Relativistic effects of the $1s\,2s\,2p\ ^4P$ of He^-

Kwong T. Chung
Department of Physics, North Carolina State University, Raleigh, North Carolina 27605
(Received 1 September 1983)

With the use of an accurate nonrelativistic wave function, the relativistic effects of the He^- $1s\,2s\,2p\ ^4P$ state are computed. These include the mass-correction term, Darwin term, and retardation and mass-polarization effects. The calculated result enables us to significantly reduce the uncertainty of the electron affinity given by Bunge and Bunge. To assist future experimental measurement on the fine structure of this ion, the expectation values of the spin-orbit, spin-other-orbit, and spin-spin operators are also calculated.

I. INTRODUCTION

The $1s2s2p\ ^4P$ of He^- ion is of particular interest both theoretically and experimentally. In the absence of a true bound state, this is the most long-lived metastable state for the He^- ion. It is extensively used experimentally in various areas of physics. Hence an accurate knowledge of the energy and lifetime of this system is very important. In 1979, Bunge and Bunge[1] made a highly precise nonrelativistic calculation for the energy of this system. However, in Ref. 1 the relativistic contributions are only estimated. Since the result of this reference is used and probably will continue to be used for calibration purposes,[2] it is highly desirable to make an actual computation of these relativistic effects.

In this work, the relativistic operators and mass polarization effect of He^- are calculated with an accurate nonrelativistic wave function. The fine structure of He^- is also calculated by computing the expectation values of the spin-orbit, spin-other-orbit, and spin-spin interactions. These results will be presented in the following sections.

II. THE ENERGY

The Hamiltonian for the quartet He^- is given by[3]

$$H=H_0+H_1+H_2+H_3+H_4\ , \tag{1}$$

where

$$H_0=\sum_{i=1}^{3}\left[-\frac{1}{2}\nabla_i^2-\frac{Z}{r_i}\right]+\sum_{i<j}^{3}\frac{1}{r_{ij}}\ , \tag{2}$$

$$H_1=\frac{1}{8c^2}\sum_{i=1}^{3}p_i^4\ , \tag{3}$$

$$H_2=\frac{Z\pi}{2c^2}\sum_{i=1}^{3}\delta(\vec{r}_i)\ , \tag{4}$$

$$H_3=-a\sum_{i<j}^{3}\vec{\nabla}_i\cdot\vec{\nabla}_j\ , \tag{5}$$

and

$$H_4=-\frac{1}{2c^2}\sum_{i<j}^{3}\frac{1}{r_{ij}}\left[\vec{\mathrm{P}}_i\cdot\vec{\mathrm{P}}_j+\frac{\vec{r}_{ij}(\vec{r}_{ij}\cdot\vec{\mathrm{P}}_i)\cdot\vec{\mathrm{P}}_j)}{r_{ij}^2}\right]\ , \tag{6}$$

where for ^4He, the factor a is

$$a=m/(m+M)=5.4859\times10^{-4}/4.002\,05$$
$$=1.3708\times10^{-4}\ , \tag{7}$$

the velocity of light $c=137.036$ a.u. and $\vec{\nabla}_i$ is the gradient operator. $\vec{\mathrm{P}}_i$ and $\vec{\mathrm{S}}_i$ are the linear and spin-angular momentum operator, respectively. The nuclear charge Z is 2. There is no contribution from the Fermi-contact term for this quartet state because the expectation value of $\delta(\vec{r}_{12})$ is zero and because of the zero magnetic moment of ^4He.

To calculate the nonrelativistic energy of the He^- system, Rayleigh-Ritz variational method is used. The basis functions are chosen in the LS coupling scheme. It is similar to that of Chung[4] except the nonlinear parameters in each partial wave are optimized individually in the present calculation. The explicit form of these basis functions will not be given here. We refer the interested reader to Ref. 4. By using a 92 linear parameter, 15 partial-wave function, we obtain an energy of $-2.178\,005\,8$ a.u. Compared with the 300-term calculation of Bunge and Bunge,[1] $-2.178\,040$ a.u., it is higher by about 0.000 034 a.u. The wave function obtained in this calculation is also checked with the virial theorem. It is found that the deviation from the virial theorem is about $0.34\times10^{-3}\%$. The energy and wave function for this nonrelativistic calculation are given in Table I.

