Design of a dynamic simulation program for the Rutherford scattering experiment based on the Euler iteration method

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Abstract. Based on the defects that the existing Rutherford scattering simulation instrument cannot be visualized, this paper designs a Rutherford scattering experimental dynamic simulation program. The simulation program mainly combines the corresponding physical formula, Euler equation iteration method and trigonometric function relationship for programming. It uses PhotoShop software, HTML, CSS, JavaScript and Python language for programming and drawing. As a result, within the same simulation time, the relationship between the number of deflected particles N and the incident energy E of alpha particles, the relationship between the number of target materials and the number of deflected particles N, and the relationship between the total number of deflected particles N and the deflected angle. This simulation program addresses the limitations of existing instruments by enabling visualization of the Rutherford scattering experiment through the innovative use of a web interface. This approach aligns with the current preferences of students. Additionally, the web-based platform allows for flexible adjustment of target nucleus types. Through this simulation program, particle scattering trajectories and the number of particles at different deflection angles are directly displayed, enabling students to better understand the Rutherford scattering experiment, enhance their learning experience, and thereby promote the development of experimental teaching and scientific research.

Keywords: Simulation, Euler method for iteration, trigonometric functions, visualization, interactive interface.

1. Introduction

The Rutherford scattering experiment was published in 1911. The results of the scattering experiment proposed an atomic nucleus model, which had a profound impact on modern physics and promoted progress in many technological applications [1]. For example, ion beam analysis technology uses the interaction between ion beams and matter to analyze the elemental composition and structure of matter, while backscattering technology uses the large-angle deflection phenomenon in Rutherford scattering to conduct material analysis.

Rutherford scattering simulation experiments have significant research value, so many teams have studied Rutherford scattering simulation experiments for teaching and research purposes. Higginson D P [2]defined a self-consistent method combining cumulative and individual scattering events, referred to as full-angle scattering (FAS), However, the article does not discuss the influence of different target nuclei on scattering. Žugec P et al [3]. Explored the shadow region in repulsive Rutherford scattering—the spatial region that completely shields any particle trajectories—as an in-depth study of Rutherford scattering experiments. Jin X et al [4]. Investigated new advances in simulating Rutherford backscattering spectra (RBS/C) using arbitrary atomic structures in the channel mode. However, there is still room for improvement in terms of algorithm accuracy, material universality, and dynamic behavior analysis. Lingis D et al [5]. proposed a new model developed using the GEANT4 simulation toolkit to simulate the Rutherford backscattering spectrum (RBS) of hydrogen (H), helium (He), and lithium (Li) ions, but the current model does not consider multiple scattering, surface roughness, and material porosity. Lichao T et al [6]. Developed a Rutherford scattering virtual simulation experiment based on Unity3D, but it lacks the presentation of particle scattering dynamic trajectories and only outputs experimental results.

The aforementioned research primarily focused on the specific details of the Rutherford scattering experiment, developed simulation programs, and designed applications in practical scenarios, thereby demonstrating the significance of the Rutherford scattering experiment and its promising future prospects. However, there are limited resources available to help students understand the program design related to the Rutherford scattering experiment. To address this issue, we have developed an interactive dynamic simulation program for the Rutherford scattering experiment. This program is accessible via a web interface, aiming to simplify experimental procedures, reduce experimental costs and the risks associated with alpha radiation sources, while enhancing experimental accuracy. The user-friendly interface provides greater convenience for educational practice, benefiting both scholars and the general public.

2. Principle of an experiment

2.1. α particle scattering theory

Let the mass of the nucleus be M, with a positive charge of +Ze, and at point O, and an α particle with a mass of m, an energy of E, and a charge of ze, incident at a speed, b is the perpendicular distance of the nucleus from the extended line of the α particle's original path, that is, the minimum straight-line distance between the incident particle and the nucleus when they are not interacting, called the aiming distance, and α is the Coulomb scattering factor. Before the derivation, a few assumptions are made: the particles only reflect once, there is only Coulomb interaction between the particles and the target nucleus, the effect of the outer electrons of the nucleus can be ignored, and the target nucleus is stationary.

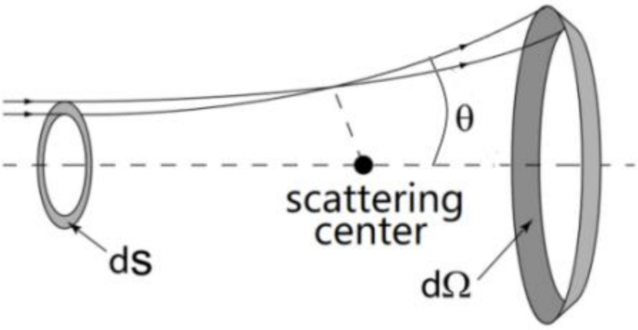


Figure 1. The scattering angle of an α particle as a function of the range.

