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Derive expression for the energy levels of a hydrogen-like ion using Bohr's semi-classical theory. Do not make an assumption that the nucleus remains at rest while the electron orbits it, and carry out your calculations in the center of mass frame of reference. Present detailed calculations, and give comments and explanations along the way. Discuss your results.

Suppose that we have two particles of mass m_1 and m_2 interacting with one another with forces F_1 and F_2 such that they satisfy the Newtonian equation:

$$\frac{d}{dt}(m_1 v_1) = F_1 \quad eq (1)$$

$$\frac{d}{dt}(m_2 v_2) = F_2 \quad eq (2)$$

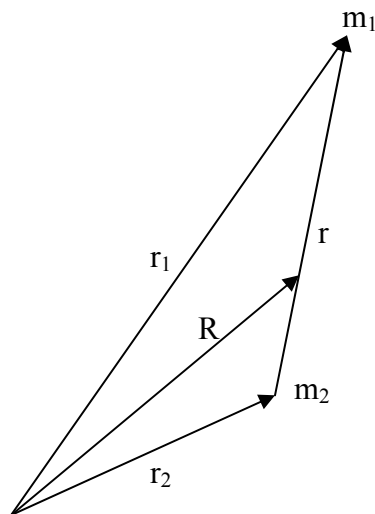
If we wish, we can set the two masses m_1 and m_2 equal to the mass of the nucleus and electron.

Then from Newton's 3rd Law, we know that

$$F_1 = -F_2$$

where F_1 and F_2 are two internal forces one particle exerts on the other, in the absence of any external forces.

In order to provide an inertial frame of reference anchored with the center of mass as the origin point, we must find the motion of the two particles relative to the center of mass at R..



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In the diagram above, we have

$$\vec{r} = \vec{r}_1 - \vec{r}_2$$
$$\vec{R} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2}$$

Therefore, the position of R is determined by the relationship between the masses of the two objects. Prior to any calculation, we already know that the mass of the nucleus is 4 orders of magnitudes larger than the electron, so the center of mass is very near the nucleus.

As a result, we can describe r_1 and r_2 :

$$\vec{r}_1 = \vec{R} + \frac{m_2}{m_1 + m_2} \vec{r}$$
$$\vec{r}_2 = \vec{R} - \frac{m_1}{m_1 + m_2} \vec{r}$$

By combining eq (1) and eq (2) and using the relation of the forces obtained from Newton's 3rd Law, we obtain:

$$m_1 m_2 \ddot{r} = (m_1 + m_2) F_1$$

For convenience, we can introduce two new variables μ and M such that

$$M = m_1 + m_2$$
$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

So the internal force of the system then becomes

$$\mu \ddot{r} = F_1$$

From dynamics, we know that the center of mass of two particles experiences no acceleration if the only forces involved are mutually attractive ones between the two particles.

However, if we wish to describe the constant velocity of the center of mass with respect to the motion of the two particles, we obtain:

$$V = \dot{R} = \frac{m_1 v_1 + m_2 v_2}{m_1 + m_2}$$
$$v = \dot{r} = v_1 - v_2$$

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If we require that the center of mass be a stationary origin, then the first equation simplifies to a conservation of linear momentum. Additionally, from the lack of external forces, angular momentum must also be conserved for the system. Where originally we have

$$L = m_1(r_1 \times v_1) + m_2(r_2 \times v_2)$$

The equation then turns into

$$L = M(R \times V) + \mu(r \times v)$$

But since we require that $V=0$, the angular momentum of the system then becomes:

$$L = \mu(r \times v) = \text{const}$$

Also, the total kinetic energy of the system must also be conserved, so we make similar substitutions

$$\begin{aligned} T &= \frac{1}{2}m_1v_1^2 + \frac{1}{2}m_2v_2^2 \\ &= \frac{1}{2}\mu v^2 \end{aligned}$$

In order for the path traveled by the nucleus and electron to form closed a conic section, typically an ellipse or circle, the angular momentum of the system must be conserved. Additionally, due to the close proximity of the nucleus to the center of mass, the low eccentricity of the electron's path makes it very nearly circular, as Bohr assumed. Thus, the distance between the electron and nucleus must also remain constant at $|\vec{r}|$, and we can use Newton's 3rd Law to equate the coulombic and centripetal forces.

$$\begin{aligned} \frac{e^2}{4\pi\epsilon_0 r^2} &= \mu \ddot{r} \\ &= \frac{\mu v^2}{r} \end{aligned}$$

Then solving for the total kinetic energy of the system yields

$$\frac{1}{2}\mu v^2 = \frac{e^2}{8\pi\epsilon_0 r}$$

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From the derivation of the center of mass, we know that the center of mass is collinear with the center of mass of the electron, and the center of mass of the nucleus. Additionally, since the orbit of the electron and nucleus is nearly circular about our origin point, the relative distance must also remain constant. Therefore we can set the potential energy from the electron to the nucleus, or the nucleus to the electron, as

$$V = -\frac{e^2}{4\pi\epsilon_0 r^2}$$

From this, we can get the expression for total energy E

$$E = T + V = -\frac{e^2}{8\pi\epsilon_0 r^2}$$

Returning to the angular momentum expression, we may find the allowed relative radial distance between the two particles if we look at the electron's and nucleus's total angular momentum around the origin point as integer multiples of Planck's constant over 2π .

$$\mu r v = n\hbar$$

We then solve for r and obtain

$$r = \frac{n^2 \hbar^2 4\pi\epsilon_0}{\mu e^2}$$

We substitute the expression for r back into the total energy equation to obtain

$$E = -\frac{\mu e^2}{2(4\pi\epsilon_0)^2 \hbar^2} \frac{1}{n^2} \quad n = 1, 2, \dots$$

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Discussion

One important note about the final expression is the nature of the μ term. From its original definition, we can state that μ is always less than the smaller of the two masses. However, we can choose to look at it in a slightly factored form as follows

$$\mu = m_1 \left(\frac{m_2}{m_1 + m_2} \right)$$

Also, we must remember that the mass of the nucleus is four orders of magnitude larger than that of the electron, so the quotient within the parenthesis is extremely close to 1. It is then safe to say that $\mu \approx m_e$. Therefore, if we compare the solution we obtained from the center of mass with that of a stationary nucleus,

$$E = -\frac{\mu e^2}{2(4\pi\epsilon_0)^2 \hbar^2} \frac{1}{n^2} \quad n = 1, 2, \dots$$
$$E = -\frac{m_e e^2}{2(4\pi\epsilon_0)^2 \hbar^2} \frac{1}{n^2} \quad n = 1, 2, \dots$$

the difference between the two will become negligible. Consequently, for the two-body particle system of the hydrogen atom, Bohr's semi-classical approach was sufficient in determining the discrete energy levels of the electron. If we were to adopt his approach for any system of more than 2 particles, then using the semi-classical approach will be much more difficult.

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References

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