In calculating the relativistic contribution for H_1 the procedure given in Ref. 3 is used. That is, we used

$$\langle\psi\,|\,H_1\,|\,\psi\rangle=-\frac{1}{8c^2}\sum_i\int(P_i^2\psi)^\dagger(P_i^2\psi)d\tau \tag{8}$$

for the mass correction term. The computation for the expectation values of H_2 and H_3 are straightforward. For H_4, some difficulties arise from the $1/r_{ij}^3$ term. By using the identity

$$\frac{\vec{r}_{12}}{r_{12}^3}\cdot(\vec{r}_{12}\cdot\vec{p}_1)\vec{p}_2=-\nabla_2\left[\frac{\vec{r}_{12}}{r_{12}}\cdot\vec{p}_1\right]\vec{p}_2$$
$$+\frac{1}{r_{12}}(\vec{r}_{12}\cdot\vec{p}_1)\nabla_2\cdot\vec{p}_2+\frac{1}{r_{12}}\vec{p}_1\cdot\vec{p}_2 \tag{9}$$

TABLE I. The energy of $(1s2s2p)^4P^o$ of He^- (in a.u.). N is the number of linear parameters and α,β,γ are the nonlinear parameters. ΔE is the binging energy contributed by adding the partial wave.

	Partial wave	N	α	β	γ	ΔE
1	$[(s,s)^3S, p]$	20	2.0	0.575	0.275	2.172 671 0
2	$[(s,p)^3P, s]$	17	1.9	0.655	0.405	0.003 509 5
3	$[(s,p)^3P, d]$	19	2.0	0.535	0.335	0.000 817 2
4	$[(p,d)^3P, s]$	5	2.2	1.055	0.305	0.000 182 6
5	$[(p,p)^3S, p]$	8	1.55	1.32	0.305	0.000 582 7
6	$[(p,s)^3P, s]$	4	2.1	0.835	0.305	0.000 130 6
7	$[(s,d)^3D, f]$	4	2.0	0.88	0.60	0.000 030 5
8	$[(d,d)^3S, p]$	4	2.05	2.3	0.255	0.000 033 5
9	$[(p,s)^3P, d]$	2	1.90	0.75	0.30	0.000 005 7
10	$[(p,p)^3S, p]$	2	1.95	2.0	2.55	0.000 002 7
11	$[(d,p)^3P, s]$	1	2.0	0.715	0.335	0.000 009 9
12	$[(p,d)^3P, d]$	1	1.9	1.2	0.4	0.000 013 4
13	$[(d,f)^3P, s]$	2	2.6	1.68	0.38	0.000 009 2
14	$[(s,f)^3F, g]$	2	2.0	0.8	0.92	0.000 003 9
15	$[(f,f)^3S, p]$	1	2.35	2.5	0.255	0.000 003 4
Total		92				2.178 005 8

and partial integration, the expectation value of H_4 can be calculated. The result of this calculation is given in Table II. The present approach, i.e., relativistic corrections are calculated as expectation value of relativistic operators, has been used to obtain highly accurate energy for the two-electron system by Pekeris and collaborators.[5]

In Ref. 1, the truncation error for full configuration interaction (CI) and for the Slater-type orbital (STO) basis is also estimated to be $-0.000\,034(10)$ a.u. which gives $-2.178\,074(10)$ a.u. for the nonrelativistic energy of the He^- $1s2s2p\ ^4P$ system. However, in this reference, the relativistic contribution is estimated to be $-0.000\,114(8)$ a.u. (if the effect of the He^+ Lamb shift is excluded). Our calculation shows that the total relativistic and mass polarization contribution is $-0.000\,115$ a.u. in excellent agreement with this reference. Hence if the estimate of the nonrelativistic energy of Bunge and Bunge is correct, then the energy for the He^- $1s2s2p\ ^4P$ should be $-2.178\,189(10)$ a.u. Compared with the energy of He $1s2s\ ^3S$, $-2.175\,344$ a.u.,[5] the electron affinity is 77.40 ± 0.28 meV. (With no extrapolation, the electron affinity from the present work would be 75.56 meV.)