A target is a very thin foil with a thickness of t and an area of s. In Figure 1, the probability that an alpha particle is scattered by a target atom in the range between θ and θ-dθ, that is, the probability that the alpha particle hits the ring ds, is:

$$\frac{ds}{s}=\frac{2\pi b\left|db\right|}{s}=\frac{2\pi\alpha^2\cos\frac{\theta}{2}}{8s\sin^2\frac{\theta}{2}}d\theta \tag{1}$$

If expressed in steradian dΩ:

$$d\Omega=2\pi\sin\theta d\theta=4\pi\sin\frac{\theta}{2}\cos\frac{\theta}{2}d\theta \tag{2}$$

So:

$$\frac{ds}{s}=\frac{\alpha^2 d\Omega}{16s\sin^4\frac{\theta}{2}} \tag{3}$$

If N_0 α particles per unit time impinge vertically on a thin foil, the number of α particles per unit time measured in the θ direction and within a solid angle dΩ is:

$$dn = N_0 \frac{ds}{s} nts = \left(\frac{1}{4\pi\varepsilon_0} \right)^2 nN_0 t \left(\frac{zZe^2}{4E} \right)^2 \frac{d\Omega}{\sin^4 \frac{\theta}{2}} \tag{4}$$

This gives us the famous Rutherford scattering formula:

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{dn}{nN_0 t d\Omega} = \left(\frac{1}{4\pi\varepsilon_0} \right)^2 \left(\frac{zZe^2}{4E} \right)^2 \frac{1}{\sin^4 \frac{\theta}{2}} \tag{5}$$

From the above formula, we can see that there is a corresponding functional relationship between the number of deflected particles N and the deflection angle, the nuclear charge number Z of the target nucleus, and the energy E of the incident α particle.

2.2. Trajectory simulation algorithm

2.2.1. Euclidean iterative method

The Euler iteration method [7] is a basic numerical integration method. Its basic idea is to use the slope (derivative) of a function at a certain point to approximate the function value near that point. The formula is as follows:

$$x_{n+1} = x_n + h \cdot f(x_n, t_n) \tag{6}$$

In this particle trajectory simulation, the Euler iteration method is used to update the speed and position of the particles. For particles subjected to forces, the Coulomb force acting on the particles is first calculated:

$$F = k \frac{q_1 q_2}{r^2} \tag{7}$$

Acceleration is calculated from the force and the particle's mass:

$$a = \frac{F}{m} \tag{8}$$

The speed is then updated via the acceleration; finally, the position is updated via the speed (The step size Δt is usually taken to be 1) .And we end up with a position function for the particles:

$$x_{x_{n+1}} = x_{x_n} + v_x \tag{9}$$

$$x_{y_{n+1}} = x_{y_m} + v_y \tag{10}$$

2.2.2. Effect of multiple scattering

The Rutherford scattering formula assumes that a particle undergoes single Coulomb scattering with only one nucleus as it passes through the target material. However, in reality, the gold foil is three orders of magnitude thicker than the atomic wire, and the particle may undergo multiple scatterings with multiple nuclei.

Therefore, in the process of programming, we simulated multiple scattering of particles. In the program, we calculate the Euclidean distance [8] d between the particle and each nucleus. But, in actual code, the square of the distance can be compared to simplify calculations:

$$d^2 = \left(x_p - x_n\right)^2 + \left(y_p - y_n\right)^2 \tag{11}$$

The size of the d determines whether the particle is scattered by the nucleus. These multiple scattering events change the particle's trajectory and energy, which causes the simulation results to deviate from the predictions of Rutherford scattering.

3. Dynamic experimental simulation programming

The Rutherford scattering simulation experiment webpage was designed using five tools: Photoshop, HTML, CSS, JavaScript, and Python.

3.1. Specific design process steps

As shown in Figure 2, first use Photoshop to draw a diagram of the instrument setup, and use HTML and CSS [9] to design the web page layout. Then use JavaScript to design the button functions, construct the Euler equation to solve for and update the alpha particle position, as well as calculate the scattering angle accordingly. Next, use Canvas to render the scattering trajectory, and use Echarts [10] to count and update the particle number and scattering angle data to display a bar chart. Finally, use Python's Flask framework to obtain the page and pass data.

