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LETTER TO THE EDITOR

CLASSICAL SPECTRUM OF AN OSCILLATORY HELIUM MODEL

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A generalization of an oscillatory two-electron atomic system, first proposed by Langmuir, has been studied numerically, by calculating electron classical orbits. By applying semiclassical quantization procedure, energy spectrum of the system is evaluated.

Nonseparable systems are subjects of extensive studies nowadays, within modern semiclassical theory, because it was there that the *Old quantum theory* failed to provide proper answers to the problem of finding reasonable correct energy spectra, beyond the hydrogen atom[1]. Apart of problems with mainly academic interest, some realistic physical systems have been treated semiclassically, e. g. coupled anharmonic oscillators[2,3], hydrogen atom in an external field[4], two-electron atomic systems[5], etc. Helium-like atoms provide a particular chalenge to the semiclassical theory, because of the strong interaction between electrons, but nevertheless a considerable improvement with respect to Bohr's original planetary model, has been achieved. On the other hand, almost all of these calculations start with Keplerian orbits, as all early planetary models did. One of exceptions was Langmuir's oscillating model[6], which has been reexamined recently in the light of the modern (semi) classical theory[7]. Here we report further examinations of the oscillating two-electron model, via numerical studies of the bounded electron motions.

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Generally, one can divide all planar two-electron models into two broad classes: (i) configurations with two electrons moving along different paths, the whole configuration being deprived of any symmetry (e. g. Lande's model); (ii) symmetric configurations with two completely equivalent electrons, e. g. Bohr's planetary and Langmuir's oscillatory models. We further subdivide symmetric configurations into two subclasses: (a) rotational and (b) oscillating models, as examplified by Bohr's and Langmuir's models mentioned, respectively.

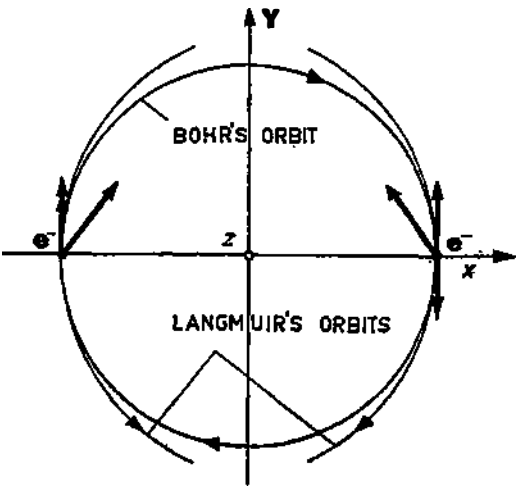

Fig. 1. Bohr's and Langmuir's ($L2$) electron orbits, for $Z = 2$. Parallel ($L2$) and antiparallel (Bohr) velocities indicate the corresponding initial conditions.

Let the electrons be initially situated on the opposite sides of the nucleus with charge Z (atomic units are used throughout), placed at the origin (see Fig. 1.). We distinguish two sets of initial conditions: (a) $\vec{v}^{(1)} = -\vec{v}^{(2)}$, with $v^{(1,2)} = v_B$, where v_B denotes Bohr's velocity, which provides for the ground state energy: $E_B = -3.0625$ a. u.; (b) $v_x^{(1)} = -v_x^{(2)}$, $v_y^{(1)} = v_y^{(2)}$. Case (b) initial values ensure the axial symmetry for all t. Standard Langmuir's model requires further: $v_x^{(1)} = v_x^{(2)} = 0$, $v_y^{(1)} = v_y^{(2)} = v_L$, with Langmuir's ($v_L$) velocity ensuring that each of electrons moves along a segment of its own circle.

We have restricted ourselves to a subclass of the oscillating models with: $v_x^{(1)} = v_x^{(2)} = 0$, but v_y different from v_L. Two cases are examined in particular:

I. $v_y = v_B$

Here, v_B means the velocity wich would initiate motion along a common circular orbit for both electrons, if $v_y^{(1)} = -v_y^{(2)}$ were taken (instead of $v_y^{(1)} = v_y^{(2)}$). The resulting trajectory of one of electrons (the other being a mirror image across Oy axis) is plotted in Fig. 2. Within numerical error, the electron paths appear closed, after 16 crossings of Oy axis. The covered part of the configuration space is clearly bounded by four caustics. The outer caustic turns out to be a part of an almost circular curve, as indicated in Fig. 2, whereas the inner caustic appears to consists of two segments of circles with centres indicated by A and B points in Fig. 2.

