Langmuir's Helium-Like Models Revisited

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Classical two-electron configurations, proposed by Langmuir in the days of Old Quantum Theory as models for helium-like atoms, have been examined making use of modern semiclassical theory for the periodic orbits quantization. Combining both analytical and numerical investigations, energy spectra for the rotor-like and oscillator-like models have been evaluated, for the nuclear charges $Z = 1, 2, 3, 6$. No essential improvement of the original result (for $Z = 2$) is obtained, signifying that either configuration turns out to be inferior to the simple Bohr's planetary model.

Stability of these systems with respect to small perturbations has been examined and a general criterion for selecting classical models as candidates for atomic orbitals within the semiclassical theory is discussed.

I. Introduction

Twelve years had passed since Planck's introduction of the energy quantization at the atomic levels before Bohr set up his theory of the hydrogen atom, the cornerstone of the Old Quantum Theory (OQT, e.g. M. Born [1]). Another twelve years elapsed before the Quantum Mechanics was set up and the semiclassical theory was virtually abandoned. In-between, leading theoreticians of the time spent much time trying to apply the Bohr-Sommerfeld quantization rule to the few-electron atoms, notably helium. As it is well known, the helium problem was satisfactorily solved (at least in principle) within the new quantum theory (which at the same time provided a conceptual explanation of why the semiclassical methods had failed), but it was only recently that we have properly understood why the OQT was so successful in explaining the energy structure of the hydrogen atom. Only after the so called *correspondence identities* for the purely Coulomb interaction have been established (see, e.g. A. Norcliffe [2]), have we realized how much the hydrogen atom is an exceptional case in many respects which at the same time have fold us where the limits of the method based on the concept of classical trajectory lie.

On the other hand, the renewed interest in the semiclassical methods (see, e.g. I. Percival [3]) has again actualized the old problem of atomic physics, which may be cast in the form of the question: What are the proper quantization rules for many-particle systems? The answer to this question is the principal achievement of the presentday semiclassical theory, in the form of the so called Einstein-Brillouin-Keller (EBK) quantization rule, which for the particular case of periodic orbits can be generalized [4] to the form (for a system with N degrees of freedom)

$$E = S^{-1}\left[2\pi\left(n + \frac{\lambda}{4}\right)\right] + \sum_{i=1}^{N-1}\left(m_i + \frac{1}{2}\right)\omega_i(E)\,, \quad n, m_i - \text{integers}\,, \qquad (1)$$

where S is the action function along the periodic orbit, λ the number of turning points and $\omega_i(E)$ are so called stability frequencies. The latter reduce to the normal mode frequencies in the case of small (harmonic) perturbations of the reference orbit [4]. In fact, first steps towards a better understanding of the two-electron atoms quantization problem have already been made [5], [6] with encouraging results. In [5] a brief review of the OQT principal helium models has been given, including those proposed by Langmuir (1921). Employing alternatively perturbational and variational methods to the so called Bohr-Kramers model, considerable improvements of the ground-state energy have been achieved [5].

Strictly speaking, from an analytical point of view, we are not fully equipped to address the problem of nonseparable systems, for it is only the quasi-one-body problem that can be fully solved analytically, both within classical and quantum

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mechanical approaches. In case of two electrons moving in the field of an (infinitely heavy) nucleus of charge Z (atomic units are used throughout, unless otherwise stated), one must resort to numerical calculations in evaluating particle trajectories, unless the system possesses a high degree of symmetry that makes it a (quasi) one-particle problem. As we shall see later on, Langmuir's models can serve as paradigms of this problem.

There is another reason which makes the search for a new insight into the semiclassical atoms appealing, and that is the question of whether one can set up a general criterion as to the selection of those classical orbits among all possible ones, that are candidates for serving as reference trajectories suitable for quantization. In the present work we attempt to give an answer to this question, by examining the stability of particle motions along particular trajectories, with respect to (small) perturbations. To this end, we make use of a recently developed classical method for evaluating the classical motion of a charged particle both in the continuum [7] and discrete spectra [8], [9]. In the latter work, autoionizing spectra for the system $(Z + e^- + e^+)$ have been evaluated, using a combined EBK procedure. In the next section we apply the same method to the $(Z + e^- + e^-)$ system and calculate the energy terms for two particular configurations of reference orbitals. As we shall see, in neither case does the improved method provide an essential improvement of the original Langmuir's results. In the last section, we discuss the problem within a broader context of the choice of reference configuration, as well as the prospects of the present method for further applications.

