Part II.

Two-Coulomb-center approximation (the first electron is regarded infinitely heavy)

Before considering the complete two-electron problem, let us consider the adiabatic approximation, when the problem is solved for definite values of R_1, and then the energy is approximated by the minimum of the curve $E(R_1)$. So, the first electron is treated classically. Such approximation was proven to have a good accuracy for asymmetrically doubly excited states under consideration. We shall be interested especially in evolution of these states with increasing of dimensionality and their large-dimensional limit.

Since the problem of two Coulomb centers is separable in prolate spherical coordinates, the states are characterized by two quantum numbers n_1, n_2 in equations depending on ξ, η. The problem in D dimensions is equivalent to three-dimensional problem with non-zero magnetic quantum number $m = (D-3)/2$. It was found in [K. Richter, J. S. Briggs, D. Wintgen, and E. A. Solov'ev, *J. Phys. B: At. Mol. Opt. Phys.* **25** (1992) 3929] that the two-center energy curves have a local minimum when $n_1 = 0$ and $n_2 \geq 5$. We reproduce these curves using 1/*D*-expansion (equivalent to 1/*m*-expansion). Our results are shown on Fig. 3

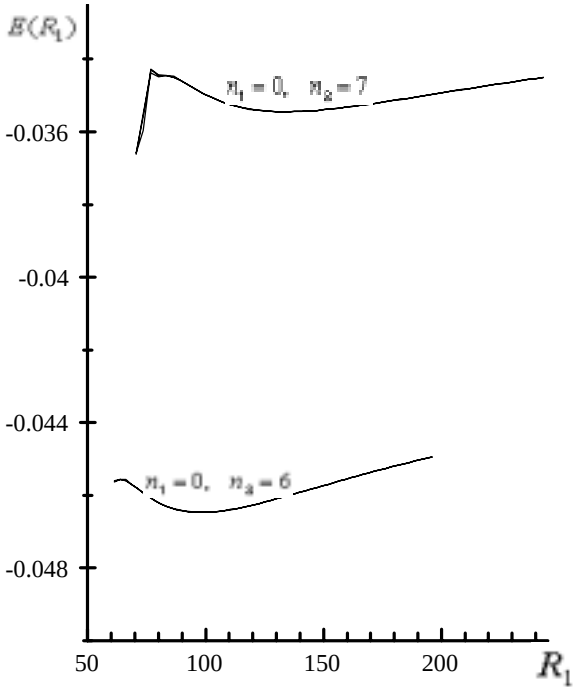

Fig. 3. Energy curves for an electron in a field of two Coulomb centers with charges $Z_1 = 2$ and

$Z_2 = -1$. R_1 is the distance between centers. Full energy is the sum of the quantum-mechanical electronic energy and the classical interaction energy $Z_1 Z_2 / R_1$. Here, $D = 3$ and $m = 0$. The electronic energy was found by an expansion over $1/N$, where $N = m + n_1 + n_2 + 1$.

Minima on the curves are evident and can be easily found numerically. The position of the scaled minimum, $r_1 = N^{-2} R_1$, as a function of N^{-1} is shown on Fig. 4.

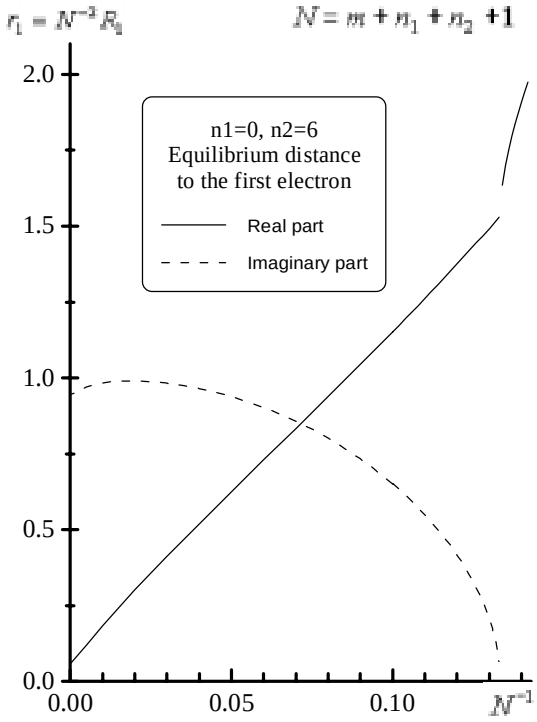

Fig. 4. A coordinate of the minimum on the energy curve $E(R_1)$ as a function of dimensionality (or a magnetic quantum number). When $N^{-1} < 0.134$ (or $m > 0.5$), the minimum turns into a complex stationary point. Here, $n_1 = 0$ and $n_2 = 6$.

