CORRECTIONS TO THE BOHR MODEL

The basic "planetary" model was based on several simplifying assumptions.

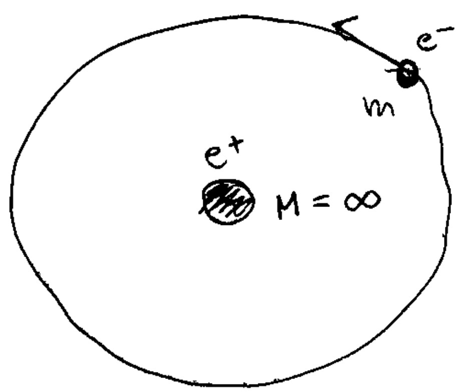
One was neglecting the relativistic and assuming that the electron energy and momentum are all described by Newtonian equations.

The model including the relativistic effects is far more complicated mathematically, and the difference between the energies E_n obtained from the relativistic model, and those obtained from the classical model, are quite small:

$$\frac{E_n(\text{relativisic}) - E_n(\text{classical})}{E_n(\text{classical})} \sim 2 \times 10^{-5}$$

So, the relative deviation due to neglecting relativistic effects is as small as 0.002%, and in most cases can be neglected.

Another simplifying assumption was taking the proton as an object of an infinite mass:

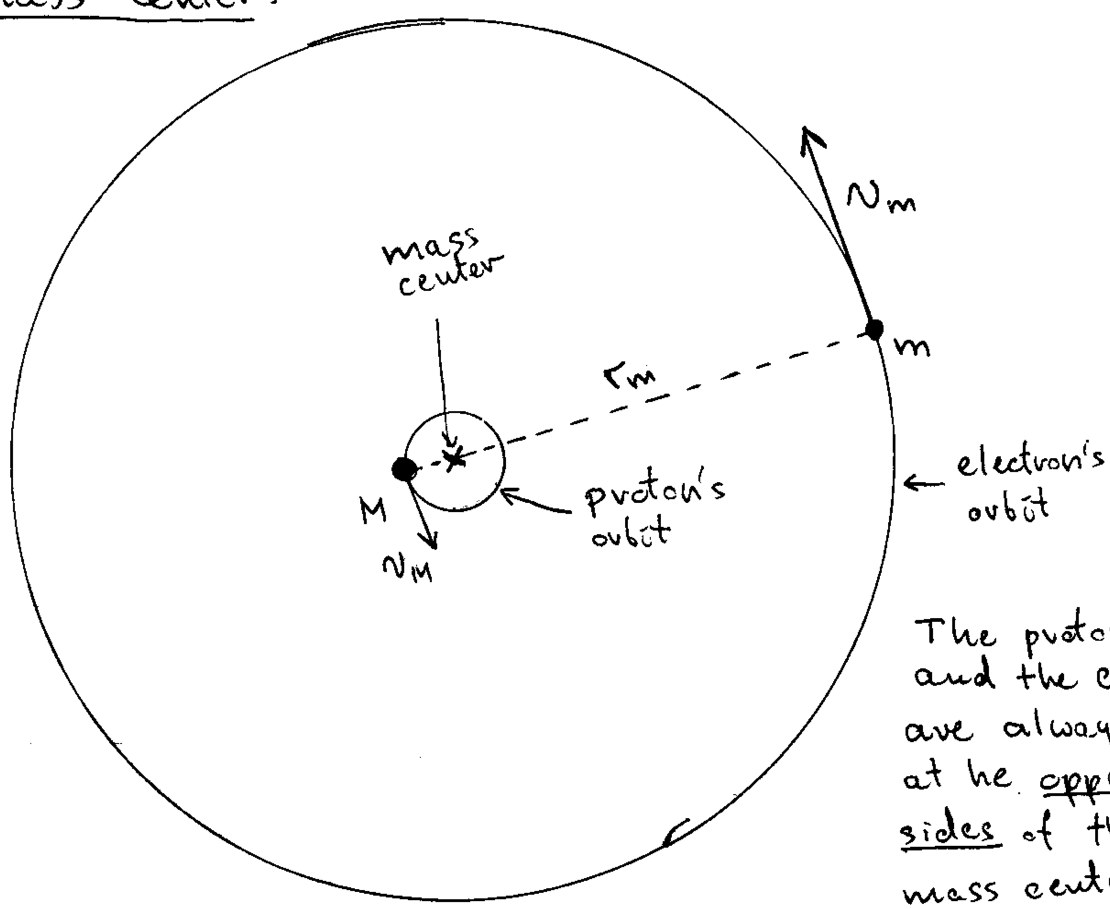


Actually, the proton is much heavier than the electron — 1836 times.