III. FINE STRUCTURE OF He^- $1s2s2p\ ^4P$

The fine structures of the Li-like $1s2s2p\ ^4P$ states have been of great interest in recent years. The accurate measurements of Levitt and Feldman,[6] Livingston and Berry,[7] and of Träbert *et al.*[8] have stimulated considerable amounts of theoretical work on this subject.[9–13] However, very few calculations have been carried out for the He^- system. Although Manson[9] investigated the He^- $1s2s2p\ ^4P$ fine structure, the wave function he used was very approximate. With the improvement of the experimental technique, the very small splitting of the fine structure of atomic systems can now be measured. For example, the long lifetime of this He^- system makes it an ideal candidate for the electron beat method.[14] It is, therefore, very important to provide accurate theoretical data

TABLE II. The electron affinity of He^- $(1s2s2p)^4P$ (in a.u.).

	This work	Bunge and Bunge (Ref. 1)	
$E_{\text{nonrelativistic}}$	$-2.178\,005\,8$	$-2.178\,040$[a]	$-2.178\,074(10)$[b]
$\langle(H_1+H_2)\rangle$	$-0.000\,112\,6$		
$\langle H_3\rangle$	$-0.000\,002\,6$		
$\langle H_4\rangle$	$0.000\,000\,5$		
Total energy	$-2.178\,120\,5$	$-2.178\,155$[c]	$-2.178\,189(10)$[c]
Electron affinity[d]	75.56 meV	76.48 meV	77.40 ± 0.28 meV
Experiment			79 ± 2 meV[e]
Experiment[f]			75 ± 5 meV

[a]300-term CI calculation.
[b]Extrapolated result.
[c]Results if the present relativistic corrections are included.
[d]Compared with the energy of He $1s2s\ ^3S$ at $-2.175\,344$ a.u. (Ref. 5) with 1 a.u. = 27.207 91 eV.
[e]Quoted in Ref. 1 from B. Brehm, M. A. Gusinow, and J. L. Hall, Phys. Rev. Lett. 19, 737 (1967).
[f]V. A. Oparin *et al.*, Zh. Eksp. Teor. Fiz. 66, 2008 (1974) [Sov. Phys.—JETP 39, 989 (1974)].

TABLE III. The fine structure of He^- $(1s2s2p)^4P$.

ΔE (10^{-6} a.u.)	$J=\frac{5}{2}$	$J=\frac{3}{2}$	$J=\frac{1}{2}$	$E_{5/2}$-$E_{3/2}$	$E_{3/2}$-$E_{1/2}$
$\langle H_{so}\rangle$	0.5100	−0.3400	−0.8500		
$\langle H_{soo}\rangle$	−0.8796	0.5864	1.4660		
$\langle H_{ss}\rangle$	0.0940	−0.3760	0.4700		
Total (in 10^{-6} a.u.)	−0.2756	−0.1296	1.0860	−0.1460	−1.2156
(in cm^{-1})	−0.06049	−0.02845	0.23837	−0.03202	−0.2668
Manson[a] (in cm^{-1})	−0.0704	−0.0251	0.261	−0.0453	−0.286

[a]See Ref. 9.

to stimulate further experimental interest.

The perturbation operators for the fine structure are coming from the spin-orbit, spin-other-orbit, and spin-spin interactions. These are[3]

$$H_{so}=\frac{Z}{2c^2}\sum_{i=1}^{3}\frac{\vec{l}_i\cdot\vec{s}_i}{r_i^3}\ , \tag{10}$$

$$H_{soo}=-\frac{1}{2c^2}\sum_{i\neq j}^{3}\left[\frac{1}{r_{ij}^3}(\vec{r}_i-\vec{r}_j)\times\vec{p}_i\right]\cdot(\vec{s}_i+2\vec{s}_j)\ , \tag{11}$$

and

$$H_{ss}=\sum_{i<j}\frac{1}{c^2r_{ij}^3}\left[\vec{s}_i\cdot\vec{s}_j-\frac{3(\vec{s}_i\cdot\vec{r}_{ij})(\vec{s}_j\cdot\vec{r}_{ij})}{r_{ij}^2}\right]\ . \tag{12}$$

The expectation value of these operators are calculated in the *LSJ* scheme. That is, the good quantum number J is formed by

$$|JJ_zLS\rangle=\sum_{S_zL_z}|LSL_zS_z\rangle\langle LSL_zS_z|JJ_z\rangle\ , \tag{13}$$

where $\langle LSL_zS_z|JJ_z\rangle$ is the Clebsch-Gordan coefficient[15] and $|LSL_zS_z\rangle$ is the angular part of the wave function obtained in the preceding section. To simplify the computation, the Wigner-Eckart theorem is also used.[15]

