New Bohr model calculates Helium ground state energy correctly

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Abstract:
The quantum mechanical methods can calculate the behavior of atoms and molecules almost correctly using the methods such as perturvation, variation, and density functional theories. But these methods can not express concretely the motion of the electron such as spin and circular movement. So in this study, we try to describe the motion of the two electrons of the helium atom using the classical methods based on the Bohr model. And using this new model, we could theoretically calculate the ground state energy of the helium, which is close to the experimental value. So it is possible that this method would be a new tool for calculating the electronic behavior.

Keywords: herium, ground state, energy, electron, classical methods, Bohr

Introduction:
In 1913, by the study of the emission spectroscopy of atomic hydrogen, Niels Bohr postulates the Bohr model by using classical mechanics and electromagnetic theory. In the Bohr model, it was hypothesized that an electron is circularly moving around the nucleus, and the orbital angular momentum is quantized in units of $\hbar = \frac{h}{2\pi}$ (h is Plank's constant $= 6.6260693 \times 10^{-34}$ Js). So we have

$$mvr = n \times \hbar \qquad (1-1)$$

where m and v are the mass ($= 9.1093826 \times 10^{-31}$ kg) and the velocity (m/sec, this "m" means meter, not mass) of the electron, and n is a positive integer. Equating the centrifugal force to the Coulomb force, we have

$$\frac{mv^2}{r} = \frac{e^2}{4\pi\epsilon r^2} \qquad (1-2)$$

where r is the circular orbital radius (m), e is the electron charge ($= 1.60217653 \times 10^{-19}C$), and ϵ is the permittivity of vacuum ($= 8.854187817 \times 10^{-12}\frac{C^2}{Nm^2}$). From the equation 1-1 and 1-2, the total energy E (J) is

$$E = -\frac{me^4}{8\epsilon^2 h^2 n^2} \qquad (1-3)$$

This results agreed with the observed hydrogen spectrum, and this model also applies to any one-electron atom. In 1923 Louis de Broglie suggested that electrons might have

a wave aspect and its wavelength λ is equal to $\frac{h}{mv}$. In 1927, Davisson and Germer experimentally confirmed de Broglie's hypothesis by reflecting electrons from metals and observing diffraction effects [1]. Recently the results of the two-slit experiment of an electron showed its wavelike properties [2].

If the circular orbital length is equal to a integer times the wavelength of the electron, we have, $2\pi r = n \times \frac{h}{mv}, mvr = n \times \frac{h}{2\pi}$, so it is consistent with the equation 1-1 of the Bohr theory. But the Bohr model could not explain about the spin of the electron and the two-electron atoms such as the helium. Because of such problems, the Bohr theory was replaced by the quantum mechanical theory based on the Schroedinger equation in 1920's. The absolute square of the wavefunction ψ gives probability density of electrons. But in quantum mechanics, it is impossible to specify both the position and the momentum of an electron at some instant of time. The solution of the Schroedinger wave equation showed that the orbital angular momentum of the electron in the ground state of the hydrogen atom is zero. So the Coulomb potential may be infinitely negative, when the electron is close to the nucleus. And the solution also showed the relation between L (the total angular momentum quantum number) and M (the quantum number of the z component of the angular momentum),

$$M = -L, -L+1, -L+2, ...L-2, L-1, L \qquad (2)$$

The relation 2 and the results of the Stern-Gerlach experiment indicated that an electron has $\pm\frac{1}{2}\hbar$ spin angular momentum (S). But we can not visualize the spin rotational motion. By equating the angular momentum of the spinnig sphere of the electron to $\pm\frac{1}{2}\hbar$, the sphere speed leads to about one hundred times the speed of light. Experimentally, the spin magnetic moment (μ) is known to be

$$\mu = -\frac{g\beta S}{\hbar} \qquad ; \beta = \frac{e\hbar}{2m} \qquad (3)$$

where g, the spin g-factor, is 2 [3], and β is the Bohr magneton ($= 9.27400949 \times 10^{-24} \frac{J}{T}$). To solve the above problem, we try forgetting quantum mechanical methods and going back to the Bohr model. We suppose that the orbital angular momentum ($S2$) of the electron in the ground state of the hydrogen atom is $\pm\hbar$ (here, spin is zero) and its g factor ($g2$) is 1. Then the magnetic moment of the electron in that state $\mu 2 = -\frac{(g2)\beta(S2)}{\hbar}$ is equal to μ of the equation 3. In this state, the problems about infinitely negative Coulomb potential and spinning sphere speed do not occur. As the magnetic moment of the electron is not changed, the splitting pattern of the energy levels in the magnetic field (Paschen-Back Effect) is also not changed.
The herium atom has two electrons and a nucleus of charge +2e. The Schroedinger equation for the helium can not be precisely solved. So the perturbation theory such as the variation method is applied to the calculation. Using the perturbation method, we can get the ground state energy of the helium atom, which is very close to the experimental value -79.0eV. But the calculation of the high order correction is very difficult.

