# Radius of convergence of the $1/Z$ expansion for the ground state of a two-electron atom

I. A. Ivanov*

*Observatoire de Paris, Section de Meudon, Département d'Astrophysique Relativiste et de Cosmologie, 92195 Meudon Cedex, France*

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An estimation of the radius of convergence of the $1/Z$ expansion ($Z$ is the charge of the nucleus) for the ground state of the two-electron atom is obtained. The calculation is based on an idea that, with certain conditions being satisfied, the radius of convergence of the $1/Z$ series can be estimated with good precision if one constructs the function $\lambda(f)$, inverse to the function $f(\lambda)=[E(\lambda)-E_0]/E_1$ ($E$ is energy, $\lambda=1/Z$, while $E_0$ and $E_1$ are the first two coefficients of the perturbation expansion of the energy). We find numerically that the nearest singularity to $f=0$ in the complex $f$ plane of the inverse function $\lambda(f)$ is at the point $f=0.8$ corresponding to the threshold point $E=-0.5$. a.u. We find also that the series for the inverse function $\lambda(f)$ converges at this point. We discuss the nature of the singularity of the inverse function $\lambda(f)$. The value for the radius of convergence of the $1/Z$ expansion of the ground state of a He-like ion obtained is $R_\lambda=1.097\,660\,79$, which we think to be the most accurate value presently available.

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## I. INTRODUCTION

Perturbation theory with the hydrogenlike zero approximation takes its origin as 1930 when Hylleraas [1] pointed out that after rescaling the space coordinates ($\mathbf{r}'=Z\mathbf{r}$) and the energy ($E'=E/Z^2$) the nonrelativistic Schrödinger equation for the two-electron atomic ion of the nuclear charge $Z$ becomes

$$\left[\frac{\mathbf{p}_1'^2}{2}+\frac{\mathbf{p}_2'^2}{2}-\frac{1}{r_1'}-\frac{1}{r_2'}+\lambda\frac{1}{r_{12}'}\right]\Psi(\mathbf{r}_1',\mathbf{r}_2')=E'\Psi(\mathbf{r}_1',\mathbf{r}_2') . \tag{1}$$

The parameter $\lambda=1/Z$ measures the strength of the electron-electron Coulomb interaction. The prime quantities denote the new coordinates and the corresponding operators of momenta. Hereafter, for simplicity, we shall omit the primes and write $E$ instead of $E'$ in (1), keeping in mind that, everywhere below, the quantity denoted by $E$ stands for the actual energy divided by $Z^2$.

The application of the Rayleigh-Schrödinger perturbation theory to the problem (1) leads to an expansion of $E$ in a power series of $\lambda$,

$$E=\sum_{i=0}^{\infty}E_i\lambda^i . \tag{2}$$

For the ground state of He-like ions the first two coefficients are $E_0=-1$ a.u., $E_1=0.625$ a.u. The coefficients of higher orders have been calculated by different authors [1–5]. In particular, in a recent paper [6], about 400 coefficients of the series (2) for the ground state of He-like ions have been tabulated.

The natural question arises as to what kind of information can be extracted from the series (2) apart from the value of the energy. If, analyzing the perturbation expansion, one can obtain some information about the exact solution of the problem (1) and its analytic properties as a function of $\lambda=1/Z$, the information of this sort, though it is interesting by itself, could also be important for the applications. It is possible that some analytic properties of the function $E(\lambda)$ (for example, the singularities of this function and its behavior near these singularities) could be shared by the more complex systems, which are also governed by the Coulomb interaction. Thus, studying the analytic properties of the exact energy of the ground state of helium, one can obtain a deeper insight into the more complex atomic systems.

Below, we discuss only the ground state of the two-electron atom. We shall recall briefly, from the literature, some rigorous results concerning the analytic properties of a function defined by the series (2) for this state. It has been rigorously proved by Kato, using the methods of the perturbation theory for unbounded linear operators [7,8], that the series for $E(\lambda)$ converges in a certain domain around $\lambda=0$, defining thus an analytic in this domain function $E(\lambda)$. Kato [8] gives an estimation for the lower bound of the radius of convergence of the series (2). Subsequent numerical analysis carried out by different authors allowed them to obtain more precise estimations for the radius of convergence of the series (2). Different methods have been used in these works, such as the ratio test [9] [that is, the numerical analysis of the sequence constructed from the ratio of two subsequent coefficients of the series (2)]. The value of the radius of convergence obtained is $R_\lambda\approx1.1184$. Padé analysis [10] of the series (2) has given $R_\lambda\approx1.118$. The Darboux function ansatz [11,12] (which consists in a presumption that the singularity is a simple branching point) has given

*Permanent address: Institute of Spectroscopy, Academy of Sciences of Russia, Troitsk, 142092, Russia.

