PHYSICAL REVIEW A VOLUME 2, NUMBER 5 NOVEMBER 1970

Transitions $(1s2p)\,^3P^o$-$(2p^2)\,^3P^e$ in He and $(2s2p)\,^3P^o$-$(2p^2)\,^3P^e$ in H$^-$

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(Received 13 July 1970)

Precision calculations of the energies of the $(2p^2)\,^3P^e$ states of He and H$^-$ are carried out with a Hylleraas-type wave function and are the lowest variational results yet obtained. The associated wave functions are used to calculate the mass polarization of the state. With the reduced mass correction, the wave numbers of the transitions $(1s2p)\,^3P^o-(2p^2)\,^3P^e$ in He and $(2s2p)\,^3P^o-(2p^2)\,^3P^e$ in H$^-$ are found to be 312 222 and 3783 cm^{-1}, respectively. This former value is in disagreement with the experiment of Kruger (1930) who obtained 312 118 cm^{-1}. The discrepency between the experimental and theoretical values of 100 cm^{-1} is large enough to encourage renewed experimental observation.

I. INTRODUCTION

The $(1s2p)\,^3P^o-(2p^2)\,^3P^e$ transition in He was observed by Kruger[1] in 1930. He obtained 312 118 cm^{-1} for this transition. The most detailed calculation of Aashamar[2] gives 312 217 cm^{-1} for this transition and it differs by 100 cm^{-1} compared to the experimental value. He calculated the eigenvalues of $(2p^2)\,^3P^e$ states in He and H$^-$ by using variational perturbation method of Hylleraas-Scherr-Knight procedure.[3] This method of calculation does not give any bound on the eigenvalues obtained. In view of the discrepancy between the theoretical and experimental results, it is appropriate to carry out a detailed variational calculation which gives an upper bound to the eigenvalues. The eigenvalues obtained are lower than the results of the other variational calculations.[4-6]

II. NONRELATIVISTIC EIGENVALUES

The most general P-wave function for even parity can be written[7]

$$\Psi(\vec{r}_1, \vec{r}_2)=[f(r_1, r_2, r_{12})+f(r_2, r_1, r_{12})]\ \mathfrak{D}_1^{0+}(\Omega), \qquad (1)$$

where the $\mathfrak{D}(\Omega)$ is the rotational harmonics, depending on the symmetric angles θ, ϕ, ψ.[7] The trial radial function $f(r_1, r_2, r_{12})$ is of Hylleraas type and is written as positive power expansions in terms of r_1, r_2, r_{12}, namely,

$$f(r_1, r_1, r_{12})=e^{-(\gamma r_1+\delta r_2)} \times \sum_{l\geq 0} \sum_{m\geq 0} \sum_{n\geq 0} C_{lmn} r_1^l r_2^m r_{12}^n . \qquad (2)$$

Since under exchange[7]

$$\mathscr{E}_{12}\, \mathfrak{D}_1^{0+}(\Omega) = -\mathfrak{D}_1^{0+}(\Omega) \ , \qquad (3)$$

the above wave function is antisymmetric in exchange and therefore refers to the triplet state. It is of even parity[7] because of

$$\mathcal{P}\, \mathfrak{D}_1^{0+}(\Omega) = +\mathfrak{D}_1^{0+}(\Omega) \ . \qquad (4)$$

The expectation value of the energy is given by

$$E=\langle \Psi H \Psi\rangle / \langle\Psi\Psi\rangle \ , \qquad (5)$$

where the Hamiltonian H (in rydbergs) is given by

$$H=-\nabla_1^2-\nabla_2^2-2Z/r_1-2Z/r_2+2/r_{12} \ . \qquad (6)$$

The eigenvalue E and the wave function Ψ are obtained variationally. The wave functions obtained are used to calculate the correction to the eigenvalue due to mass polarization, which is given by

$$E_M=-(2m/M)\langle \Psi \nabla_1 \cdot \nabla_2 \Psi\rangle \ . \qquad (7)$$

The resultant eigenvalue is given by

$$E_T=E+E_M \ . \qquad (8)$$

TABLE I. Variational nonrelativistic energy E and the mass-polarization correction E_M for He in units of rydberg (R_M). The nonlinear parameters are $\gamma=0.786$ and $\delta=1.390$.

