OSCILLATOR STRENGTHS OF THE $1s2s\ ^1S^e \rightarrow 1s2p\ ^1P^o$ TRANSITION IN He

S.N. TIWARY* AND P. KUMAR

International Centre for Theoretical Physics 34 100 Trieste, P.O.B. 586, Italy

(Received August 29, 1990)

The paper presents configuration interaction (CI) calculations of both the length and velocity forms of the oscillator strengths for $1s2s\ ^1S^e \rightarrow 1s2p\ ^1P^o$ transition in the He atom. For the first time the agreement between the length and velocity values to within about 0.045% has been achieved.

PACS numbers: 31.10.+z

1. Introduction

Helium is an abundant element in the universe and has been of growing interest for both experimentalists as well as theorists. Knowledge of accurate optical oscillator strengths is needed in laser physics, plasma physics, astrophysics, atmospheric physics, and fusion research. It is also required in testing the accuracy wave functions involved in the transition matrix elements. The agreement between the length (f_L) and velocity (f_V) forms of the oscillator strengths reflects the accuracy of the wave functions. Exact wave functions are exact solutions of the exact Schrödinger wave equation. In practice, it is not possible to solve Schrödinger wave equation except for the hydrogen atom. Alternative to solving the Schrödinger equation, the configuration interaction method is widely used in atoms, molecules, ions, clusters and solids.

Tiwary and his coworkers [1–13] have extensively investigated both the length and velocity forms of both the relativistic and non relativistic optical oscillator strengths in several atoms and ions using Hartree–Fock (HF) and configuration interaction (CI) wave functions. Most recently, Tiwary [11–13] has shown that the choice of configurations and orbitals employed in configurations plays an extremely important role in order to have a very compact CI calculation which yields an excellent agreement between f_L and f_V. Recently, Berrington et al.[14]

*A part of this work was done when the author was Research Director and Professor, CNRS Laboratory, University of Paris-Sud, Paris; Observatoire de Paris, Meudon, France.

have calculated the length and velocity forms of the oscillator strengths for He. Considerable disagreement between the length and velocity values exists. Weise et al.[15] have reported the experimental value of the oscillator strength for the He atom.

The primary purpose of this paper is to extend our earlier calculations based on the Tiwary approach, which is very convenient, economic, compact and promising, to evaluate the length and velocity values of the optical oscillator strengths for the $1s2s\ ^1S^e \rightarrow 1s2p\ ^1P^o$ transition in the He atom.

2. Method

We have carried out our calculations using the computer CIV3 of Hibbert [16] in the same way as in our earlier work [1–13]. The CI wave function is written as

$$\Psi(LS) = \sum_{i=1}^{M} a_i \Phi_i(\alpha_i LS). \tag{1}$$

Each of the M single-configuration function Φ_i is constructed from one-electron functions, whose orbital and spin momenta are coupled to form the common total angular momentum quantum number L and S according to the prescription denoted in (1) by α_i.

We express the radial parts of the one-electron functions in analytical form as a sum of Slater-type orbitals, following Clementi and Roetti[17]:

$$P_{nl} = \sum_{j=1}^{k} C_{jnl} r^{I_{jnl}} e^{-\xi_{jnl} r}. \tag{2}$$

The parameters in (2) can be varied to optimize the energy of any state, subject to orthonormality condition

$$\int_0^\infty P_{nl}(r) P_{n'l}(r) \mathrm{d}r = \delta_{nn'}. \tag{3}$$

Once wave functions of the form (1) have been determined in this way, they can be used to obtain the optical oscillator strengths, f_L and f_V, for the transition between the initial and final states Ψ^i and Ψ^f with energies E^i and E^f respectively:

$$f_L = \frac{2\Delta E}{3g_i} |\langle \Psi^i | \sum_{p=1}^{N} r_p | \Psi^f \rangle|^2 \tag{4}$$

and

$$f_V = \frac{2}{3g_i \Delta E} |\langle \Psi^i | \sum_{p=1}^{N} \nabla_p | \Psi^f \rangle|^2, \tag{5}$$

whereas $\Delta E = E^f - E^i$ and $g_i = (2L_i + 1)(2S_i + 1)$ is the statistical weight of the lower state Ψ^i. For the exact wave functions, (4) and (5) give identical results.

