Part I.

Asymmetric stationary points in a helium effective potential

Here, we use the basic formulas for *D*-dimensional three-particle systems that can be found in [*Sov. J. Nucl. Phys*. **50** (4), 1989 or *Sov. Phys. JETP* **70** (1), 1990]. Helium-like scaled Hamiltonian in *D* dimensions for S-states is

$$H = -\frac{1}{2(D-3)^2}\sum_{i,j=1}^{3}\frac{\partial}{\partial r_i}A_{ij}(r_1,r_2,r_3)\frac{\partial}{\partial r_j} + V_{\rm eff}(r_1,r_2,r_3) \qquad (1)$$

where

$$\mathbf{A} = \begin{pmatrix} \frac{1}{2} & 0 & \frac{r_1^2+r_3^2-r_2^2}{2r_1r_3} \\ 0 & \frac{1}{2} & \frac{r_2^2+r_3^2-r_1^2}{2r_2r_3} \\ \frac{r_1^2+r_3^2-r_2^2}{2r_1r_3} & \frac{r_2^2+r_3^2-r_1^2}{2r_2r_3} & 1 \end{pmatrix} \qquad (2)$$

is a symmetric matrix (off-diagonal elements equal to $\cos\theta_1$ and $\cos\theta_2$ expressed via distances), and

$$V_{\rm eff}(r_1,r_2,r_3) = -\frac{1}{r_1}-\frac{1}{r_2}+\frac{\lambda}{r_3}+\frac{1}{4}\frac{r_1^2+r_2^2}{r_1^2r_2^2+r_2^2r_3^2+r_3^2r_1^2-r_1^4/2-r_2^4/2-r_3^4/2} \qquad (3)$$

is an effective potential. Here, $r_3 = r_{12}$.

<u>Calculation of all asymmetric stationary points in the effective potential</u>

Here, we find all solutions (r_1,r_2,r_3) with $r_1 \neq r_2$ of the system of equations

$$\partial V_{\rm eff}/\partial r_1 = \partial V_{\rm eff}/\partial r_2 = \partial V_{\rm eff}/\partial r_3 = 0\,. \qquad (4)$$

Let us introduce variables

$$x = (r_1 + r_2)/r_3,\ y = r_1 r_2 / r_3^2,\ \text{and}\ z = r_3. \tag{5}$$

The following relation between derivatives holds:

$$\begin{pmatrix} \dfrac{\partial V_{\text{eff}}}{\partial r_1} \\ \dfrac{\partial V_{\text{eff}}}{\partial r_2} \\ \dfrac{\partial V_{\text{eff}}}{\partial r_3} \end{pmatrix} = \begin{pmatrix} \dfrac{1}{r_3} & \dfrac{r_2}{r_3^2} & 0 \\ \dfrac{1}{r_3} & \dfrac{r_1}{r_3^2} & 0 \\ -\dfrac{r_1 + r_2}{r_3^2} & -\dfrac{2r_1 r_2}{r_3^3} & 1 \end{pmatrix} \begin{pmatrix} \dfrac{\partial V}{\partial x} \\ \dfrac{\partial V}{\partial y} \\ \dfrac{\partial V}{\partial z} \end{pmatrix}, \tag{6}$$

where

$$V(x,y,z) = \frac{\lambda y - x}{yz} + \frac{1}{4z^2} \frac{x^2 - 2y}{x^2 - 2y + 2x^2 y - 1/2 - x^4/2} \tag{7}$$

is the effective potential, expressed in terms of variables (5).

The determinant of the transformation matrix (Jacobian) is $(r_1 - r_2)/r_3^3 \neq 0$. So, the system of equations (4) is equivalent to

$$\partial V/\partial x = \partial V/\partial y = \partial V/\partial z = 0. \tag{8}$$

Note, that solving (8), we miss some symmetric stationary points since (4) does not follow from (8) when $r_1 = r_2$ (Jacobian equals to zero).

