Rutherford Scattering with Adaptive Runge-Kutta

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An adaptive time-step Runge-Kutta algorithm calculates the trajectory of incident electrons approaching a single gold proton and compares the resulting N *vs.* θ data to Rutherford's scattering formula.

I. INTRODUCTION

Using an adaptive time-step Runge-Kutta algorithm, the trajectory of an incident electron approaching a gold proton can be modeled. The scattering angles can then be tallied and the resulting count can be compared to Rutherford's theoretical results.

In Sec. II the theory behind Rutherford scattering and its application within a Runge-Kutta computational model is discussed. Sec. III discusses the intricacies of the program modeling the above theory. The computational results are described in Sec. IV and we conclude in Sec. V.

II. THEORY

The behavior of particles acting upon one another is a crucial concept in the field of modern physics. The 20th century saw numerous developments in the area, one of the more significant discoveries being made by Ernest Rutherford in 1909 [1, pp. 119]. Rutherford's discoveries, that protons and the majority of atomic mass lay within the nucleus of an atom, were the result of his particle scattering experiments [1, pp. 120]. In this experiment, Rutherford beamed alpha particles through gold foil which consequently scattered them as a result of the gold atom's positively charged nucleus [1, pp. 121]. Consequently, Rutherford derived an equation relating the number of particles hitting the detector, N, to the scattering angle, θ:

$$N = \frac{(ke^2)^2 Z^2 N_i n A}{4R^2 (KE)^2 sin^4(\frac{\theta}{2})} \tag{1}$$

where k is Coulomb's constant, e is the charge of an electron, Z is the atomic number of gold, N it the "number of nuclei per unit area of foil," n is the number of incident particles, A is the "area of the detector," KE is the kinetic energy of the incident particle, and θ is the scattering angle [1, pp. 122].

Rutherford's scattering equation can be measured computationally by calculating the scattering angle and tallying the number of detector hits for each given value of θ. In order to calculate the scattering angle, Coulomb's law can be used:

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

where k is Coulomb's constant, q_1 and q_2 are the charges interacting, and r is the distance between the two charges [2, pp. 7].

Given that Coulomb's law is the force between two charged particles, the trajectory of one particle can be easily computed using a fourth order Runge-Kutta algorithm based on Newton's Second Law. The basic fourth order Runge-Kutta algorithm can be written as:

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k4) \tag{3}$$

where k_2 depends on k_1, k_3 on k_2, and k_4 on k_3 [3, pp. 369]. By combining the Runge-Kutta algorithm with Newton's Second Law utilizing Coulomb's law for the force, Rutherford's scattering angle formula can be observed computationally.

III. COMPUTATIONAL EXPLANATION

In general, **rutherford.cpp** begins by asking for numerous variables required for the various processes to run. The gold proton is considered to reside at the origin, the x-axis running from left to right and the y-axis running from bottom to top. The incident particle is given an initial x_0, y_0, x_{v0}, and y_{v0}. The distance from the target particle to the detector is also recorded. Two time steps are required, one large and one small, that will alternate depending on how close the incident particle is from the target particle. Finally, a number of incident particles is specified which are released between two y_{range} values either randomly or in an evenly dispersed pattern.

A trajectory is calculated for each initial y_0 either chosen randomly or evenly spaced between two y_{range} values. The trajectory uses a modified version of the fourth order Runge-Kutta algorithm to use a smaller time step when the incident particle is close to the target particle. The Runge-Kutta function uses a custom derivative function that computes Coulomb's law in a modified system of units:

$$a_x = \beta\frac{x}{r^3}, a_y = \beta\frac{y}{r^3} \tag{4}$$

where r is the distance between the two particles and:

$$\beta = \frac{-197\alpha e^2 Z}{m} \tag{5}$$

After the Runge-Kutta algorithm completes for each y_0, the scattering angle is calculated using the following

equation:

$$\theta_{scattering} = \arctan(\frac{y}{x}) \times \frac{180}{\pi} \tag{6}$$

Where y is the vertical distance between the target particle and point of detection and x is the distance between the target particle and the detector.

The count is then recorded by first normalizing θ and incrementing its value within an array. The array is then iterated to tally up the number of particles hitting the detector for a given θ. A theoretical value is calculated using θ and Equation 1. The resulting plot of $\theta_{computational}$ *vs. N* is graphed along with $\theta_{theoretical}$ *vs. N*.

