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AN ALTERNATIVE METHOD FOR CALCULATING THE QUANTUM STATES OF HELIUM

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I. Introduction

To calculate the energy of stationary states of electrons in atoms with more than one electron, Bohr's theory cannot be modified in principle, if only because it is based on the study of the mechanical energy of electrons moving along closed trajectories. The main drawback of Bohr's theory is considered to be its inability to explain the properties of more complex atoms. Even the problem of the energy levels of the helium atom has not been solved. When an electron moves along closed orbits, electrodynamics assumes continuous emission of an electron and its fall onto the nucleus, that is, it assumes the instability of atoms.

Like Bohr's theory, quantum mechanics also studies the mechanical properties of electrons in atoms, but hides this problem of the instability of atoms behind the Heisenberg uncertainty relation. An electron does not move along closed trajectories, but can be anywhere in the atom. The question of the physical mechanisms of such transitions is not even raised, and the Heisenberg uncertainty relation addresses this problem to the Creator.

After the discovery of the wave properties of the electron by de Broglie, and in fact the reformulation of Bohr's postulates, it became possible to describe the behavior of electrons in atoms using the wave function. The complex exponent allows us to describe both the circular orbits of the electron and the plane waves of quantum mechanics. And the Schrödinger equation is the law of conservation of energy written in operator form.

Both theories have significant shortcomings. They do not take into account the magnetic field in atoms, considering it to be negligible compared to the electric field. As it turned out, the energy of the electric and magnetic fields is the same in magnitude, that is, it is an electromagnetic field that circulates around the nucleus [1, 2]. The circulating electromagnetic field ensures the stability of atoms.

To calculate the spectral terms of a helium atom, we will use an approach based on the electroneutrality of the atom. Electroneutrality means that the electric field created by the nucleus at each point outside the outer electron shell of the atom is exactly equal to the field created by the outer electron shell and has the opposite direction. The resulting field at each point outside the atom is zero. In this case, we can ignore the nucleus and calculate the energy of the electric field created by the electron shell outside the atom. The energy of this field will be the ionization energy of the electron shell. This allows us to study the behavior of the electron shell regardless of the presence of the nucleus. The proposed approach allows us to substantiate the concept of an "artificial atom". The properties of an artificial atom correspond to the properties of a real atom with the same number of electrons.

We will demonstrate the application of this method using the example of a helium atom. The nucleus of a helium atom has a positive charge of +2, and there are two electrons around the nucleus. These electrons are arranged in such a way as to ensure that the atom is electrically neutral, i.e. the electric field created by the nucleus outside the atom is compensated by the electric field of the electron shell. The ionization energy of the atom will be determined by the energy of the electric field outside the atom.

II. Justification of the calculation method

For an artificial atom and a real atom with one electron (a hydrogen atom), the stationary states are spheres of radius r_n, on the surface of which there is a unit charge e [1]. The ionization energy of the stationary state is equal to the energy of the electric field in the entire space outside the atom, that is, from the radius r_n to infinity:

$$E_n = \frac{\varepsilon_0}{2}\int_V \vec{E}\,\vec{E}\,dV, \quad (1)$$

where $\vec{E}$ is the electric field strength of the charge e placed on a spherical surface of radius r_n.

After calculating the integral, it can be seen that the ionization energy of the stationary state is equal to the energy of a spherical capacitor, the radius of the inner shell of which is rn, and the outer shell is infinity:

$$E_n = \frac{q^2}{8\pi\varepsilon_0 r_n}. \quad (2)$$

For a helium atom q = 2e, where *e* is the electron charge; r_n is the radius of the sphere on the surface of which a charge q is placed. In this case, the energy of interaction between electrons is not taken into account. In a helium atom, two electrons are in the $1s^2$ state, i.e. placed on a spherical surface with radius r_n, and their energy is the same and is ½ E_n.