Explicitly, equations (8) are

$$\begin{gathered} \frac{xy(-1 + x^4 - 4x^2 y + 8y^2) - (1 - x^2)^2 (1 - x^2 + 4y)^2 z}{yz^2 (1 - x^2)(1 - x^2 + 4y)} = 0 \\ \frac{-y^2 (1 + x^2) - x(1 - x^2)(1 - x^2 + 4y)^2 z}{y^2 z^2 (1 - x^2)(1 - x^2 + 4y)^2} = 0 \\ \frac{y(x^2 - 2y) + (x - \lambda y)(1 - x^2)(1 - x^2 + 4y) z}{yz^3 (1 - x^2)(1 - x^2 + 4y)} = 0 \end{gathered} . \tag{9}$$

All denominators in (9) should be non-zero, i. e. $y \neq 0$, $z \neq 0$, $1 - x^2 \neq 0$, and $1 - x^2 + 4y \neq 0$ (we shall prove below that $x \neq 0$, $1 + x^2 \neq 0$, and $\lambda(1 + x^2)(1 - 5x^4) - 8x(1 - 3x^2) \neq 0$ also). In terms of distances it means that $r_1 \neq 0$, $r_2 \neq 0$, $r_3 \neq 0$, $r_1 + r_2 + r_3 \neq 0$, $r_1 + r_2 - r_3 \neq 0$, $-r_1 + r_2 + r_3 \neq 0$, and $r_1 - r_2 + r_3 \neq 0$. If it is the case, then (9) is equivalent to the system of polynomial equations

$$\begin{gathered} xy(-1 + x^4 - 4x^2 y + 8y^2) - z' = 0 \\ -y^2(1 - x^4) - xz' = 0 \\ y(x^2 - 2y)(1 - x^2)(1 - x^2 + 4y) + (x - \lambda y)z' = 0 \end{gathered}, \tag{10}$$

where

$$z' = \left(1 - x^2\right)^2 \left(1 - x^2 + 4y\right)^2 z. \tag{11}$$

From (10), it follows that

$$z' = xy(-1 + x^4 - 4x^2 y + 8y^2) \tag{12}$$

together with a system of equations

$$\begin{gathered} x^2 - x^6 - y + 5x^4 y - 8x^2 y^2 = 0 \\ 2(-x^4 + x^6 - y + 4x^2 y - 5x^4 y - 4y^2 + 8x^2 y^2) + \lambda xy(1 - x^4 + 4x^2 y - 8y^2) = 0 \end{gathered}. \tag{13}$$

Note that $x \neq 0$ (proof: if $x = 0$ then $y = 0$, but such (x, y) does not satisfy equations (9)).

Solving (13) is straightforward, but rather cumbersome.

Replacing the second equation in (13) by $\lambda y(\text{first equation}) - x(\text{second equation})$, we arrive to an equivalent system of equations

$$\begin{gathered} x^2 - x^6 - y + 5x^4 y - 8x^2 y^2 = 0 \\ 2x^5 - 2x^7 + (2x - 8x^3 + 10x^5)y + (-\lambda + 8x - 16x^3 + \lambda x^4)y^2 = 0 \end{gathered}. \tag{14}$$

Replacing the second equation in (14) by $(-\lambda + 8x - 16x^3 + \lambda x^4)(\text{first equation}) + 8\text{x}^2(\text{second equation})$, we arrive to an equivalent system of equations

$$\begin{gathered} x^2 - x^6 - y + 5x^4 y - 8x^2 y^2 = 0 \\ -\lambda x^2 + 8x^3 - 16x^5 + 2\lambda x^6 + 8x^7 - \lambda x^{10} + (\lambda - 8x + 32x^3 - 6\lambda x^4 - 24x^5 + 5\lambda x^8)y = 0 \end{gathered}. \tag{15}$$

Dividing the second equation in (15) by non-zero common factor $1-x^2$, we obtain

$$\begin{aligned} x^2 - x^6 - y + 5x^4 y - 8x^2 y^2 = 0 \\ -\lambda x^2\left(1-x^2\right)\left(1+x^2\right)^2 + 8x^3\left(1-x^2\right) + \left[\lambda(1+x^2)(1-5x^4) - 8x(1-3x^2)\right]y = 0 \end{aligned} . \tag{16}$$