II. Helium-like classical models

II.1. Preliminary considerations

Generally, two-electron atom classical configurations can be classified into three main categories: (a) rigid-body (rotor-like) models, (b) oscillating models, (c) mixed cases. The original Bohr's model of the ground-state energy of He belongs to category (a), and though the simplest of all classical configurations, it yielded an energy closest to the experimental one among old models (see [4], [5]). Linear oscillating (excited) helium states, based on the so called *free fall* models, have been discussed by Dimitrijević et al. [10]. Here, zero angular momentum configurations cannot be quantized, however, without referring to related plane configurations, or to more refined quantization rules, like EBK (which was one of the reasons why Bohr discarded them in his hydrogen semiclassical theory [1]). Mixed models are generally much more involved, like Lande's and the Bohr-Kramers model (see [4], [5]; see also Van Vleck's even more complicated model [11]).

The general ideas in determining an energy spectrum in the OQT was to solve first the (classical) problem of (quasi) periodic motion, express the trajectories in terms of action-angle variables and then to quantize the action *along the actual trajectory*. The modern semiclassical theory differs from the old one in two important respects (see [3]): (i) It introduces semiinteger quantum numbers (Maslow indices); (ii) the evaluation of the (canonically invariant) sum under the integral for the action [5] along a curve C_k need not correspond to an actual orbit. The latter feature of the EBK quantization condition enables one to treat nonseparable, aperiodic systems with very complicated trajectories. As we shall see below, one of Langmuir's models [12] belongs to the separable class of Hamiltonians, whereas for the other one can find an approximate analytical solution (at least for $Z = 2$). Here we restrict ourselves to the case of periodic orbits (but see concluding remarks).

II.2. Rotator model of helium-like systems. L1

Let an infinitely heavy charge Z be situated at the origin, with two electrons at

$$\boldsymbol{r}_1 = r\,\hat{\boldsymbol{r}}_1\,, \quad \boldsymbol{r}_2 = r\,\hat{\boldsymbol{r}}_2\,. \tag{2}$$

We allow the system to rotate around the axis through the origin, parallel to the vector $\boldsymbol{r}_1 - \boldsymbol{r}_2$ (see Fig. 1), with an angular velocity Ω. From the balance of the centrifugal and Coulomb forces, one has the relation

$$r = (4Z)^{1/3}\,b\,. \tag{3}$$

For $Z = 2$ it follows that $\Phi = \pi/6$ and the three charges form an equilateral triangle which rotates around the $0y$ axis. Since we have here a purely rotational motion, (1) reduces to the standard Bohr-Sommerfeld condition*, and the distance from the

* We disregard for the moment the second term of (1).

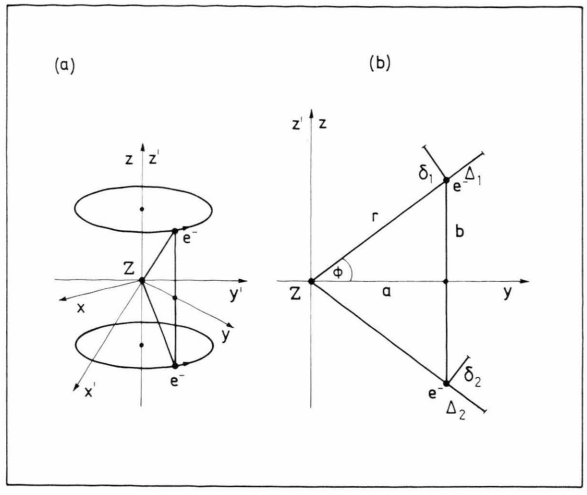

Fig. 1. Langmuir's rotating helium-like model (L1). Primed quantities refer to the laboratory and unprimed to the body-fixed reference systems.

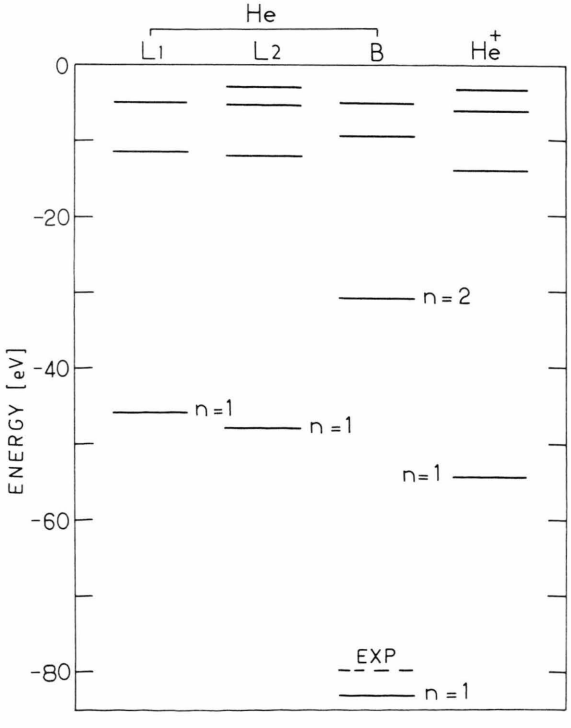

Fig. 2. Helium atom energy level schemes for Langmuir's models L1 and L2 (see text) and Bohr's planetary model B. He^+ levels are shown for comparison, too.