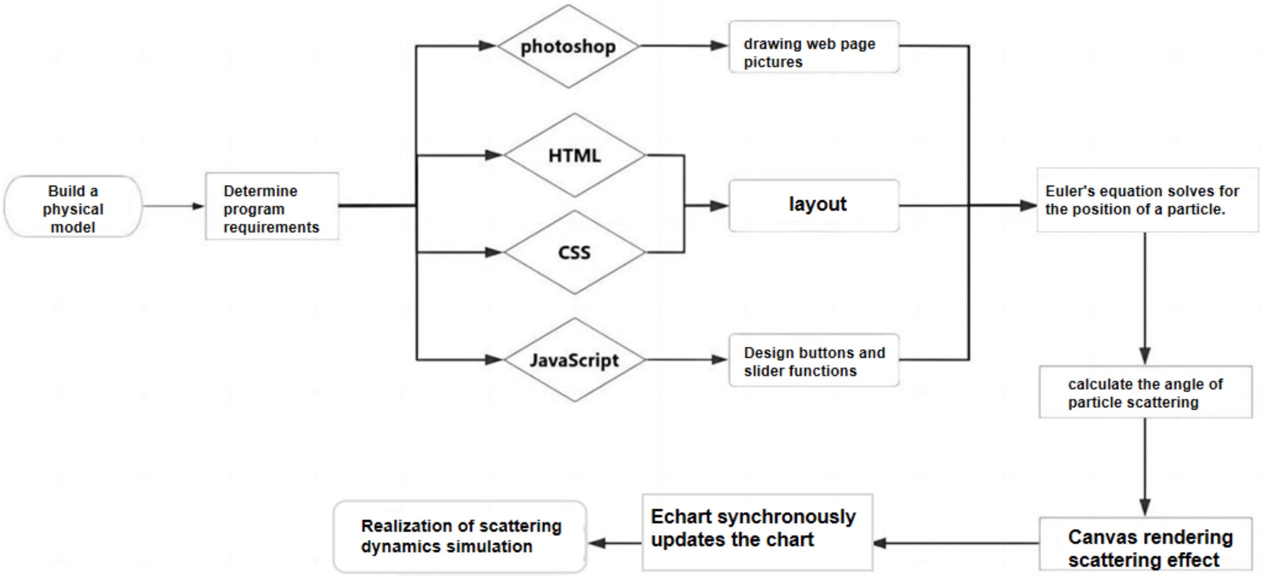


Figure 2. Program design flowchart.

3.2. Introduction to procedural implementation techniques

The main points of the program implementation are: determining the velocity and position of αparticles, real-time updating of the particle position to form a dynamic trajectory and dynamic bar chart, and the dynamic trajectory's timely response to changes in various parameters.

3.2.1. Determine the speed and position of the α particle

To achieve the function of determining the position and speed of alpha particles, we mainly combined the corresponding physical formulas, the Euler equation iteration method, and trigonometric function relationships to program it. First, define the user-defined function 'IsOffset', and then set up a loop to determine the distance between the particle and the target nucleus. When the particle enters the atom, calculate the Coulomb force it receives; then define the Coulomb constant, elementary charge, target nuclear charge from the proton number slider, alpha particle charge number, alpha particle mass, Coulomb force, acceleration (where 100 is the unit conversion factor), define the formula for calculating the sine, cosine and tangent values; finally, calculate the acceleration components a_x and a_y, and use the static ratio k_v and static speed v_{static} to calculate v_x and v_y and update the actual speed.

3.2.2. Create dynamic charts and column charts

Create a particle array, set ‘requestId’ to store the animation frame request ID to control the start and stop of the animation, and set ‘showtrail’ to control whether to display particle trails, with the default being no display. Define the ‘InitalParticle’ function to initialize particles and add them to the particle array. Define the ‘IschangeColor’ function to mark particles when their horizontal velocity vx is negative to determine color changes. Define the ‘drawParticles’ function to draw particle trajectories. This function includes a counter that increments by 1 each time it is called, then clears the canvas and draws the background. When the counter ‘Count equals’ 400 or 1, call the ‘InitalParticle’ function to initialize the particles. Finally, set a loop to iterate through the particle array and update each particle's trajectory, achieving the particle movement animation effect through recursive calls to ‘drawParticles’.

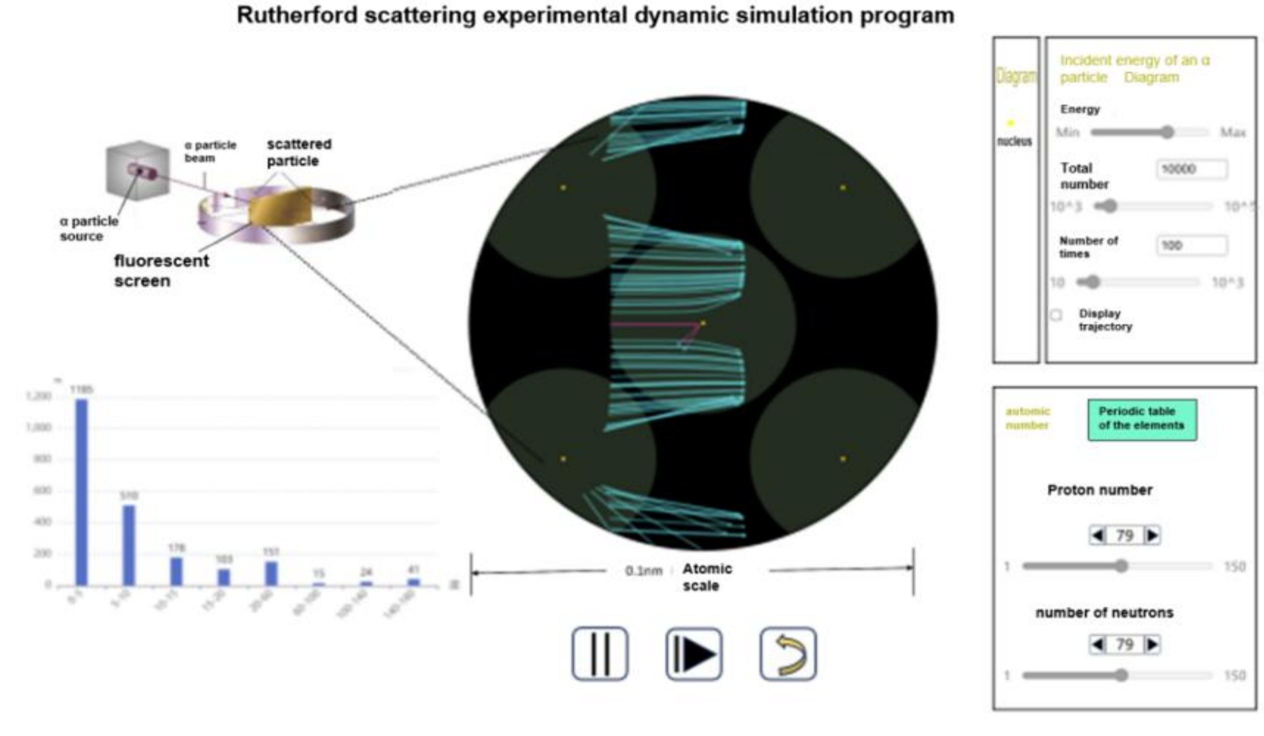
3.2.3. Dynamic trajectory: timely response to changes in various parameters

