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The Three Body Problem and the Runge-Lenz Equivalent Constant of the Motion

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I. SYNOPSIS

The Runge-Lenz equivalent for the H_2^+ (and the Earth, Moon and Sun) problem is obtained

II. INTRODUCTION

The simplest three body problems of solar interest are the Sun-Earth-Moon system, where the Moon is considered small relative to the Sun and the Earth, and the Earth-Moon-rocket system (see M. C. Gutwiller, Rev. Mod. Phys., 70, 589 (1998) for an up-to-date review of this three body problem.) If we ignore the Sun, and consider the Earth-Moon-rocket system, a three body system, we begin to encounter (even ignoring the Sun) extraordinary difficulties which makes analysis so difficult as to border on the impossible. Certainly, we will not achieve such clean and aesthetic results as we did with the two body Kepler problem.

Three things are moving in this system, the Earth, the Moon, and the rocket. In order of mass, the Earth is the most massive, followed by the Moon and trailed (distantly) by the rocket. The effect of the rocket on either the Earth or the Moon is negligible and we will ignore it. Thus, concentrating on the rocket, we will argue that the rocket travels in the field of forces set up by the Moon and the Earth. It therefore might make sense to place our coordinate system on the center of gravity of the Earth-Moon system (ignoring the rocket) and we will temporarily do this now. Technically, we are not on the center of gravity of the entire system!

We recognize that the entire system, Earth, Moon, and rocket, might be tumbling "about the center of gravity" and to be able to concentrate on what interests us, let us arbitrarily agree to place the Moon on the +z axis, and the Earth on the -z axis of our system, treating the Earth Moon system as a non-rigid two body rotor. From our perspective "on the center of gravity", the Earth and the Moon are sometimes approaching us, sometimes fleeing from us, i.e., oscillating in some strange way against each other. For very short rocket flights, it might be of interest to study the rocket assuming the Earth-Moon distance was fixed. This implies that the rocket moves very much faster than the Earth or the Moon.

Now the Moon is at a place on the $+z$ axis, and the Earth is at another place on the -z axis, and the rocket is located at x,y,z in the same coordinate system. For the purposes of our discussion, the Earth and Moon positions are fixed. Now substitute for Earth, nucleus B, and for the Moon substitute nucleus A, and for the rocket let's substitute an electron. The forces which were gravitational are now Coulombic, but by an irony of nature, the form of these forces is retained. Thus, gravitational or Coulombic, it makes no difference at our level of treatment.

The situation is shown in Figure 1.

Let the charge on nucleus A be called $Z_A e$, where Z_A is the atomic number of nucleus A and e is the magnitude of the elementary electron charge. The charge on nucleus B will then be $Z_B e$, while the charge on the electron will be -e.

If $Z_A = Z_B$ then we are talking about a homonuclear diatomic, while when $Z_A \neq Z_B$ we are talking about a heteronuclear diatomic. For the homonuclear case, when $Z_A = Z_B = 1$ we are talking about ${H_2}^+$ the prototypical 1-electron chemical bonding situtation. H_2^+ and H_2 (neutral) are the kernel problems which shape our thinking about the chemical bond!

Interstellar interest in H_2^+ continues unabated even if chemists tend to ignore it. A hydrogen molecule ($H_2(g)$) can be ionized by cosmic radiation to form H_2^+ which then can collide with another hydrogen molecule to cause the reaction

$$H_2^+ + H_2 \rightarrow H_3^+ + H$$

This H_3^+ is very reactive, and can transfer a proton to a wandering oxygen atom, giving

$$H_3^+ + O \rightarrow OH^+ + H_2$$

Next, the OH^+ ion can steal a H atom from H_2 to give

$$OH^+ + H_2 \rightarrow H_2O^+ + H$$

and so it goes (Physics World, October 1996, page 39).

Because the internuclear distance in diatomics is a measureable, we prefer to couch our discussion in terms of that variable, so we define the positions of the two nuclei to be +R/2 and -R/2 on the z axis, as shown in Figure 2.

This means that we abandon the center of gravity concept entirely now. In this final coordinate system, we will study the motion of the electron in the field of the two fixed nuclei. This is truly a restricted three body problem, isn't it? We abandon the idea of using the center of mass and writing the total energy in terms of the mass motion

$$m_{total} v_{c.of.m}^2$$

and terms in vibration, rotation, etc., in the center of mass system.

It is very convenient to introduce two distance which appear relevant. These are called r_A and r_B the distances from the electron to nucleus A and B respectively.

From this drawing, it is clear that the magnitude of these two distances are

$$r_A = \sqrt{x^2+y^2+\left(z-\frac{R}{2}\right)^2}\ ;\ r_B = \sqrt{x^2+y^2+\left(z+\frac{R}{2}\right)^2} \tag{2.1}$$

(using the Pythagorous Theorem) and we see that the forces on the electron due to the nuclei lie in these two directions (see Figure 3).