origin is

$$r_n = \frac{4(4Z)^{1/3}}{[(4Z)^{2/3}-1]^2}\, n^2, \quad n = 1, 2, 3, \ldots . \tag{4}$$

The total energy of the system is then

$$E_n = \frac{[1-(4Z)^{2/3}]^3}{n^2}. \tag{5}$$

For $Z = 2$, one has for the lowest level ($n = 1$):

$$E_1 = -45.917\ \text{eV}, \tag{6}$$

which yields the first ionization potential: $E_{\text{ion}} = -8.5$ eV (see Fig. 2) for Langmuir's first model (L1). Being negative, the last value signifies that the system is imbedded into the continuum (autoionizing level) and can decay into He^+ and a free electron. The reason for this too high energy level, as compared with planetary Bohr's model, is obvious: the electrons appear too close to each other and their repulsion dominates. As the charge Z increases, Φ becomes smaller (see (3)) and the electrons approach each other even more closely. For large Z, r_n behaves as n^2/Z, i.e. similarly to the planetary model.

We now examine the behaviour of the system under small perturbations of the reference orbits. Let the radius vectors in the body fixed frame of reference be now

$$\boldsymbol{r}_1 = (r + \Delta_1)\,\hat{\boldsymbol{n}}_1 + \delta_1 \hat{\boldsymbol{m}}_1 + \nabla_1 \hat{\boldsymbol{i}}, \tag{7}$$

$$\boldsymbol{r}_2 = (r + \Delta_2)\,\hat{\boldsymbol{n}}_2 + \delta_2 \hat{\boldsymbol{m}}_2 + \nabla_2 \hat{\boldsymbol{i}}, \tag{8}$$

$$\hat{\boldsymbol{n}}_{1,2} = \frac{1}{(4Z)^{1/3}}\,[\sqrt{(4Z)^{2/3}-1}\,\hat{\boldsymbol{j}} \pm \hat{\boldsymbol{k}}], \quad \hat{\boldsymbol{n}}_{1,2} \parallel \boldsymbol{r}_{1,2}, \tag{9}$$

$$\hat{\boldsymbol{m}}_{1,2} = \frac{1}{(4Z)^{1/3}}\,[\hat{\boldsymbol{j}} \pm \sqrt{(4Z)^{2/3}-1}\,\hat{\boldsymbol{k}}], \quad \hat{\boldsymbol{m}}_{1,2} \perp \boldsymbol{r}_{1,2}, \tag{10}$$

where $\Delta_1, \Delta_2, \ldots$, are small deviations from the leading trajectories. Substituting (7) and (8) into Newton's equations [13]

$$\frac{\mathrm{d}^2 \boldsymbol{r}_1}{\mathrm{d}t^2} = -Z\frac{\boldsymbol{r}_1}{r_1^3} + \frac{\boldsymbol{r}_1 - \boldsymbol{r}_2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|^3} \tag{11}$$

and retaining terms linear in Δ_1/r, etc. (see [13]), one obtains, taking account of the constraints

$$\Delta_1 + \Delta_2 = \delta_1 + \delta_2 = \nabla_1 + \nabla_2 = 0, \tag{12}$$

the following equations for the deviations:

$$\frac{r^3}{Z}\frac{\mathrm{d}^2\nabla_1}{\mathrm{d}t^2} = 0\,, \quad a = \sin\Phi\,, \quad b = \cos\Phi\,, \tag{13a}$$

$$\frac{r^3}{Z}\frac{\mathrm{d}^2\Delta_1}{\mathrm{d}t^2} = (2+b^2)\,\Delta_1 - 3\,a\,b\,\delta_1\,, \tag{13b}$$

$$\frac{r^3}{Z}\frac{\mathrm{d}^2\delta_1}{\mathrm{d}t^2} = -\,a\,b\,\Delta_1 - 3\,b^2\,\delta_1\,. \tag{13c}$$

Equation (13a) is decoupled from the rest and is solved to give

$$\nabla_1 = A\,t + B\,, \quad \nabla_2 = -\,\nabla_1\,. \tag{14}$$

Solution (14) signifies that the system is unstable with respect to perturbations along the reference trajectories of the electrons, with one of the particles advancing and the other legging behind. In order to see what is the behaviour of the atom with respect to the perpendicular deviations, we write (13b)–(13c) in the matrix form

$$\frac{r^3}{Z}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\begin{Bmatrix}\Delta_1\\ \delta_1\end{Bmatrix} = \begin{Bmatrix}2+b^2-3\,a\,b\\ -\,a\,b \quad -3\,b^2\end{Bmatrix}\begin{Bmatrix}\Delta_1\\ \delta_1\end{Bmatrix} = \mathbf{BF}\,, \tag{15}$$

