Modeling of α-particle scattering off a gold foil as a simulation of Geiger and Marsden's experiment

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Abstract

A simulation of Geiger and Marsden's experiment was constructed in Python modeling the scattering distribution of α-particles on a gold atom. Thompson's structure of the atom was initially assumed and rejected due to small scattering angles. Rutherford's model was then assumed, accepted and numerically explored further in terms of scattering distribution.

Introduction

During the early twentieth century, there was controversy about the structure of the atom. Thompson initially proposed the famous "plum pudding model" [1]. This model describes the atom as a collection of uniformly spread particles across the whole atom. Therefore, the charge density of protons and electrons in the volume of the atom would be extremely small. In a paper published in 1909, Geiger and Marsden reported observations of α-particles which strike on a gold foil and scatter in angles greater than 90^o [2]. This did not agree with Thompson's model due to the uniform spreading of the protons which allows only for slight repulsion of a striking α-particle which can thus scatter no more than a fraction of a degree.

The above disagreement between theory and experimental results led Rutherford to propose a new model of the atom two years later. Specifically, he suggested that "the theory of Sir J. J. Thomson ... and the particular structure assumed for the atom does not admit of a very large deflexion of an α-particle in traversing a single atom, unless it be supposed that the diameter of the sphere of positive electricity is minute compared with the diameter of the sphere of influence of the atom" [3]. This "sphere of positive electricity" is of course the nucleus.

The model developed in this report, simulates the encounter of an α-particle with a single gold atom assuming both Thompson's and Rutherford's structure of the atom. The scattering distribution for this encounter in both cases is analysed and Rutherford's model is extended to simulating the encounter of an α-particle with a gold foil, ignoring multiple scattering. This extension also investigates the accuracy of the numerical approximations as compared to analytical values. The simulation is made using Python's libraries SciPy and NumPy [4].

Theory

In order to investigate the models, a system of coupled differential equations of two-dimensional motion were set up and then solved by the *odeint* function of SciPy. The idea is that the positive

α-particle is repelled due to an electric force exerted by the protons of the gold atom, while gravitational effects and electron contribution are assumed negligible.

The centre of the atom is the origin of the coordinate system used. The physical constants and unchanged parameters of the simulation, along with necessary derivations are explained in appendix A to which the reader is referred. Although they are essential for understanding the equations that follow, they were left out of the theory section due to their overwhelming bulkiness. It is most important to understand that the quantities used are made dimensionless and hence constants disappear from the equations.

Rutherford's model assumption of the nucleus suggests that the equations of motion should be

$$v_x = \frac{dx}{dt}, \qquad \frac{dv_x}{dt} = \frac{x}{d^3} \tag{1}$$

$$v_y = \frac{dy}{dt}, \qquad \frac{dv_y}{dt} = \frac{y}{d^3}, \tag{2}$$

where v is the velocity of the α-particle and $d = \sqrt{x^2 + y^2}$.

Thompson's model assumption of uniformity implies that $\frac{q}{D_0^3} = \frac{Q}{D^3}$ within the atom, where Q, D are the charge and radius of the atom and q, D_0 are the charge and diameter of any smaller sphere contained by the atom. Therefore, an α-particle inside the gold atom obeys a different set of equations:

$$v_x = \frac{dx}{dt}, \qquad \frac{dv_x}{dt} = \frac{8x}{D^3} \tag{3}$$

$$v_y = \frac{dy}{dt}, \qquad \frac{dv_y}{dt} = \frac{8y}{D^3} \tag{4}$$

In both models, the α-particle is scattered at an angle θ from the gold atom and the dependence of the scattering angle on the impact parameter b is investigated.

The conservation of total energy

$$\frac{1}{2}mu(v \times v_a)^2 + \frac{2Zq_e^2}{d \times a} = 8.0 \times 10^{-13}\ J, \tag{5}$$

is also investigated as a test for the accuracy of the numerical approximations used.

Rutherford further predicted the following dependences between various parameters [3],[5]

$$b = \frac{kZq_e^2}{T}\sqrt{\frac{1+\cos\theta}{1-\cos\theta}} \tag{6}$$

$$d_{min} = \frac{b\cos\frac{\theta}{2}}{1-\sin\frac{\theta}{2}} \tag{7}$$

$$f = \frac{\pi N_A L \varrho k^2 q_e^2 Z^2}{2T^2 M} \times 10^{-9} \times \left(\frac{1+\cos\theta}{1-\cos\theta}\right), \tag{8}$$

which are tested in the simulation. Thus, the right-hand side of (6) and (7) are called test function 1 and 2 respectively. The last equation predicts the fraction of scattered α-particles at an angle greater or equal to θ and thus describes the scattering distribution of the particle on a gold foil. Multiple scattering in this case is assumed statistically impossible due to the minute size of the nucleus.