In order to achieve the function of responding to changes in various parameters in time for dynamic tracking, our program mainly uses the tool of adding event listeners for programming. Add input event listeners to the speed slider speedmySlider, the total number slider TotalNumberSlider, the text box TotalNumberText, the count slider EveryNumberSlider, and the text box EveryNumberText to update the corresponding variables and related text box contents when the sliders are dragged to change their values, and to update the corresponding slider positions and related variable values when the text box values are changed, thereby responding to changes in speed, total number, and count.

4. Method of use and result analysis

4.1. Program installation and page introduction

The specific steps of the usage process are as follows: open the mainpage → adjust the controllable parameters (energy, total number, number of times(Figure3), periodic table of elements(Figure4), proton number, etc.) → click on the alpha particle launcher → the canvas forms a scatter dynamic simulation diagram(Figure5) → a dynamic bar chart is generated(Figure6) → click on the pause button to pause → click on the next button to move the alpha particle one step → click on the reset button to reset the simulation.



Total number 10000

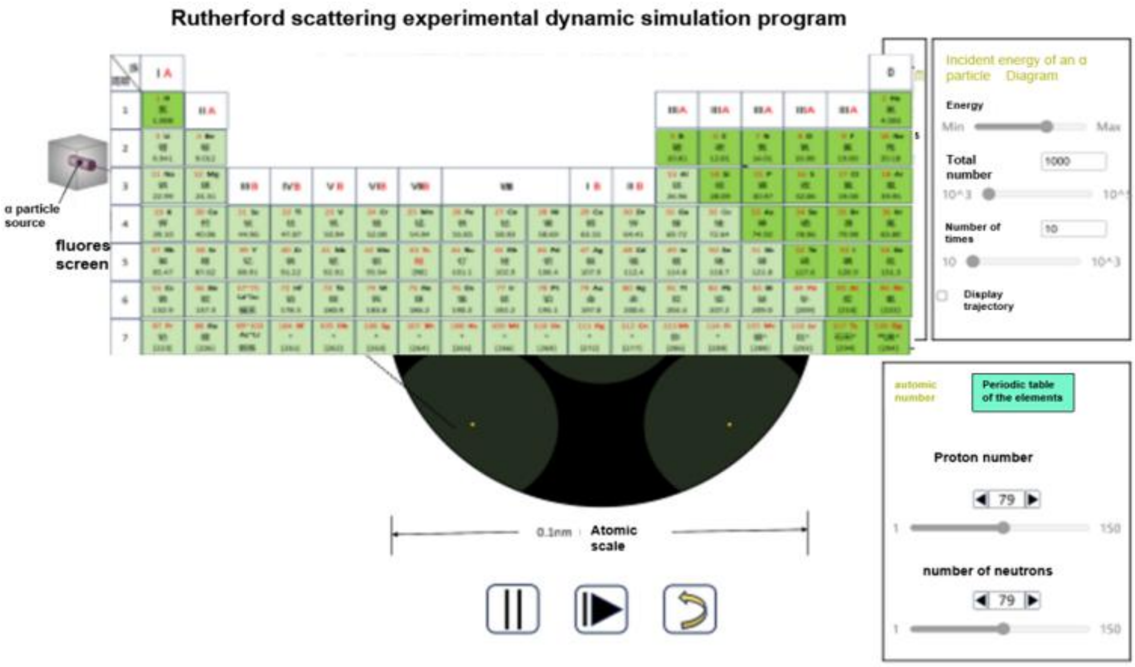
Number of times 100

Proton number 79

number of neutrons 79

Figure 3. Page layout.

The entire page includes the following parts: the alpha particle initiator (top left), the alpha particle controllable parameters (top right), the controllable parameters of the target nucleus element (bottom right), the button tool (bottom center), the dynamic scattering canvas (centered), and the dynamic bar chart (bottom left).