Now, let a matrix $\mathbf{T}$ be such that

$$\mathbf{T}_0^{-1}\,\mathbf{B}\mathbf{T} = \mathbf{\Lambda} = \begin{Bmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{Bmatrix}. \tag{16}$$

Then (15) becomes

$$\frac{r^3}{Z}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\begin{Bmatrix}G_1\\ G_2\end{Bmatrix} = \mathbf{\Lambda}\begin{Bmatrix}G_1\\ G_2\end{Bmatrix},$$

$$\mathbf{G} = \begin{Bmatrix}G_1\\ G_2\end{Bmatrix} = \mathbf{T}^{-1}\,\mathbf{F}\,. \tag{17}$$

From the corresponding secular equations one easily finds the characteristic values of $\mathbf{B}$:

$$\lambda_{1,2} = \frac{1}{\zeta^2} \pm \left(\frac{1}{\zeta^4} - \frac{9}{\zeta^2}\right)^{1/2}, \quad \zeta = (4\,Z)^{1/3}, \tag{18}$$

so that one has from (17) (noticing that $\lambda_1 > 0$, $\lambda_2 < 0$, $Z > 1$):

$$G_1 = C_1^{(1)}\,e^{\alpha t} + C_2^{(1)}\,e^{-\alpha t}\,, \tag{19a}$$

$$G_2 = C_1^{(2)}\,e^{i\omega t} + C_2^{(2)}\,e^{-i\omega t} \tag{19b}$$

with

$$\alpha = \frac{1}{r}\left(\frac{Z\lambda_1}{r}\right)^{1/2}, \quad \omega = \frac{1}{r}\left(-\frac{Z\lambda_2}{r}\right)^{1/2}. \tag{20}$$

We do not write the explicite expression for $\mathbf{T}$ but only note that it appears nonunitary, because $\mathbf{B}$ is non-Hermitean. From (17) we obtain

$$\Delta_1 = F_1 = T_{11}[C_1^{(1)}\,e^{\alpha t} + C_2^{(1)}\,e^{-\alpha t}] + T_{12}[C_1^{(2)}\,e^{i\omega t} + C_2^{(2)}\,e^{-i\omega t}]\,, \tag{21}$$

$$\delta_1 = F_2 = T_{21}[C_1^{(1)}\,e^{\alpha t} + C_2^{(1)}\,e^{-\alpha t}] + T_{22}[C_1^{(2)}\,e^{i\omega t} + C_2^{(2)}\,e^{-i\omega t}]\,. \tag{22}$$

We see that the solutions are mixtures of terms growing (decreasing) with time and oscillatory terms (with angular frequency ω). In order to get an insight into the actual contributions of these qualitatively different terms, we write down numerical values of T_{ij} for $Z = 2$ ($\zeta = 2$):

$$T_{11} = -\,0.99643\,, \quad T_{12} = 0.24637\,,$$
$$T_{21} = 0.08444\,, \quad T_{22} = 0.96917\,. \tag{23}$$

Evidently, $\mathbf{T}$ is almost unitary (and quasidiagonal) and as dominant term in (21) appears that with T_{11}, while for δ_1 nonoscillatory admixture (with T_{21}) turns out to be negligible. Hence, for this particular case, the system is also unstable with respect to radial perturbations, and (almost) stable concerning $\delta_{1,2}$ deviations. The situation is similar for other Z-values, since one has from (18)

$$2.76 < \lambda_1 < 3\,, \quad -3 < \lambda_2 < -1.96\,, \quad 1 \leqq Z\,. \tag{24}$$

δ-oscillations provide additional kinetic energy to the atom, which can be evaluated by the standard formula [9]

$$\Delta E_v^{(n)} = (v + \tfrac{1}{2})\,\omega_n\,, \quad \omega_n = \omega(r_n)\,. \tag{25}$$

These oscillations possess the (classical) amplitudes

$$A_v^{(n)} = \frac{\sqrt{2\,\Delta E_v^{(n)}}}{\omega_n} = \frac{\sqrt{2v+1}}{\omega_n}\,. \tag{26}$$

However, from the condition $\delta \ll r$ (linear approximation) it follows that only levels with large n can have these normal mode excitations. To fix the idea how much this restriction is severe, we take the case: $Z = 2$, $v = 0$, and evaluate from $A_0^{(n)} \ll r_n$:

$$\sqrt{n} \gg 3\,. \tag{27}$$

It is interesting to note that from (3) and (4) one has the limiting configuration

$$\lim_{Z\to+\frac{1}{4}} \Phi = \pi/2\,, \quad \lim_{Z\to+\frac{1}{4}} r_n \to \infty\,. \tag{28}$$