These forces are

$$\vec{F}_A = -Z_A e^2 \frac{(\vec{r}-\vec{R}/2)}{{r_A}^3}$$

$$\vec{F}_B = -Z_B e^2 \frac{(\vec{r}+\vec{R}/2)}{{r_B}^3}$$

where $\vec{R}/2$ points directly at nucleus A. If you check the units, you will see this is inverse square, just hidden under flowers.

How wonderful it would have been if, relative to the Kepler problem, the problem under study here reduced to two nuclei at the two foci of the ellipse, with the path still elliptical. Where before we had the Sun (nucleus) at the focus of an ellipse, it would have been pleasing to just stick the other nucleus at the other focus and preserve the orbit. Such is not to be. In fact, we can not, even under the super restrictive conditions used here, write down the formula for the path of the electron (classical) as a function of either time, or angle. We are at the end of the analytical mathematical road (for us).

Why? The easiest way to see what is wrong is to ask, is the angular momentum of the electron (rocket) constant? That is, what is the time derivative of $\vec{L}$?

$$\frac{d\vec{L}}{dt} = \frac{d[\vec{r}\times\vec{p}]}{dt} = \vec{r}\times\vec{F}$$

which equals

$$\frac{d\vec{L}}{dt} = \vec{r}\times(-Z_A e^2(\vec{r}-\vec{R}/2)/r_A^3)+\vec{r}\times(-Z_B e^2(\vec{r}+\vec{R}/2)/r_B^3) \tag{2.2}$$

since $\vec{F} = \vec{F_A} + \vec{F_B}$. Looking at the numerator of the first term in this expression we have

$$\vec{r}\times(\vec{r}-\vec{R}/2) = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ x & y & \left(z-\frac{R}{2}\right) \end{vmatrix}$$

which can be expanded to be:

$$= \hat{i}\left(y\left(z-\frac{R}{2}\right)-yz)+\hat{j}(xz-x\left(z-\frac{R}{2}\right)\right)+\hat{k}(xy-yx)$$

which equals

$$= \hat{i}\left(-y\frac{R}{2}\right)+\hat{j}\left(+x\frac{R}{2}\right)+zero\ \hat{k} \tag{2.3}$$

We get a similar expression for the other (the plus) term, i.e.,

$$\vec{r}\times(\vec{r}+\vec{R}/2) = \hat{i}\left(y\frac{R}{2}\right)+\hat{j}\left(-x\frac{R}{2}\right) \tag{2.4}$$

Therefore, for the time derivative of $\vec{L}$ (substituting Equations 2.3 and 2.4 into Equation 2.2)we obtain

$$\frac{d\vec{L}}{dt} = -(Z_A e^2/r_A^3)\left[\hat{i}\left(-y\frac{R}{2}\right)+\hat{j}\left(x\frac{R}{2}\right)\right] - \frac{Z_B e^2}{r_B^3}\left[\hat{i}\left(y\frac{R}{2}\right)+\hat{j}\left(-x\frac{R}{2}\right)\right]$$

Written in components we have

$$\frac{d\vec{L}}{dt} = e^2\left(\hat{i}y\left[\frac{Z_A}{r_A^3}-\frac{Z_B}{r_B^3}\right]+\hat{j}x\left[-\frac{Z_A}{r_A^3}+\frac{Z_B}{r_B^3}\right]\right)$$

which is, sob, sob, not zero! $\vec{L}$ is not a constant of the motion.

III. ONE CONSTANT OF THE MOTION FOR ANGULAR MOMENTUM

Only the z component (the component in the $\hat{k}$ direction) of the time derivative of $\vec{L}$ vanishes, and therefore, only the component of $\vec{L}$ along the $\hat{k}$ direction is constant in time. Where before we had three constants in $\vec{L}$ (in the Kepler problem), here we have only one constant, the z-component of $\vec{L}$, called usually L_z . The fact that $\vec{L}$ is not constant does not mean however that there are only two constants of the motion for this problem, E and L_z.