For approximate wave functions the two equations may yield different results. The reliability of either depends on the closeness of f_L and f_V. The orbital parameters are given in Table I, and the configurations, eigenvalues and eigenvectors are shown in Table II.

TABLE I

Orbital	Clementi-type coefficient	Slater-type coefficient	Power of r	Exponent
1*s*	0.7683746	2.5925207	1	1.4171400
	0.2234582	1.6376495	1	2.3768196
	0.0408197	0.7525371	1	4.3962803
	−0.0099399	−0.3314993	1	6.5269899
	0.0023000	0.1029656	1	7.9425201
2*s*	0.6509011	0.8069327	1	0.7269900
	−1.4337626	−0.5081150	2	0.6234567
3*s*	0.7648256	0.2992656	1	0.3370100
	−1.7828140	−0.2852873	2	0.4536100
	1.6303940	0.0175190	3	0.3504700
4*s*	0.8293958	4.1807432	1	1.8520002
	−1.4844770	−2.0038538	2	1.0644598
	1.5559158	0.0670743	3	0.5212400
	−0.9731816	−0.0020540	4	0.4131600
2*p*	0.9999984	0.2525131	2	0.5444100
3*p*	1.0273581	0.1118024	2	0.3887800
	−1.6455326	−0.0137661	3	0.3262800
4*p*	0.8165703	1.2150021	2	1.1067400
	−4.7213602	−0.0193060	3	0.2659300
	4.7835064	0.0025682	4	0.3047900
3*d*	0.9999996	0.0090422	3	0.3336100

TABLE II

Eigenvalues			
0.15806031	−0.19589573	−0.25147843	−0.27560341
Eigenvectors			
0.04079726	−0.02400953	0.00065881	−0.00062717
0.07248473	−0.00097271	0.01833319	0.00655191
0.12160408	0.01192556	0.03794486	−0.00998447
0.22682041	0.32660192	−0.47904712	0.78044623
0.34985387	0.52506173	−0.46953279	−0.60262746
0.33175260	0.56233323	0.73981160	0.12476432
0.75448149	−0.53275615	0.02153911	0.03535789
0.33152992	−0.09800667	0.01471848	−0.10096729
0.00414367	−0.00988289	−0.00142995	0.00164838
0.00308820	−0.01484744	0.01627476	−0.02436458
0.12335235	0.08341360	−0.00362617	0.00081825
Eigenvalues			
−0.32496315	−0.51877910	−0.66916490	−1.62146854
Eigenvectors			
−0.00647475	0.00255906	−0.00353335	−0.01475137
−0.02745869	0.53957993	−0.83187890	0.01490863
−0.10852885	0.81941342	0.54762793	−0.01517044
−0.04392256	−0.01646160	0.00567848	0.00258452
0.13296682	−0.02415534	−0.00517827	−0.00211096
0.07031196	−0.07651496	−0.00644495	0.00066703
0.34062368	−0.06705791	0.00708818	−0.14861274
−0.91970563	−0.14751071	−0.03686330	−0.02457336
0.01264475	−0.06551158	0.07706523	−0.04746114
0.00711230	−0.00246042	−0.00362650	−0.00117549
−0.02800527	0.01239579	−0.02475663	−0.98710841
Eigenvalues			
−2.00556278	−2.09898376	−2.86817265	
Eigenvectors			
−0.00075378	0.00069020	−0.99874216	
0.01016305	−0.10036153	0.00719863	
0.00578633	−0.01130393	0.00578961	
0.03240103	0.00426215	0.00077057	
0.00093062	−0.00100374	0.00086157	
−0.00037473	0.00029970	−0.00019551	
−0.01058970	0.02381424	0.04343308	
0.00304885	−0.00115770	0.02204642	
0.11374962	−0.98706824	−0.00018459	
0.99284047	0.11451381	−0.00043560	
−0.00497466	0.04242749	0.00786655	

3. Results and discussion

Table III displays our present calculated configuration interaction oscillator strengths, of both f_L and f_V, of the $1s2s\ ^1S^e \rightarrow 1s2p\ ^1P^o$ transition in the He atom with other available theoretical results of Berrington et al.[14] and experimental value reported by Weise et al.[15].