The system acquires infinite dimensions at zero energy, with two electrons aligned along a straight line through the nucleus. Hence, in this (unphysical) limit, Bohr's planetary and Langmuir's models merge ("hypo-Bohrean model"), with the only difference that Bohr's planetary system is a zero-energy atom for any (properly quantized) r_n. In the other extreme limit of an infinitely charged nucleus, one has

$$\lim_{Z \to \infty} \Phi = 0 \tag{29}$$

and the system becomes an "anti-Bohrean" case, with two electrons almost in contact, revolving around the charge Z.

II.3. Oscillating model of helium-like systems: L2

Let two electrons be situated on opposite sides of the heavy charge Z, as shown in Fig. 3, with equal distance r_0 from the nucleus. We endow the electrons with initial velocities $v_1^{(0)}$ and $v_2^{(0)}$ and seek a periodic motion solution. If one chooses $v_1^{(0)} = -v_2^{(0)}$, the solution is the well-known Bohr's planetary model with the ground-state energy $E_B = -3.0625$ a. u. Langmuir started with the initial condition

$$v_1^{(0)} = v_2^{(0)} \tag{30}$$

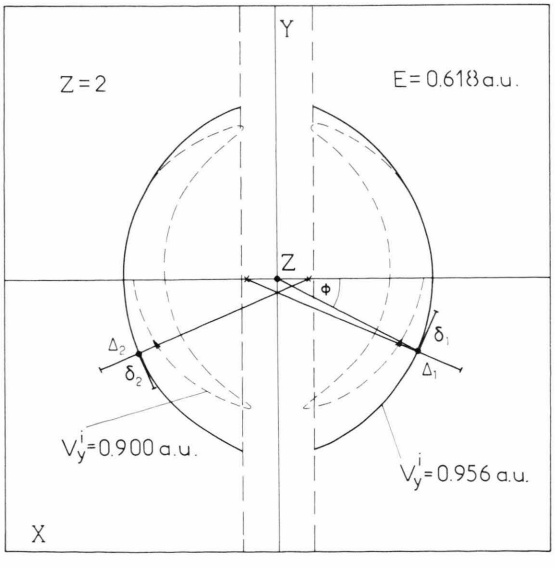

Fig. 3. Langmuir's oscillating helium model (L2)-numerical results for two sets of initial conditions (see text).

searching for periodic orbits with axial symmetry. The Hamiltonian of the system is

$$H = -\frac{2Z}{r} + \frac{1}{2r\cos\Phi}, \tag{31}$$

which is nonseparable. Langmuir solved the corresponding classical equation numerically and found two remarkable features of the model: (i) the orbits appear almost exactly as parts of circles centred at points displaced from the origin by a distance $\varrho \approx 0.19\, r_0$; (ii) if the configuration is scaled so that the angular momenta satisfy $l_1^{(0)} = l_2^{(0)} = \hbar$, radii of the circles are identical with that of Bohr's ground-state atom.

With property (ii) considered as quantization condition, Langmuir obtained for the ionization potential $I = 25.62$ eV, which at the time was fairly close to that measured experimentally (25.4 ± 0.25) eV. Nevertheless, Langmuir was unable to formulate a convincing quantization rule for this nonseparable system. Two attempts to quantize the atom *via* the Sommerfeld condition

$$\oint p\, \mathrm{d}q = n h\,, \quad n = 1, 2, 3, \ldots, \tag{32}$$

with the alternative choices 1) $q = \Phi$, 2) $q =$ distance from the medium point (at $y = 0$ in Fig. 3) along the orbits, failed even to provide the proper sign of the ionization potential, the latter turning out to be -4.58 eV and -5.55 eV, respectively.

In order to reexamine the L2 model, we solved (11) numerically, with the initial condition (30), by varying, at a fixed r_0, v_0. The results are shown in Fig. 3 for $r_0 = 2.2857\, a_0$ and two values of v_0. As can be infered from Fig. 3, numerical calculations fully confirm Langmuir's findings, with $\varrho/r_0 \approx 0.2$ (Langmuir's more accurate result was 0.1953). From these numerical results one can evaluate configurations of any energy E', making use of the scaling laws for Coulomb interaction [14]:

$$E \to \frac{1}{\lambda} E\,, \quad r \to \lambda r\,, \quad t \to \lambda^{3/2} t\,, \quad s \to \sqrt{\lambda}\, S\,, \tag{33}$$

where λ is the real scaling parameter (not to be confused with the number of turning points in (1)).