N	$-E$	$E_M\times 10^4$
20	1.420 913 411 81	0.125 189 18
35	1.420 995 752 67	0.125 260 75
56	1.421 000 099 87	0.125 267 76
70	1.421 000 281 02	0.125 268 33
84	1.421 000 285 53	0.125 268 24
90	1.421 000 299 90	0.125 268 26
95	1.421 000 302 00	0.125 268 26
96	1.421 000 303 03	0.125 268 25
97	1.421 000 304 14	0.125 268 24

TABLE II. Variational nonrelativistic energy E and the mass-polarization correction E_M for H$^-$ in units of rydberg (R_M). The nonlinear parameters are $\gamma=0.48$ and $\delta=0.153$.

N	$-E$	$E_M\times 10^5$
20	0.250 633 9181	0.831 938 36
35	0.250 679 3267	0.829 078 73
56	0.250 704 3288	0.819 861 73
70	0.250 707 0029	0.818 446 92
84	0.250 707 1403	0.818 391 41
90	0.250 709 4102	0.816 452 84

TABLE III. Comparison of the calculated values of nonrelativistic energies with previous calculations and experiment.

Author/System	He		H⁻		Remarks
	E (R_M)	Transition $(1s2p)^3P^0 - (2p^2)^3P^e$ (cm^{-1})	E (R_M)	Transition $(2s2p)^3P^0 - (2p^2)^3P^e$ (cm^{-1})	
Drake[a]			−0.250 7008	3670	Variational, two nonlinear parameters
Drake and Dalgarno[b]	−1.420 999	312 220.99			Variation, two nonlinear parameters
Holøien[c]	−1.421 000 299 0	312 220.85	−0.250 702 012		Variational, one nonlinear parameter
Present calculations	−1.421 000 304 14	312 222.22[d]	−0.250 709 4102	3787.03[d]	Variational, two nonlinear parameters
Aashamar[e]	−1.421 000 311 20	312 217[f]	−0.250 653 6415		Variational Perturbation[g]
Experiment[h]		312 118[i]			

[a]Reference 4.
[b]Reference 5.
[c]Reference 6.
[d]Includes mass polarization corrections.
[e]Reference 2.
[f]Includes mass polarization and relativistic corrections.
[g]Reference 3.
[h]Reference 1.
[i]See Note added in Manuscript.

III. RESULTS AND DISCUSSION

The nonrelativistic energy E and the mass-polarization correction E_M are given in the Tables I and II as a function of the number of terms for He and H^-, respectively. In Table III the present results are compared with other calculations and also with experiment. The present results for the eigenvalues are lower than the other variational calculations.

The sharp line in far-uv region with wave number 312 118 cm^{-1}, corresponding to a wave length 320.392 Å, has been observed by Kruger[1] and is ascribed by Wu[8] to the transition $(1s2p)\ ^3P^o - (2p^2)\ ^3P^e$ in He. In order to compare with experiment, we use the Pekeris[9] value $-4.266\,556\,218 R_M$ for the energy of the $(1s2p)\ ^3P^o$ state of helium in combination with our theoretical value of the $(2p^2)\ ^3P^e$ state. This gives rise to a line with wave number 312 222 cm^{-1}, corresponding to a wavelength 320.284 Å. This number differs by that of Aashamar by 5 cm^{-1}, which is the contribution due to relativistic corrections.[2] The discrepancy between the experimental and theoretical values is nearly 100 cm^{-1}. As noted by Aashamar also, this discrepancy cannot be accounted for on theoretical grounds and should be ascribed to the experimental errors. It will be worthwhile to repeat the experiment to observe this transition in question.

The state $(2p^2)\ ^3P^e$ in H^- can decay radiatively into $(1sKp)\ ^3P^o$ continuum or to the $(2s2p)\ ^3P^o$ autoionization state with a lifetime of 10^{-12} sec. The position and width of the autoionization state of H^- have been calculated accurately[10] and are $-0.285\,194\,02 R_M$ and 0.006 eV, respectively. Combining with energy of the state $(2p^2)\ ^3P^e$, we find after reduced mass correction, the transition should give rise to a line of wave number 3783 cm^{-1}. The width of the line is dominated by the autoionization width of $(2s2p)\ ^3P^o$ state and, therefore, should be of the order of 0.006 eV, corresponding to 50.9 cm^{-1}.

Note added in manuscript. The transition $(1s2p)\ ^3P^o - (2p^2)\ ^3P^e$ in He is under reinvestigation by Dr. J. L. Tech and J. Ward of the National Bureau of Standards. The preliminary results appear to agree very closely with the theoretical calculations. More details will be given in their publication.

ACKNOWLEDGMENTS

I would like to thank Dr. W. C. Martin for pointing out the discrepancy between the experimental and theoretical results for helium. I wish to thank Dr. A. Temkin for helpful discussions and critical reading of the manuscript.

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