Let us consider two different opportunities. The first one: $\lambda(1+x^2)(1-5x^4) - 8x(1-3x^2) = 0$. Then from the second equation of (16) it follows that $-\lambda\left(1+x^2\right)^2 + 8x = 0$. These equations have the only solutions $x = 0$ when $\lambda = 0$ or $x = \pm 1$ when $\lambda = \pm 2$, but they don't satisfy (9). So, we consider only the second opportunity: $\lambda(1+x^2)(1-5x^4) - 8x(1-3x^2) \neq 0$. Then from the second equation of (16) it follows that

$$y = \frac{x^2(1-x^2)\left[\lambda(1+x^2)^2 - 8x\right]}{\lambda(1+x^2)(1-5x^4) - 8x(1-3x^2)} . \tag{17}$$

Eliminating y from (16), we arrive to an equation for x

$$x^5(x^2-1)^2(x^2+1)(2\lambda - 16x - \lambda^2 x + 16\lambda x^2 - 3\lambda^2 x^3 + 6\lambda x^4 - 3\lambda^2 x^5 - \lambda^2 x^7) = 0 . \tag{18}$$

Note that $x^2 + 1 \neq 0$ (proof: if $x^2 + 1 = 0$ then $y = -1/2$, and $1 - x^2 + 4y = 0$, but it does not satisfy (9)). Then, (18) is equivalent to the seventh-order algebraic equation

$$\lambda^2 x(1+x^2)^3 - 2\lambda(1+8x^2+3x^4) + 16x = 0 \tag{19}$$

that appears cannot be simplified further. So, there are generally (for $\lambda \neq 0$) seven stationary points corresponding to seven roots of the polynomial in lhs of (19).

<u>Summary of the computation of all asymmetric stationary points</u>

First, solve Eq. (19) in respect to x. Second, find y according to Eq. (17). Third, find z by the formula

$$z = \frac{xy(-1+x^4-4x^2y+8y^2)}{(1-x^2)^2(1-x^2+4y)^2} \tag{20}$$

that follows from (11) and (12). Finally, compute distances by the formulas

$$r_1 = \frac{z}{2}\left[x \pm (x^2 - 4y)^{1/2}\right]$$
$$r_2 = \frac{z}{2}\left[x \mp (x^2 - 4y)^{1/2}\right]. \qquad (21)$$
$$r_3 = z$$

(if a symbol " m " does not look here as a minus-plus sign, then please change it to a minus-plus sign manually).

Explicit expressions in terms of x are presented here also:

$$r_1 = \left(\frac{1+12x^2+58x^4+36x^6+5x^8}{32x(x^2-1)(x^2+1)^3} - \frac{1+8x^2+3x^4}{64(x^2-1)}\lambda\right)\left[x \pm \left(\frac{1+4x^2+x^4}{2x^2} - \frac{(1+x^2)^3}{4x}\lambda\right)^{1/2}\right]$$
$$r_2 = \left(\frac{1+12x^2+58x^4+36x^6+5x^8}{32x(x^2-1)(x^2+1)^3} - \frac{1+8x^2+3x^4}{64(x^2-1)}\lambda\right)\left[x \mp \left(\frac{1+4x^2+x^4}{2x^2} - \frac{(1+x^2)^3}{4x}\lambda\right)^{1/2}\right]. \qquad (22)$$
$$r_3 = \frac{1+12x^2+58x^4+36x^6+5x^8}{16x(x^2-1)(x^2+1)^3} - \frac{1+8x^2+3x^4}{32(x^2-1)}\lambda$$

<u>Choice of a proper stationary point</u>

Below, we list all seven stationary points for helium ($\lambda = 1/Z = 1/2$):