 

$R_\lambda \approx 1.119$ and 1.1056, respectively. In a recent paper of Baker *et al.* [6] the authors have performed extensive high-precision calculations of the coefficients of the series (2) for the ground state of He-like ions, and by the analysis of the asymptotic behavior of these coefficients, they have obtained the value $R_\lambda \approx 1.097\,66$ for the radius of convergence. These authors concluded also that the nearest singularity to $\lambda=0$ in the $\lambda$ plane is of a complex nature. According to these results this singularity is an essential singularity (that is, neither a pole nor a branching point). The authors thus explained the reason why the Padé analysis and the Darboux function ansatz could not give very precise results, since both methods cannot describe essential singularities.

We shall present another estimation of the radius of convergence of the series (2), which we have obtained by a rather different method but, to our opinion, by a more straightforward one. This method does not rely on any particular ansatz for the investigated function, which allowed us to achieve a sufficiently high accuracy in our calculation. The value obtained for the radius of convergence of the $1/Z$ expansion for the ground state of He-like ions is $R_\lambda = 1.097\,660\,79$. We expect that eight digits are valid, at least. We thus confirm the results of Baker *et al.* and add a few more digits to their result.

## II. THEORY

The following method for the determination of the radius of convergence of the expansion (2) relies on two basic facts. First, as was rigorously proved by Reinhardt [13], if the radius of convergence of $1/Z$ expansion (2) is determined by a singularity on the positive $\lambda$ axis, then if we denote this value as $\lambda_s$, the energy $E$ becomes for this value of $\lambda$ degenerate with a threshold. In other words, $E(\lambda_s) = -\frac{1}{2}$ (energy in atomic units of the remaining $1s$ electron after the ionization of the other electron). Second, as was shown by Baker *et al.* [6], for the expansion (2), the nearest singularity to $\lambda=0$ in the $\lambda$ plane is in fact on the positive real axis. Thus, the value of $E(\lambda_s)$ is known. We rewrite expansion (2) in the following form, introducing a new function $f(\lambda)$:

$$f(\lambda) = \frac{E(\lambda)-E_0}{E_1} = \sum_{i=1}^{\infty} \frac{E_i}{E_1}\lambda^i . \tag{3}$$

For $\lambda=0$, $f(\lambda)=0$, $df(\lambda)/d\lambda=1$; hence around the point $\lambda=0$ the inverse function $\lambda(f)$ exists and is analytic in some domain containing the point $f=0$. The series expansion of $\lambda(f)$ in the vicinity of the point $f=0$ is obtained from the Lagrange formula [14], which gives the coefficients of the expansion of the inverse function once the series for $f(\lambda)$ is known:

$$\lambda(f) = \sum_{k=1}^{\infty} \frac{f^k}{k!}\left[\frac{d^{k-1}}{d\lambda^{k-1}}\left\{\frac{\lambda}{f(\lambda)}\right\}^k\right]_{\lambda=0} = \sum_{k=1}^{\infty} \lambda_k f^k . \tag{4}$$

The series (4) converges in some domain around $f=0$. We note now that, according to the results of Reinhardt and Baker *et al.* cited above, the value of $f$ is known at the singular point $\lambda_s$. Substituting the known values of $E(\lambda_s)$, $E_0$, $E_1$ in (3), we have $f(\lambda_s) = (-\frac{1}{2}+1)/0.625 = 0.8$. Hence, if the series (4) converged for $f=0.8$, we could directly obtain the value of $\lambda_s$ by summing up the series (4). *A priori,* the convergence, of course, cannot be guaranteed. According to the general theory the radius of convergence of the series (4) is equal to the distance to the nearest to $f=0$ in the complex $f$-plane singularity of the function $\lambda(f)$. The question of the value of the radius of convergence of the series (4) is thus related to the location of the singularities of the function $\lambda(f)$ in the complex $f$ plane. Results of Baker *et al.* [6] demonstrate that the point $\lambda_s$ is an essential singularity of the function $f(\lambda)$, this function exhibiting a very complicated behavior around this point. We can expect therefore that the point $f(\lambda_s)=0.8$ is also a singular point (and, most probably, this is an essential singularity) of the inverse function $\lambda(f)$. Besides this possible singularity, the inverse function $\lambda(f)$ can have other singularities situated closer to $f=0$ in the complex $f$ plane. For example, any point in the $\lambda$ plane where $df/d\lambda=0$ produces a singularity of the inverse function $\lambda(f)$. We can therefore expect that the radius of convergence of the series (4) is equal to 0.8 or less, if the function $\lambda(f)$ has the singularities situated closer to $f=0$ than $f=0.8$. This reasoning will help us in the numerical investigation of the series (4) presented in the next chapter. Our numerical analysis of the series (4) gives for the radius of its convergence the value which is very close to 0.8. Since we expect the function $\lambda(f)$ to have the singularity at the point $f=0.8$ in the complex $f$ plane, we can conclude that the value of the radius of convergence does equal 0.8. The point $f=0.8$ thus lies on the boundary of the circle of convergence. Numerical analysis shows that the series (4) converges at this point, allowing us to thus determine $\lambda_s$ summing up the series (4) at the point $f=0.8$.