To compute the above theory, an adaptive form of Runge-Kutta needed to be created. The traditional fourth order Runge-Kutta algorithm depends on a fixed time step, which can be decreased for more accurate results at the expense of time or increased for quick computations at the expense of accuracy. To counteract this issue, a custom algorithm was developed that changes the time step depending on the distance between the incident particle and the target particle. If the approaching particle is within some user-defined x radius of the target particle after the current Runge-Kutta step finishes, the adaptive time step algorithm begins to function. A temporary time step is created to bring the particle as close to the radius as possible without entering it, and the Runge-Kutta step is rerun. After this transitionary step, the smaller time step is adopted until the particle is outside the radius of the target particle where it finally reverts to the original, larger time step. This adaptive time step model essentially allows for the particle to approach the target at a relatively fast rate, favoring time over accuracy until it is close to the target particle where it then favors accuracy over time. Since the scattering angle is defined heavily by the computations occurring close to the particle (where the force between the charges is greatest), the smaller time step results in more accurate scattering angles.

The units used in the computational work were derived to be reasonable despite convention. For instance, all distances are measured in nm as opposed to m. Coulomb's law includes a constant k which, given our system of units, needed to be changed accordingly. As a result, the following was derived:

$$F = \frac{kq^2}{r^2} = \frac{ke^2}{r^2} = \frac{1}{r^2}\frac{e^2}{4\pi\epsilon_0} = \frac{1}{r^2}\alpha\bar{h}c \tag{7}$$

Where $\bar{h}c$ is a constant equal to 197 and α, the fine structure constant, can be written as:

$$\alpha = \frac{e^2}{4\pi\epsilon_0\bar{h}c} \tag{8}$$

IV. RESULTS

The results of the trajectory utilizing an adaptive time step are favorable. When the incident particle is within some threshold of the target particle, the smaller time step is used. Once the incident particle is then outside this threshold, the larger time step is reverted. Consequently, the most accurate results occur closest to the particle. As seen in FIG. 1, the trajectory of the particle is determined when the two particles are closest together. Since the smaller time step is used at this point, the resulting scattering angle is more accurate.

The behavior of the incident particle is modeled accurately by FIG. 1. Between $-4000 < x < 0$, the force on the electron due to the proton is not large enough to make a difference in the electron's trajectory. Once the electron is within a threshold of the proton, in this figure a threshold of $100nm$, the smaller time step is uti-

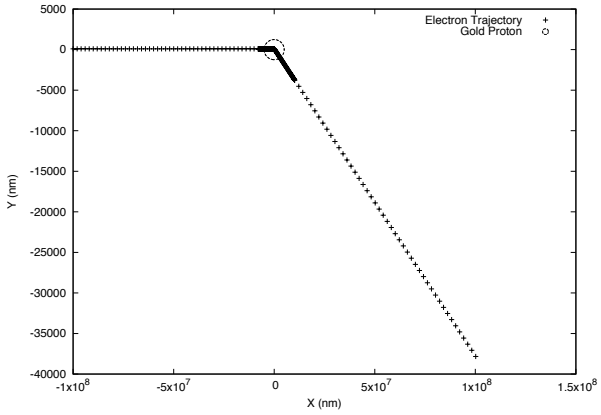

FIG. 1: The trajectory of an incident electron approaching a gold proton.

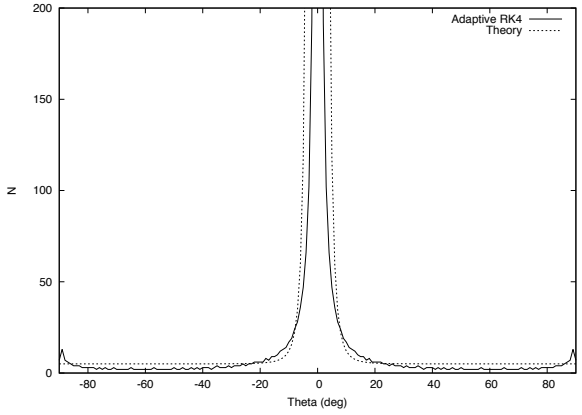

FIG. 2: A graph of Theta vs. N where the theoretical value is shifted up to account for the error in the computational result.

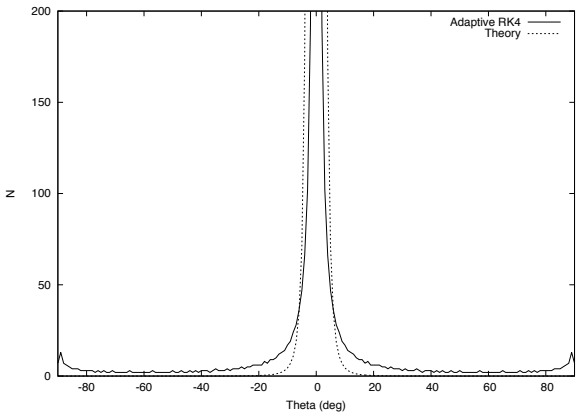

FIG. 3: A graph of Theta vs. N showing the discrepancies between theory and computational results.

lized and more accurate descriptions of the motion are recorded. The particle is then scattered in the negative y direction as it started above the proton and is being attracted down by it. The larger time step is then used once the force is negligible, as the particle will continue more or less in a straight line after its initial deflection. Finally, the electron hits the detector and the incident angle can be calculated with its final y position and distance from the proton to the detector. To be clear, the circle representing the gold proton is not an indication of the proton's radius, but is merely a marker to describe where the target particle is located.