TABLE III
Optical oscillator strengths (OOS) of the $1s2s\ ^1S^e \rightarrow 1s2p\ ^1P^o$ transition in the He atom.

OOS	Present results	Berrington et al.	Weise et al.
f_L	0.36155194	0.3662	
f_V	0.36171776	0.3445	0.3764

Several features of importance emerge from Table III. First, there is an excellent agreement (within 0.045%) between our present compact CI length and velocity forms of the oscillator strengths which reflects the quality of the wave functions employed in the transition matrix elements and indicates the validity of the Tiwary approach. Second, Berrington et al. have achieved the agreement between the length and velocity values to within about 5.926% which is considerably larger than our prediction. Our present values of the oscillator strengths are close to the length form of the oscillator strengths of Berrington et al. which indicates that the length value is more reliable than the velocity value of the oscillator strengths. Third, the experimental value of the oscillator strength reported by Weise et al. differs from the theoretical values. However, the disagreement between the experimental observation and theoretical predictions is not too large. Finally, our experience of extensive theoretical investigations of both the relativistic as well as non relativistic optical oscillator strengths shows that a huge number of configurations and orbitals in the configurations are needed in order to obtain an excellent agreement between the length and velocity forms of the oscillator strengths. This makes the CI calculation very cumbersome as well as very expensive from the computational point of view. Using the suitable choice of the basis orbitals which leads to a very compact CI calculation and also yields an excellent agreement, we have for the first time obtained the agreement between f_L and f_V to within about 0.045%.

4. Conclusion

Our present results demonstrate that the Tiwary approach is capable of producing an excellent agreement between the length and velocity forms of the optical oscillator strengths. The present CI wave function may be of use for calculations of scattering cross sections for the excitation process in the helium atomic system. We hope that this work will stimulate further experimental as well as theoretical investigations.

Acknowledgments

The author would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO, for hospitality at the International Centre for Theoretical Physics, Trieste, Italy and Swedish Agency for Research Cooperation with Developing Countries (SAREC) for financing my current Associateship visit. He is also grateful to Professors Dujardin, Hellner, Le Rouzo, Combet Fernoux, Gaillard (Director), Remy (Adj. Director) and Hibbert for encouragement and discussion. Finally, he wishes to express his thanks to Bihar University, India, for leave and UGC for Major Research Project.

References

[1] S.N. Tiwary, *Chem. Phys. Lett.* **93**, 47 (1982).

[2] S.N. Tiwary, *Chem. Phys. Lett.* **96**, 333 (1983).

[3] S.N. Tiwary, A.E. Kingston, A. Hibbert, *J. Phys. B* **16**, 2457 (1983).

[4] A. Hibbert, A.E. Kingston, S.N. Tiwary, *J. Phys. B* **15**, L643 (1982).

[5] S.N. Tiwary, *Astrophys.* **269**, 803 (1983).

[6] S.N. Tiwary, *Astrophys.* **272**, 781 (1983).

[7] A.E. Kingston, A. Hibbert, S.N. Tiwary, *J. Phys. B* **20**, 3907 (1987).

[8] S.N. Tiwary, *Atomic and Molecular Physics*, World Scientific Publisher Co, Singapore 1987.

[9] S.N. Tiwary, A.P. Singh, D.D. Singh, R.J. Sharma, *Can. J. Phys.* **66**, 1076 (1988).

[10] S.N. Tiwary, *Ph. D. Thesis on Structure and Scattering Calculations in Atoms and Ions,* Bihar University, Muzaffarpur, Bihar 1989.

[11] S.N. Tiwary, ICTP, Trieste, IC/90/243.

[12] S.N. Tiwary, ICTP, Trieste, IC/91/111.

[13] S.N. Tiwary, *Nuovo Cimento* (in press).

[14] K.A. Berrington, P.G. Burke, L.C.G. Freitas, A.E. Kingston, *J. Phys. B* **18**, 4135 (1985).

[15] W.L. Weise, M.W. Smith, B.M. Gennon, *Atomic Transition Probabilities,* NSRDS-NBS, US Government Printing Office, Washington 1966.

[16] A. Hibbert, *Comput. Phys. Commun.* **9**, 141 (1975).

[17] E. Clementi, C. Roetti, *At. Data Nucl. Data Tables* **14**, 177 (1974).