Classical Collapse of Bohr Atom

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In this work, we will compare two integration algorithms, the Runge-Kutta 4 and the Velocity Verlet algorithms, and use them to describe two-body orbital motion and, most importantly, to simulate Bohr Hydrogen atom and show its theoretical collapse. The successful simulation allows us to validate the unphysicality of this collapse.

I. INTRODUCTION

In 1913, Niels Bohr, a Danish physicist, modified Rutherford's atomic model due to the 1911 theory incompleteness. Indeed, despite of proving the presence of mostly vaccuum as well as a positively charged nucleus, the New Zealander scientist was unable to explain the orbital motion of the negatively charged electron around this nucleus. Therefore, Bohr realized that such model would need to rely on quantum mechanics rather than simply classical physics.

Bohr postulated the existence of energy levels, the presence of electrons at specific energy levels, and the possibility of them transitioning from one to another by absorbing or emitting energy. However, his model included two major drawbacks: first, it was only accurate for the configuration of Hydrogen. It could not predict the behavior of heavier atoms. Second, as moving electrons emit energy, they should collapse into the nucleus.

This work will focus on mathematically explaining and simulating this collapse of Bohr atom by comparing the two different types of algorithms we will study.

In Sec. II we will introduce and derive the Velocity Verlet Algorithm. In order to do so, we will briefly discuss the basic Verlet algorithm. Following that, in Sec. III we will compare the two types of algorithms we used, the Runge-Kutta 4 and the Velocity Verlet, for simple orbital, circular motion. In Sec. IV we will dive into Bohr atom. We will derive Larmor's Formula and use it as the electron's change in radiation energy, allowing us to find the acceleration, velocity, and position expressions describing the orbital path. Additionally, we will analytically find the theoretical time of the collapse. Our results for our Bohr atom simulation will be described in Sec. V and we will conclude in Sec. VI.

II. INTEGRATION ALGORITHMS

A. Verlet Algorithm

Introduced by the French physicist, Loup Verlet in 1967 and used in molecular dynamics, this algorithm allows more stability than the more elementary Euler Method as well as preserving physical properties of the system. It is, in fact, called *symplectic* as it preserves phase space and time-reversibility.

The Verlet algorithm can be derived by Taylor expanding the position at two different times $r\left(t+\Delta t\right)$ and $r\left(t-\Delta t\right)$ about an arbitrary position $r(t)$. This allows us to find the update in position $r\left(t+\Delta t\right)$ and in velocity $dr(t)/dt$ by respectively adding and subtracting those.

$$\begin{aligned} r(t+\Delta t) &= 2r(t)-r(t+\Delta t) \\ &\quad +\frac{\mathrm{d}^2 r(t)}{\mathrm{d}t^2}\Delta t^2+O(\Delta t^4) \end{aligned} \tag{1}$$

$$\frac{\mathrm{d}r(t)}{\mathrm{d}t} = \frac{r(t+\Delta t)-r(t-\Delta t)}{2\Delta t}+O(\Delta t^2) \tag{2}$$

Some issues with the Verlet algorithm are that because of the velocity being of order of 2, the alogrithm is of order 2, position and velocity are not described at the same step, the acceleration must be dependent on the position, and it is not *self-starting*. It requires a first position value based on the initial condition in order to run. [1] [2] [3]

B. Velocity Verlet Algorithm

Contrarily to what the Verlet algorithm might have implied, in classical mechanics, at any time during a motion, the position and velocity of all particles in the system are known. This is related to the classical predictability of a known force, not respected by the Verlet algorithm.

Therefore, in the 80's, a new, self-starting algorithm, which includes the velocity at each step, is born. This Velocity Verlet algorithm still remains equivalent to its predecessor as it will describe the same predictions.

The Velocity Verlet algorithm can once again be derived by Taylor expanding $r\left(t+\Delta t\right)$ around $r(t)$, but this time, its first and second derivatives will be expanded as well.

$$\begin{aligned} r(t+\Delta t) &= r(t)+\frac{\mathrm{d}r(t)}{\mathrm{d}t}\Delta t+\frac{1}{2}\frac{\mathrm{d}^2 r(t)}{\mathrm{d}t^2}\Delta t^2 \\ &\quad +O(\Delta t^3) \end{aligned} \tag{3}$$

Now, if we consider $\frac{\mathrm{d}r(t)}{\mathrm{d}t}$ as being $v(t)$ and $\frac{\mathrm{d}^2 r(t)}{\mathrm{d}t^2}$ as being $a(t)$, we can expand $v(t+\Delta t)$ around $v(t)$ and $a(t+\Delta t)$ around $a(t)$ and use the latter to rewrite the expansion for the velocity.