Total number: 1000
Number of times: 10
Proton number: 79
number of neutrons: 79

Figure 4. Periodic table page image.

In the controllable parameters of the target nucleus element, you can control the number of protons in the nucleus, the number of neutrons in the nucleus, and the Periodic Table of Elements button. When you click the Periodic Table of Elements and then click the desired element, the corresponding numbers of protons and neutrons will be automatically generated, as shown in Figure 4.

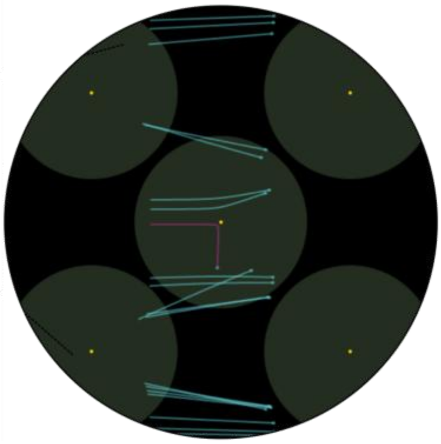


Figure 5. Dynamic scattering image.

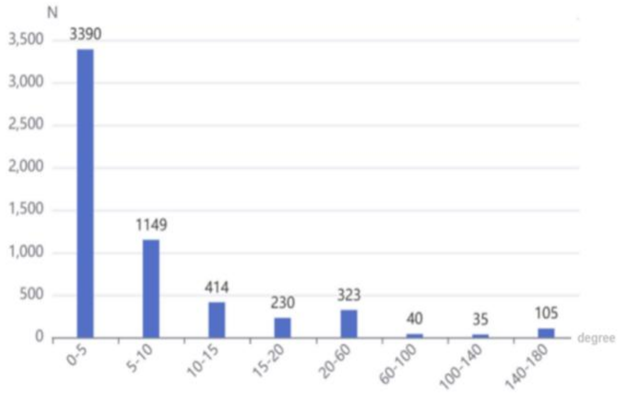


Figure 6. Bar chart.

The dynamic scattering image is shown in Figure 5. When the display track is selected, the scattering simulation diagram displays the trajectory of the alpha particle. The histogram chart is illustrated in Figure 6. After the simulation starts, the histogram is generated immediately when the first group of α particles leaves the canvas, dynamically displaying the particle distribution at different scattering deflection angles.

4.2. Results and analysis

4.2.1. Relationship between N and θ

In order to explore the relationship between N and θ, we performed theoretical calculations of Rutherford scattering formula $N = a \times \frac{1}{\sin^4\left(\frac{\theta}{2}\right)}$ with corresponding values, and selected simulated data with the parameters of Z = 79 (i.e., gold nucleus) for the target nucleus, $N = 10^4$ for the total number of particles, and E = default for the energy value. The specific simulated data obtained are shown in Table 1:

Table 1. Select simulated data for N-θ.

angle range /°		0-5	5-10	10-15	15-20	20-60	60-100	100-140	140-180
experimental count	N	5880	1589	987	568	600	200	96	80

The result is shown in Figure 7:

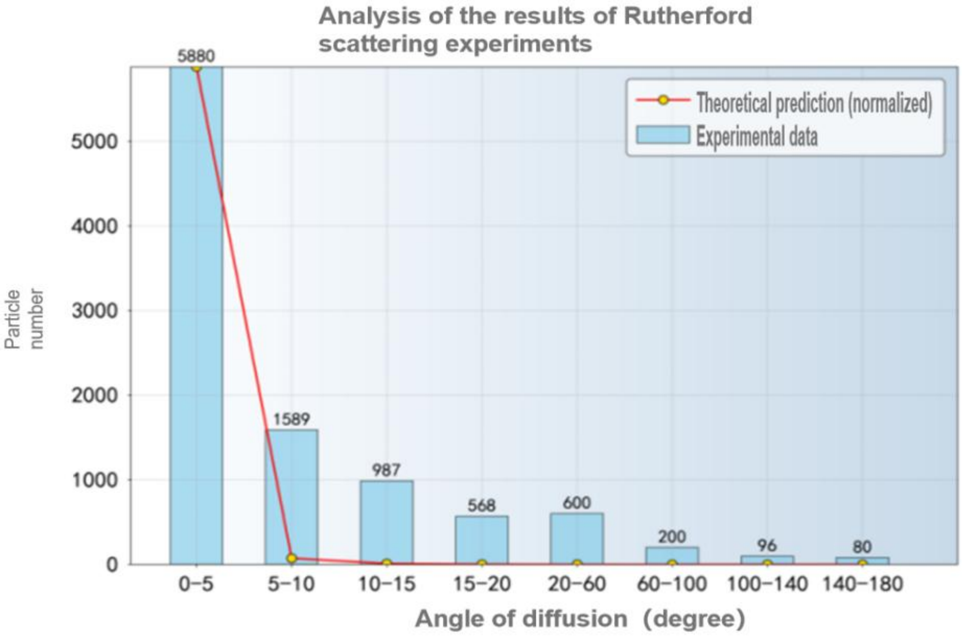


Figure 7. Histogram of the relationship between N and θ.

