs pose significant challenges for such calculations. This study recognizes the limitations of analytical calculations and introduces the GA method as a powerful tool to address the complexity of lens designs. By focusing on electrostatic lenses, the research offers valuable information and techniques for improving the performance and design of electrostatic lens systems. Additionally, the introduction of new methodologies and approaches expands the range of tools available to researchers and practitioners in the field, encouraging further advancements and discoveries.

By utilizing the GA, the design of lens systems for electron collision studies can be optimized. By leveraging the power of genetic algorithms, the resolution and performance of optical devices used in electron collision studies can be improved.

Understanding how aberration coefficients vary with magnification can help in the design and optimization of optical systems. By characterizing the aberration coefficients across different magnification settings, it becomes possible to calibrate the system to achieve more accurate and precise imaging results. This calibration can involve adjusting lens positions, introducing compensating elements, or implementing software-based corrections. By measuring aberration coefficients at different magnifications, manufacturers can verify if the resulting optical systems meet the desired performance specifications. Any deviations from the expected aberration behavior can be flagged for further investigation or adjustments in the manufacturing process. Adaptive optics techniques are employed to correct aberrations in real-time, particularly in applications such as astronomy or laser systems. The knowledge of the aberration dependence on magnification can guide the adaptive optics system in adjusting its corrective measures dynamically based on the desired magnification level. This can enhance the overall imaging or beam quality, compensating for the specific aberration characteristics at different magnifications. These are just a few examples of how the obtained information on the dependence of aberration coefficients on magnification can be utilized in real-world applications. By leveraging this knowledge, it becomes possible to optimize optical systems, enhance imaging quality, and enable more precise control over aberrations, leading to improved performance in various domains that rely on optical systems and imaging technologies.

The performance of the GA method can be influenced by the choice of algorithmic parameters, such as population size, mutation rate, and selection criteria. Future research could

focus on developing multi-objective GA algorithms or hybrid approaches that integrate the GA method with other optimization techniques to tackle the complexities of multi-objective aberration optimization for electrostatic lenses.

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