$$a(t+\Delta t) \;=\; a(t) + \frac{\mathrm{d}a(t)}{\mathrm{d}t}\Delta t + O(\Delta t^2) \tag{4}$$

$$v(t+\Delta t) \;=\; v(t) + \frac{1}{2}(a(t+\Delta t) + a(t))\Delta t + O(\Delta t^3) \tag{5}$$

This allows us to find the following algorithm:

Given x_n, v_n and a_n

Step 1: $v_{n+1/2} = v_n + \frac{1}{2}a_n\Delta t$

Step 2: $x_{n+1} = x_n + v_{n+1/2}\Delta t$

Step 3: Evaluate a_{n+1}

Step 4: $v_{n+1} = v_{n+1/2} + \frac{1}{2}a_{n+1}\Delta t$

Step 5: Equalize all n quantities to their updates. [1] [2] [3]

III. ALGORITHMS COMPARISON

A. Circular Orbital Motion with Runge-Kutta 4

For the Runge-Kutta 4 Method, we did not alter the algorithm that we already work with previously. We simply reused the same initial conditions with the position being $(1, 0)$ in Cartesian coordinates and the initial velocity being $(0, 2\pi)$.

What we did add is an internal clock which allows us to determine the execution time of our code. In this case, the running time was of 133498 microseconds, corresponding to approximately 0.13 second.

From Fig. 1, we can see that with a time step of 0.01 of a second, after 10 full orbits, and only 0.13 second, we obtain a reasonably accurate circle depicting our orbit. From Fig. 2, we can observe that Law of Conservation of Energy, which should hold in this case, was perfectly respected. E/m is perfectly stable up until the end.

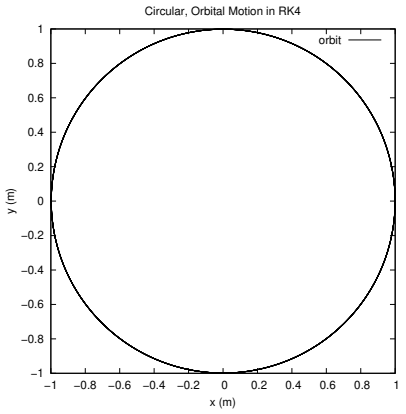

FIG. 1: RK4 orbit of radius 1 around the origin.

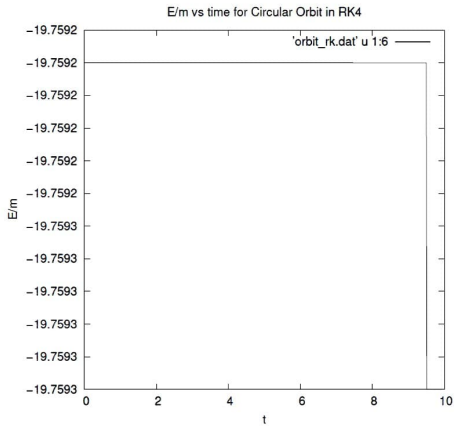

FIG. 2: Change in Energy during RK4 simulation.

B. Circular Orbital Motion in Velocity Verlet

For the Velocity Verlet algorithm, we implemented the expression we derived in Sec. II. We made sure that the acceleration used was the gravitational acceleration obtained from Newton's Law of Gravitation and that it was in terms of vectors. This means that we had an x and y directions as we did in the RK4 algorithm.

However, contrarily to the Runge-Kutta method, which requires intermediary functions to run, the Velocity Verlet algorithm, being a close variant of Euler algorithm, can be directly executed in the main function, at least for simple orbital motion.

Once again, we created a clock which would allow us to determine the execution time of our code. In this case, the running time was of 147539 microseconds, corresponding to approximately 0.15 second.

When simulating with the same amount of orbits, the same time step, and only 0.02 second more, the Velocity Verlet algorithm gives us an equivalently accurate circular orbital motion. From Fig. 3, we can briefly wonder about the stability of the energy of our system as E/m keeps oscillating throughout the motion. Nonetheless, this energy is still enclosed between two values. This can be understood as a conservation of energy.

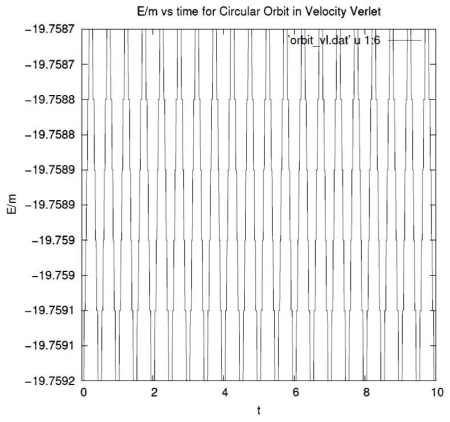

FIG. 3: Change in Energy during Velocity Verlet simulation.