In this paper, we try to calculate the ground state energy of the herium atom using the new theory based on the Bohr model, and check if the calculation value is equal to the experimental value -79.0eV.
First, suppose we have the following model (Fig.1). In that model, two electrons of the helium are on the opposite sides of the nucleus and moving on the same circular orbital.

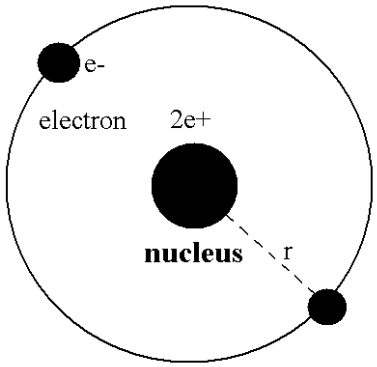

Fig.1 The two electrons are moving on the opposite sides.

Equating the centrifugal force to the Coulomb force (the magnetic force is too small to be considered), we have

$$\frac{mv^2}{r} = \frac{2e^2}{4\pi\epsilon r^2} - \frac{e^2}{4\pi\epsilon(2r)^2} \qquad (4-1)$$

The circular orbital length is supposed to be an integer times the wavelength of the electron, we have

$$2\pi r = \frac{h}{mv} \times n \qquad (4-2)$$

The total energy E of the electrons is the sum of the kinetic energy and the Coulomb potential energy, so

$$E = 2 \times \frac{mv^2}{2} - 2 \times \frac{2e^2}{4\pi\epsilon r} + \frac{e^2}{4\pi\epsilon(2r)} \qquad (4-3)$$

Solving the above three equations (4-1, 4-2, 4-3), the ground state energy (n=1) is -83.33eV. The value is lower than the experimental value -79.0eV. In this model, as the two electrons are on the same orbital, it is possible that the two electronic waves interfere with each other and their motions are affected, so the equations (4-1, 4-2, 4-3) may not be satisfied.
To avoid such problems, we suppose another model as shown in Fig.2 and Fig.3. In that model, the planes of the two same-shaped orbitals are perpendicular to each other. Any point on the electron 1 orbital is at the same distance from the points on the

both-side(± z) electron 2 orbital. On the electron 1 orbital, the wave of electron 2 may interfere with itself and vanish, so the motion of electron 1 may not be affected by the wave of electron 2.

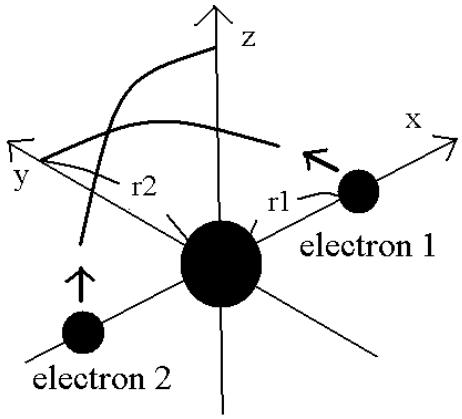

Fig.2: The two same-shaped orbital planes are perpendicular to each other. This figure shows one quarter of the orbitals.

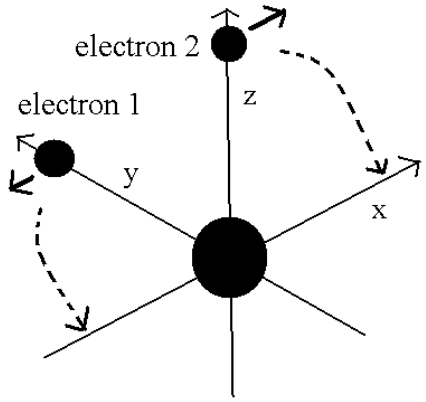

Fig.3: The electrons have moved one quarter of their orbitals.

Here we investigate how the electrons of the helium atom are moving by calculating the Coulomb force among the two electrons and the nucleus at short time intervals.