In fact, there is another (H. A. Erikson and E. L. Hill, Phys. Rev., 75,29(1949)). To find it, we begin by defining the angular momentum as measured about nucleus A (and later we will do the same about nucleus B). If we are sitting on nucleus A, and we wished to define the angular momentum, referring to shows how to define $\vec{L}_A$ e.g.,

$$\vec{L}_A \equiv \vec{r}_A \times \vec{p}$$

where $\vec{r}_A$ is the vector from nucleus A to the electron. Similarly, we have

$$\vec{L}_B = \vec{r}_B \otimes \vec{p}$$

$$\vec{r}_A + \frac{\vec{R}}{2} = \vec{r}\ ;\ \vec{r}_B - \frac{\vec{R}}{2} = \vec{r}$$

In components (comparing to Equation 2.1), this means that

$$\vec{r}_A = x\hat{i} + y\hat{j} + \left(z - \frac{R}{2}\right)\hat{k}$$

$$\vec{r}_B = x\hat{i} + y\hat{j} + \left(z + \frac{R}{2}\right)\hat{k}$$

If we restrict ourselves to motion in the y-z plane (set x=0, and since the forces then would have no x component, and hence no x-acceleration, x would remain zero!) the problem at hand simplifies a bit. Now we can expand the two defined angular momemta into components. We obtain:

$$\vec{r}_A \otimes \vec{p} = \vec{L}_A = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 0 & y & (z - \frac{R}{2}) \\ 0 & p_y & p_z \end{vmatrix}$$

which means that there is only an $\hat{i}$ component of this angular momentum, i.e.,

$$\vec{L}_A = \hat{i}\left[y p_z - \left(z - \frac{R}{2}\right)p_y\right]$$

and, analogously,

$$\vec{L}_B = \hat{i}\left[y p_z - \left(z + \frac{R}{2}\right)p_y\right]$$

Notice that, rearranging, we have

$$\vec{L}_A = \hat{i}\left(\vec{L}_x + \frac{R}{2}p_y\right) \tag{3.1}$$

$$\vec{L}_B = \hat{i}\left(\vec{L}_x - \frac{R}{2}p_y\right) \tag{3.2}$$

and that $\vec{L}_A$ and $\vec{L}_B$ (as defined) only have components in the x direction, and that these components are themselves related to L_x , the component of angular momentum for the electon when measured from the origin itself.

The constant of the motion we seek is related to $\vec{L}_A \cdot \vec{L}_B$, where

$$\vec{L}_A \cdot \vec{L}_B = L_x^2 - \left(\frac{R}{2}\right)^2 p_y^2$$

where we have explicitly used Equations 3.1and 3.2.

What is the time behaviour of $\vec{L}_A \cdot \vec{L}_B$? To answer this question we take the time derivative, i.e.,

$$\frac{d\left(L_A \cdot L_B\right)}{dt} = \underbrace{2L_x\frac{dL_x}{dt}}_{1} - \underbrace{2\left(\frac{R}{2}\right)^2 p_y\frac{dp_y}{dt}}_{2} \tag{3.3}$$

Both of these terms admit of simple substitutions. Take the first term (1 above). Starting with

$$\frac{dL_x}{dt} = \frac{d[yp_z - zp_y]}{dt} = \frac{dy}{dt}p_z + y\frac{dp_z}{dt} - \frac{dz}{dt}p_y - z\frac{dp_y}{dt}$$

we obtain

$$\frac{dL_x}{dt} = p_y\frac{p_z}{m} + y\dot{p}_z - p_z\frac{p_y}{m} - z\dot{p}_y = yF_z - zF_y \tag{3.4}$$

where F_z and F_y are the z and y components of the force on the electron. But that force was

$$\vec{F} = \vec{F}_A + \vec{F}_B = -Z_A e^2\frac{(\vec{r} - \vec{R}/2)}{{r_A}^3} - Z_B e^2\frac{(\vec{r} + \vec{R}/2)}{{r_B}^3}$$

Since the term in Ze^2 will appear frequently, we will substitute Q for it. Then, from Equation 3.4 we have

$$\frac{dL_x}{dt} = yF_z - zF_y = y\left[-Q_A\frac{(z - \frac{R}{2})}{{r_A}^3} - Q_B\frac{(\frac{R}{2} + z)}{{r_B}^3}\right] - z\left[-Q_A\frac{y}{{r_A}^3} - Q_B\frac{y}{{r_B}^3}\right]$$

This means that, returning to term 1 in Equation 3.3,

$$L_x\frac{dL_x}{dt} = (yp_z - zp_y)\left(-y\left[-Q_A\frac{(z - \frac{R}{2})}{{r_A}^3} - Q_B\frac{(z + \frac{R}{2})}{{r_B}^3}\right] - z\left[-Q_A\frac{y}{{r_A}^3} - Q_B\frac{y}{{r_B}^3}\right]\right)$$

The last two terms cancel the leading parts of the first two terms, leading to

$$L_x \frac{dL_x}{dt} = L_x \frac{R}{2} y \left[\frac{Q_A}{r_A^3} - \frac{Q_B}{{r_B}^3} \right]$$