C. Runge-Kutta 4 vs. Velocity Verlet

The RK4 algorithm is the most efficient algorithm.

It requires less resources than the Velocity Verlet as the latter has to determine one more velocity and acceleration in order to complete each iteration. The more steps each iteration requires, the more memory the process needs. Additionally, as we decided to implement this algorithm as an update the the Euler one, it cannot deallocate memory as it goes, using space the machine could benefit from. Those issues result into a net increase in the execution time of our **simple** program. In this case, it represents 15% of margin, a number which cannot be neglected. In more complex and larger scale computations, this will result into irregularities, large errors, or even instabilities.

Lastly, on a macroscopic level, the oscillation of the Velocity Verlet's energy show some conservation. Nevertheless, if now we look at a smaller level, from one time step to the other, the energy is constantly changing. It is never stable, contrarily to the RK4 algorithm which proved it was possible.

We can thus say that at macroscopic and microscopic levels, the Velocity Verlet algorithm is far less efficient that the Runge-Kutta algorithm, but still a good update to Euler algorithm.

IV. BOHR AND THE CLASSICAL LIFETIME OF AN HYDROGEN ATOM

Bohr, in the description of his newly found atomic model, based his theory and explanation on three postulates. [4]

Postulate I: The electron is moving in circular orbit around the nucleus and the electrostatic, attractive force between the positively charged nucleus and the negatively charged electron creates the centripetal force needed for this motion.

$$\frac{mv^2}{r} = \frac{e^2}{4\pi\epsilon_0 r^2} \tag{6}$$

With ϵ_0 being the electrical permittivity of free space.

Postulate II: the electron can only resolve in some selected orbit in which the angular momentum is equal to an integral multiple of the Planck's constant divided by 2π.

$$L = I\omega = mrv = \frac{nh}{2\pi} \tag{7}$$

With n, principal quantum number, being a positive integer and h, Planck's constant.

Postulate III: the electron can jump from one orbit to another by radiating some energy in the form of a photon.

$$E_n - E_p = hv \tag{8}$$

With E_n being the energy at the n^{th} orbit, E_p being the energy at the p^{th} orbit, $n > p$, and v being the frequency of radiation.

As we focus on the classical electron, we will have to use $[Eq.\,(6)]$ as well as determine the radiation energy of this electron. To do so we need Larmor's Formula. [5]

A. Larmor's Formula

As represented in Fig. 4, we start with a charged particle placed at the origin. We call this X. We accelerate it up until a time Δt. We call this X'. We let the particle go for an arbitrary time t. We call it X"

We consider the distance $|XX"|$ as being vt with v being a constant velocity. This implies $\Delta t \ll t$.

We can find the radius of equipotential lines around X and X'. We have $r = ct$ for X' and $r = c(t + \Delta t)$ for X as those were emitted earlier.

Now, if we consider an arbitrary direction for the Electric Field at X, at X", the direction will be the same but the radial vector will be different up until it touches the X' equipotential line. After that moment, the Electric Field changes direction until it reaches the original radial vector, at the X equipotential line. The region of this change in direction is our region of interest.

Based on the geometry of Fig. 4, we can decompose vt into $v_\perp t$ and $v_\parallel t$ and E into $E_\perp$ and $E_\parallel$. Additionally, as v is constant, we can say

$$v = a\Delta t \tag{9}$$

$$v_\perp = a_\perp \Delta t \tag{10}$$

Now as the E's and v's vectors form similar triangles, we can write $E_\perp$ in terms of $E_\parallel$ and then of E by Gauss's Law

$$E_\perp = -\frac{a_\perp r}{c^2} E = -\frac{a_\perp q}{c^2 4\pi\epsilon_0 r} \tag{11}$$

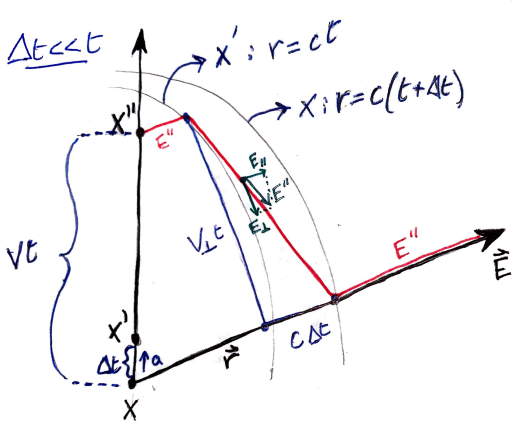

FIG. 4: Geometry of an accelerating, then coasting charged particle and the consequences on its Electric Field.

