

## Nonrelativistic ionization energy for the helium ground state

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(Received 19 March 2002; published 12 August 2002)

The helium ground-state nonrelativistic energy with 24 significant digits is presented. The calculations are based on variational expansion with randomly chosen exponents. This data can be used as a benchmark for other approaches for many-electron and/or three-body systems.

DOI: 10.1103/PhysRevA.66.024501

PACS number(s): 31.15.Pf, 31.15.Ar

From the early days of quantum mechanics the ground-state ionization energy of the helium atom was a benchmark for approximate methods of solving the nonrelativistic Schrödinger equation for a few-body system. One of the earliest variational calculations has been performed by Hylleraas [1] in 1929 and it yields about five significant digits for the nonrelativistic ionization potential. In 1957, Kinoshita [2] presented a seven digit number obtained with a 39-parameter function, which, along with higher-order corrections including the Lamb shift calculations, confirmed a very good agreement with the best experimental value. Since that time, with the development of computer power, the accuracy has grown very rapidly. We would like to mention here the two most recent calculations. The first [3] is aimed to elaborate an efficient variational method for the many-electron atoms. The second [4] is to find an effective and economical way for studying the helium and heliumlike two-electron atoms.

In this short report we want to present a very accurate value for the nonrelativistic energy of the helium ground state. In our calculations we strictly follow a method described in [6]. The two modifications are to be stated. First, sextuple precision arithmetic (about 48 decimal digits) implemented as a FORTRAN90 module has been used instead of a multiprecision package written by Bailey. The use of this module gives about fivefold improvement in computational time and allows one to increase significantly the length of a basis set. The module is based on a representation of a sextuple precision number by a set of three double precision numbers. It is assumed that an *exact* sum of these double precision numbers is some sextuple precision number [5].

Second, we have taken a multilayer variational wave function with five independent sets of variational parameters (instead of four as in [6]), which consecutively approximates one after another smaller and smaller distances of electrons with respect to a nucleus.

A variational wave function is expanded in the form [6]

$$\psi_0 = \sum_{i=1}^{N/2} \{U_i \operatorname{Re}[\exp(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12})] + W_i \operatorname{Im}[\exp(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12})]\}, \quad (1)$$

where  $\alpha_i$ ,  $\beta_i$ , and  $\gamma_i$  are complex parameters generated in a quasirandom manner:

$$\alpha_i = \left[ \frac{1}{2} i(i+1) \sqrt{p_\alpha} (A_2 - A_1) + A_1 \right] + i \left[ \frac{1}{2} i(i+1) \sqrt{q_\alpha} (A'_2 - A'_1) + A'_1 \right]. \quad (2)$$

$[x]$  designates the fractional part of  $x$ ,  $p_\alpha$  and  $q_\alpha$  are some prime numbers,  $[A_1, A_2]$  and  $[A'_1, A'_2]$  are real variational intervals which need to be optimized. Parameters  $\beta_i$  and  $\gamma_i$  are obtained in a similar way. The actual values of these parameters for the calculation with the largest basis set of 5200 functions are presented in Table I. As is seen from the table fine tuning of variational parameters is not required, which greatly facilitates calculations.

TABLE I. Variational parameters and number of basis functions ( $n_i$ ) for different subsets of the variational wave function with  $N=5200$ . Intervals  $[A_1, A_2]$  and  $[A'_1, A'_2]$  correspond to real and imaginary parts of a randomly chosen parameter  $\alpha_i$  [see Eq. (2) for details], intervals  $[B_1, B_2]$  and  $[B'_1, B'_2]$  to  $\beta_i$ , and intervals  $[G_1, G_2]$  and  $[G'_1, G'_2]$  to  $\gamma_i$ . Prime numbers are  $p_\alpha=2$ ,  $p_\beta=3$ ,  $p_\gamma=5$ , and  $q_\alpha=7$ ,  $q_\beta=11$ ,  $q_\gamma=13$ .

	$n_i$	$A_1$	$A_2$	$A'_1$	$A'_2$	$B_1$	$B_2$	$B'_1$	$B'_2$	$G_1$	$G_2$	$G'_1$	$G'_2$
$i=1$	1160	0.70	3.10	0.00	0.60	0.95	3.35	0.00	0.50	0.00	0.80	0.00	0.75
$i=2$	1160	1.00	9.35	0.00	1.05	0.60	7.60	0.00	0.70	0.00	0.70	0.00	1.80
$i=3$	1020	3.00	14.0	0.00	0.00	3.50	14.0	0.00	0.00	0.00	1.60	0.00	1.60
$i=4$	950	16.0	48.0	0.00	0.00	16.0	48.0	0.00	0.00	0.00	10.0	0.00	5.50
$i=5$	910	45.0	200.0	0.00	0.00	45.0	200.	0.00	0.00	0.00	30.0	0.00	11.0

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TABLE II. Nonrelativistic energies for the ground state of a helium atom  ${}^{\infty}\text{He}$ .  $N$  is the number of basis functions. The last digits of the difference in energy between two successive calculations are shown in a third column.

$N$	$E_{nr}$ (in a.u.)	$\Delta E$
3400	-2.9037243770341195983110931	
3800	-2.9037243770341195983111421	490
4200	-2.9037243770341195983111540	119
4600	-2.9037243770341195983111572	32
5200	-2.9037243770341195983111587	15
Extrap.	-2.9037243770341195983111594(4)	

Table II demonstrates a convergence of the variational expansion with the number of basis functions. An extrapolated value has been obtained by means of the simple extrapolation formula

$$E_{\text{extrap}} = E(N) - CN^{-\nu}, \quad (3)$$

TABLE III. Comparison with other calculations.

	$N$	$E$ (a.u.)
Goldman [7]	8066	-2.903724377034119594
Chuluunbaatar <i>et al.</i> [8]	5669	-2.90372437703411959829
Sims and Hagstrom [3]	4648	-2.9037243770341195982999
Drake <i>et al.</i> [4]	2358	-2.903724377034119598305
	Extrap.	-2.903724377034119598311(1)
This work	5200	-2.903724377034119598311159

where parameters  $C$  and  $\nu$  are taken from the best fit of the last four or five calculations.

In Table III a comparison with the most recent and most accurate values is presented. Our result extends the accuracy of the previous calculations by more than three orders of magnitude.

The author would like to thank J. S. Sims and G. W. F. Drake for stimulating this work.

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