We now evaluate the action function along the trajectory [3] (see Fig. 3), with $\lambda = 4$ the number of turning points in (1).

$$S = \oint (p_x\, \mathrm{d}x + p_y\, \mathrm{d}y) = 2\pi n\,, \quad n = 1, 2, 3, \ldots, \tag{34}$$

which, in combination with (33), provides for $n = 1$

$$E_1 = -48.0 \text{ eV} . \tag{35}$$

Hence, the EBK quantization rule yields an even worse ionization potential (-6.24 eV) than that obtained originally by Langmuir. It turns out, therefore, that it is an improper model which precludes it from being an adequate configuration for the ground-state helium, and not only an inappropriate quantization procedure, as employed by Langmuir.

We now attempt to answer a more fundamental question: why is the L2 model inferior to Bohr's planetary system? The question is more interesting in view of the common features of the two models quoted above. We examine, therefore, the stability of the oscillating model, similarly to the analysis in Section II.2. One observes, first, that an approximate relation holds (see Fig. 3):

$$r \approx R_0 - \varrho \cos \Phi . \tag{36}$$

Further, from the conservation of the total angular momentum

$$\boldsymbol{l}_1 + \boldsymbol{l}_2 = 0 , \tag{39}$$

one has the following constraints:

$$\delta_1 + \delta_2 = 0 , \quad \Delta_1 - \Delta_2 = 0 , \tag{40 a, b}$$

$$\nabla_1^2 + \nabla_2^2 + 2 \nabla_1 \nabla_2 \cos 2\Phi = 0 . \tag{40c}$$

From (40 c) we see that

$$\nabla_1 = \nabla_2 = 0 , \quad \Phi \neq 0 , \tag{41}$$

which means that the L2 model is essentially a plain configuration. Writing

$$\boldsymbol{r}_{1,2} \approx (R_0 - \varrho \cos \Phi + \Delta_{1,2}) \, \hat{\boldsymbol{n}}_{1,2} + \delta_{1,2} \hat{\boldsymbol{m}}_{1,2} , \quad \hat{\boldsymbol{n}}_{1,2} \parallel \boldsymbol{R}_0^{(1,2)} , \quad \hat{\boldsymbol{m}}_{1,2} \perp \boldsymbol{R}_0^{(1,2)} \tag{42}$$

one has

$$\frac{\mathrm{d}^2 \Delta_1}{\mathrm{d}t^2} = \frac{\Delta_1}{(R_0 - \varrho \cos \Phi)^3} \left(2Z - \frac{1}{2 \cos \Phi} \right) - \frac{\delta_1 \sin \Phi}{4 \cos^2 \Phi \, (R_0 - \varrho \cos \Phi)^3} , \tag{43 a}$$

$$\frac{\mathrm{d}^2 \delta_1}{\mathrm{d}t^2} = - \frac{\Delta_1 \sin \Phi}{2 \cos^2 \Phi \, (R_0 - \varrho \cos \Phi)^3} - \frac{\delta_1}{(R_0 - \varrho \cos \Phi)^3} \left(Z - \frac{1}{4 \cos \Phi} \right) . \tag{43 b}$$

The system (43) cannot be solved by the procedure applied to Equations (13). This can be seen by rewriting (43) in the matrix form

$$(R_0 - \varrho \cos \Phi)^3 \frac{\mathrm{d}^2}{\mathrm{d}t^2} \begin{Bmatrix} \Delta_1 \\ \delta_1 \end{Bmatrix} = \begin{Bmatrix} 2Z - \dfrac{1}{2 \cos \Phi} - \dfrac{\sin \Phi}{4 \cos^2 \Phi} & \\ - \dfrac{\sin \Phi}{2 \cos^2 \Phi} & - \left(Z - \dfrac{1}{4 \cos \Phi} \right) \end{Bmatrix} \begin{Bmatrix} \Delta_1 \\ \delta_1 \end{Bmatrix} . \tag{44}$$

A matrix diagonalizing the matrix on rhs of (44) would have time-dependent elements, *via* the (yet undetermined) function $\Phi(t)$. Hence, this matrix would not commute with the $I \mathrm{d}^2/\mathrm{d}t^2$ operator on the lhs of (44), and the diagonalization procedure fails. One may attempt to make use of an iterative procedure (see, e.g. [15], [16]), but such an elaboration would not help much, in particular in view of the absence of an exact analytical expression for $r(t)$.