Without worrying about the direction, this gives us the Electric field, Magnetic Field, and Pointing vector

$$E(r,t) = -\frac{a_\perp q}{c^2 4\pi\epsilon_0 r} \tag{12}$$

$$B(r,t) = \frac{E}{c} = -\frac{a_\perp q}{c^3 4\pi\epsilon_0 r} \tag{13}$$

$$S(r,t) = \frac{E\times B}{\mu_0} = \frac{a^2(\sin\theta)^2 q^2}{c^3(4\pi)^2\epsilon_0 r^2} \tag{14}$$

By determining the spatial average of the pointing vector, we can obtain Larmor's Formula

$$\begin{aligned} P &= \frac{a^2q^2}{c^3(4\pi)^2\epsilon_0}\int_0^{2\pi}\int_0^{\pi}\frac{(\sin\theta)^2}{r^2}r^2\sin\theta d\theta d\phi \\ &= \frac{a^2q^2}{c^3 8\pi\epsilon_0}\frac{4}{3} = \frac{2ka^2q^2}{3c^3} \end{aligned} \tag{15}$$

B. The Differential Equation of the Collapse

With Larmor's Formula, we can now express the loss in energy of the electron. We set k to 1, and use Bohr's first postulate as well as the relationship between radius, charge, and energy. [6] [7] [8]

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -P = -\frac{2e^2}{3c^3}\frac{e^4}{r^4 m_0^2} = -\frac{2r_0^3(m_0c^2)c}{3r^4} \tag{16}$$

With $r_0 = e^2/m_0c^2 = 2.8\times10^{-15}$ m being the classical electron radius. Using the classical expression for Energy

$$E = -\frac{e^2}{r} + \frac{1}{2}m_0v^2 = -\frac{e^2}{2r} = -\frac{r_0(m_0c^2)}{r} \tag{17}$$

Now, we can take the derivative of [$Eq.$ (17)] and equal it to the change we found thanks to Larmor's Formula

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \frac{r_0(m_0c^2)}{2r^2}\frac{\mathrm{d}r}{\mathrm{d}t} = -\frac{2r_0^3(m_0c^2)c}{3r^4} \tag{18}$$

We isolate $\frac{\mathrm{d}r}{\mathrm{d}t}$ and obtain v_r, the radial velocity

$$v_r = -\frac{4}{3}\frac{r_0^2 c}{r^2} \tag{19}$$

As for the azimuthal velocity, v_θ, we have to realize that the velocity present in the centripetal force of Bohr's first postulate is the azimuthal one.

$$v_\theta = r\frac{\mathrm{d}\theta}{\mathrm{d}t} = \sqrt{\frac{e^2}{m_0 r}} = \sqrt{\frac{r_0}{r}}c \tag{20}$$

Thanks to those velocities, we can determine $d\theta/dt$, d^2r/dt^2 and $d^2\theta/dt^2$, essential to find the expressions for the accelerations.

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = \sqrt{\frac{r_0}{r^3}}c \tag{21}$$

$$\frac{\mathrm{d}^2r}{\mathrm{d}t^2} = \frac{8r_0^2}{3r^3}\frac{\mathrm{d}r}{\mathrm{d}t}c = -\frac{32r_0^4}{9r^5}c^2 \tag{22}$$

$$\frac{\mathrm{d}^2\theta}{\mathrm{d}t^2} = -\frac{3}{2}\sqrt{\frac{r_0}{r^5}}\frac{\mathrm{d}r}{\mathrm{d}t}c = 2\sqrt{\frac{r_0}{r}}\frac{r_0^2}{r^4}c^2 \tag{23}$$

Which gives us the following accelerations

$$a_r = \frac{\mathrm{d}^2r}{\mathrm{d}t^2} - r(\frac{\mathrm{d}\theta}{\mathrm{d}t})^2 = -\frac{32r_0^4}{9r^5}c^2 - \frac{r_0}{r^2}c^2 \tag{24}$$

$$a_\theta = 2\frac{\mathrm{d}r}{\mathrm{d}t}\frac{\mathrm{d}\theta}{\mathrm{d}t} + r\frac{\mathrm{d}^2\theta}{\mathrm{d}t^2} = -\frac{8}{3}\sqrt{\frac{r_0}{r}}\frac{r_0^2}{r^3}c^2 \tag{25}$$

Thus now, we know our accelerations and velocities in terms of polar coordinates. This will allow us to create the algorithm to simulate such motion.