Simulation data shows that in the dynamic simulation of Rutherford scattering, the number of scattered particles (N) and the scattering angle (θ) show an inverse relationship, which is in good agreement with the conclusion of the Rutherford scattering experiment that “very few particles experience large angle deflection, while the vast majority experience small angle deflection or even almost no deflection.”

In order to further verify the applicability of the theoretical model, the linear regression analysis was used to calculate the correlation coefficient R, the determination coefficient R^2, the standard error SE, and the significance level P value of the experimental data and theoretical prediction. The specific values are shown in Table 2:

Table 2. Experimental error in the relationship between N and θ.

Error indicator	R	R^2	SE	P
value	0.968	0.936235	0.096333	8.3×10^{-5}

$R^2\approx0.936$ Explanation 93.6% of the experimental data variation can be explained by the theoretical model, and the scattering simulation results have high explanatory and predictive power for the N-θ relationship. The SE is small, which shows that the estimation of the Rutherford scattering N-θ relationship through simulated experimental data is relatively accurate, and the results of the statistical analysis of the data are more reliable. And $P < \mathbf{1}\times10^{-3}$, it can be seen that the regression result is statistically significant, that is, the model parameters significantly affect the data.

4.2.2. Relationship between N and Z

To explore the N-Z relationship, we selected experimental data for four metals: aluminum, copper, silver, and gold (with nuclear charges Z of 13, 29, 47, and 79, respectively). We then plotted the N-Z relationship for different angle ranges based on theoretical fits to the number of scattered particles within each range using the fitting function $N = a \times \frac{Z^2}{\sin^4\left(\frac{\theta}{2}\right)} + b$. The results are shown in Figure 8:

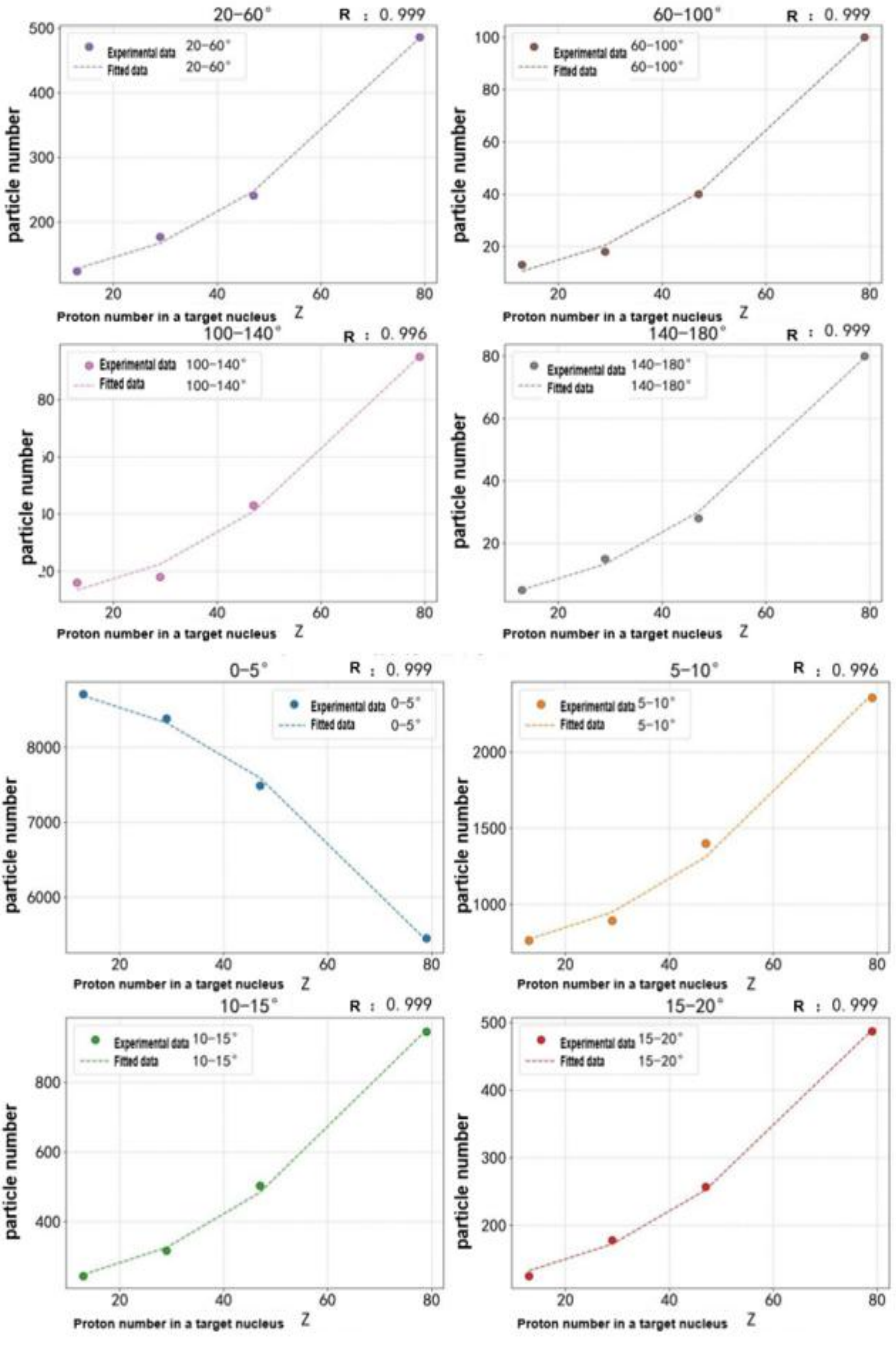


Figure 8. N-Z relationship diagram in different angle ranges.