Since Equation 3.3 is only partially addressed so far, we have (after adding the second (term 2) force)

$$\frac{d\vec{L}_A \cdot \vec{L}_B}{dt} = 2L_x \frac{R}{2} y \left[\frac{Q_A}{r_A^3} - \frac{Q_B}{{r_B}^3} \right] - 2\left(\frac{R}{2}\right)^2 p_y \left[-Q_A \frac{y}{{r_A}^3} - Q_B \frac{y}{{r_B}^3} \right]$$

which becomes

$$= 2L_x \frac{R}{2} y \left[\frac{Q_A}{{r_A}^3} - \frac{Q_B}{{r_B}^3} \right] - 2\left(\frac{R}{2}\right)^2 p_y \left[-Q_A \frac{y}{{r_K}^3} - Q_B \frac{y}{{r_B}^3} \right]$$

$$= 2L_x \frac{R}{2} y \left[\frac{Q_A}{{r_A}^3} - \frac{Q_B}{{r_B}^3} \right] - 2\left(\frac{R}{2}\right)^2 p_y \left[-Q_A \frac{y}{{r_A}^3} - Q_B \frac{y}{{r_B}^3} \right] \tag{3.5}$$

You were hoping for more? Nature isn't kind.

IV. CONTINUING

We now investigate a special vector pair defined through special vectors:

$$\frac{\frac{\vec{R}}{2} \cdot \vec{r}_A}{r_A} \quad ; \quad \frac{\frac{\vec{R}}{2} \cdot \vec{r}_B}{r_B}$$

We ask what are the time derivatives of these two special vectors? Taking the time derivatives explicitly we have

$$\frac{d\left[\frac{\vec{R}}{2} \cdot \frac{\vec{r}_A}{r_A}\right]}{dt} = \frac{\vec{R}}{2} \cdot \frac{d\left[\frac{\vec{r} - \frac{\vec{R}}{2}}{r_A}\right]}{dt} \tag{4.1}$$

where

$$\frac{(\vec{r} - \frac{\vec{R}}{2})}{r_A} = \frac{(0\hat{\imath} + y\hat{\jmath} + (z - \frac{R}{2})\hat{k})}{\sqrt{(0^2 + y^2 + (z - \frac{R}{2})^2)}}$$

(remember, $\vec{R}$ points in the z-direction here, we restricted the motion to the y-z plane, remember?) so that

$$\frac{d\left[\frac{\vec{R}}{2} \cdot \frac{\vec{r_A}}{r_A}\right]}{dt} = \frac{\vec{R}}{2} \cdot \left(\frac{\dot{0}}{r_A} + \frac{\dot{y}}{r_A} + \frac{\dot{z}}{r_A} \right) + \left[\frac{\vec{R}}{2} \cdot \left(y\hat{\jmath} + \left(z - \frac{R}{2}\right)\hat{k} \right) \right] \frac{d\left\{{r_A}^{-1}\right\}}{dt}$$

so

$$\frac{R}{2}\frac{p_z}{mr_A} + \frac{\vec{R}}{2} \cdot (y\hat{\jmath} + (z - \frac{R}{2})\hat{k}) \frac{d\left[y^2 + (z - \frac{R}{2})^2\right]^{-1/2}}{dt}$$

Since $\vec{R}$ is parallel to $\hat{k}$ (i.e., $\frac{\vec{R}}{2} = \frac{R}{2}\hat{k}$ and $p_z = m\dot{z}$ and, finally, $\vec{R} \cdot \dot{\hat{\jmath}} = 0$), we obtain

$$= \frac{R}{2}\frac{p_z}{mr_A} + \frac{R}{2}\left(z - \frac{R}{2}\right) \frac{d\left[y^2 + \left(z - \frac{R}{2}\right)^2\right]^{-1/2}}{dt}$$

$$= \frac{R}{2}\frac{p_z}{mr_A} + \frac{R}{2}\left(z - \frac{R}{2}\right) \left(-\frac{1}{2}\left(y^2 + \left(z - \frac{R}{2}\right)^2 \right)^{-3/2} \right) 2\left(y\dot{y} + \left(z - \frac{R}{2}\right)\dot{z} \right)$$

$$= \frac{R}{2}\frac{p_z}{mr_A} - \frac{R}{2}\left(z - \frac{R}{2}\right) \frac{\left(y\dot{y} + \left(z - \frac{R}{2}\right)\dot{z}\right)}{r_A^3}$$

$$= \frac{R}{2}\frac{p_z}{mr_A} - \frac{R}{2}\left(z - \frac{R}{2}\right)\frac{\left(yp_y + (z - \frac{R}{2})p_z\right)}{m{r_A}^3} \tag{4.2}$$

We obtain a similar result for B, i.e.,

$$\frac{d[\frac{\vec{R}}{2}\cdot\frac{\vec{r}_B}{r}]}{dt} = \frac{\frac{R}{2}p_z}{mr_B} - \frac{R}{2}\left(z + \frac{R}{2}\right)\left(\frac{yp_y + \left(z + \frac{R}{2}\right)p_z}{m{r_B}^3}\right)$$