The result of the present calculation is given in Table III. It is interesting to note that the $J=\frac{1}{2}$, $\frac{3}{2}$, and $\frac{5}{2}$ levels are completely inverted as predicted by Manson.[9] The fine-structure splitting is predicted to be −0.03202 and −0.2668 cm^{-1} for $E_{5/2}$-$E_{3/2}$ and $E_{3/2}$-$E_{1/2}$, respectively. The calculated splitting of the $E_{5/2}$-$E_{3/2}$ of this work differs from that of Ref. 9 by about 30% but the difference between the two results for $E_{3/2}$-$E_{1/2}$ is less than 8%. In view of the approximate nature of the wave function used in Ref. 9 this agreement is rather remarkable.

IV. SUMMARY

The purpose of this work is to provide a more accurate relativistic correction to the energy of Bunge and Bunge, thus, to obtain a more reliable electron affinity energy for He^- $1s2s2p\ ^4P$. To this end, we have used an accurate nonrelativistic wave function to evaluate the relativistic contributions. If the calculation presented in this work is reliable, the electron affinity calculated by Bunge and Bunge can be quoted with an uncertainty of ±0.28 meV rather than the ±0.5 meV given in Ref. 1.

The Lamb shift for low-Z atomic system is expected to be small; it is not considered in this work. Since the electron affinity is the energy difference of the He $1s2s\ ^3S$ and He^- $1s2s2p\ ^4P$ states and the energy of He $1s2s\ ^3S$ quoted from Ref. 5 does not include the Lamb shift, the error on the calculated affinity is probably negligible. Hence if the nonrelativistic estimate from Ref. 1 is correct, the electron affinity of He^- is 77.40±0.28 meV. It should be pointed out here that the nonextrapolated result in this work would be 75.56 meV.

To stimulate further experimental interest on the measurement of very small fine-structure splitting of atomic systems, the expectation value for the spin-orbit, spin-other-orbit, and spin-spin operators are also calculated. We hope these results can be compared with that of the experiment in the near future.

ACKNOWLEDGMENTS

I wish to thank Professor W. Mehlhorn and Dr. R. Bruch for the hospitality they extended to me at the University of Freiburg where part of this research was carried out. This work is supported by the National Science Foundation Grant No. 82-06490 and by the Deutsche Forschungsgemeinschaft (DFG).

[1]A. V. Bunge and C. F. Bunge, Phys. Rev. A 19, 452 (1979).
[2]R. V. Hodges, M. J. Coggiola, and J. R. Peterson, Phys. Rev. A 23, 59 (1981).
[3]H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer, Berlin, 1957), p. 181.
[4]K. T. Chung, Phys. Rev. A 20, 724 (1979).
[5]Y. Accad, C. L. Pekeris, and B. Schiff, Phys. Rev. A 4, 516 (1971); C. L. Pekeris, Phys. Rev. 112, 1649 (1958).
[6]M. Levitt and P. Feldman, Phys. Rev. 180, 48 (1969); M. Levitt, R. Novick, and P. D. Feldman, Phys. Rev. A 3, 140 (1971).
[7]A. E. Livingston and H. G. Berry, Phys. Rev. A 17, 1966 (1978).
[8]E. Träbert, H. Hellman, P. H. Heckman, S. Bashkin, H. A. Klein, and J. D. Silver, Phys. Lett. 93A, 76 (1982).
[9]S. T. Manson, Phys. Rev. A 3, 147 (1971).
[10]K. T. Cheng, J. P. Desclaux, and Y. K. Kim, J. Phys. B 11, L359 (1978).
[11]M. H. Chen, B. Crasemann, and H. Mark, Phys. Rev. A 27, 544 (1983).
[12]R. Glass, J. Phys. B 11, 3469 (1978).
[13]J. Hata and I. P. Grant, J. Phys. B 16, 915 (1983).
[14]R. Bruch and H. Klar, J. Phys. B 13, 2885 (1980).
[15]A. Messiah, *Quantum Mechanics* (Wiley, New York, 1961), Vol. II.