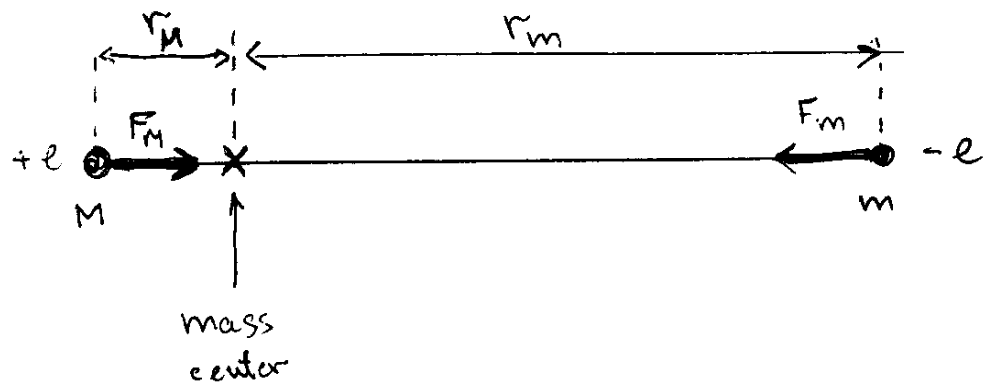
However, if we take into account the finite proton mass, it leads to a much larger energy difference ~~than~~ than the relativistic effects — about 0.05%, i.e. ~250 times larger than the relativistic correction.

It's perhaps worth to show how we carry out the calculations for finite proton mass:

Now it is not the electron orbiting a stationary proton, but both particles are orbiting the mass center:



The proton and the electron are always at he opposite sides of the mass center.



m – electron mass; r_m – electron orbit radius

M – proton " r_M – proton " "

F_M and F_m are the Coulomb attraction forces acting on the proton and the electron, respectively. According to the III Newton Law, $\vec{F}_M = -\vec{F}_m$ (so, $|\vec{F}_M| = |\vec{F}_m|$, of course).

Step 1. The forces $\vec{F}_M$ and $\vec{F}_m$ play the role of <u>centripetal forces</u> causing the orbital motion of the particles. So, we can write:

$$F_M = \frac{M v_M^2}{r_M} = M \omega^2 r_M \qquad (\omega \text{ – angular speed})$$

$$F_m = \frac{m v_m^2}{r_m} = m \omega^2 r_m \qquad (\text{Eq. } 1)$$

The angular speed ω is, of course, the <u>same</u> for both particles.

Since $F_M = F_m \Rightarrow M\omega^2 r_M = m\omega^2 r_m$

ω^2 cancels out: $M r_M = m r_m$

$$\Rightarrow \quad r_M = r_m \cdot \left(\frac{m}{M}\right) \qquad \text{(Eq. 2)}$$

Step 2) Let's calculate the total <u>kinetic</u> energy, which now is the sum of the electron energy (K_m) and the proton energy (K_M):

$$K = K_m + K_M = \frac{m v_m^2}{2} + \frac{M v_M^2}{2}$$

Let's again use the angular velocity: $v_m = \omega \cdot r_m$
$v_M = \omega \cdot r_M$

So:

$$K = \frac{m\omega^2 r_m^2}{2} + \frac{M\omega^2 r_M^2}{2}$$

Use Eq. 2:

$$= \frac{m\omega^2 r_m^2}{2} + \frac{M\omega^2 r_m^2}{2}\left(\frac{m}{M}\right)^2$$

$$= \frac{\omega^2 r_m^2}{2}\left(m + \frac{Mm}{M^2}\right) = \frac{m v_m^2}{2}\left(1 + \frac{m}{M}\right) \qquad \text{(Eq. 3)}$$

Step 3. Now, take the Coulomb force:

$$F_c = |F_M| = |F_m| = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{(r_m + r_M)^2}$$

Note that now the distance between the particles is equal to the sum of the orbit radii, $r_m + r_M$.

But again we can use Eq. 2, $r_M = r_m \cdot \left(\frac{m}{M}\right)$:

$$F_c = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{\left(r_m + r_m \cdot \frac{m}{M}\right)^2} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_m^2\left(1 + \frac{m}{M}\right)^2}$$

This force is equal to the centripetal force acting on the electron, given by Eq. 1.
We can then write:

$$\frac{m v_m^2}{r_m} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_m^2\left(1 + \frac{m}{M}\right)^2}$$

Multiply both sides by $r_m/2$

We obtain:

$$\frac{m v_m^2}{2} = \frac{1}{8\pi\varepsilon_0}\frac{e^2}{r_m\left(1 + \frac{m}{M}\right)^2} \qquad \text{(Eq. 4)}$$