Now the "fun" begins.

$$\frac{\frac{R}{2}p_z}{mr_A} = \frac{\frac{R}{2}{r_A}^2 p_z}{m{r_A}^3}$$

having multiplied top and bottom by the same item (p^2/r^2).

$$\frac{\frac{R}{2}p_z}{mr_A} = \frac{\frac{R}{2}(0^2 + y^2 + (z - \frac{R}{2})^2)p_z}{m{r_A}^3} \tag{4.3}$$

(in the y-z plane, i.e. x=0) we have substituting, into Equation 4.1 and using Equations 4.2 and 4.3,

$$\frac{d[\frac{\vec{R}}{2}\cdot\frac{\vec{r_A}}{r_A}]}{dt} = \frac{R}{2}\frac{y^2p_z}{m{r_A}^3} + \frac{R}{2}\frac{(z-\frac{R}{2})^2p_z}{m{r_A}^3} -$$

$$\frac{R}{2}\frac{y(z-\frac{R}{2})p_y}{m{r_A}^3} - \frac{R}{2}\frac{(z-\frac{R}{2})^2p_z}{m{r_A}^3}$$

so

$$\frac{d\left[\frac{\vec{R}}{2}\cdot\frac{\vec{r}_A}{r_A}\right]}{dt} = \frac{R}{2}\frac{y\left(yp_z - (z-\frac{R}{2})p_y\right)}{m{r_A}^3}$$

$$\frac{d\left[\frac{\vec{R}}{2}\cdot\frac{\vec{r}_A}{r_A}\right]}{dt} = \frac{R}{2}\frac{yL_x}{m{r_A}^3} + \left(\frac{R}{2}\right)^2\frac{yp_y}{m{r_A}^3}$$

Notice the similarity to the "A" terms in the expression for the time derivative of $\vec{L}_A\cdot\vec{L}_B$ (Equation 3.5) which was

$$\frac{d[\vec{L_A}\cdot\vec{L_B}]}{dt} = 2\,L_x\frac{R}{2}y\left[\underbrace{\frac{Q_A}{{r_A}^3}}\; - \frac{Q_B}{{r_B}^3}\right] - 2\underbrace{\left(\frac{R}{2}\right)^2 p_y\left[-Q_A\frac{y}{{r_A}^3}\right.}\; \left. -Q_B\frac{y}{r_B^3}\right]$$

We conclude that

$$\frac{1}{2}\frac{d[\vec{L_A}\cdot\vec{L_B}]}{dt} - \left[\frac{Q_A}{m}\frac{d[\frac{\vec{R}}{2}\cdot\vec{r_A}/r_A]}{dt}\right] - \left[\frac{Q_B}{m}\frac{d[\frac{\vec{R}}{2}\cdot\vec{r_B}/r_B]}{dt}\right] = 0$$

so that

$$\frac{d\left(\vec{L_A}\cdot\vec{L_B} - \frac{Q_A}{m}[\vec{R}\cdot\frac{\vec{r_A}}{r_A}] - \frac{Q_B}{m}[\vec{R}\cdot\frac{\vec{r_B}}{r_B}]\right)}{dt} = 0$$

Therefore

$$\vec{L}_A\cdot\vec{L}_B - \frac{Q_A}{m}\left[\frac{\vec{R}\cdot\vec{r}_A}{r_A}\right] - \frac{Q_B}{m}\left[\frac{\vec{R}\cdot\vec{r}_B}{r_B}\right]$$