No	x	r_1	r_2	r_3	V_0
1	0.064	-5.644	5.580	-1.008	-0.249
2	$-1.375-1.741i$	$-0.018+0.111i$	$0.055+0.020i$	$-0.057-0.024i$	$-11.043+8.764i$
3	$-1.375+1.741i$	$-0.018-0.111i$	$0.055-0.020i$	$-0.057+0.024i$	$-11.043-8.764i$
4	$0.295+2.137i$	$0.036+0.109i$	$-0.178+0.110i$	$0.110+0.051i$	$2.540+4.522i$
5	$0.295-2.137i$	$0.036-0.109i$	$-0.178-0.110i$	$0.110-0.051i$	$2.540-4.522i$
6	$1.638-0.257i$	$0.123+0.354i$	$0.186+0.001i$	$0.151+0.240i$	$-2.654+0.529i$
7	$1.638+0.257i$	$0.123-0.354i$	$0.186-0.001i$	$0.151-0.240i$	$-2.654-0.529i$

The second column is a list of all roots of a polynomial equation (19), and the third, fourth, and fifth columns are distances calculated by (22) using upper sign (another seven configurations can be obtained by interchange r_1 and r_2). In the last column of the table we give also the classical energy $V_0 = V_{\text{eff}}(r_1, r_2, r_3)$.

The first configuration is real and corresponds to a minimum at non-physical negative distances. It is interesting to note, that $(-r_1, r_2, -r_3)$ represents a physical saddle point for a system in which Coulomb repulsion between electrons is changed to attraction (with the same constant) and attraction between the first electron and a nucleus is replaced by repulsion.

Another six configurations are complex, and they are arranged in three complex-conjugate pairs.

We believe that an appropriate configuration that corresponds to asymmetrically doubly excited two-electron atoms ("planetary" atoms) studied in [K. Richter, J. S. Briggs, D. Wintgen, and E. A. Solov'ev, *J. Phys. B: At. Mol. Opt. Phys*. **25** (1992) 3929] in a large-dimensional limit is the seventh configuration. The first argument in favor of our hypothesis: it is the only configuration that has all positive real parts of distances, and so the wavefunction condenses in the physical range of arguments. The second argument: it is the only complex configuration that has relatively small imaginary part of classical energy, that is typical for quasi-stationary states. The third argument: a ratio $|r_1|/|r_2| = 2.011$ is approximately the same as for "planetary" atoms.

Asymmetric stationary point	Symmetric minimum
$r_1 = 0.123 - 0.354i$ $r_2 = 0.186 - 0.001i$ $r_3 = 0.151 - 0.240i$	$r_1 = r_2 = 0.303$ $r_3 = 0.449$
$\|r_1\|/\|r_2\| = 2.011$	$r_1 / r_2 = 1$
$\theta_{23} = (72.07 - 50.54i)^\circ$ $\theta_{31} = (18.30 + 33.12i)^\circ$ $\theta_{12} = (89.64 - 17.42i)^\circ$	$\theta_{23} = \theta_{31} = 42.35^\circ$ $\theta_{12} = 95.30^\circ$
$\omega_1 = 14.667 - 4.188i$ $\omega_2 = 11.792 + 5.748i$ $\omega_3 = 2.263 + 4.284i$	$\omega_1 = 11.763$ $\omega_2 = 5.426$ $\omega_3 = 3.549$
$V_0 = -2.654 - 0.529i$	$V_0 = -2.738$
$q_1 = (-0.675 + 0.270i)\Delta r_1 + (0.465 - 0.119i)\Delta r_2 + (0.496 - 0.279i)\Delta r_3$ $q_2 = (0.875 - 0.027i)\Delta r_1 + (0.647 + 0.390i)\Delta r_2 + (-0.745 - 0.343i)\Delta r_3$ $q_3 = (0.840 + 0.205i)\Delta r_1 + (0.002 + 0.216i)\Delta r_2 + (0.200 - 0.176i)\Delta r_3$	$q_1 = 0.811\Delta r_1 + 0.811\Delta r_2 - 1.048\Delta r_3$ $q_2 = -0.667\Delta r_1 - 0.667\Delta r_2 - 0.053\Delta r_3$ $q_3 = -0.707\Delta r_1 + 0.707\Delta r_2$

Above, we compare the asymmetric stationary point with the symmetric minimum for helium. There, q_1, q_2, and q_3 are normal-mode coordinates. It is interesting that the real part of the energy for asymmetric stationary point is only slightly greater than the energy for symmetric minimum.