Step 4: Combine Eq. 3 and Eq. 4 to obtain the total kinetic energy:

$$K = \frac{1}{8\pi\varepsilon_0}\frac{e^2}{r_m\left(1+\frac{m}{M}\right)^2} \times \left(1+\frac{m}{M}\right)$$

$$= \frac{1}{8\pi\varepsilon_0}\frac{e^2}{r_m\left(1+\frac{m}{M}\right)} \qquad \text{(Eq. 5)}$$

Step 5: Take the electrostatic potential energy:

$$U = -\frac{1}{4\pi\varepsilon_0}\cdot\frac{e^2}{(r_m + r_M)}$$

[$r_m + r_M$ is the distance between the two charges]

Again, use Eq. 2:

$$U = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{\left(r_m + r_m\frac{m}{M}\right)} = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_m\left(1+\frac{m}{M}\right)} \qquad \text{(Eq. 6)}$$

Step 6: Add K (Eq. 5) and U (Eq. 6) to obtain the total energy of the atom:

$$E = K + U = \frac{1}{8\pi\varepsilon_0}\frac{e^2}{r_m\left(1+\frac{m}{M}\right)} - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_m\left(1+\frac{m}{M}\right)}$$

$$= -\frac{1}{8\pi\varepsilon_0}\frac{e^2}{r_m\left(1+\frac{m}{M}\right)} \qquad \text{(Eq. 7)}$$

Note that the equation for the total energy is very similar to that we obtained for the $M = \infty$ case:

$$M = \infty : \qquad E = -\frac{1}{8\pi\varepsilon_0}\frac{e^2}{r}$$

$$M \text{ finite:} \qquad E = -\frac{1}{8\pi\varepsilon_0}\frac{e^2}{r_m\left(1+\frac{m}{M}\right)}$$

If $M \to \infty$, then $\frac{m}{M} \to 0$ and the second equation becomes identical with the first one.

Step 7. In this step, we use the <u>Bohr postulate</u> that the <u>angular momentum</u> can only take values $n\hbar$, where $n = 1, 2, 3 \ldots$

In the $M = \infty$ model, the proton is stationary and it does not contribute to the total momentum. Now, we have to take the <u>sum</u> of angular momenta of both particles:

$$L_{TOT} = m v_m \cdot r_m + M v_M r_M =$$

$$= m\omega r_m^2 + M\omega r_M^2$$

Use Eq. 2:

$$L = m\omega r_m^2 + M\omega r_m^2\left(\frac{m}{M}\right)^2$$

$$= m\cdot\omega\cdot r_m^2\left(1+\frac{m}{M}\right) = m v_m r_m\left(1+\frac{m}{M}\right)$$

But $L = n\hbar$

So:

$$m v_m r_m\left(1+\frac{m}{M}\right) = n\hbar$$

And:

$$v_m = \frac{n\hbar}{m\cdot r_m\left(1+\frac{m}{M}\right)} \qquad (\text{Eq. } 8)$$

Step 8

First, insert Eq. 8 into Eq. 3:

$$K = \underbrace{\frac{m v_m^2}{2}\left(1+\frac{m}{M}\right)}_{\text{Eq. } 3} = \frac{m}{2}\left[\frac{n\hbar}{m r_m\left(1+\frac{m}{M}\right)}\right]^2\left(1+\frac{m}{M}\right)$$

$$= \frac{n^2\hbar^2}{2 m r_m^2\left(1+\frac{m}{M}\right)}$$

Now, take Eq. 5 that also gives the kinetic energy K, and equate the two expresions for K:

$$\frac{n^2\hbar^2}{2m r_m^2\left(1+\frac{m}{M}\right)} = \frac{1}{8\pi\varepsilon_0}\,\frac{e^2}{r_m\left(1+\frac{m}{M}\right)}$$

Lot of things cancel out, and we solve the above for r_m:

$$\boxed{r_m = \frac{4\pi\varepsilon_0\hbar^2}{me^2}\,n^2} \qquad \text{(Eq. 9)}$$

Equation 9 give us the allowed values of the electron orbit radius r_m – note that the result is the same as in the $M=\infty$ case!