Method

Initially, Thompson's model was built and then Rutherford's was built and extended. The following chart represents the flow of logic in the simulation. Trajectories are symbolised by T. The number of trajectories created in each model is arbitrary and only satisfies two conditions; taking enough measurements for precise graphs and cover both the cases in which the α-particle crosses or passes by the atom.

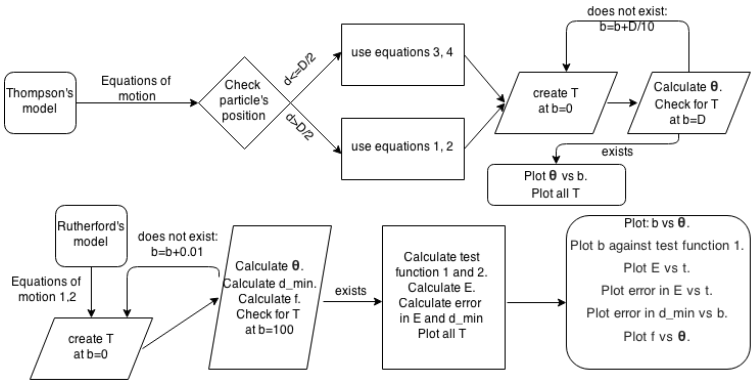
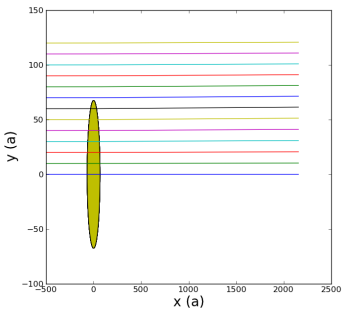


Figure 1: The steps taken in the simulation after defining the constants

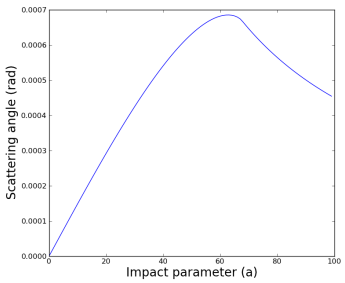
In Thompson's model θ was plotted against b, while in Rutherford's model it was the other way round, for reasons obvious in the Results section. The plots of errors in the terminal of the second branch of the chart were meant to check the accuracy of the model. The rest of the plots gave insight into the scattering distributions.

Results

Thompson's model produced trajectories with only small scattering angles as seen in figure (2a) It is clear in figure (2b) that the largest scattering angle $\theta \approx 0.0007\ rad$ is observed when the α-particle passes tangentially from the atom. Therefore, Thompson's model clearly does not



(a) Trajectories

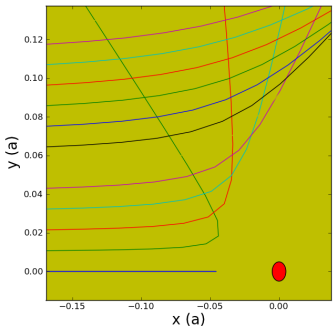


(b) The scattering angle is too small

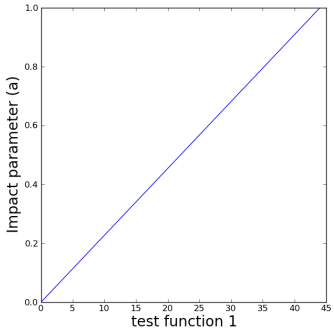
Figure 2: Thompson's model

satisfy Geiger and Marsden's experiment [6].

The simulation of Rutherford's model, though, produced trajectories of α-particles which were scattered even more than 90 degrees, as in figure (3a). No α-particle penetrates the atom very close to its centre like in Thompson's model, confirming Rutherford's suggestion of a strongly charged nucleus [3]. The trajectories are zoomed in and look segmented reminding that the numerical method used is just an approximation.



