

LETTER TO THE EDITOR

Analytical determination of stable configurations in doubly excited atoms and ions

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Abstract. A simple approach is proposed to determine analytically the classically stable configurations of doubly excited states in atoms and Z ions, in the case when both electrons are located on one side of the nucleus. An analytical formula gives the ratio between the electron distances within the 1% accuracy of the existing numerical computations.

Recently new classical configurations of electrons in the helium atom have been discovered in numerical simulations [1–3]. The main unusual feature of these states is that both electrons are located on one side of the charged centre and the inner electron does not allow the outer electron to come close to the nucleus. The numerical calculations carried out in [1–3] show that corresponding classical trajectories are stable in the one-dimensional model of helium and that this stability persists in the three-dimensional atom. It was also demonstrated numerically that such a stable orbit exists also for an ion with charge $Z > 1$ [3]. In the quantum case the existence of stable classical orbit leads to the appearance of long lived excited states which for the outer electron are located near the position of classical equilibrium [3]. While the numerical analysis of such configurations in the classical and quantum cases was quite extensive the analytical investigation is much less developed. Here I introduce a simple analytical approach which allows us to find analytically the equilibrium positions for arbitrary Z values and provides a better understanding of the underlying physics. This understanding gives explanations for some numerical observations of [3] and can be useful for future investigations of these interesting states.

The physical basis for the analytical approach can be discovered from the picture of classical electron motion presented in [1]. First, we see that the stable classical configurations exist even for the one-dimensional helium atom and that these 1D orbits are preserved in the 3D case. Second, we remark that the outer electron is located at a much larger distance from the nucleus than the size of the orbit of the inner electron (approximately 3 times larger). Due to that the frequency of the inner electron motion must be much faster than the frequency of outer electron. Therefore, it is possible to expect that the motion of outer electron goes in some effective averaged potential created by inner electron. In the following we will consider the one-dimensional model of the helium atom (or ion with charge Z) in which both electrons move on one line which pass through the nucleus. As we will see the geometrical configuration corresponds to the picture in which the inner electron makes fast oscillations almost as in the one-electron one-dimensional atom with the charge

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Z. The one-dimensional classical atom orbit can be parametrically presented in the form [4, 5]: $a_{\text{in}}(t) = a(1 - \cos \xi)$, $t = T(\xi - \sin \xi)/2\pi$ where $a_{\text{in}}(t)$ is the distance between the centre and the inner electron, a is the large half-axis of the ellipse and T is the period of motion (this solution is obtained from the standard equations [5] by taking eccentricity $e = 1$). At the same time the outer electron makes small oscillations on the same line in the minimum of averaged potential created by the inner electron and the charged centre. The graphic picture of such a one-dimensional configuration is presented in the figure in [1]. In the quantum system such a situation corresponds to the case when the inner electron in the excited state has one parabolic quantum number n_1 much larger than another n_2 (the limiting case is $n_1 = n - 1$, $n_2 = m = 0$). For such states the orbital momentum l is of the order of \sqrt{n} so that the eccentricity $e = (1 - l^2/n^2)^{1/2} = 1$ in the classical limit $n \gg 1$ (see also [4]).

Table 1. Comparison of numerical data [3] (marked by subscript nu) with the theory of this paper (marked by subscript th).

Z	$2a_{\text{th}}$	R_{th}	$R_{\text{nu}}/R_{\text{th}}$	$a_{\text{no}}/a_{\text{th}}$
1.01	1.010	151.24	0.9999	1.000
1.10	1.103	16.243	1.0018	0.997
1.50	1.550	4.2219	0.9948	1.000
2.00	2.220	2.7024	0.9965	0.968
3.00	3.673	1.9258	0.9950	0.944
4.00	5.237	1.6579	0.9970	0.929
5.00	6.870	1.5197	0.9995	0.919
10.0	15.53	1.2746	1.0130	0.896

To obtain an expression for the effective potential in the one-dimensional model of the Z ion we can assume that the inner electron is moving in the same way as in a Coulomb field with a maximal distance from the nucleus in the aphelion equal to $2a$. Then using the solution for the Kepler motion we can average the interaction between the electrons $V_{\text{int}} = 1/(x - a_{\text{in}}(t))$ over the period of motion of the inner electron and to obtain in this way an effective potential U_{eff} in which the outer electron moves. Here x is the distance between the nucleus and the outer electron and $a_{\text{in}}(t)$ gives the position of the inner electron at time t . The averaging over Kepler orbit is given by the integral $\langle V_{\text{int}} \rangle = 1/T \int_0^T dt/(x - a_{\text{in}}(t))$, where T is the period of the motion. Using the standard parametric representation for the 'eccentric anomaly' in the Kepler motion [5] we can write $a_{\text{in}}(t) = a(1 - \cos \xi)$ and $dt/T = (1 - \cos \xi)d\xi/2\pi$ where we took into account that in our one-dimensional case the eccentricity $e = 1$. This reduces the integral to the form $\langle V_{\text{int}} \rangle = 1/2\pi \int_0^{2\pi} (1 - \cos \xi)d\xi/(x - a + a \cos \xi)$ in which it can be computed analytically. Finally we get effective potential which describes the motion of the outer electron:

$$U_{\text{eff}} = -\frac{Z}{x} + \frac{x}{a(x^2 - 2ax)^{1/2}} - \frac{1}{a}. \quad (1)$$

Here the first term gives the interaction of the outer electron with the charged centre while the other terms represent the averaged interaction $\langle V_{\text{int}} \rangle$ between the electrons. From the expression for U_{eff} it is clear that the distance x between the outer electron and the nucleus is always larger than $2a$ due to strong repulsion between the electrons. For $Z > 1$ the

minimum of the effective potential for the outer electron is defined from the condition $dU_{\text{eff}}/dx = 0$ and is given by

$$R_{\text{th}} = \frac{x_{\text{min}}}{2a} = \frac{Z^{2/3}}{Z^{2/3} - 1}. \quad (2)$$

The comparison of this theoretical value of this ratio with the numerical results (R_{nu}) [3] demonstrates agreement within 1% accuracy (see table 1). This is comparable with the accuracy of the numerical data presented in [3]. Let us mention that the ratio R is energy independent.