Methods and results:
The computer program (class filename: MathMethod) written in the JAVA language (version 1.5.0) to calculate the electronic orbital of the herium is shown in Fig.4.
As shown in Fig.2 and Fig.3, the herium nucleus is at the origin, the orbital plane of the electron 1 is the xy-plane, and the orbital plane of the electron 2 is xz-plane. The

electron 1 initially at (r1, 0, 0) (Fig.2) moves one quarter of its orbital to (0, r2, 0) (Fig.3), while the electron 2 initially at (-r1, 0, 0) (Fig.2) moves to (0, 0, r2) (Fig.3). Meter and second are rather large units for measurement of atomic behavior, here we use new convenient units MM (1 MM = 1×10^{-14} meter), SS (1 SS = 1×10^{-21} second) and MM/SS (1 MM/SS = 1×10^{7} meter/second).

Fig.4: The program to calculate the electronic orbital of the helium.

```
import java.util.Scanner;
class MathMethod {
public static void main(String[ ] args) {
Scanner stdIn=new Scanner(System.in);              // input r1 and |E |
System.out.println("r1 between nucleus and electron 1 (MM) ?");
double r=stdIn.nextDouble( );
System.out.println("total energy |E |in the helium (eV) ?");
double E=stdIn.nextDouble( );
for (int i=1; i<100; i++) {                        // repeat until r1=initial r1+100
                                                   // calculate initial VY from E and r1
double vya= -(E*1.602177e-19)+(8.07477705e-14/r); //vya=total E-potential energy
if (vya>0) {
double vyb=Math.sqrt(vya/(9.1093826*1.0e-31)); //velocity from kinetic energy
double VY=vyb*1.0e-7;                              // m/sec to MM/SS
double prexx=r; double VX=0.0; double WN=0.0;
double preyy=0.0; double xx, yy, vk, preVY, preWN, midWN;
do {
xx=prexx+VX; yy=preyy+VY;                          // electron 1 position after 1 SS
preVY=VY; preWN=WN;
vk=VX*VX+VY*VY;                                    // calculate WN from VX, VY
WN=WN+1.374779252e-4*vk;                           // WN=WN + Eq.(7)
                                                   // calculate VX, VY from Coulomb force
double ra=Math.sqrt(prexx*prexx+preyy*preyy);
double rb=Math.sqrt(4.0*prexx*prexx+2.0*preyy*preyy);
VX=VX+506.5276876*prexx*(-1.0/(ra*ra*ra)+1.0/(rb*rb*rb)); //+Eq(5-1) ×10^-28
VY=VY+506.5276876*preyy*(-1.0/(ra*ra*ra)+0.5/(rb*rb*rb)); //+Eq(5-2) ×10^-28
prexx=xx; preyy=yy;
} while (xx>0);                                    // repeat above until electron 1 arive at y axis
if (VY>-0.001 && VY<0.001) {                       // last VY condition
System.out.print("r1: "+r+"          ");
System.out.printf("VY:% .5f          ", VY);
System.out.printf("preVY:% .5f          ", preVY);
midWN=(WN+preWN)/2; System.out.printf("midWN:% .5f \n ", midWN);
}
```

} r=r+1:
} } }

In this program, we first input the initial x-coordinate r1 (in MM) of the electron 1, and the absolute value of the total energy E (in eV) of the helium. From the inputted value, we calculate the initial velocity of the electron 1. And at intervals of 1 SS we calculate the Coulomb force among the two electrons and the nucleus. When the electron 1 is at (xx, yy, 0), the electron 2 is at (-xx, 0, yy) (in MM). Change MM to meter as follows; x (m) = xx $\times 10^{-14}$. y (m) = yy $\times 10^{-14}$. So the x component of the acceleration (m/sec^2) of the electron 1 is as follows;

$$-\frac{2e^2x}{4\pi\epsilon m(x^2+y^2)^{\frac{3}{2}}}+\frac{e^2\times(2x)}{4\pi\epsilon m(4x^2+2y^2)^{\frac{3}{2}}} \qquad (5-1)$$

where the first term is by the Coulomb force between the nucleus and the electron 1, and the second term is by the force between the two electrons.
In the same way, the y component of the acceleration (m/sec^2) is as follows;

$$-\frac{2e^2y}{4\pi\epsilon m(x^2+y^2)^{\frac{3}{2}}}+\frac{e^2\times y}{4\pi\epsilon m(4x^2+2y^2)^{\frac{3}{2}}} \qquad (5-2)$$