We were able to trace the stationary point up to a large-dimensional limit $N \to \infty$ when it tends to $2(0.029 - 0.472i)$. We also performed an analytic continuation of stationary points in a helium potential (listed in the table in the first section of this text) from $m_1 = 1$ to $m_1 \to \infty$. Results are given in a following table.

No	r_1	r_2	r_3	V_0
1	-1.398	1.345	-0.529	-0.468
2	$-0.018+0.136i$	$0.085+0.060i$	$-0.070-0.057i$	$-5.588+8.149i$
3	$-0.018-0.136i$	$0.085-0.060i$	$-0.070+0.057i$	$-5.588-8.149i$
4*	$-0.220+0.106i$	$0.030+0.196i$	$0.122+0.119i$	$2.510+2.351i$
5*	$-0.220-0.106i$	$0.030-0.196i$	$0.122-0.119i$	$2.510-2.351i$
6	$0.029+0.472i$	$0.234+0.052i$	$0.011+0.363i$	$-2.082+0.818i$
7	$0.029-0.472i$	$0.234-0.052i$	$0.011-0.363i$	$-2.082-0.818i$

* Note. The forth and the fifth stationary points were evolved from the corresponding configurations given in the table for $m_1 = 1$ (see the first section) with interchange of r_1 and r_2. Another stationary points were evolved without interchange (configurations with interchange have no definite limit at $m_1 \to 0$).

It can be seen from Fig. 5 by checking the value of r_1, that the system condenses to the seventh configuration in the large-dimensional limit (our present scaling differs by a factor 2). This numerical experiment confirms our choice of the stationary point that was done in the first section.

The dependence of the energy on dimensionality is shown on Fig. 6.

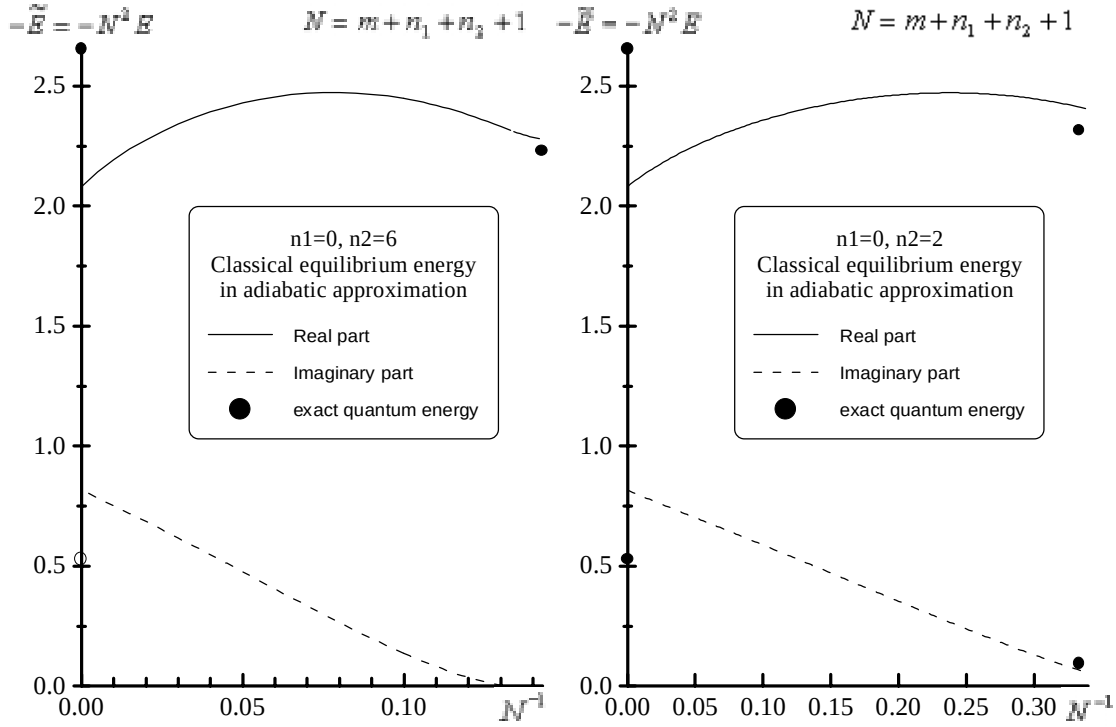

Fig. 6. A minimum on the energy curve $E(R_1)$ as a function of dimensionality. When $n_2 = 2$ (the left figure), the real minimum does not exist even for three-dimensional problem. Nevertheless, the

complex stationary point gives a good approximation to the energy.