One can estimate, however, the stability of the electron motion by making use of an approximate expression for $\Phi(t)$. One such simple form is

$$\Phi_1(t) = \Phi_{\max} \sin \left\{ 2\pi \frac{t}{T} \right\} , \tag{45}$$

where $\Phi_{\max} = \Phi(T/4)$, and T is the period of motion. A better approximation is found to be

$$\Phi_2(t) = \left\{ 1 + 2 (\Phi_{\max} - 1) \left(\frac{t}{T} \right)^{1/2} \right\} \sin \left\{ 2\pi \frac{t}{T} \right\} . \tag{46}$$

Both (45) and (46) are plotted in Fig. 4, together with the (exact) numerical solution. As can be seen from Fig. 4, (46) follows the exact curve very well, with $\Phi_{\mathrm{ex}}(0) = \Phi_2(0)$, $\Phi_{\mathrm{ex}}(T/4) = \Phi_2(T/4)$, and the relative deviations of the time derivatives turn out to be at the end points

$$\left. \frac{\delta \dot{\Phi}}{\dot{\Phi}_{\mathrm{ex}}} \right|_{t=0} = 0.0273 , \quad \left. \frac{\delta \dot{\Phi}}{\dot{\Phi}_{\mathrm{ex}}} \right|_{t=T/4} = 0.0414 . \tag{47}$$

In estimating the stability of the system, however, neither Φ_1 nor Φ_2 appear simple enough for allowing (44) to be solved analytically. One can estimate the "local stability" at a particular point on the electron path by assuming $\Phi = \Phi_0 = \text{const}$ and then solve (44) for the motion around Φ_0 in a similar

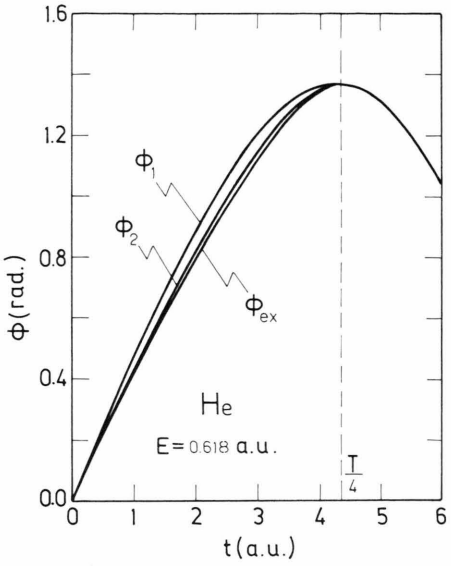

Fig. 4. Electron angular coordinate (see Fig. 3) as function of time (T-period). Exact numerical (Φ_{ex}), approximate (Φ_1 (45)), and improved approximate (Φ_2 (46)) solutions.

manner as it was done for (15). One obtains a general solution of the form (21) and (22), with increasing contribution from the terms with T_{12}, T_{21} as $\Phi \to \Phi_{max}$. However, since these solutions are valid only for $t \ll T/4$, there is no practical difference between the exponential (T_{11}, T_{21}) and oscillatory (T_{12}, T_{22}) terms. Hence, no long-term behaviour can be infered from such a piecewise analysis. On the other hand, the latter indicates that no sharp distinction can be drawn between Δ and δ deviatons in the L2 model, as opposed to the case with the L1 system from Section II.

$Z \neq 2$ configurations

In order to see whether the general behaviour of the L2 system changes with Z, we have calculated numerically electron orbits for $Z = 1, 3, 6$, also. These computations have revealed a number of interesting features common to the L2 helium-like models (see Fig. 5): (i) the electron orbits are again segments of circles, as for the neutral, (ii) the centres of these circles approach each other as Z increases, merging in the limit $Z \to \infty$, (iii) Φ_{max} increases and eventually reaches $\pi/2$, thus making electron orbits to contact each other on the $0y$ axis. Hence, for $Z \to \infty$ both electrons move along a common circle, but in a very different way compared with Bohr's planetary model. Here, one has a sort of an "oscillatory dipole", instead of Bohr's "rotating quadrupole". This limiting case may be called "meta-Bohrian" configuration.

In the same way as for $Z = 2$, the ground-state energies for $Z = 1, 3, 6$ have been evaluated and plotted in Fig. 6, against the nuclear charge, together with Bohr's planetary model values. The energies of the helium ion are shown too. As can be seen from Fig. 6, the E_{L2} energies appear embedded into the continuum, i.e. unstable against the decay

$$\mathrm{He}\,(n = 1) \to \mathrm{He}^+ + \mathrm{e} \tag{48}$$

for $Z < Z_0$, $Z_0 \approx 2.75$, and tend to merge with Bohr's values in the limit: $Z \to \infty$.

The principal objection to the L2 model is that, although the system possesses no angular momentum, individual particles do, and, what is a more serious shortcoming in view of the importance of adiabatic invariants in the OQT, those momenta are time-dependent.