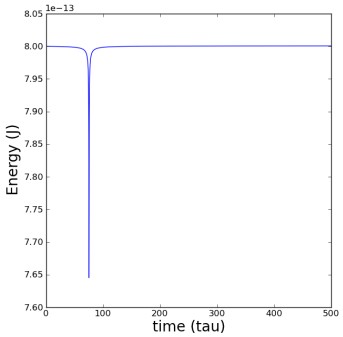
(a) Trajectories



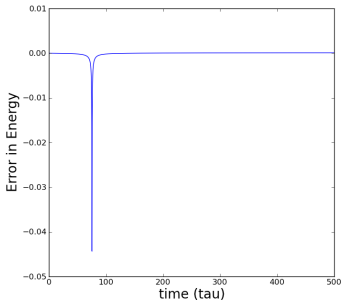
(b) The scattering angle as a function of impact parameter

Figure 3: Rutherford's model

The relation between scattering angle and impact parameter is indeed given by equation (6). The slope of the graph is about 0.0227 m which agrees with the analytical value within a negligible fractional error of the order of 10^{-5}.



(a) Energy over time



(b) Fractional error in total energy

Figure 4: Energy conservation

Although the results seem accurate, the conservation of energy for the system was tested to confirm this. Figure (4) suggests that energy is conserved at the value calculated analytically throughout the simulation except for the time interval $68 - 82\ \tau$ during which the fractional error rises above 0.1% and even reaches 4.4%. At this time interval, the α-particle is closest to the

nucleus and thus the speed changes slightly because the trajectory is approximated by segments.

Finally, measurements of the minimum distance of each trajectory to the centre of the atom were plotted against the test function 2. The behaviour of this graph is very similar to the behaviour of figure (4b). The minimum distance reaches no more than 1.3% error but fluctuates over a greater interval. The early maximum in the graph can be justified again by the segmented nature of the trajectories observed in figure (3a). For small impact parameters the edges on the trajectory affect minimum distance measurements.

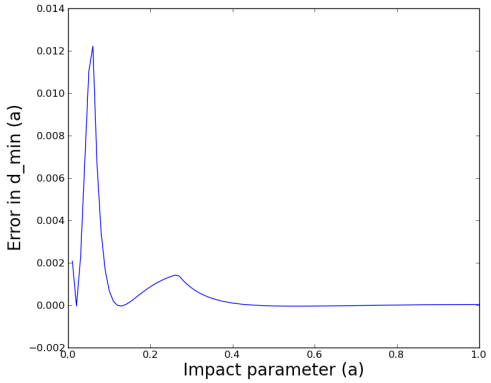


Figure 5: Fractional error in minimum distance

Having established the accuracy of the simulation, equation (8) can be trusted to model the scattering pattern of α-particles on a gold foil. The equation essentially suggests the probability of a particle to be scattered at angles greater than a desired one.

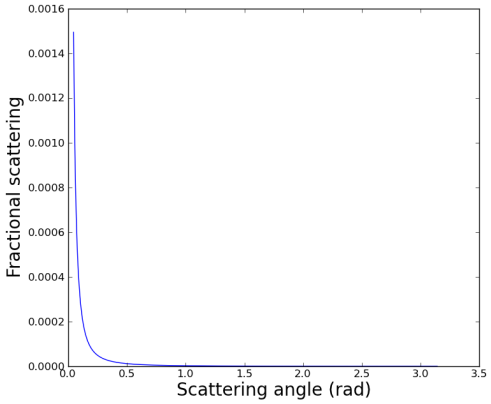


Figure 6: Scattering pattern. The fractional scattering rapidly drops to values near 0

Conclusion

The main aim of the simulation was to model scattering of an α-particle on a gold atom using both Thompson's and Rutherford's structure of the atom. The modeling allowed for comparison between the two opposing structures and for investigation of the accuracy of NumPy and SciPy. The simulation proved to be very accurate considering some analytical solutions to the model. It also modeled the trajectories and provided numerically relations between the scattering angle and the impact parameter of α-particles for both models.

The result of 0.0227 m for the slope of graph (3b) was exact. However, errors arose due to the non-continuous nature of the results, as is evident in the graphs (5) and (4b). Using more computer power, more iterations for time can be done so that the results are closer to the analytical. The deviation of $4,4\%$ in energy measurements is certainly not negligible.

The simulation can be extended in various ways. Geiger and Marsden carried out the experiment with different independent variables [6], like different atomic mass instead of scattering angle. It can also be extended to other situations in which equations of motion can be explored numerically, as in orbital motion [4]. It can prove very useful in cases in which the equations of motion cannot be solved analytically, like in the famous case of the three-body problem.