It can be seen that the number of particles N increases with the increase of the nuclear charge number Z of the target nucleus, and there is a proportional relationship between the two. In the small angle range, due to the stronger Coulomb repulsion between the target nucleus with a high nuclear charge number and the alpha particle, more particles are deflected at a larger angle. Therefore, when the total number remains unchanged, an increase in the number of particles deflected at a large angle will inevitably lead to a decrease in the number of particles deflected at a small angle. The results of the simulation experiment are in agreement with the theoretical fitting curve, and the N-Z relationship is reasonably explained.

Similarly, a linear regression analysis was performed on the simulated experimental data and the fitted data for the N-Z relationship, and the correlation coefficient between the simulated experimental count and the fitted count was calculated one by one. Some of the data are displayed (Table 3), and the SE, P value, and linear regression coefficients a and b are determined. See Table 4 for details.

Table 3. Correlation coefficient between the experimental count and the fitted total count for different Z values.

	z value	experimental count	proposed total	relative error
angle 0-5°	13	8710	8691	0.22%
	29	8384	8329	0.66%
	47	7488	7592	1.39%
	79	5450	5422	0.51%
		......		
angle 60-100°	13	13	12	7.69%
	29	18	20	11.11%
	47	40	40	0.00%
	79	100	100	0.00%
		......		
angle140-180°	13	5	5	0.00%
	29	15	14	6.67%
	47	28	30	7.14%
	79	80	80	0.00%

Table 4. Experimental error in the relationship between N and Z.

Error indicator	R^2	SE	P	slope :a	intercept :b
value	0.996	275.611	0.002	5836.316	-690.158

Table 3, 4 shows that the linear regression $R^2 = 0.996$ indicates that 99.6% of the experimental data variation can be explained by the theoretical model. The small standard error SE indicates that the fitted parameters are estimated with high accuracy. P= 0.002 indicates that the regression result is statistically significant, i.e., the model parameters significantly affect the data.

4.2.3. Relationship between N and E

From the Rutherford scattering formula, it can be seen that the relationship between the number of scattered particles N and the energy of the incident α particles E is $\mathbf{N}\propto\frac{1}{E^2}$. Therefore, we directly adjusted the simulated experimental data with different energy values, and fitted the data with different incident energies according to the Rutherford scattering formula to plot the N-E relationship diagram in different angular ranges. The results are shown in Figure 9.