According to the law of conservation of energy, E_n must be equal to the work of transferring the charge 2e from infinity to the surface of a sphere of radius r_n, which in turn is equal to the kinetic energy of the mass $m = 2m_0$:

$$E_{nk} = \frac{mv_n^2}{2}. \quad (3)$$

Since the kinetic energy of the charge q is the source of the magnetic field in the atom, the energy of the magnetic field must be exactly equal to the energy of the electric field. This can be verified by direct calculation. The energy of the magnetic field in the volume of a sphere of radius r is equal to:

$$E_{nB} = \frac{\varepsilon_0 c^2}{2}\int_r^\infty \vec{B}\vec{B}\,dV. \quad (4)$$

A charge q, moving along the surface of a sphere of radius r_n with a speed v_n, creates a magnetic field regardless of the trajectory. The orientation of the orbit in space is oriented in any direction with equal probability. The magnetic field covered by the plane of the orbit can be determined simply [2]. On the one hand, the flux is the product of the magnetic field on the area covered by the orbit of the electron in the quantum state n. On the other hand, this flux is equal to n quanta of the magnetic flux h / e [1]. Equating these expressions, we determine the induction of the magnetic field in the state n:

$$B = \frac{nh}{2\,e\,2\,\pi\,r_n^2} = \frac{n\hbar}{q\,r_n^2}.$$

Because the magnetic field lines are closed, integration in the orbital plane gives the same result as integration in the whole space outside the orbit. For the element of the area $4\pi r^2 dr$ the energy of the magnetic field:

$$E_{nB} = \frac{\pi\,\varepsilon_0\,n^2\hbar^2c^2}{q^2r_n}.$$

Since the source of the magnetic field is an electron, instead of the speed of light, the formula should include the orbital speed of the electron:

$$E_{nB} = \frac{\pi\varepsilon_0 n^2\hbar^2 v_n^2}{q^2 r_n}. \quad (5)$$

Solving the system of equations (2, 3 and 5), we determine the unknown quantities v_n and r_n:

$$v_n = \frac{q^2\sqrt{2}}{8\pi\varepsilon_0 n\hbar},$$

$$r_n = \frac{8\pi\varepsilon_0 n^2\hbar^2}{m\,q^2}.$$

In these equations q = 2e, $m = 2m_0$, n – takes only even values. Calculation according to the above formulas allows us to determine the energy values corresponding to the total energy of two electrons, which is distributed equally between the electrons. Excited states can be obtained by giving the principal quantum number n even values. As in the ground state, we will assume that the charge q = 2 e is placed on the spherical surfaces corresponding to the excited states. The results of the calculation are presented in (Table 1).

Table 1

Parameters of stationary states in a helium atom

State	r_n, Å	v_n, 10^6 m/c	$E_{nB}=E_{nE}=E_{nk}$, eV	E_n, eV exp.	$\cos^2 \alpha$
$1s^2$	0.5296	3.093	54,4	24,5876	0,904
$2s^2$	2.118	1.547	13,6	3,972	0,584
$3s^2$	4.765	1.031	6,046	1,668	0,552
$4s^2$	8.472	0.7733	3,401	0,918	0,540
$5s^2$	13.24	0.6187	2,176	0,578	0,531
$6s^2$	19.06	0.5156	1,511	0,398	0,527

In the basic stationary state of a helium atom, both electrons are in the $1s^2$ state and have the same ionization energy 27.2 eV. The orbital magnetic moments of both electrons are parallel, but they can be oriented in any direction with equal probability. Therefore, the average value of the resulting moment is zero, and the ground state is a singlet (shell state $1S^2$). If both electrons of a helium atom are in an excited state, then this state is as stable as the ground state, i.e. orthohelium is a quasi-stationary excited state of a helium atom. Transition to the ground state is possible only with the simultaneous emission of two photons (the lifetime of an orthohelium atom due to the two-photon decay $2^3S_1 \to 1^0S_1 + 2\gamma$ is 2.49×10^8 s, or 7.9 years). Since such transitions are unlikely, the corresponding state is quasi-stationary.

The method used to calculate the stationary states in a helium atom automatically excludes the interaction between electrons, since we have only one charge of magnitude 2e and mass $2m_0$. The magnetic moment is zero, since a closed orbit of the charge acquires all possible orientations with equal probability. In an external magnetic field, the magnetic moment is nonzero, since the orbit acquires a predominant orientation along or against the external magnetic field. This phenomenon it is manifested when observing the Zeeman effect. It is explained by the splitting of energy levels.