References

[1] Thompson, J. J., "On the Structure of the Atom: an Investigation of the Stability and Periods of Oscillation of a number of Corpuscles arranged at equal intervals around the Circumference of a Circle; with Application of the Results to the Theory of Atomic Structure" (extract of paper), 1904, Philosophical Magazine, 7, p237.

[2] Geiger, H. & Marsden, E., "On a Diffuse Reflection of the -Particles", 1909, Proc. Roy. Soc., 82, p495

[3] Rutherford, E., "The Scattering of α and β Particles by Matter and the Structure of the Atom", 1911, Philosophical Magazine, 21, p669.

[4] Colling, D. *et al*, Imperial College Y1 Introduction to Python (v0.1), 2014

[5] Beiser, A., "Concepts of Modern Physics" (6th edition), 2003

[6] Geiger, H. & Marsden, E., "The Laws of Deflexion of a Particles through Large Angles", 1913, Philosophical Magazine, 25, 148

Appendix A

The physical constants used throughout are Coulomb's constant $k = 8.99 \times 10^9\ Nm^2C^{-2}$, electron's charge $q_e = 1.60 \times 10^{-19}\ C$, the atomic mass unit $u = 1.66 \times 10^{-27}\ kg$ and Avogadro's number $N_A = 6.02 \times 10^{23}\ {}^{mol^{-1}}$. The atomic number for α-particles is 2, while for a gold atom it is $Z = 79$. The mass of an α-particle is $4.00u$, while for a gold atom $196.97u$. Care has been taken to use similar symbols for all quantities in the code.

In figure (7), a gold atom with its nucleus at its centre lies on the origin of the coordinate system. As depicted in the figure, the impact parameter b is the vertical distance of the initial

position of the α-particle to the centre of the atom, while the minimum distance of the particle's trajectory to the centre is called d_{min}. The scattering angle θ is the angle between the initial and final velocity vectors. The area spanned by the impact parameter is the scattering cross section. Obviously, a particle following a trajectory within this area, is scattered at an angle is greater or equal to θ. The fraction f turns out to depend on πb^2 as equation (8) suggests [5].

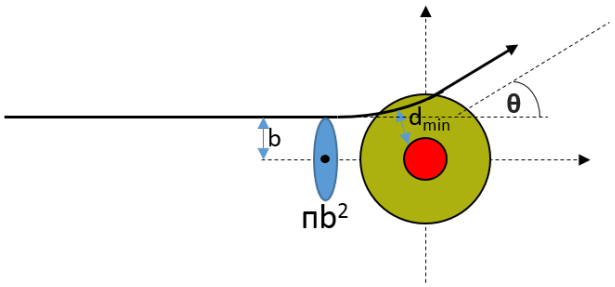


Figure 7: Depiction of the most important parameters for the simulation. The gold atom and its nucleus are the yellow and red circles respectively. The nucleus' size is clearly not to scale.

All projectiles start at initial x-position $x_i = -500$ with 0 vertical velocity. They all have initial kinetic energy $T = 5\ MeV$, thus giving an analytically calculated constant total energy $E_{an} = 8 \times 10^{-13}\ J$. The diameter of a gold atom is $D = 135\ pm$, while the diameter of the nucleus is $D_n \approx 10\ fm$. The modeling in the case of the gold foil assumes separation $r = 288\ pm$ between atoms and thickness of foil $L = 0.08\ \mu m$. [4] The density of the foil is estimated by $\varrho = \frac{1}{2}\frac{14mu}{r^3} \approx 2000\ kg\ m^{-3}$ by assuming that the volume element is a cube which turns out to contain 14 gold atoms each one contributing half its mass to the cube.

The repulsive acceleration exerted on the projectile by the atom is actually $\mathbf{a} = \frac{2kZq_e^2}{mud^3}\mathbf{d}$. The constant $C = \frac{2kZq_e^2}{mu}$ has units of $[m^3 s^{-2}]$. Therefore, by defining an arbitrary unit of measurement for length $a = 1\ pm$ and then using $\tau = \sqrt{\frac{a^3}{C}}$ and $v_a = \frac{a}{\tau}$ for measurement of time and speed respectively, the equations of motion do not need constants.

Apendix B

The code of the simulation follows in the next page.