Nonetheless, what we were interested in was the time it should take for the electron to fall and collapse. Looking back at the expression we had for the radial velocity,

$$r^2\frac{\mathrm{d}r}{\mathrm{d}t} = 1/3\frac{\mathrm{d}r^3}{\mathrm{d}t} = -\frac{4}{3}r_0^2 c \tag{26}$$

We solve the differential equation with t going between 0 and t, and Bohr's radius a_0 at $t = 0$,

$$r^3 = a_0^3 - 4r_0^2 ct \tag{27}$$

Equaling r to 0 and solving for t,

$$t = \frac{a_0^3}{4r_0^2 c} \tag{28}$$

With $r_0 = 2.8\times10^{-15}$ m and $a_0 = 5.3\times10^{-11}$ m, $t = 1.55\times10^{-11}$ s.

V. RESULTS OF SIMULATION

First of all, from our derivations above, we realized we were working with extremely small numbers: r_0 is in fm, a_0 in 10^{-11} m. Yet, we were also working with very large number as the speed of light c, in the 10^8.

For these reasons, we chose fm for our units of distance, 10^{-23} s, which we called *RVLs*, for our time, allowing us to equal c to 3, radians for angles, and 1 for k.

What our simulations of the collapse showed us was three different stages in the progression of the electron. With our current knowledge of Quantum Physics, none of them are truly physical as an electron would simply not fall in such a fashion. Nevertheless, even if we accept the classical assumption that it would, this would leave us with one physical stage, the fall, and two unphysical ones, close to and beyond the nucleus.

First, the fall itself. In our simulations using both algorithms, in order to reach the nucleus, the classical electron has to go through an enormous amount of circular orbits. This was expected as to derive our differential equation, we assumed not only the electron having a circular path but also, the radial acceleration being much larger than the azimuthal one. In fact, as we increase the radius to reach Bohr's, the orbits started to form one black disk. Fig. 6, Fig. 5.

Paying attention to Fig. 5, we can observe a curious S-shaped pattern close to the origin. This is our first unphysical stage, when the electron goes inside the nucleus. Interestingly enough, in that region, the accelerations keeps changing direction.

The second unphysical stage was also "unmathematical." Indeed, we came to learn that our code needed a time boundary to stop at the origin. Otherwise, it would eventually run for negative radii. This "displacement" seemed random as the direction of its path, its length, as well as the linear relationship between x- and y-coordinates changed when changing the initial conditions. Interestingly however, the orbit would always eventually stop seemingly arbitrarily.

Concerning the time of the collapse of the Bohr atom, we encountered some difficulties with our choice of time step. Indeed, balancing out efficiency and accuracy is no easy task, especially when in this case, we needed both to determine the time of the collapse.

Nonetheless, as we increased the starting radius, progressively reaching Bohr's radius, we realized that using the same time step would be impossible as the radius would ultimately have an order of 10^4 larger than its final stage. We thus drastically increased the time step used. This gave us a time of 2.68×10^{-14} s.

We tried smaller time steps, but our computer would not get anywhere. It would either run forever until shutting down, or give us back emptiness.

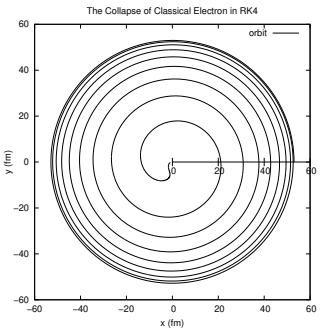

FIG. 5: Collapse of electron from a close distance.

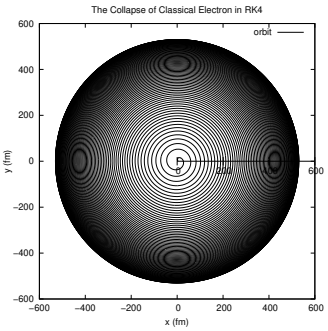

FIG. 6: Collapse of electron from medium range distance.

VI. CONCLUSION

In conclusion, we believe that through this work, we were able to fully explain the new algorithm that we discovered, the Velocity Verlet algorithm, and to apply it to simple computation. We were able to compare this new method to the RK4 one we already knew and critically judge the efficiency and practically of them both.

Additionally, we were able to explain the physics behind the unphysical collapse of a classical electron of circular orbit, as well as derive the necessary functions needed to simulate such a motion.

Lastly, we were able to predict through simulation the path of a classical electron collapsing to a certain degree of accuracy via both algorithm. Nonetheless, this also showed us more unphysical properties than one might think as its motion had three phases.

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