Step 9:

Now, the only thing that remains to be done is to plug Eq. 9 into Eq. 7, and we will obtain the expression for the ~~tot.~~ energy of the allowed states:

$$E = -\frac{1}{8\pi\varepsilon_0}\,\frac{e^2}{r_m\left(1+\frac{m}{M}\right)} =$$

$$= -\frac{1}{8\pi\varepsilon_0} \frac{e^2}{\frac{4\pi\varepsilon_0\hbar^2 n^2}{me^2}\left(1+\frac{m}{M}\right)}$$

$$= -\frac{me^4}{32\pi^2\varepsilon_0^2\hbar^2\left(1+\frac{m}{M}\right)} \cdot \frac{1}{n^2}$$

$$= -\frac{e^4\left(\frac{mM}{m+M}\right)}{32\pi^2\varepsilon_0^2\hbar^2} \frac{1}{n^2}$$

$$\boxed{E_n = -\frac{e^4 \cdot \mu}{32\pi^2\varepsilon_0^2\hbar^2} \cdot \frac{1}{n^2} \quad \text{where } \mu = \frac{m \cdot M}{m+M}} \quad \text{(Eq 10)}$$

$\mu = \frac{mM}{m+M}$ is called the <u>reduced mass</u>

Note that the final equation we got is essentially identical with the expression for the E_n in the case of $M = \infty$, except that instead of m_e, the electron mass, ~~[illegible]~~ there is μ, the reduced mass.

In fact, both equations are equivalent, because if in Eq. 10 we put $M = \infty$, then

$$\mu = \frac{mM}{m+M} \xrightarrow[M \to \infty]{} m$$

and we get an identical equation as we obtained on Page 186.

Let's calculate μ for the H atom: $M = 1836\,m$, so

$$\mu = \frac{m \cdot 1836m}{m + 1836m} = \frac{1836}{1837} m = 0.99946\,m$$

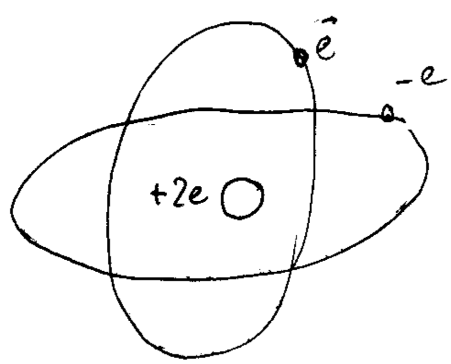
So, all energies ~~should be multiplied by~~ obtained from the "simpler" model should be multiplied by 0.99946

All equations for the energy differences – too. For instant, the equation 6.37 in the book, corrected for finite proton mass, should now read:

$$\lambda = \frac{64\pi^2 \varepsilon_0^2 \hbar^3 c}{0.99946\,m e^4} \left(\frac{n_1^2 n_2^2}{n_1^2 - n_2^2} \right)$$

Other applications of the Bohr model:

Bohr and his co-workers tried to apply the "planetary model" to Helium atom, which has a nucleus consisting of two protons and two neutrons. Neutrons have no electric charge, so the charge of the nucleus is $+2e$:

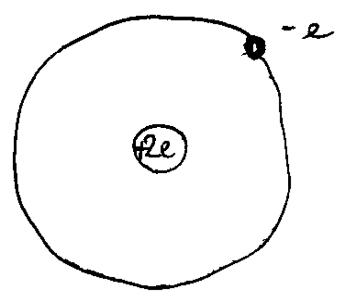


However, all efforts of solving such a system led to a complete failure. The reason is that there is also electrostatic interaction between the electrons, and no way was found to include it into the equations.

So, the Bohr model had a limited success, being appropriate only for systems consisting a single electron.

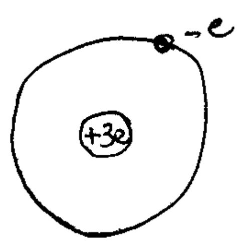
Is the H atom the only single-electron system known? No!

If we remove one electron from the helium atom, we obtain a He^+ ion, which is a single-electron system:



He^+ ion

The next atom is Lithium (Li), which has three protons in its nucleus. If we remove two electrons from the Li atom, we obtain a Li^{2+} ion:



All these systems can be solved using the same approach - only then we have to take the nucleus charge not as $+e$, but as $+Ze$ where Z is the number of protons in the nucleus. We get then:

$$E_n = -\frac{m Z^2 e^4}{32\pi^2 \varepsilon_0^2 \hbar^2} \cdot \frac{1}{n^2}$$

Where $Z = 2$ for He^+ ion, $Z = 3$ for Li^{2+} ion

More accurately, we should replace m by the reduced mass $\mu = \frac{mM}{m+M}$. For He atom, the nucleus mass is $M \approx 7300\, m$

The model for <u>finite nucleus mass</u> can also be applied to the so-called "exotic atoms" – "positronium" or "muonium".

In <u>muonium</u>, or "muonic atom", the electron is replaced by a negatively charged particle called <u>muon</u>, with mass equal 207 electron masses.
In <u>positronium</u>, the proton is replaced by a <u>positron</u>, a particle of charge $+e$ and the same mass as electron.