It's worth noting how important initial conditions are when running these trials. For instance, the starting conditions for the referenced figure are:

$x_{detector} = 100000000\ nm$

$dt_{large} = 2000$

$dt_{small} = 100$

$x_0 = -100000000\ nm$

$y_0 = 100.0\ nm$

$v_{x0} = 1000\ \frac{nm}{s}$

If the incident particle's velocity is not great enough, it will not have sufficient momentum to overcome the target particle. This could be negated by increasing the mass of the incident particle, however since we are using a custom system of units, it remains 1 throughout all trials. The distance between the target particle and the detector is equally important. If this distance is too small, the incident particle experiences incorrect results when close to the target, often scattering at a nonsensical value or bouncing backwards. Consequently, the input values must be chosen deliberately for accurate results.

The results of the Rutherford scattering calculations are interesting and are highly dependent upon initial conditions.

It's worth noting that between the two max N values on the computational graphs, a value of zero N is measured for θ = zero. Rutherford's theory says that this area should reach infinity, but given the limitations of the code, infinity is recorded as zero. Consequently, this seemingly random discrepancy between the two adjacent maxima can be seen as the area where calculations are impossible to obtain without more accurate methods/equipment.

When comparing the theoretical to computational result, a clear difference can be seen between the two plots. This difference appears almost functionally different, as the computational result appears to have a different dependence on θ than Rutherford's formula. Regardless, there are still similarities between the two plots. For instance, both plots show that when θ is close to zero, the number of counts tends towards infinity. As θ increases or decreases, the number of counts begins to symmetrically decrease. This is in line with theory, as the smaller the scattering angle, the larger the number of scattered incident particles. Inversely, the larger the scattering angle the smaller the number of particles striking the detector. The salient difference, once again, is the rate at which these occur.

There are many possibilities as to why this rate is inconsistent. FIG. 2 shows the relation between θ and N when the detector is close to the proton. Here the theory seems relatively accurate compared to the computational results. In FIG. 3, however, there is a much clearer distinction. The theoretical value seems like it could have a functional difference than the computational result, which can be explained in a few different ways. One potential reason is that in this simulation, there is only one proton that the incident particle approaches. Consequently, the electron might not have the same trajectory as Rutherford theorized as the gold foil in his example had a plethora of protons. The cumulative force of all these protons on the incident particle would therefore alter the scattering angle and resulting N value. Another possibility is the omission of A in Eq. 1. This value is technically unknown computationally, but can be approximated to match the theory. Using the following initial conditions:

$x_{detector} = 100000000\ nm$

$dt_{large} = 100$

$dt_{small} = 0.001$

$x_0 = -100000000\ nm$

$-20 < y_0 < 20\ nm$

$v_{x0} = 1000\ \frac{nm}{s}$

$N_i = 2000$

$r_{threshold} = 100\ nm$

and an A value of 10^{19}, a slightly smaller difference between the theoretical results and computational results can be achieved. With this value of A, the curve approaching ∞ is slightly similar if the theoretical results were shifted up by 5 counts of N to match the computational results. This shift could almost be thought of as an error threshold in the computational results. This value of A, however, appears to depend on θ in some regard but cannot be generally determined without further testing.

V. CONCLUSION

Using an adaptive time step model of Runge-Kutta, an approximation of Rutherford scattering can be achieved. The trajectory of incident electrons approaching a gold proton can be calculated with a greater accuracy when using the adaptive time step. The resulting θ values can then be determined and tallied, eventually being compared to the theoretical result given by Eq. 1.

The accuracy of this approximation depends on numerous factors. The initial starting conditions **must** be chosen carefully and within physical limitations in order to effectively compare the computational results to the theoretical results. Similarly, greater precision should be utilized when tallying up N for each θ, an issue that could be improved by using a different counting system. The program could be improved by including more target particles placed at randomly dispersed locations, ideally allowing a more accurate result of θ *vs.* N to be calculated and subsequently compared to theory.

Regardless, the above method shows the essential point of Rutherford's experiment: particles are scattered at a much greater degree when closer to an atom's nucleus, disproving earlier atomic models by suggesting the atom actually consisted of a positive nucleus surrounded by orbiting electrons.

[1] R. Serway, C. Moses, and C. Moyer, *Modern Physics* (Brooks Cole, 2004), 3rd ed., ISBN 0534493394.

[2] E. Purcell and D. Morin, *Electricity and Magnetism* (Cambridge University Press, 2014), 3rd ed.

[3] D. Zill, *A First Course in Differential Equations with Modeling Applications* (Brooks/Cole, 2013), 3rd ed.