Discussion

The three-dimensional problem was generalized to arbitrary dimensionality. The adiabatic solution was analytically continued to the large-dimensional limit. It was found that the large-dimensional limit is associated with the seventh complex stationary point of the effective potential. Within the adiabatic approximation, the energy was found as a function of dimensionality. We believe that the dependence of the exact energy on dimensionality is approximately the same. It was found that the width decreases linearly in the wide range of the parameter N^{-1}, see Fig. 6. So, it is expected that only two terms of the expansion over $1/N$ are sufficient to reproduce the width with a reasonable accuracy. Since the shape of the curves for a real part of the energy is almost parabolic, it is expected that only three terms of the expansion over $1/N$ may be sufficient to obtain a real part. However, the behavior of the energy is non-analytic when dimensionality is close to three (an imaginary part disappears, and a real part has a discontinuity in the second derivative). It means that the convergence of the $1/N$-expansion may be slower in this case, and more coefficients of the expansion are needed.

Below, we present for reference a table of the stationary points for different λ and for $m_1 = \infty$ (non-helium two-electron atoms).

λ	r_1	r_2	r_3	V_0
0.050	-0.07946 - 0.27265*I	0.15509 - 0.11373*I	-0.03285 - 0.08908*I	-1.69498 - 2.98071*I
0.100	-0.06894 - 0.29848*I	0.16972 - 0.10833*I	-0.03745 - 0.12494*I	-1.83599 - 2.55919*I
0.150	-0.05805 - 0.32146*I	0.18191 - 0.10232*I	-0.03789 - 0.15612*I	-1.92615 - 2.22704*I
0.200	-0.04669 - 0.34307*I	0.19251 - 0.09580*I	-0.03574 - 0.18550*I	-1.98713 - 1.94710*I
0.250	-0.03486 - 0.36396*I	0.20186 - 0.08889*I	-0.03158 - 0.21415*I	-2.02857 - 1.70359*I
0.300	-0.02261 - 0.38458*I	0.21012 - 0.08167*I	-0.02573 - 0.24265*I	-2.05593 - 1.48789*I
0.35	-0.01001 - 0.40529*I	0.21740 - 0.07426*I	-0.01842 - 0.27141*I	-2.07276 - 1.29462*I
0.40	0.00288 - 0.42649*I	0.22376 - 0.06673*I	-0.00979 - 0.30082*I	-2.08153 - 1.12012*I
0.45	0.0160 - 0.4486*I	0.22928 - 0.05919*I	- 0.33132*I	-2.08411 - 0.96181*I
0.50	0.0293 - 0.4723*I	0.23401 - 0.05173*I	0.01089 - 0.36345*I	-2.08195 - 0.81775*I
0.55	0.0427 - 0.4982*I	0.23798 - 0.04442*I	0.02274 - 0.39794*I	-2.07623 - 0.68650*I
0.60	0.0561 - 0.5274*I	0.24127 - 0.03735*I	0.03548 - 0.43580*I	-2.06794 - 0.56696*I
0.65	0.0696 - 0.5613*I	0.24393 - 0.03060*I	0.0490 - 0.4785*I	-2.05793 - 0.45831*I
0.70	0.0831 - 0.6024*I	0.24601 - 0.02425*I	0.0634 - 0.5284*I	-2.04698 - 0.36000*I
0.75	0.0967 - 0.6544*I	0.24757 - 0.01838*I	0.0784 - 0.5894*I	-2.03579 - 0.27169*I
0.80	0.1102 - 0.7243*I	0.24868 - 0.01306*I	0.0942 - 0.6685*I	-2.02502 - 0.19333*I
0.85	0.1238 - 0.8267*I	0.24940 - 0.00840*I	0.1108 - 0.7804*I	-2.01534 - 0.12519*I
0.90	0.1376 - 0.9993*I	0.24981 - 0.00451*I	0.1282 - 0.9632*I	-2.00743 - 0.06814*I
0.95	0.1538 - 1.3628*I	0.24996 - 0.00162*I	0.1486 - 1.3381*I	-2.00202 - 0.02415*I

Note that all distances have positive real parts when $\lambda > 0.45$.