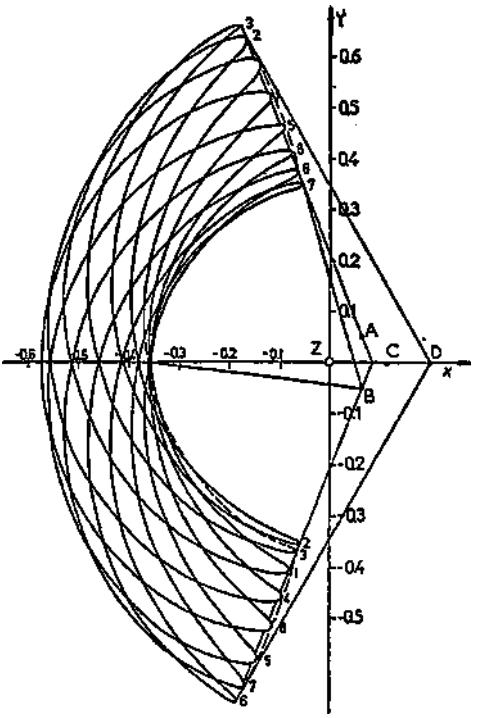

Fig. 2. Periodic orbit of one of the electrons for $v_l = v_B$, for $Z = 2$. Points A and B indicate centres of circles, whose segments the inner caustic consists of. Point C denotes the centre of circle for the corresponding Langmuir's orbit (see text), while D is the centre of the circle which approximates the outer caustic. Lateral caustics are indicated by dashed lines.

We now attempt to quantize the system energy by imposing approximate quantization conditions on the corresponding action function. We first observe that, after imposing constraints:

$$x^{(1)} = -x^{(2)}, \quad v_x^{(1)} = -v_x^{(2)}, \quad y^{(1)} = y^{(2)}, \quad v_y^{(1)} = v_y^{(2)}$$

via corresponding initial conditions, our system becomes two-dimensional and we restrict ourselves to a single electron orbit, as shown in Fig. 2. The Einstein-Brillouin-Keller quantization rule requires that action A_k satisfies

$$A_k = \oint_{C_k} \vec{p} \cdot \mathrm{d}\vec{q} = \left(n_k + \frac{\alpha_k}{4}\right) 2\pi, \quad n_k = (0), 1, 2, \ldots, \; k = 1, 2, \ldots N \qquad (1)$$

where N is number of degrees of freedom, α_k is so called Maslov index and integration is carried out along topologically distinct curves C_k in the configuration space. The choice of α_k depends on the type of motion. Generally, it assumes value 0 for rotational and 2 for vibrational motion, but in practice some ambiguities

appear. Our case is not a proper one for *EBK* theory, since we restrict ourselves in advance to periodic motion. Hence, the system appears more classical than semiclassical.

In quantizing electron motion we follow closely the procedure due to Delos et al.[7], applied to the hydrogen atom in a (strong) magnetic field. Eq. (1) reads:

$$S_i = \oint_{C_k} (p_x \, dx + p_y \, dy), \qquad i = 1, 2, \ldots, 8 \tag{2}$$

where C_i is a part of the electron orbit which starts, say, at a point on Oy axis, then crosses once again the same axis and ends up at a point on Oy axis, not far away from the starting point (see Fig. 2). Since S_i varies somewhat with i, as shown in Table 1, we take an average value for the action S_i:

$$S = \langle S_i \rangle_i = 4.6520 \tag{3}$$

with standard deviation:

$$\sqrt{\sigma} = 0.1505. \tag{4}$$

TABLE 1

i	1	2	3	4	5	6	7	8
S_i	4.799	4.6286	4.5242	4.4722	4.7495	4.8723	4.4379	4.7325

Partial actions S_i (see text) along the curve from Fig. 2.