The stationary point, frequencies, and normal-mode coordinates as functions of nuclear charge and mass of the first electron

The dependence of this stationary point on λ was studied in detail. We give two tables, showing the behavior in a full range $0<\lambda<1$ and near a symmetry-breaking point $0.805<\lambda<0.817$ (a symmetry-breaking point ≈ 0.814 is defined here as a value of λ when the symmetric equilibrium configuration becomes unstable). The third table demonstrates approximate separability in terms of prolate spheroidal coordinates (see details below in this section). So, this system behaves as a problem of two Coloumb centers, that was found earlier for "planetary" states. We investigate also a system in which the mass of the first electron was varied from one to infinity (the last two tables). It was shown that the stationary point tends to a definite limit when the mass tends to infinity. This limit corresponds to a molecular-like system when the motion of the first electron can be described classically. Such adiabatic-approximation approach was proven to be appropriate for "planetary" atoms.

The tables contain also squares of frequencies and coefficients of transformation of displacements of distances into normal modes, $q_i = \sum_j T_{ij}\Delta r_j$. Squares of frequencies were calculated as roots of an equation

$$\det(\mathbf{AB}-\omega^2\mathbf{I})=0\,. \tag{23}$$

where a matrix $\mathbf{A}$ was defined by (2), and $B_{ij}=\dfrac{\partial^2 V_{\mathrm{eff}}}{\partial r_i \partial r_j}(r_1,r_2,r_3)$. A matrix of transformation to normal modes $\mathbf{T}$ was calculated as follows. First, we calculated eigenvectors of the matrix $\mathbf{A}$. They were arranged as raws of a matrix $\mathbf{S}$. Then, a matrix of normalized eigenvectors was calculated as $\mathbf{S}_{\mathrm{n}}=(\mathbf{SS}^{\mathrm{T}})^{-1/2}\mathbf{S}$, so that $\mathbf{S}_{\mathrm{n}}\mathbf{S}_{\mathrm{n}}{}^{\mathrm{T}}=\mathbf{I}$ and $\mathbf{S}_{\mathrm{n}}\mathbf{AS}_{\mathrm{n}}{}^{\mathrm{T}}=\Lambda$ is a diagonal matrix of eigenvalues. After that, a matrix $\mathbf{B_1}=\Lambda^{1/2}\mathbf{S}_{\mathrm{n}}\mathbf{BS}_{\mathrm{n}}{}^{\mathrm{T}}\Lambda^{1/2}$ was calculated and its eigenvectors were found and were arranged as raws of a matrix $\mathbf{S_1}$. A matrix of normalized eigenvectors was calculated as $\mathbf{S}_{1\mathrm{n}}=(\mathbf{S}_1\mathbf{S}_1{}^{\mathrm{T}})^{-1/2}\mathbf{S}_1$, so that $\mathbf{S}_{1\mathrm{n}}\mathbf{S}_{1\mathrm{n}}{}^{\mathrm{T}}=\mathbf{I}$ and $\mathbf{S}_{1\mathrm{n}}\mathbf{B}_1\mathbf{S}_{1\mathrm{n}}{}^{\mathrm{T}}=\Omega^2$ is a diagonal matrix of squares of frequencies. Finally, a transformation matrix was obtained as $\mathbf{T}=\left(\left(\mathbf{S_{1}}_{\mathrm{n}}\Lambda^{1/2}\mathbf{S}_{1\mathrm{n}}\right)^{\mathrm{T}}\right)^{-1}$. When we used another set of coordinates (s_1, s_2, s_3), a new transformation matrix was obtained as $\mathbf{T}' = \mathbf{TR}$, where $R_{ij} = \dfrac{\partial r_i}{\partial s_j}$.