If the constraint (39) is relaxed and nonzero values for the total angular momentum are allowed, the L2 configuration becomes the rotator-oscillator model, which might be called the "hyper-Bohrean" case. This sort of configuration has been examined

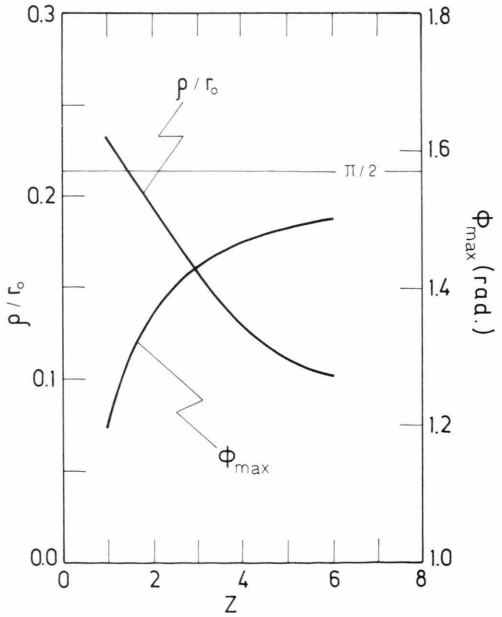

Fig. 5. Helium-like L2 atoms. ϱ-distance of the centre of a circle from the origin, r_0-initial (minimum) distance of the electron from the origin.

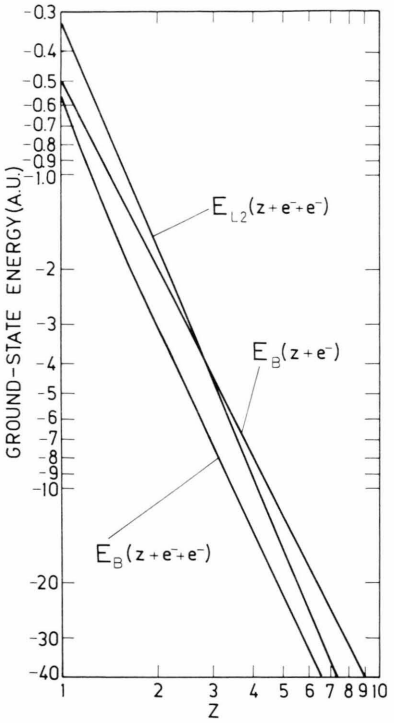

Fig. 6. Ground-state energies (see text) against nuclear charge Z.

in the study of the doubly excited helium atom (see, e.g. [17] and references therein). In fact, the L1 model cal also be transformed to this mixed case by rotation of the rotating triangle around the $0y$ axis (with $\Phi \to \pi/2$).

In view of the analytical difficulties in studying L2 stability, one obviously should resort to numerical investigations. These would, presumably, give an additional insight into the relevant distinction between regular and irregular spectra [18].

III. Concluding remarks and discussions

After the advance of Quantum Mechanics we know that the OQT is applicable only for states with large angular momenta of individual particles of the system, at least of those systems for which no correspondence identities are known. Therefore it is not surprising that the most straightforward extension of the hydrogen atom to helium-like systems, Bohr's planetary model, yields the best value for the ground energy. From that point of view both L1 and L2 may be candidates for the two-electron system doubly excited states at best. However, since there is no unique type of configuration to be adopted even for these excited atoms, the question arises as to which of the many different models is to be singled out and, if there are two or more equivalent alternatives, which one can be adopted *a priori* as the best for the ground state? This may be regarded as the principal aim of our attempt to classify possible configurations with respect to their instabilities.

In II.2. we have seen that the L1 model possesses a much higher energy than the corresponding Bohr's planetary configuration. Further, compared to the latter, L1 has one more unstable degree of freedom. We may, therefore, regard L1 as an unstable configuration, which easily colapses into Bohr's planetary case. Unfortunately, because we have been unable to solve the equation of motion for the unperturbed L2 case, and because of the additional difficulties with system (44), we could not complete this sort of analysis for the second Langmuir's model.

In view of the fact that in the ground state helium-like systems have both electrons with zero angular momentum, it is of interest to set up a hierarchy of models according to their (classical) resemblence with the ground-state (classical) configuration. It is clear that all rotating models lie the furthest from the classical picture of a quantum ground state. Oscillatory models, like L2, are better in that respect, since their angular momentum is zero, although individual momenta are not. Finally, so called *free fall* models, like the examined in [10], are the closest to the picture which a classical physicist may have of the zero-angular momenta systems. It is of interest, therefore, to examine such models and see what a set of the energy-level scheme they provide. Another interesting problem is the L2-like case with (quasi) periodic orbits, which fill a part of the two-dimensional configuration space. Some calculations along these lines are in progress and results will be published elsewhere.

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