Now, as can be infered from Fig. 2, C_i touches four caustics, and as each is supposed to contribute $\pi/2$ to the phase of a corresponding wave function, one has:

$$S = 2\pi n, \qquad n = 1, 2, \ldots \tag{5}$$

In order to obtain the lowest energy level: E_1, we scale the configuration which has provided S (Eq. (3)), by applying the so called similarity transformations:

$$E \to \lambda E, \quad \vec{r} \to \frac{1}{\lambda} \vec{r}, \quad S \to \frac{1}{\sqrt{\lambda}} S \tag{6}$$

what yields for the total ground-state energy:

$$E_1 = -1.6788 \text{ a. u. } (-45.68 \text{ eV}) \tag{7}$$

This is to be compared with $L2$ configuration[7], which possesses: $E_1 = -48.0$ eV. The latter case is achieved by increasing v_y until $v_y = v_B$ is reached, when the outer and inner caustics merge and coincide with the very (degenerated) orbit. By further increasing v_y, nonperiodic motion reappears, until eventually new perio-

dic orbit shows up. Numerical calculations have revealed the existence of at least one of these configurations, namely, one has for:

II. $v_y = v_L/v_B$

similar configuration, as shown in Fig. 3. The covered part of the configuration space lies now on the outer part (relative to the $L2$ orbit) of the entire configuration space. By repeating the procedure once again (this time, however, only S_1 has been evaluated), we get for the lowest energy level:

$$E_1 = -1.6768 \text{ a. u. } (-45.62 \text{ eV}) \tag{8}$$

which coincides, approximately, with the value found for case I.

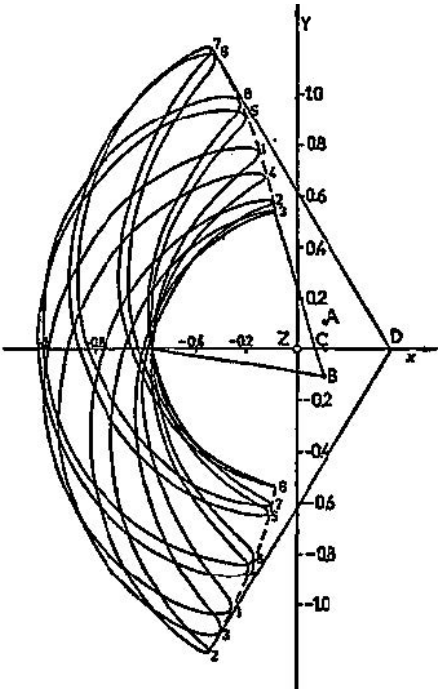

Fig. 3. The same as in Fig. 2, for $v_t = v_L/v_B$. Note that the radius of the Langmuir's orbit is the segment from the inner caustic to the point C, whereas in Fig. 2 it goes from C to the outer caustic.

Numerical analysis has made, therefore, an interesting feature of the oscillatory model comes out: by varying the initial velocity v_y around Langmuir's initial value v_L, new periodic orbits appear, but E_{L2} turns out to be minimum (ground state) energy. Note that we have not examined intermediate values: $v_B < v_y < v_{L2}$, $v_{L2} < v_y < v_{L2}/v_B$ where additional periodic orbit may appear, but the above conclusion seems reasonably safe against this possibility. Langmuir's configuration thus turns out stable against neighbouring *modes* of oscillation.

Strictly speaking, the above analysis is applicable only for highly excited states, which, according to the scaling laws, have the energies:

$$E_n = E_1/n^2, \qquad n = 2, 3, 4, \ldots \tag{9}$$

making the higher overtones appear. This is the same as with Bohr's planetary atom and is a general feature of Coulombic systems[8].

The present calculations confirm the earlier findings[7] that oscillating models are much inferior to Bohr's planetary model in providing ground-state energy of two-electron atoms.

Acknowledgments

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KLASIČNI SPEKTAR JEDNOG OSCILATORNOG MODELA HELIJUMA

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Jedno uopštenje Langmuirovog dvoelektronskog oscilatornog atomskog modela proučavano je numerički, računajući klasične putanje elektrona. Primenjujući modernu teoriju semiklasične kvantizacije, dobijen je energetski spektar sistema.