The first table shows that $\mathrm{Re}\, r_1$ becomes negative for sufficiently small $\lambda < 0.21$ that agrees with the fact that "planetary" atoms don't exist for large charges. It shows also that the fastest first two modes are almost stable because ω_1 and ω_2 have relatively small imaginary parts, but the slowest third mode is unstable ($\mathrm{Im}\,\omega_3 > \mathrm{Re}\,\omega_3$). In total, the stationary points are relatively stable, because the decay occurs mainly along the fastest modes.

The second table shows that the complex stationary point turns into a local minimum and a real saddle point when $\lambda > \lambda_* \approx 0.809585$. The saddle point disappears at the symmetry-breaking point $\lambda = \lambda_{**} \approx 0.814389$. The local minimum becomes an absolute minimum at $\lambda > \lambda_c \approx 0.810776$, and it turns more and more asymmetric, $r_1 / r_2 \to \infty$ when $\lambda \to 1$.

The third table refers to use of prolate spheroidal coordinates $s_2 = (r_2 + r_3) / r_1$ and $s_3 = (r_2 - r_3) / r_1$ instead of distances r_2 and r_3. It shows that the slowest-mode motion occurs mainly along the coordinate $s_1 = r_1$ since $|T'_{32}|, |T'_{33}| << |T'_{31}|$. For $\lambda < 0.7$, the motion along the first mode occurs mainly along r_1 and s_2, and the motion along the second mode occurs mainly along r_1 and s_3 (in the table, there is interchange of modes between $\lambda = 0.6$ and $\lambda = 0.7$). So, this problem resembles a two-center-Coulomb problem when the normal-mode coordinates are: $\xi - \xi_0(r_1)$ and $\eta - \eta_0(r_1)$ where $\xi = s_2 = (r_2 + r_3) / r_1$ and $\eta = s_3 = (r_2 - r_3) / r_1$ that depend only on r_1 and s_2 or on r_1 and s_3. The last table reflects the fact that this approximate separability becomes more exact when the mass of the first electron increases.

Let us consider the behavior of parameters of the stationary point in two limiting cases.

For $\lambda \to 1$

$$
\begin{aligned}
x &= 1+\varepsilon+\varepsilon^2+2\varepsilon^3+O(\varepsilon^4),\\
r_1 &= \tfrac{1}{4}\varepsilon^{-1}-\tfrac{3}{8}-\tfrac{11}{16}\varepsilon+O(\varepsilon^2),\\
r_2 &= \tfrac{1}{4}+\tfrac{1}{4}\varepsilon^3+O(\varepsilon^4),\\
r_3 &= \tfrac{1}{4}\varepsilon^{-1}-\tfrac{3}{8}-\tfrac{9}{16}\varepsilon+O(\varepsilon^2),\\
\omega_1 &= 8+4(1+\sqrt{10})\varepsilon^2+O(\varepsilon^3),\\
\omega_2 &= 8+4(1-\sqrt{10})\varepsilon^2+O(\varepsilon^3),\\
\omega_3 &= 8\varepsilon^2+12\varepsilon^3+23\varepsilon^4+O(\varepsilon^5),\\
V_0 &= -2-2\varepsilon^2+O(\varepsilon^3).
\end{aligned}
, \qquad (24)
$$

where $\varepsilon = 1-\lambda$. So, the configuration becomes very asymmetric, $r_1/r_2 \sim \varepsilon^{-1}$, and the first electron is almost ionized, $r_1 \to \infty$. The classical energy V_0 tends to the large-dimensional energy for He^+ ion.