(where $Q_i = Z_ie^2$) is a constant of the motion. QED

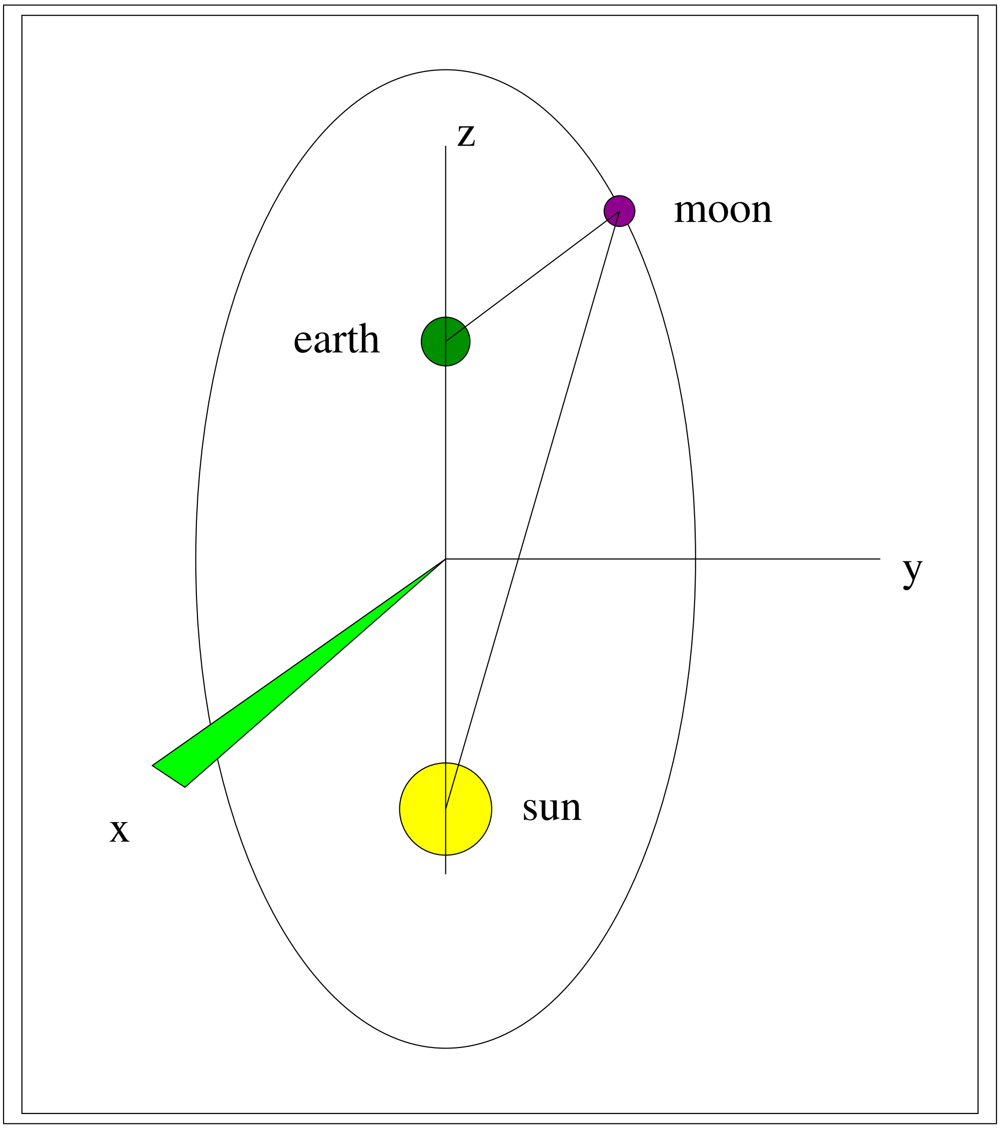

FIG. 1: The Sun-Earth-Moon the Earth-Moon-Rocket and the A-B-electron systems in the coordinate system in which the z-axis connects the two heavy bodies. The two heavy particles are located on the z-axis at +R/2 and -R/2.

