Electron Orbits: in atoms and molecules

Objectives

In this activity you will model the motion of an electron orbiting a single proton and two protons. You'll start with the program you wrote in PHYS 1311, Space Voyage 2. To simplify the model, we'll assume that the two protons remain fixed in position, and only the electron moves. Before doing this activity you should have read Section 13.9 of the *Matter & Interactions 4e* textbook, which discusses the structure of a computational model that includes the Coulomb force and electric field.

After completing this activity you should be able to:

- Write a program to model the motion of three or more objects interacting through the Coulomb force
- By varying initial speed, generate several very different electron trajectories
- Discuss the issue of sensitivity to initial conditions

1 Electron motion around the proton

In Space Voyage: Part 2 you wrote a program to model the behavior of a spacecraft that was initially launched from a location 10 Earth radii to the left of the Earth and traveled to the moon. Starting with this program:

⇒ Replace the gravitational force by the Coulomb force and all masses by charges (except for the momentum)
⇒ The Earth and the Moon are replaced by protons and the spacecraft by an electron
⇒ Initially place proton 1, proton 2, and the electron at $\vec{r}_{P1} =< 0, 0, 0 >$, $\vec{r}_{P2} =< 10.0, 0, 0 >$ Å, and $\vec{r}_e =< -0.529, 0, 0 >$ Å
⇒ Give the electron an initial velocity of $\vec{v}_e =< 0, v_i, 0 >$ to create a circular orbit around P1. You should be able to use Newton's 2nd law to determine this value
⇒ For the while loop you will need to calculate a reasonable time for a complete orbit, a reasonable time step Δt, and a value for the vpython rate function to visualize the orbit.
⇒ Optimize the values of v_i and Δt to get a stable circular orbit. Report these values in your code

Check your work before continuing.

2 Electron motion around two protons

Now consider the orbits around two protons. This situation mimics the H_2^+ diatomic molecular ion.
⇒ Bring the second proton closer to P1 by setting $\vec{r}_{P2} =< 1.052, 0, 0 >$ Å
⇒ Change initial $\vec{r}_e$ and $\vec{v}_e$ until you find a stable elliptical orbit about both protons. Report these values in your code.
⇒ You might also add vector arrows for the electric field at the location of the electron and for its momentum. You'll have to find the best scale factors.

3 Optional: Re-aiming the Camera

If you would like to center the scene better in the window, you can insert the following line just before the loop. This line tells the camera to point at a location midway between the two protons

```
scene.center = (proton1.pos + proton2.pos)/2
```

Check your work before continuing.

4 Exploring Complex Trajectories

⇒ Add a check to stop the program if the electron crashes into a proton. Remember the radius of a proton is about a femtometer. So, is this necessary?
⇒ Find initial speeds that produce the following trajectories. Record each one as a comment in your program:
⇒ An initial speed that yields a "figure-8" orbit that loops around the two protons
⇒ The minimum initial speed that allows the electron to just escape from the proton in Part 1
⇒ The minimum initial speed that allows the electron to just escape from the molecule in Part 2.
⇒ In the last two cases, calculate the additional energy (in eV) that is needed to increase the kinetic energy of the electron from its value for the stable orbits.

Check your work before continuing.

5 Turn in Your Program

⇒ Unless your instructor specifies otherwise, restore your program to use the initial velocity from Part 2.
⇒ Email your final program to me at pstancil@uga.edu. Turn in your answers to the questions posed above within your code or place a written copy into my mailbox, all by Monday Nov. 14, 2022, 11:59pm. One copy per lab group.