For small λ

$$
\begin{aligned}
x &\sim \left(3+i\sqrt{7}\right)^{1/3}\lambda^{-1/3} = (1.542+0.379i)\lambda^{-1/3},\\
r_1 &\to -0.063-0.194i,\\
r_2 &\to 0.094-0.054i,\\
r_3 &\to (-0.018-0.156i)\lambda^{1/3},\\
\omega_1 &\to (30.046+11.064i)\lambda^{-1/6},\\
\omega_2 &\to (11.064-30.046i)\lambda^{-1/6},\\
\omega_3 &\to 7.260-24.205i,\\
V_0 &\to -3.250-4.630i.
\end{aligned}
. \qquad (25)
$$

Note that there is no stationary configuration without repulsion between electrons ($\lambda = 0$), but it exists for arbitrary small λ and tends to a definite limit at $\lambda \to 0$. Since $r_3 \to 0$, the repulsion between electrons does not cease in a limit $\lambda \to 0$. The ratio $|r_1|/|r_2| = 1.883$ remains approximately the same as for helium (2.011).

Now let us determine the critical parameter λ_* when a pair of the complex-conjugate stationary points turns into a local minimum and a real saddle point. The critical parameter is one of roots of the discriminant of the polynomial in lhs of (19) lying in the interval $[0,1]$. This discriminant represents a tenth order polynomial in λ. After dividing it by non-zero factor λ^2+4 we obtain an equation for λ_*

$$729\lambda^8 - 30888\lambda^6 + 592297\lambda^4 - 1901151\lambda^2 + 1000188 = 0\,. \tag{26}$$

Its root lying in the interval $[0,1]$ is

$$\lambda_* = \left[\frac{286}{27} - \frac{\sqrt{c}}{2} - \frac{1}{2}\left(3c_1 - c + \frac{825626}{81\sqrt{c}}\right)^{1/2}\right]^{1/2}, \tag{27}$$

where $c_1 = -\dfrac{203042}{2187}$ and

$$c = c_1 + \frac{1}{2187}\left(\frac{183397124569\cdot 2^{1/3}}{c_2} + \frac{c_2}{2^{1/3}}\right)$$
$$c_2 = \left(168354536727788381 + 740874556833075\sqrt{6685}\right)^{1/3}.$$

Numerically, $\lambda_* = 0.809585316$. It differs slightly from a value 0.8097 given in a paper of D. Z. Goodson et al. [J. Chem. Phys. 1992, **97**, 8481].

To find the symmetry-breaking point λ_{**} (where a saddle point collides with the symmetric minimum), we express λ via x solving (19) as a quadratic equation for λ:

$$\lambda = \frac{1 + 8x^2 + 3x^4 \pm (1 + 22x^4 - 7x^8)^{1/2}}{x(1+x^2)^3}\,. \tag{28}$$

Then, using (22) we obtain

$$(r_1 - r_2)^2 = x^2 - 4y = \frac{1 - x^4 \mp (1 + 22x^4 - 7x^8)^{1/2}}{4x^2}\,. \tag{29}$$

Putting $r_1 - r_2$ to zero, we find $x = 3^{1/4}$ with the lower sign before $(1 + 22x^4 - 7x^8)^{1/2}$. Inserting it into (28), we find $\lambda_{**} = 8\cdot 3^{-1/4}(1+3^{1/2})^{-2} = 0.814389$. This result is identical to $\lambda_0 = 2^{5/2}\left[(4/3)^{1/4} - (3/4)^{1/4}\right]$ that was found previously by L. D. Mlodinow and N. Papanicolaou [*Ann. Phys. (N. Y.)* **131**, 1 (1981)].

Plot of the effective potential for different λ and mass m_1

Here, we give plots of the effective potential as a function only the first variable r_1 and minimized over another variables:

$$V_1(r_1) = \min_{r_2, r_3} V_{\text{eff}}(r_1, r_2, r_3). \tag{30}$$

Such function is more easier for plotting than a complete function of all three variables.

Qualitatively, a graph of the function V_1 has different shapes when $0 < \lambda < \lambda_*$, $\lambda_* < \lambda < \lambda_{**}$, and $\lambda_{**} < \lambda < 1$. These three different shapes are shown on the following figure for some specific values of λ.