## III. NUMERICAL PROCEDURE

All our calculations have been performed in quadruple precision. Using the tabulated data for the first 400 coefficients of $1/Z$ expansion (2) given by Baker *et al.* for the ground state of He-like ions, we calculate 400 terms of the series of the function $\lambda(f)$, using formula (4). In Table I, we present the first 50 coefficients of this series. To determine the radius of convergence of this series, we have performed a Neville-Richardson analysis of ratios $r_k = \lambda_{k-1}/\lambda_k$ of two successive coefficients of a series $\lambda(f)$. The limit of this ratio, as is well-known, gives the value of the radius of convergence. We recall briefly the idea of this analysis. If asymptotically, when $k$ tends to infinity, this ratio satisfies an expansion of the type

$$r_k = r_0 + \frac{r_1}{k} + \frac{r_2}{k^2} + \cdots , \tag{5}$$

then the sequence $r_k^{(1)} = kr_k - (k-1)r_{k-1}$ also satisfies an expansion of the type (5), where $r_0$ remains unchanged but the term of order $k^{-1}$ is eliminated. One can iterate this procedure, constructing the sequence $r_k^{(2)}$ in the same

TABLE I. Coefficients of series for $\lambda(f)$.

| $k$ | $\lambda_k$ | $k$ | $\lambda_k$ |
|---|---|---|---|
| 1 | 1.000 000 000 000 0 | 26 | 0.080 170 627 289 5 |
| 2 | 0.252 266 287 150 6 | 27 | 0.091 688 520 995 4 |
| 3 | 0.113 358 108 820 7 | 28 | 0.105 175 564 462 8 |
| 4 | 0.064 135 115 189 8 | 29 | 0.120 982 387 367 6 |
| 5 | 0.042 488 555 073 8 | 30 | 0.139 525 575 540 8 |
| 6 | 0.031 811 781 810 6 | 31 | 0.161 300 325 241 7 |
| 7 | 0.026 181 922 720 4 | 32 | 0.186 895 607 200 3 |
| 8 | 0.023 135 734 481 9 | 33 | 0.217 012 342 365 5 |
| 9 | 0.021 544 392 125 5 | 34 | 0.252 485 194 504 7 |
| 10 | 0.020 855 023 351 5 | 35 | 0.294 308 709 176 2 |
| 11 | 0.020 784 797 469 7 | 36 | 0.343 668 678 618 7 |
| 12 | 0.021 186 660 024 1 | 37 | 0.401 979 793 199 0 |
| 13 | 0.021 986 630 175 0 | 38 | 0.470 930 858 770 0 |
| 14 | 0.023 153 132 351 1 | 39 | 0.552 539 123 549 0 |
| 15 | 0.024 681 525 807 1 | 40 | 0.649 215 577 536 3 |
| 16 | 0.026 586 234 609 7 | 41 | 0.763 843 473 695 3 |
| 17 | 0.028 896 890 506 7 | 42 | 0.899 872 787 225 8 |
| 18 | 0.031 656 734 404 5 | 43 | 1.061 433 894 412 9 |
| 19 | 0.034 922 399 045 6 | 44 | 1.253 474 436 486 6 |
| 20 | 0.038 764 633 321 4 | 45 | 1.481 924 161 917 3 |
| 21 | 0.043 269 757 692 6 | 46 | 1.753 893 543 192 1 |
| 22 | 0.048 541 767 132 2 | 47 | 2.077 913 178 544 4 |
| 23 | 0.054 705 074 230 3 | 48 | 2.464 222 460 471 8 |
| 24 | 0.061 907 936 230 7 | 49 | 2.925 117 776 016 9 |
| 25 | 0.070 326 649 167 3 | 50 | 3.475 372 665 303 2 |

way, which again satisfies an expansion of the type (5) with the same $r_0$, the terms of order $k^{-1}$, $k^{-2}$ being eliminated. This procedure can be continued. Of course, *a priori* it is difficult to state whether the ratios for the given series satisfy an expansion of the type (5), but in general the Neville-Richardson procedure does help to accelerate the convergence, even if the asymptotic expansion of $r_k$ is different from (5) (for example, when the powers are fractional; see [6]). In Table II, the values of the ratio $r_k=\lambda_{k-1}/\lambda_k$ and the sequences $r_k^{(2)},r_k^{(3)}$ are presented—correspondingly, the second and the third iterations of the Neville-Richardson procedure are presented. In Table II, one can see that the limit of the