III. Stationary states of the helium atom

The calculations given in the previous section show that the total ionization energy of an electron in the ground state is 27.2 eV, which is significantly different from the experimental value of 24.5876 eV. When a helium atom is irradiated with a quantum of light whose energy is equal to the ionization energy, one electron will leave the atom. The He^+ ion is formed, the experimental value of the ionization energy is 54.418 eV. Therefore, the total energy of electrons in the stationary state in a helium atom is exactly equal to the energy of the stationary state of the helium ion, which is important for the interpretation of the concept of "stationary state".

The interaction energy between electrons will have the minimum possible value if the electrons are located on opposite sides of the orbit and have the same direction of rotation clockwise or counterclockwise. Due to the arbitrary orientation of the orbit, the magnetic moment will be zero. Electrons placed on opposite sides of the electron orbit create a field that is not radial. At an arbitrary point P, electron 1 creates an electric field that has a tangential E_{t1} and a radial component E_{r1} (Fig. 1). The second electron creates fields E_{t2} and E_{r2}, respectively. The tangential components are mutually compensated, and the radial components are added. The energy of the electric field is determined by the sum of only the radial components.

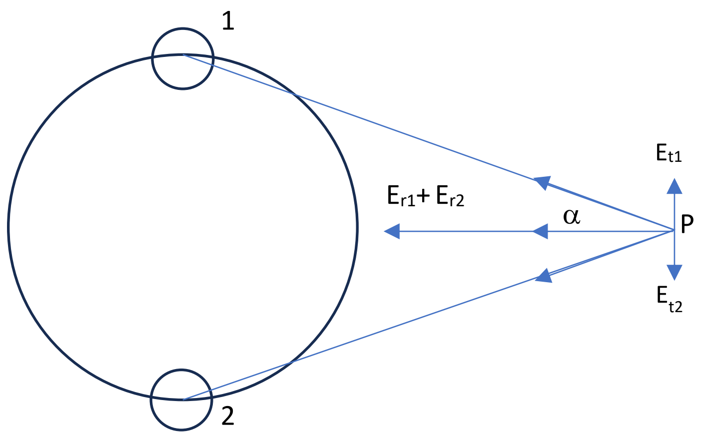

Fig. 1 **Mutual compensation of the tangential component of the electric field created by electrons in a helium atom**

Since the electrons are always at the greatest possible distance from each other, the magnitude of the radial component will depend both on the position of each electron on the trajectory and on the location of point P. When bypassing the trajectory, the tangential components of the electric field will be mutually compensated. The radial components can be characterized by the average value for each point P. The averaged value of the radial component of the electric field can be defined as $E \cos \alpha$. The energy of the electric field in the entire space outside the atom will be determined by the integral of the quantity $4 E^2 \cos^2 \alpha$. Moreover, we will assume that the value of $\cos^2 \alpha$ = const (Table 1).

With an increase in the principal quantum number, the radius of the sphere on which electrons move increases. This leads to an increase in the tangential and decrease in the radial components of the field. At the same time, with an increase in the radius of the spherical surface, the electric field strength outside the atom decreases sharply, and accordingly, the electric field energy. Both effects lead to a decrease in the average value of $\cos^2 \alpha$. Moreover, for the $2s^2$ state, the decrease in $\cos^2 \alpha$ is very significant.

Thus, the use of an alternative approach based on the electroneutrality of the atom allows us to obtain accurate values of the ionization energy of energy levels. At the same time, each step of the proposed algorithm has a logical physical justification.

IV. Conclusions

An alternative method for calculating stationary states is proposed, which based on the electroneutrality of the atom. Stationary states arise as a result of the quantization of the magnetic flux in atoms. The quantum of the magnetic flux is equal to h/e for each electron of the atom. In excited states, the number of magnetic flux quanta captured by the orbit of each electron is proportional to the principal quantum number. The stability of atoms is ensured by the electromagnetic field circulating around the nucleus.

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