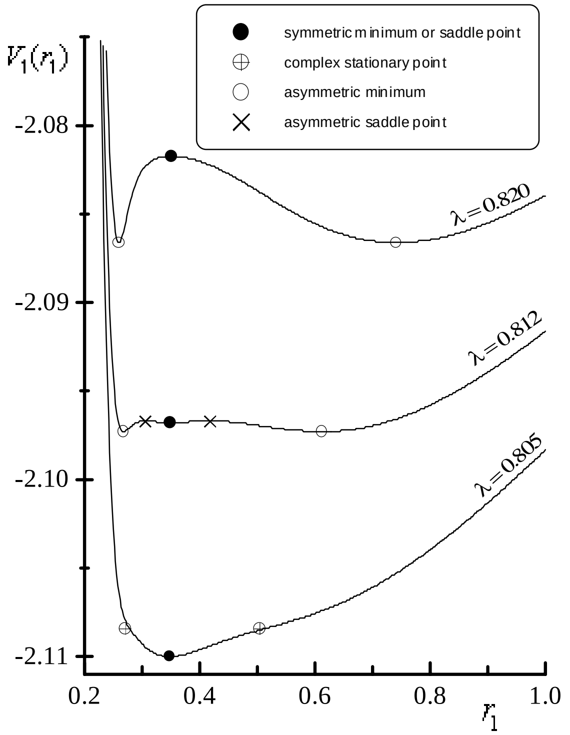

Fig. 1. Possible shapes of the potential $V_1(r_1)$. The lower curve refers to the case $0 < \lambda < \lambda_*$. It has a single minimum corresponding to a symmetric configuration. Asymmetric complex stationary points are shown on the figure by two points with coordinates $(\mathrm{Re}\, r_1, \mathrm{Re}\, V_1(r_1))$. The intermediate curve refers to the case $\lambda_* < \lambda < \lambda_{**}$. Here, the symmetric minimum still exists, but complex stationary points turn into a pair of asymmetric minima and a pair of saddle points. For $\lambda_{**} < \lambda < 1$ (the upper curve on the figure), the symmetric minimum turns into a saddle point, and asymmetric saddle point

disappears.

Graphs of the function V_1 with increased mass of the first electron are shown on Fig.2.

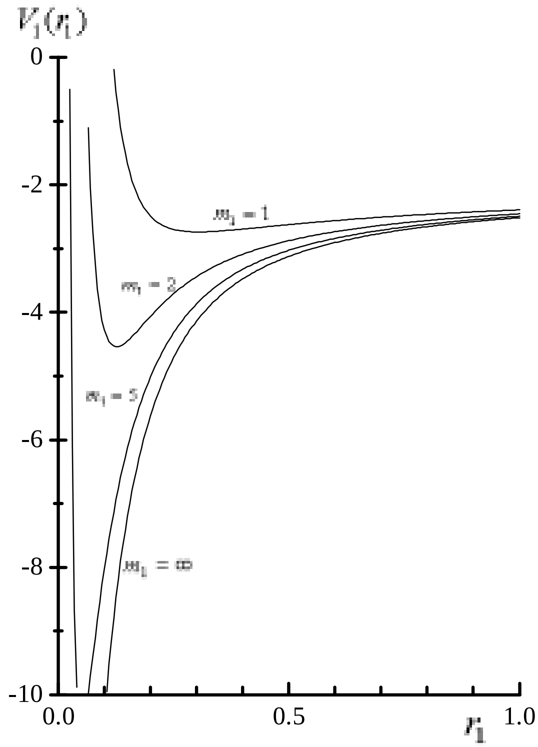

Fig. 2. Changing of the shape of the potential $V_1(r_1)$ when the mass of the first electron is increased. The lower curve refers to the adiabatic approximation when the first electron is treated classically.

In the limit $m_1 \to \infty$, coordinates of the minimum tend to zero, so the system collapses. However, the complex stationary point is weakly dependent on m_1, r_1 varies from $0.123 - 0.354i$ to $0.029 - 0.472i$ when m_1 varies from zero to infinity (see the attached table). So, the complex equilibrium configuration does not collapse, and adiabatic approximation is possible.