TABLE II. Ratio test for the series $\lambda(f)$.

| $k$ | $r_k$ | $r_k^{(2)}$ | $r_k^{(3)}$ |
|---|---|---|---|
| 10 | 1.033 055 3 | 1.154 832 6 | 1.486 653 2 |
| 40 | 0.851 087 3 | 0.807 360 7 | 0.796 888 2 |
| 70 | 0.830 988 6 | 0.803 872 3 | 0.800 156 5 |
| 100 | 0.822 932 8 | 0.802 842 7 | 0.800 561 8 |
| 130 | 0.818 518 2 | 0.802 303 3 | 0.800 578 7 |
| 160 | 0.815 701 2 | 0.801 992 5 | 0.800 587 6 |
| 190 | 0.813 733 0 | 0.801 744 4 | 0.800 308 9 |
| 220 | 0.812 271 8 | 0.801 550 4 | 0.800 373 4 |
| 250 | 0.811 138 8 | 0.801 416 9 | 0.800 479 4 |
| 280 | 0.810 231 5 | 0.801 315 6 | 0.800 439 5 |
| 310 | 0.809 486 4 | 0.801 223 7 | 0.800 286 2 |
| 340 | 0.808 862 1 | 0.801 132 9 | 0.800 113 4 |

sequence $r_k$ is a number that is very close to 0.8. More elaborate methods of the acceleration of convergence would probably be more accurate, but since from the results of Reinhardt and Baker *et al.* we expect to find a singularity of the function $\lambda(f)$ at the point $f=0.8$, the numbers presented in Table II give enough evidence that the value of radius of convergence is indeed equal to 0.8. Having established this fact we can proceed to the analysis of the convergence properties of the series $\lambda(f)$ at the point $f=0.8$. This point lies on the boundary of the circle of convergence of the series (4). Generally speaking, the series can converge or diverge at this point. Our analysis of a sequence of the partial sums of the series (4) indicates that it converges for $f=0.8$. In Table III, the first column contains the sequence of the partial sums of the series (4) for $f=0.8$. Recalling that according to (4) the sum of this series gives directly the value of the radius of convergence of the $1/Z$ expansion, we see that even simple direct summation gives the expected result, which is very close to that of Baker *et al.*: $\lambda_s=1.097\,66$. The series converges rather slowly; to obtain a better precision we have to use some methods of acceleration of convergence. Among those found especially useful for our problem are the Aitken transformation and the $\epsilon$ algorithm. The Aitken transformation consists of transforming the original sequence $a_k^{(0)}$ into a new sequence $a_k^{(1)}$ according to the following rule:

$$a_k^{(1)}=\frac{a_k^{(0)}a_{k+2}^{(0)}-a_{k+1}^{(0)2}}{\Delta^2 a_k^{(0)}} . \tag{6}$$

Here, $\Delta^2 a_k^{(0)}=a_k^{(0)}-2a_{k+1}^{(0)}+a_{k+2}^{(0)}$ is the second difference of the original sequence $a_k^{(0)}$. It is not difficult to show that if the original sequence converges geometrically to some limit (i.e., $a_k^{(0)}=\alpha+\beta^k$), all the terms of a sequence $a_k^{(1)}$ constructed according to (6) will be identically equal to $\alpha$. For the geometric sequences, the Aitken transformation therefore accelerates perfectly the convergence, giving the correct limit at each step. It can be shown that this transformation accelerates also the convergence of the more complex sequences. The $\epsilon$ algorithm is another well-known accelerator of convergence; it consists also in a prescription according to which from the original sequence the new sequence is constructed, having the same limit but converging in some cases more rapidly. For lack of space, we shall not give more details about the $\epsilon$ algorithm. A detailed discussion of these methods is given in [15,16]. In our calculation, we have used the subroutine available in the NAG library of computer programs, which performs the calculations according to the prescriptions of the $\epsilon$ algorithm. The second column of Table III contains the sequence that is the result of the Aitken transformation applied to the sequence of the partial sums of the series (4) (first column Table III). The third column contains the results of the second iteration of the Aitken transformation and the fourth one contains the result of the application of the $\epsilon$ algorithm to the sequence obtained as a result of the second iteration of the Aitken transformation. The numbers in the fourth column reveal already a good convergence to the limit, which is approximately equal to 1.097 660 79, with