For the case when the outer electron is located in the minimum of U_{eff} we can easily find the total energy of the atom. For that we substitute the value of x_{min} from (2) in the expression (1) and taking into account that the energy of the inner electron is $-Z/2a$ we get

$$E_{\text{at}} = (-2Z + 3Z^{1/3} - 2)/2a. \quad (3)$$

This formula allows us to determine the size of the inner orbit $2a$ for a given energy and given Z . The comparison with the numerical results [3] at $E_{\text{at}} = -1$ (table 1) demonstrates 5–10% agreement. The reason due to which (3) is less accurate than (2) is probably connected with some oscillations of the outer electron (about 3%) that are well averaged when we compute the minimum position x_{min} (which was defined as the average value for the data presented in [3]) while the contribution of this uncertainty in the E_{at} is apparently more important. Analogous to the derivation of (3) it is easy to find that the ionization energy for the outer electron is $I = (Z + 2 - 3Z^{1/3})/2a$.

Another point which can be seen from the data of table 1 is that the agreement becomes worse for larger values of Z . Also numerical results of [3] show that the stable position for the outer electron seems to disappear for $Z > 12.5$. This could be understood from the comparison of the frequency of inner electron $\omega_{\text{inn}} = Z^{1/2}/a^{3/2}$ with the frequency ω_{out} of small oscillations of outer electron near the minimum x_{min} :

$$S = \frac{\omega_{\text{inn}}}{\omega_{\text{out}}} = \frac{4}{\sqrt{3}} \frac{Z}{(Z^{2/3} - 1)^2}. \quad (4)$$

For not large values of Z this ratio is quite large which justifies the averaging approximation over inner electron motion. For helium $S = 13.4$ that is in a good agreement with the numerical value 14.78 of [6]. However, with the increase of Z the ratio in (4) decreases and it becomes equal to the golden mean value 1.618 at $Z \approx 11$. Due to that for large $Z > 11$ the average field approximation starts to be violated and the point x_{min} becomes unstable. This is probably the reason why the numerical experiments show disappearance of the stable state for $Z > 12.5$.

It is interesting to note that for $Z < 1$ the effective potential still has the stable point at x_{min} given by (2) but this point now corresponds to the maximum of the potential and is unstable. In this case x_{min} is negative. This means that the outer electron for $Z > 1$ is now located on the other side of the nucleus (let us say at the left-hand side, while the inner electron remains on the right-hand side from the centre). If we replace the electron on the left by a positron then the sign of the potential will be changed to the opposite one. In that case the effective potential for the positron has a minimum at x_{min} and therefore such a configuration for this unusual 'ion' is stable. Such a 'posion' consists of the nucleus with charge $Z < 1$, electron moving at the right side and positron located at the minimum

given by (2) at the left side. The ratio of the electron frequency to the frequency of small oscillations of the positron is equal to $S = 4Z/\sqrt{3}(1 - Z^{2/3})^2$. For Z close to 1 this ratio is large and utilization of averaging over fast electron oscillations is well justified. However, for $Z < 0.2$ the ratio S becomes less than 1. This indicates that for $Z < 0.2$ the 'posion' becomes unstable and fast ionization takes place. Let us mention that the 'posion' structure is quite different from the standard positronium ($Z = 0$). In the posion the positron is fixed and the electron is doing fast oscillations around the ion Z . While in the positronium both particles are always moving in the symmetric way around the centre of mass. Since only relative charge is important the discussed situation can be realized for charged particles when the charge in the centre $|Z_1|$ is less than the charge of the particles $|Z_2|$ moving around the centre.

In conclusion, the analytical approach based on the derivation of effective potential by averaging over fast oscillations of the inner electron allowed us to determine the equilibrium positions for the slow outer electron which are in 1% agreement with the numerical results [3]. The effective potential (1) is quite similar to the molecular potential and therefore the appearance of the molecular series of levels discussed in [7] (corresponding to excitations in this potential) seems to be quite natural. The conditions of applicability of this averaged potential are also defined ($S \gg 1$). It is shown that for the charge $Z < 1$ the ion has a stable configuration if the slow ('outer') electron is replaced by a positron ('posion').

References

- [1] Richter K and Wintgen D 1990 *Phys. Rev. Lett.* **65** 1965
- [2] Richter K and Wintgen D 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** L565
- [3] Richter K, Briggs J S, Wintgen D and Solov'ev E A 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 3929
- [4] Casati G, Guarneri I and Shepelyansky D L 1989 *IEEE J. Quantum Electron.* **24** 1420 equation (48)
- [5] Landau L D and Lifshitz E M 1973 *Mechanics* (Moscow: Nauka)
- [6] Richter K, Tanner G and Wintgen D 1993 *Phys. Rev. A* **48** 4182
- [7] Ostrovsky V and Prudov N 1993 *J. Phys. B: At. Mol. Opt. Phys.* **26** L263