Change m/sec^2 to MM/SS^2 using the next relation;

$$1m/sec^2 = 1\times 10^{-28} MM/SS^2 \qquad (6)$$

Based on that calculation value we change the velocity vector and the position of the electrons. We suppose electron 1 moves only on the xy-plane, so the z component of the acceleration of the electron 1 is neglected. We also calculate the wavelength of the electron from the velocity ($\lambda = \frac{h}{mv}$) at intervals of 1 SS. The number of that wave (λ in length) contained in that short movement section (The sum of them is WN) is,

$$\frac{\sqrt{VX^2+VY^2}\times 10^{-14}}{\frac{h}{m\sqrt{VX^2+VY^2}\times 10^7}} \qquad (7)$$

where (VX, VY) are the velocity of the electron 1 (in MM/SS), the denominator is the wavelength (in m), and the numerator is the movement distance (in m) for 1 SS.
When the electron 1 has moved one quarter of the orbital and its x-coordinate is zero (Fig.3), this program checked the y-component of the electron 1 velocity (last VY). As we want the last VY value which is close to zero in Fig.3, only when -0.001 < VY < 0.001 (MM/SS) is satisfied, the program displays the following values on the screen, r1, VY, preVY (VY 1SS ago), and (mid)WN (the total number of the electronic wave contained in one quarter of the orbital). The initial inputted x-coordinate of the electron 1 is automatically increased by 1 MM per above calculation to +100 MM.

E (eV)	r1 (MM)	WN	WN × 4
-77.0	3155.7	0.25333	1.01332
-77.5	3135.5	0.25250	1.01000
-78.0	3115.4	0.25170	1.00680
-78.5	3095.5	0.25089	1.00356
-79.0	3075.9	0.25010	1.00040
-79.5	3056.6	0.24932	0.99728
-80.0	3037.4	0.24854	0.99416
-80.5	3018.6	0.24777	0.99108
-81.0	3000.0	0.24699	0.98796

Fig.5: The results in which VY in Fig.3 is the closest to zero

Fig.5 shows the results in which the last VY is the closest to zero. Fig.6 graphs the results in Fig.5. As shown in Fig.5 and Fig.6, when the total energy of the helium (E) is -79.0 eV (the experimental value), WN x 4 is the closest to 1.

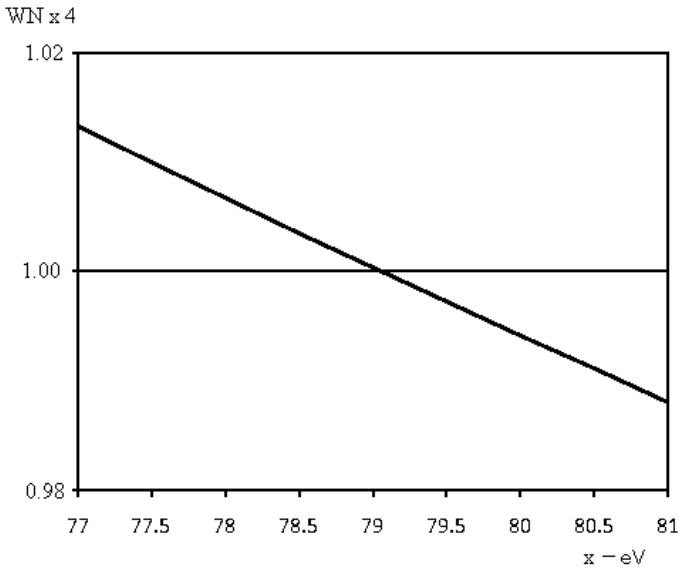

Fig.6: Plots of the number of the electronic wave contained in one orbital at various energy levels.

This results demonstrate that two electrons in the ground state of the helium may be actually moving around the nucleus on the orbitals of one electronic wave length as shown in Fig.2 and Fig.3.

In this study, we do not use the quantum mechanical method such as the Schroedinger equation. It is a very meaningful and astonishing thing that the calculation value by this new method based on the Bohr model is about the same as the experimental value. In the future, this method will be possibly to be a new useful tool for calculating electronic behavior.

References:

[1] C. Davisson, and L. H. Germer, Nature 119, 558, 1927
[2] A. Tonomura, J. Endo, T. Matsuda, et al., Am. J. Phys., 57, 117, 1989
[3] G. Gabrielse, D. Hanneke, T. Kinoshita, et al., Phys. Rev. Lett., 97, 030802, 2006

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