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Nonrelativistic energy levels of helium atom

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The nonrelativistic energy levels of a helium atom are calculated for S, P, D and F states. The calculations are based on the variational method of "exponential" expansion. The convergence of the calculated energy levels is studied as a function of the number of basis functions N. This allows us to claim that the obtained energy values (including the values for the states with a nonzero angular momentum) are accurate up to 28-35 significant digits.

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1. Introduction

The quantum problem of three bodies with Coulomb interaction is one of the most notable nonintegrable problems in quantum mechanics. At the same time, extremely accurate numerical solutions for the problem of bound states for a system of three particles may be obtained with modern computers. For example, the nonrelativistic energy of the ground state of helium with a nucleus of an infinite mass is now known accurately to 46 significant digits [1].

In the present study, a version of the variational method (the so called "exponential" expansion) [2] that allows to numerically solve the quantum Coulomb three-body bound state problem with a very high precision, which is easily applicable as well to the states with a nonzero angular momentum, is considered. This method is used to calculate the nonrelativistic energies of a helium atom for S, P, D, and F states. It is shown that the developed method is an efficient and flexible instrument for studying Coulomb systems. An analysis of convergence proves that the method is highly accurate and demonstrates that nonrelativistic energies accurate up to 28-35 significant digits may be obtained with rather moderate efforts.

Developing of such high precision methods is of importance for the reason that it may help solving a wide variety of problems that are of interest in physics. For example, antiprotonic helium atoms are of particular interest, which allows for high precision studies of energy spectrum of this exotic system and inferring of various properties of an antiproton from comparison of theory and experiment [3, 4]. Here it is worthy to mention a recent interest to the antiprotonic helium as a tool for constrains on various fifth forces [5, 6] to set general limits on new interactions beyond the Standard Model.

2. Generalized Hylleraas expansion

Let us consider the generalized Hylleraas expansion for the states of arbitrary total orbital momentum L [7]:

$$\psi(r_1,r_2)=\sum_{l_1+l_2=\mathscr{L}}\mathscr{Y}_{LM}^{l_1l_2}(r_1,r_2)\left[e^{-\alpha r_1-\beta r_2-\gamma r_{12}}\sum_{l,m,n\geq 0}C_{lmn}r_1^l r_2^m r_{12}^n\right], \tag{2.1}$$

$\mathscr{L}=L$ for the states of "normal" spatial parity $\Pi=(-1)^L$, and $\mathscr{L}=L+1$ for the states of "anomalous" spatial parity $\Pi=(-1)^{L+1}$. The complex parameters in the exponent are generated in a pseudorandom way. The $\mathscr{Y}_{LM}^{l_1l_2}$ functions are regular bipolar spherical harmonics [8] that depend on two angular coordinates:

$$\mathscr{Y}_{LM}^{l_1l_2}(r_1r_2)=r_1^{l_1}r_2^{l_2}\{Y_{l_1}(\hat{r}_1)\otimes Y_{l_2}(\hat{r}_2)\}_{LM},$$

where $Y_l(\hat{r})=Y_{lm}(\theta,\varphi)=\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos(\theta))e^{im\varphi}$, $P_l^m(\cos(\theta)$ are associated Legendre polynomials. Spatial parity operator $P\psi=\pi\psi$ acts on the spatial coordinates in the following way: $P(r_1,r_2)\rightarrow(-r_1,-r_2)$. The ease of use of the $\mathscr{Y}_{LM}^{l_1l_2}$ functions stems from the fact that they correctly reproduce the behavior of the wave function at $r_1\rightarrow 0$ (or $r_2\rightarrow 0$), and retain the reasonable requirement of boundedness of the function within the domain of variables for the expression within square brackets in Eq. (2.1).

Table 1: Convergence of the nonrelativistic energy of the ground state of a helium atom.

Basis (N)	E_{nr}
10000	−2.90372 43770 34119 59831 11592 45193 9
14000	−2.90372 43770 34119 59831 11592 45194 398
18000	−2.90372 43770 34119 59831 11592 45194 40432
22000	−2.90372 43770 34119 59831 11592 45194 40443

3. Results and discussion

In Table 1 we check the convergence of energy for the ground state of helium versus increasing basis sets of the variational expansion. The structure of "layers" of basis functions is very similar to what was used in our previous calculations [9], where it was explicitly published (see Table I in [9]). In present case we optimized the variational basis with $N = 10\,000$ functions and 8 layers. For the final calculation with $N = 22\,000$ functions we used 12 layers, and for the last four layers the ends of intervals $[A_1, A_2]$ and $[B_1, B_2]$ grew exponentially: $A_1(j) = B_1(j) = 10^{j-4}$, $A_2(j) = B_2(j) = 10^{j-3}$ for $j = 9, \ldots, 12$. Computations were performed in the duodecimal arithmetics (about 100 decimal digits). Programs of duodecimal precision were developed by our group in order to overcome the problem of the numerical instability of calculations at large values of N.

Results of numerical calculations of the nonrelativistic energies for S, P D, and F states of a helium atom are presented in Table 2. Variational parameters were optimized manually. It should be noted that the optimal variational parameters for different states differ significantly, and the calculation accuracy depends to a considerable extent (5-8 digits) on the particular choice of optimal variational parameters for a given bound state. Basis sets with $N = 10\,000$ functions were used to optimize the variational parameters. When the non S states listed in the table were calculated, 4 to 6 "layers" of basis functions were used, while for the S states calculations were done in the similar way as for the ground state. The results in Table 2 are presented for two subsequent calculations with increasing basis sets, what allows to demonstrate convergent digits. The third line shows the results of variational calculations by Drake and Yan [10] performed in year 1992, where the Rydberg states (excluding S states) of helium were studied. Comparison between two calculations demonstrates excellent agreement. The largest set for each particular state has been chosen by the reason that further increase of the basis gives rise to numerical instability of calculations within given duodecimal arithmetics. As may be seen numerical precision for triplet states is slightly higher, probably that is due to smaller effect of the logarithmic singularity. For higher orbital angular momentum states we have managed to achieve precision of 27-28 digits. Still that is the best known data for these states. All the calculations were performed on the Linux mainframe computers of our Laboratory.