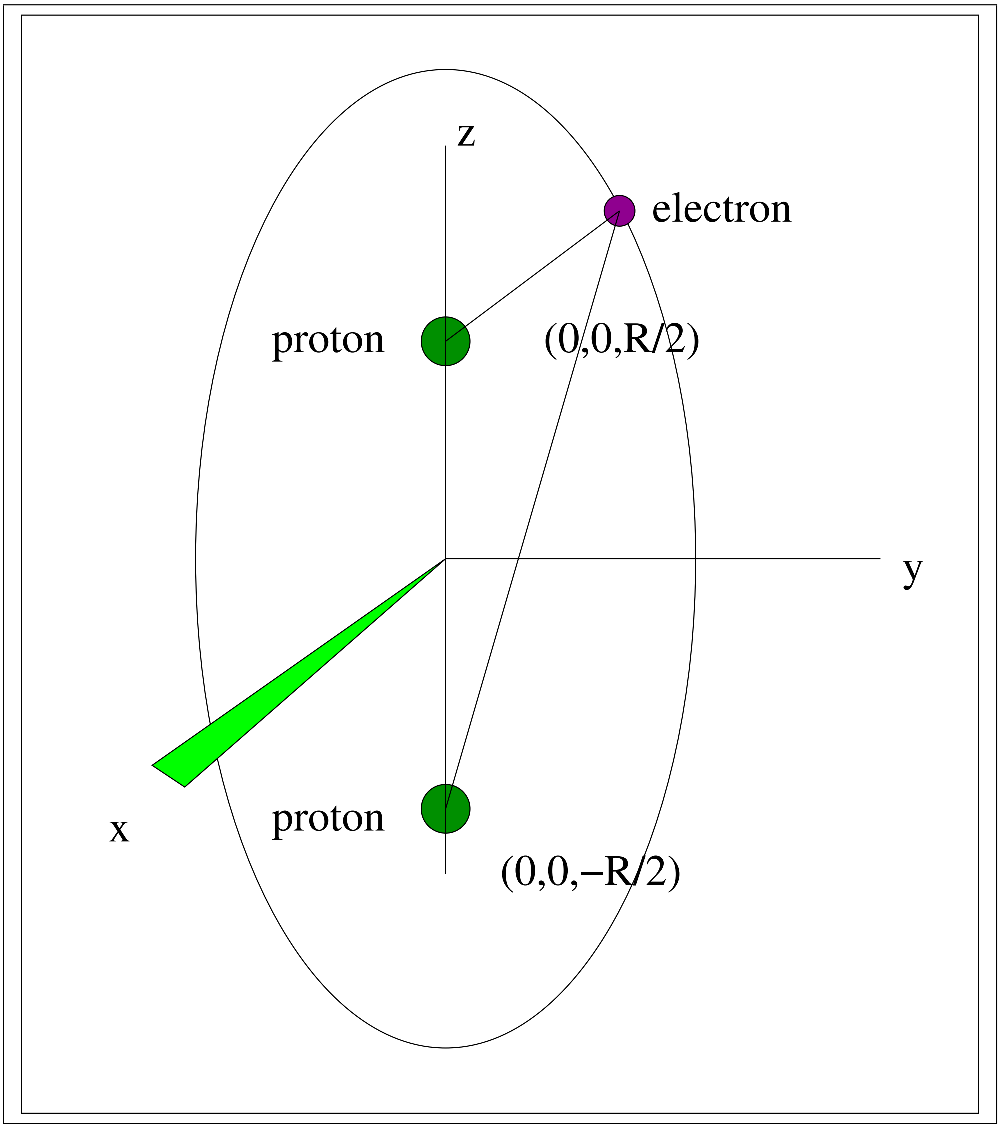

FIG. 2: The coordinate system for H_2^+

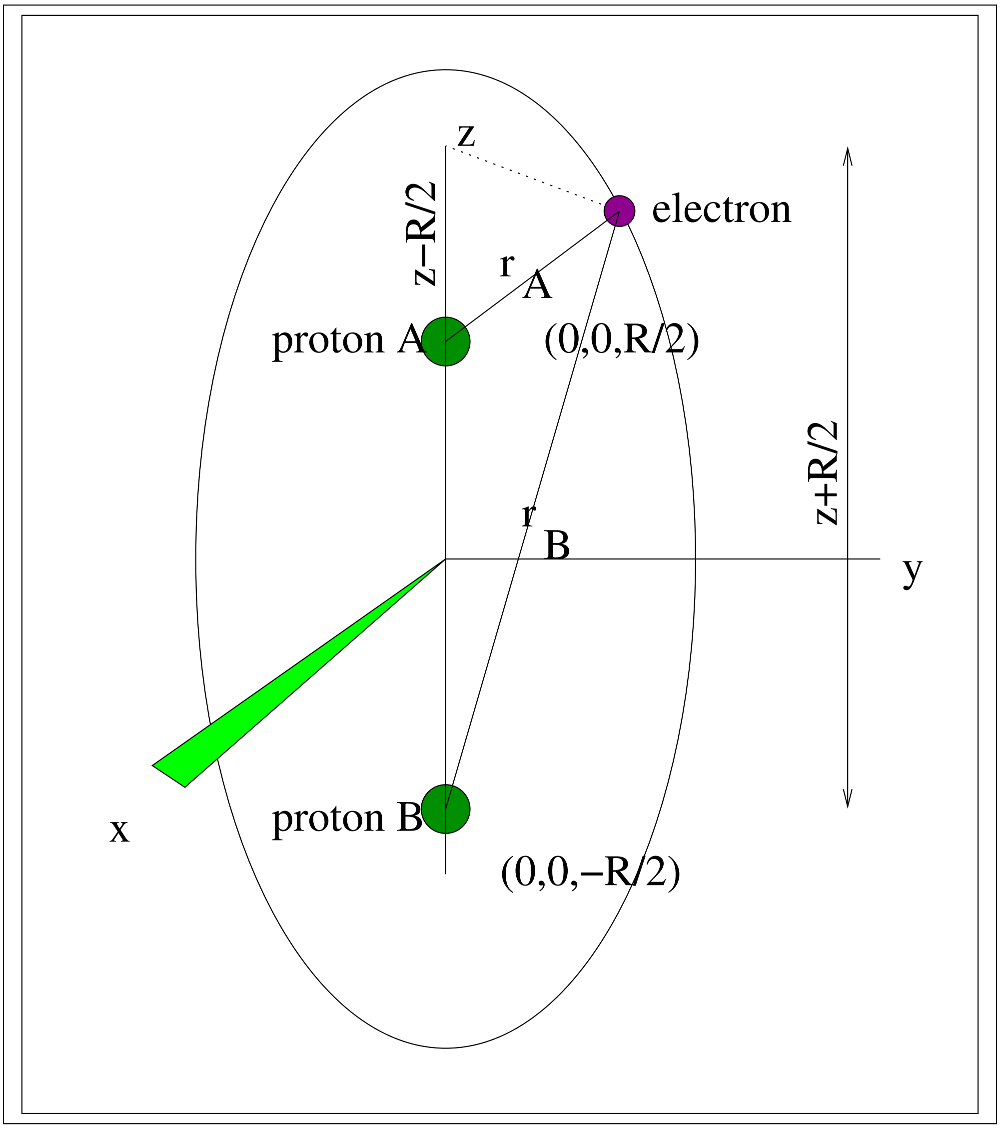

FIG. 3: The coordinate system for H_2^+. The two important distances r_A and r_B are shown explicitly.

