*International Journal of Theoretical Physics, Vol. 30, No. 6, 1991*

# Effect of Relativity on the Oscillator Strengths of $2p^6 3s\ ^2S^e_J \rightarrow 2p^5 3s^2\ ^2P^o_{J'}$ Transition in $Cu^{18+}$, $Zn^{19+}$, $Br^{24+}$, and $Kr^{25+}$ ions

**S. N. Tiwary**[1]

*Received August 31, 1990*

We report Hartree-Fock and configuration-interaction calculations of both the length and velocity forms of the oscillator strengths for the resonance excitation $1s^2 2s^2 2p^6 3s\ ^2S^e_J \rightarrow 1s^2 2s^2 2p^5 3s^2\ ^2P^o_{J'}$ transition, which leads to autoionization (Auger transition), in the $Cu^{18+}$, $Zn^{19+}$, $Br^{24+}$, and $Kr^{25+}$ ions of the sodium isoelectronic sequence both in *LS* and intermediate coupling schemes. Our present results demonstrate that relativity has a substantial influence on the oscillator strengths.

## 1. INTRODUCTION

Knowledge of both the length ($f_L$) and velocity ($f_V$) forms of the optical oscillator strengths is needed in astrophysics, plasma physics, atmospheric physics, laser physics, and fusion research; it is also required in testing the accuracy of the wave functions involved in the transitions under consideration. The agreement between $f_L$ and $f_V$ indicates the accuracy of the wave functions. Accurate wave functions are needed for the reliable study of collision processes in atoms, molecules, and ions.

It is well known that relativistic effects play an extremely important role in obtaining accurate results, especially in heavy ions. Consequently, it is indispensable to incorporate the relativistic effects in order to obtain reliable results.

The primary purpose of this work is to examine the effects of (1) relativity, (2) correlation, and (3) inclusion of $3p$ and $3d$ orbitals taken from Clementi and Roetti (1974) [smaller exponents of the $2p$ orbital of Clementi and Roetti are used for $3p$ and $3d$ orbitals exactly in the same way as we did in our earlier work (Tiwary, 1990)] in our present CI

[1]International Centre for Theoretical Physics, Trieste, Italy.



0020-7748/91/0600-0825$06.50/0 

calculations on both the length and velocity forms of the optical oscillator strengths for the inner-shell excitation, which leads to autoionization and plays an important role in explaining the structure observed in the total ionization cross-section curve by electron impact, the $1s^2 2s^2 2p^6 3s\ ^2S_J^e \rightarrow 1s^2 2s^2 2p^5 3s^2\ ^2P_{J'}^o$ transition in the $Cu^{18+}$, $Zn^{19+}$, $Br^{24+}$, and $Kr^{25+}$ ions of the sodium isoelectronic sequence.

## 2. METHOD

We have performed our $J$-independent and -dependent calculations using the general configuration-interaction (CI) code CIV3 of Hibbert (1975) and Glass and Hibbert (1978). The $LS$ wave functions are written in the form

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

The coefficients $a_i$ are the eigenvector components of the Hamiltonian matrix with typical element

$$H_{ij} = \langle \Phi_i | H | \Phi_j \rangle \tag{2}$$

$\Phi_j$ are single-configuration functions constructed from one-electron functions, whose orbital and spin momenta are coupled to form the common total angular momentum quantum numbers $L$ and $S$ according to a prescription denoted in (1) by $\alpha_i$.

We express the radial parts of the one-electron functions in analytical form as a sum of Slater-type orbitals, following Clementi and Roetti (1974):

$$P_{nl} = \sum_{j=1}^{k} C_{jnl} r^{I_{jnl}} e^{-\xi_{jnl} r} \tag{3}$$

The parameters in (3) can be varied to optimize the energy of any state, subject to the orthonormality conditions

$$\int_0^\infty P_{nl}(r) P_{n'l}(r)\, dr = \delta_{nn'} \tag{4}$$

Once the radial wave functions are determined, relativistic effects may be added to the Hamiltonian in the form of the Breit–Pauli interaction, of which we include the spin–orbit, spin–other-spin, spin–spin, mass correction, and one-body Darwin terms. The first three terms split $LS$ states into $J$-dependent levels, while the last two effect the overall energy of each term. The expansion (1) is then replaced by

$$\Psi(J) = \sum_i a_i \Phi_i(LSJ) \tag{5}$$

where the summation now includes single configurations with different $L$ and $S$ (which can couple to form a common $J$ value). The matrix which is diagonalized to give the eigenenergies and eigenvector components $a_i$ now contains the Breit–Pauli operators as well as the previous nonrelativistic terms in the Hamiltonian.