For the ground state energy we compare our best obtained value with previously published results in Table 3. Indeed, explicit inclusion of the logarithmic singularity into a variational expansion may seriously improve precision of the results. On the other hand, with our variational basis function we can easily extend calculations to the states with excited electronic orbital as well as

Table 2: Convergence of the nonrelativistic energies of the S, P, D, and F states of a helium atom. N is the number of basis functions. The two lines represent two consecutive calculations with the largest basis sets to show convergent digits. The third line presents calculations by Drake and Yan [10].

State	N	E_{nr}	State	N	E_{nr}
1^1S	18000	−2.90372 43770 34119 59831 11592 45194 40432	4^1S	14000	−2.03358 67170 30725 44743 92926 44363 64
1^1S	22000	−2.90372 43770 34119 59831 11592 45194 40443	4^1S	18000	−2.03358 67170 30725 44743 92926 44363 87
2^1S	18000	−2.14597 40460 54417 41580 50289 75461 918	4^3S	14000	−2.03651 20830 98236 29958 03780 71617 853
2^1S	22000	−2.14597 40460 54417 41580 50289 75461 921	4^3S	16000	−2.03651 20830 98236 29958 03780 71617 874
	[10]	−2.14597 40460 5443(5)			
2^3S	14000	−2.17522 93782 36791 30573 89782 78206 81124	4^1P	18000	−2.03106 96504 50240 71475 89314 36090 3
2^3S	16000	−2.17522 93782 36791 30573 89782 78206 81125	4^1P	22000	−2.03106 96504 50240 71475 89314 36094 1
	[10]	−2.17522 93782 367912(1)		[10]	−2.03106 96504 5024(3)
2^1P	18000	−2.12384 30864 98101 35924 73331 42354	4^3P	18000	−2.03232 43542 96630 33195 38824 67087
2^1P	22000	−2.12384 30864 98101 35924 73331 42374	4^3P	22000	−2.03232 43542 96630 33195 38824 67103
	[10]	−2.12384 30864 98092(8)		[10]	−2.03232 43542 9662(2)
2^3P	16000	−2.13316 41907 79283 20514 69927 63793	4^1D	22000	−2.03127 98461 78684 99621 39438 073
2^3P	18000	−2.13316 41907 79283 20514 69927 63806	4^1D	26000	−2.03127 98461 78684 99621 39438 143
	[10]	−2.13316 41907 7927(1)		[10]	−2.03127 98461 78687(7)
3^1S	18000	−2.06127 19897 40908 65074 03499 37089 2816	4^3D	18000	−2.03128 88475 01795 53802 34920 591
3^1S	22000	−2.06127 19897 40908 65074 03499 37089 2824	4^3D	22000	−2.03128 88475 01795 53802 34920 630
				[10]	−2.03128 88475 01795(3)
3^3S	14000	−2.06868 90674 72457 19199 65329 11291 75048	4^1F	18000	−2.03125 51443 81748 60863 20824 071
3^3S	16000	−2.06868 90674 72457 19199 65329 11291 75049	4^1F	22000	−2.03125 51443 81748 60863 20824 079
				[10]	−2.03125 51443 81749(1)
3^1P	18000	−2.05514 63620 91943 53692 83410 913	4^3F	18000	−2.03125 51684 03245 39350 49887 2817
3^1P	22000	−2.05514 63620 91943 53692 83410 921	4^3F	22000	−2.03125 51684 03245 39350 49887 2846
	[10]	−2.05514 63620 9195(3)		[10]	−2.03125 51684 032454(6)
3^3P	18000	−2.05808 10842 74275 33134 26965 47197			
3^3P	22000	−2.05808 10842 74275 33134 26965 47203			
	[10]	−2.05808 10842 7428(4)			
3^1D	18000	−2.05562 07328 52246 48939 00994 819			
3^1D	22000	−2.05562 07328 52246 48939 00994 825			
	[10]	−2.05562 07328 52245(6)			
3^3D	18000	−2.05563 63094 53261 32711 49601 65840			
3^3D	22000	−2.05563 63094 53261 32711 49601 65851			
	[10]	−2.05563 63094 53261(4)			

nonzero angular momentum states with large L.

Variational wave functions of bound states are obtained by solving the Schrodinger equation for the quantum three-body problem with Coulomb interaction using a variational approach based on exponential expansion with the parameters of exponents being chosen in a pseudorandom way. The results of these studies demonstrated that the energy values were accurate to 27–35 significant digits.

Table 3: Comparison of the nonrelativistic energies of the ground state of a helium atom.

Author (year)	Ref.	N	Energy (in a.u.)
Drake *et al.* (2002)	[11]	2358	−2.90372 43770 34119 598311
Korobov (2002)	[9]	5200	−2.90372 43770 34119 59831 1159
Schwartz (2006)	[1]	24099	−2.90372 43770 34119 59831 11592 45194 40444 66969 25310
Nakashima, Nakatsuji (2007)	[12]	22709	−2.90372 43770 34119 59831 11592 45194 40444 66969
this work	[2]	22000	−2.90372 43770 34119 59831 11592 45194 40443

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