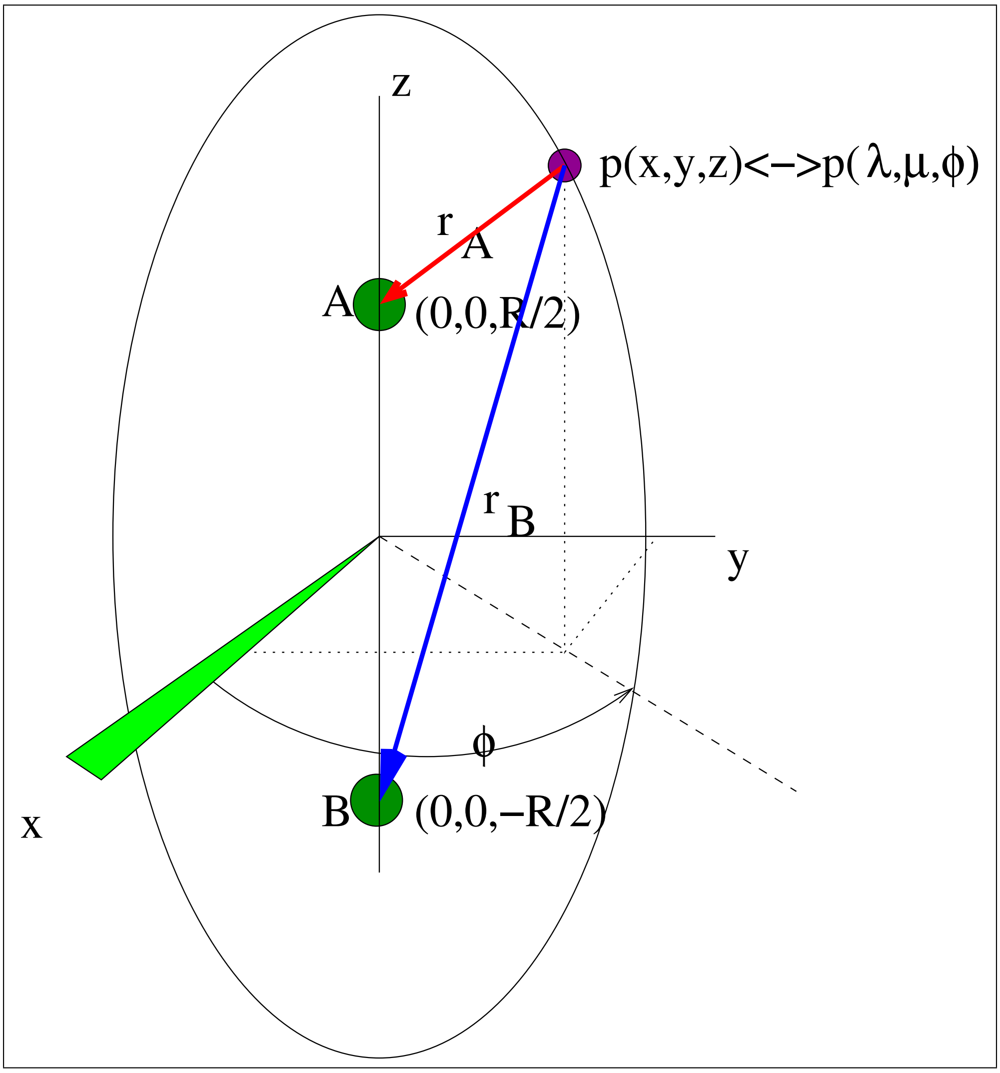

FIG. 4: The coordinate system for H_2^+. r_A and r_B in terms of the differing z coordinate are shown. Also, the forces are shown explicitly as a red and a blue vector (attractive).