TABLE III. Sequence of partial sums of series $\lambda(f)$ and results of acceleration of its convergence.

| $k$ | Partial sums of series (4) | Aitken transformation | Iteration of Aitken transformation | $\epsilon$ algorithm |
|---|---|---|---|---|
| 305 | 1.097 637 727 408 | 1.097 656 561 016 | 1.097 660 077 099 | 1.097 660 077 099 |
| 308 | 1.097 638 389 612 | 1.097 656 696 387 | 1.097 660 103 028 | 1.097 660 717 311 |
| 311 | 1.097 639 028 752 | 1.097 656 826 597 | 1.097 660 127 910 | 1.097 660 801 650 |
| 314 | 1.097 639 645 787 | 1.097 656 951 878 | 1.097 660 151 795 | 1.097 660 783 213 |
| 317 | 1.097 640 241 627 | 1.097 657 072 449 | 1.097 660 174 730 | 1.097 660 798 311 |
| 320 | 1.097 640 817 141 | 1.097 657 188 521 | 1.097 660 196 760 | 1.097 660 798 806 |
| 323 | 1.097 641 373 153 | 1.097 657 300 290 | 1.097 660 217 928 | 1.097 660 798 599 |
| 326 | 1.097 641 910 452 | 1.097 657 407 944 | 1.097 660 238 272 | 1.097 660 798 685 |
| 329 | 1.097 642 429 786 | 1.097 657 511 663 | 1.097 660 257 831 | 1.097 660 798 271 |
| 332 | 1.097 642 931 870 | 1.097 657 611 616 | 1.097 660 276 640 | 1.097 660 797 224 |
| 335 | 1.097 643 417 385 | 1.097 657 707 963 | 1.097 660 294 733 | 1.097 660 796 626 |
| 338 | 1.097 643 886 981 | 1.097 657 800 858 | 1.097 660 312 141 | 1.097 660 793 998 |
| 341 | 1.097 644 341 277 | 1.097 657 890 447 | 1.097 660 328 893 | 1.097 660 798 169 |
| 344 | 1.097 644 780 866 | 1.097 657 976 868 | 1.097 660 345 020 | 1.097 660 789 942 |
| 347 | 1.097 645 206 313 | 1.097 658 060 252 | 1.097 660 360 547 | 1.097 660 789 986 |
| 350 | 1.097 645 618 157 | 1.097 658 140 726 | 1.097 660 375 500 | 1.097 660 795 749 |

an error that we estimate as one unit of the last digit. We thus confirm the result given by Baker *et al.*: 1.097 66, all digits of which, given in [6], are correct. We have performed also the preliminary numerical investigations of the nature of the singularity $f=0.8$ of the inverse function $\lambda(f)$ [which can give some insight into the problem of the nature of the singularity of the energy at a point $\lambda_s=\lambda(0.8)\approx 1.097\,066\,079$]. Our analysis, with the help of the Padé approximant and Darboux function ansatz of the function $\lambda(f)$ in a singular point $f=0.8$, indicates that, as could be expected, the singularity of the inverse function $\lambda(f)$ is of the same type as that of the function $f(\lambda)$—essential singularity.

## IV. REMARKS AND PROSPECTS

A knowledge of the precise value of the radius of convergence of the $1/Z$ expansion is important for the second part of the problem—an investigation of the analytic behavior of the exact energy around the singular point. Baker *et al.* give the ansatz that reproduces the coefficients of the perturbation series for the ground-state energy of He-like ions with very good precision. However, the question as to what extent this ansatz is unique (as Baker *et al.* remark in their paper) remains open.

One idea advocated in the present paper is that the study of the function inverse to the exact energy could be an easier task than directly studying the function $E(\lambda)$. Our results show that at least for the determination of the radius of convergence this procedure works. We can hope that this approach will allow us to make some progress in the determination of the nature of the singularity. Usually, in the numerical investigations of the given series, the most difficult part of the problem is to locate numerically the singularity. Only afterwards can one start to investigate numerically the nature of the singularity. Of course, the results that one obtains on this second step crucially depend on the precision with which the location of the singular point is known. Our approach has an advantage: that for the inverse function we know the location of the singularity with absolute accuracy. This can help us perhaps to make some further progress in the investigation on the nature of the singularity and to obtain some information about the analytic properties of the exact energy of the ground state of the two-electron system.

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