## 3. RESULTS AND DISCUSSION

Table I displays the $J$-independent and -dependent Hartree–Fock (HF) and configuration-interaction (CI) optical oscillator strengths, of both the length ($f_L$) and velocity ($f_V$) forms, of the resonance excitation (the inner-shell excitation which leads to autoionization), the $1s^2 2s^2 2p^6 3s\ ^2S^e_J \rightarrow 1s^2 2s^2 2p^5 3s^2\ ^2P^o_{J'}$ transition in the $Cu^{18+}$, $Zn^{19+}$, $Br^{24+}$, and $Kr^{25+}$ ions of the sodium isoelectronic sequence.

Several features of importance emerge from Table I. First, relativistic effects lead to an increase of $f_L$ values in the CI calculations, whereas the situation is reversed in the case of the $f_V$ values. Second, correlation effects enhance both $f_L$ and $f_V$ values. Our present CI $f_L$ is smaller than the CI $f_V$, whereas the HF $f_L$ is larger than the HF $f_V$. Third, it is clear from Table I that the relativistic $f_L$ and $f_V$ values for the $\Delta J = 0$ transition are significantly smaller compared to the $f_L$ and $f_V$ values for the $\Delta J = 1$ transitions. Values of the oscillator strengths decrease with increase of the atomic number $Z$.

**Table I.** $J$-Independent and -dependent Oscillator Strengths of $1s^2 2s^2 2p^6 3s\ ^2S^e_J \rightarrow 1s^2 2s^2 2p^5 3s^2\ ^2P^o_{J'}$ in the $Cu^{18+}$, $Zn^{19+}$, $Br^{24+}$, and $Kr^{25+}$ Ions of the Sodium Isoelectronic Sequence

| Systems | Function | $f_L$ | $f_V$ | $2J+1$ | $2J'+1$ | $f_L$ | $f_V$ |
|---|---|---|---|---|---|---|---|
| $Cu^{18+}$ | HF | 0.062 | 0.058 | 2 | 2 | 0.021 | 0.019 |
| | | | | 2 | 4 | 0.041 | 0.039 |
| | CI | 0.080 | 0.082 | 2 | 2 | 0.029 | 0.026 |
| | | | | 2 | 4 | 0.057 | 0.053 |
| $Zn^{19+}$ | HF | 0.061 | 0.058 | 2 | 2 | 0.021 | 0.019 |
| | | | | 2 | 4 | 0.041 | 0.038 |
| | CI | 0.079 | 0.081 | 2 | 2 | 0.029 | 0.026 |
| | | | | 2 | 4 | 0.057 | 0.052 |
| $Br^{24+}$ | HF | 0.058 | 0.055 | 2 | 2 | 0.019 | 0.018 |
| | | | | 2 | 4 | 0.039 | 0.037 |
| | CI | 0.074 | 0.076 | 2 | 2 | 0.029 | 0.024 |
| | | | | 2 | 4 | 0.055 | 0.047 |
| $Kr^{25+}$ | HF | 0.057 | 0.055 | 2 | 2 | 0.019 | 0.018 |
| | | | | 2 | 4 | 0.038 | 0.037 |
| | CI | 0.073 | 0.076 | 2 | 2 | 0.028 | 0.023 |
| | | | | 2 | 4 | 0.054 | 0.046 |

Finally, our present results clearly demonstrate that both relativity and correlation have substantial influence on the oscillator strengths, of both the length and velocity forms, of the inner-shell excitation, which leads to autoionization in the $Cu^{18+}$, $Zn^{19+}$, $Br^{24+}$, and $Kr^{25+}$ ions of the sodium isoelectronic sequence. This suggests that it is indispensable to incorporate the relativistic and correlation effects simultaneously in order to obtain the most reliable results.

## 4. CONCLUSION

Our present theoretical relativistic and nonrelativistic investigations of both the length and velocity forms of the optical oscillator strengths demonstrate the importance of correlation, relativity, and our new approach to choose the basis functions in the Hartree-Fock as well as configuration-interaction calculations. We hope that this work will stimulate experimental and other more elaborate theoretical investigations.

## ACKNOWLEDGMENTS

The author would like to thank Prof. Abdus Salam, the International Atomic Energy Agency, and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste, Italy, and the Swedish Agency for Research Cooperation with Developing Countries (SAREC) for financing my current Associateship visit. He is also grateful to Profs. Denardo, Dujardin, Hellner, le Rouzo, Combet Fernoux, Gaillard (Director), Remy (Adj. Director), and Hibbert for encouragement and suggestions. Finally, he wishes to express his thanks to Bihar University, India, for leave. Part of this work was done while the author was Research Director and Professor, CNRS Laboratory, University of Paris-Sud, and Observatoire de Paris, Meudon, Paris, France.

## REFERENCES

Clementi, E., and Roetti, C. (1974). *Atomic Data Nuclear Data Tables*, **14**, 177.
Glass, R., and Hibbert, A. (1978). *Comput. Physics Communications*, **16**, 19.
Hibbert, A. (1975). *Comput. Physics Communications*, **9**, 141.
Tiwary, S. N. (1990). ICTP, Trieste, Italy, preprint.