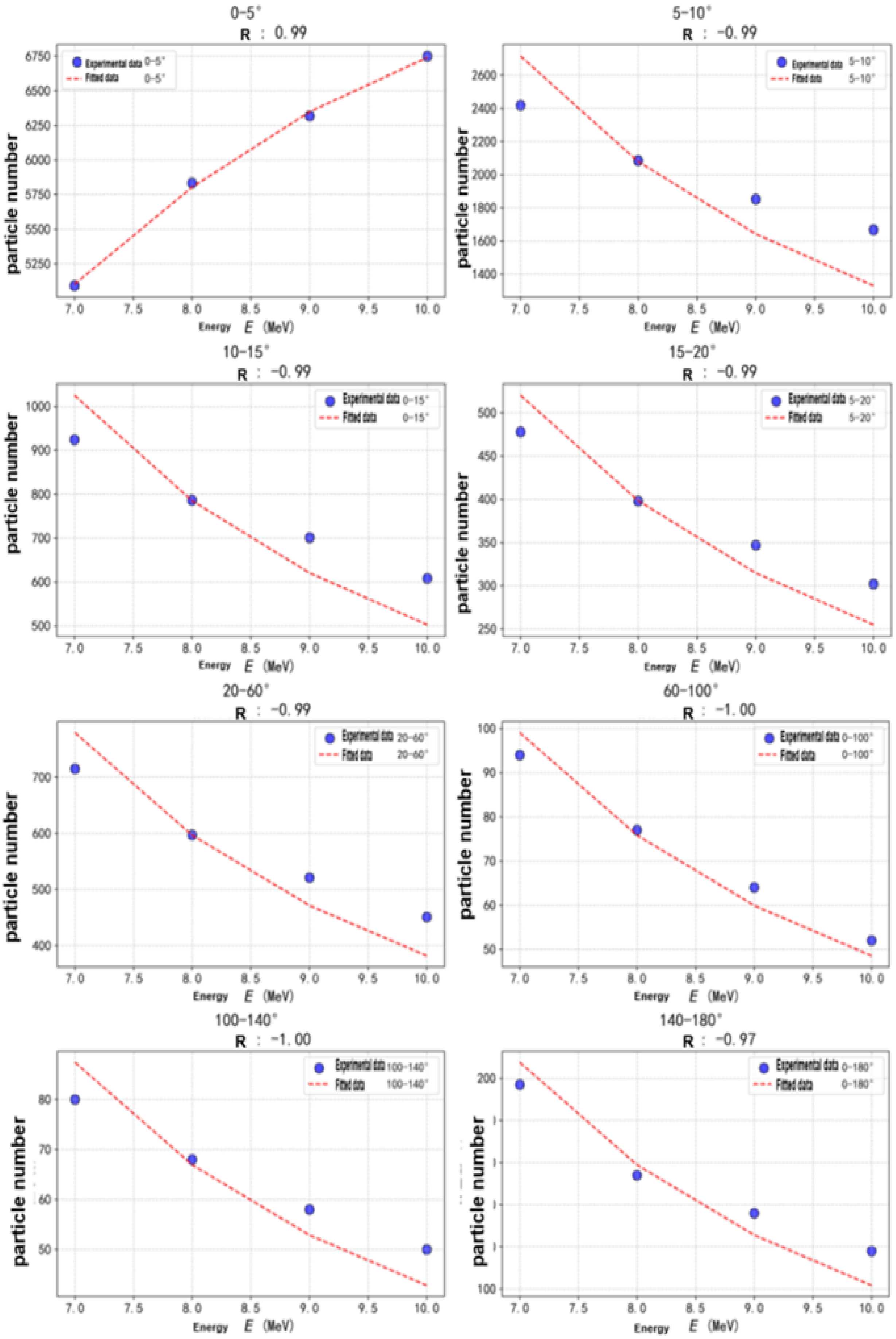


Figure 9. N-E relationship diagram in different angle ranges.

As can be seen from the figure, the simulated experimental data and the fitted curve trend are consistent, and the number of particles N increases with increasing energy E, and there is an inverse relationship between the two. In the small angle range, as the incident particle energy E increases, the time for the particles to be acted on by the Coulomb repulsive force is shortened, so that more particles are scattered at smaller angles, that is, as the energy E increases, the number of particles scattered at small angles increases accordingly. Moreover, the results of the simulation experiment are consistent with the theoretical fitting curve, and the N-E relationship is also reasonably explained.

Similarly, a linear regression analysis was performed on the simulated experimental data and the fitted data for the N-E relationship, and the correlation coefficient between the simulated experimental count and the fitted count was calculated one by one (Table 6), and the R^2, SE, and P values of the two as well as the linear regression coefficients a and b were determined. The specific values are as follows:

Table 5. Correlation coefficient between the experimental count and the proposed total count for different E values.

	E value	experimental count	proposed total	relative error
angle0-5°	7	5092	5102	0.20%
	8	5833	5803	0.51%
	9	6319	6349	0.47%
	10	6750	6740	0.15%
		......		
angle60-100°	7	94	99	5.32%
	8	77	76	1.30%
	9	64	60	6.25%
	10	52	49	5.77%
		......		
angle140-180°	7	197	207	5.08%
	8	154	158	2.06%
	9	136	126	7.35%
	10	118	102	13.56

Table 6. Experimental error in the relationship between N and E.

Error indicator	R^2	SE	P	slope :a	intercept :b
value	0.997	255.312	0.002	5836.316	-690.158

The data in Table 5, 6 shows that the linear regression $R^2 = 0.997$ indicates that 99.7% of the experimental data variation can be explained by the theoretical model, and the model has a strong explanatory power for the data. The standard error SE = 255.312 is small, indicating that the estimated accuracy of the fitted parameters is high. The significance level P = 0.002 indicates that the regression results are statistically significant, that is, the model parameters significantly affect the data.

5. Experimental teaching and significance

The Rutherford scattering virtual simulation experiment project proposed in this paper uses Photoshop to draw the content of the page pictures, HTML and CSS to draw the page layout, and JS code to construct the scattering Euler equation. After designing the functions of each button, the scattering effect is designed using the canvas. Finally, the ECharts is used to display the chart in real time, which realizes the simulation of the dynamic trajectory of multiple particle scattering in the software. In the simulation process of particle scattering, we combined the corresponding physical formulas, Euler equation iteration method and trigonometric function relationship to program, and used Photoshop, HTML, CSS, JavaScript and Python to program and draw. The final conclusion is that the number of scattered particles N and the scattering angle θ show an inverse relationship, that is, with the increase of scattering angle θ, in the same simulation time, the number of incident particles N decreases; secondly, the number of scattered particles N is proportional to the nuclear charge number Z of the target nucleus, that is, as the number of protons in the target material increases, the number of incident particles N increases during the same simulation time; and the number of scattered particles N is inversely proportional to the energy E of the incident α particles, that is, as the incident energy E of the α particles increases, the number of incident particles N decreases during the same simulation time.

The Rutherford scattering experiment dynamic simulation program provides new ideas and methods for teaching nuclear physics experiments, helps cultivate students' scientific research spirit and practical ability, and makes a positive contribution to the development of experimental teaching and scientific research.

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