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Relativistic and Nonrelativistic Oscillator Strengths in the Na Isoelectronic Sequence

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We report the general trend of the nonrelativistic Hartree–Fock relativistic Hartree–Fock, nonrelativistic configuration-interaction, and relativistic configuration-interaction length form of the oscillator strengths for the resonance excitation $1s^22s^22p^63s\ {}^2S^e_J \rightarrow 1s^22s^22p^53s^2\ {}^2P^o_{J'}$ transition, which leads to autoionization (Auger transition), in Na, Mg^{1+}, Al^{2+}, Si^{3+}, P^{4+}, S^{5+}, Cl^{6+}, Ar^{7+}, K^{8+}, Ca^{9+}, Sc^{10+}, Ti^{11+}, Fe^{15+}, Cu^{18+}, Zn^{19+}, Br^{24+}, and Kr^{25+} ions of the sodium isoelectronic sequence.

1. INTRODUCTION

Knowledge 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. Accurate wave functions are needed for the reliable study of collision processes in atoms, molecules, and ions.

More recently, I have shown (Tiwary, 1991) that the 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 general trend and the effects of (1) relativity, (2) correlation, and (3) inclusion of 3*p* and 3*d* orbitals taken from Clementi and Roetti (1974) (smaller exponents of the 2*p* orbital of Clementi and Roetti are used for 3*p* and 3*d* orbitals) in our present Hartree–Fock (HF) and configuration-interaction (CI) calculations of the optical oscillator strengths for the inner-shell excitation, which

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leads to autoionization and plays an important role in explaining the structure observed in the total ionization cross section curve by electron impact, $1s^2 2s^2 2p^6 3s\ ^2S^e_J \rightarrow 1s^2 2s^2 2p^5 3s^2\ ^2P^o_{J'}$, transition in Na, Mg^{1+}, Al^{2+}, Si^{3+}, P^{4+}, S^{5+}, Cl^{6+}, Ar^{7+}, K^{8+}, Ca^{9+}, Sc^{10+}, Ti^{11+}, Fe^{15+}, 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 eigenvectors components of the Hamiltonian matrix with typical element

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

Φ_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 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 (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 the 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 affect 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 given the eigenenergy 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

Figure 1 displays the general trend of the nonrelativistic Hartree–Fock (HF), relativistic Hartree–Fock (RHF), nonrelativistic configuration-interaction (CI), and relativistic configuration-interaction (RCI) length form (f_L) of the optical oscillator strengths of the inner-shell excitation, which leads to autoionization, in Na, Mg^{1+}, Al^{2+}, Si^{3+}, P^{4+}, S^{5+}, Cl^{6+}, Ar^{7+}, K^{8+}, Ca^{9+}, Sc^{10+}, Ti^{11+}, Fe^{15+}, Cu^{18+}, Zn^{19+}, Br^{24+}, and Kr^{25+} ions of the sodium isoelectronic sequence.

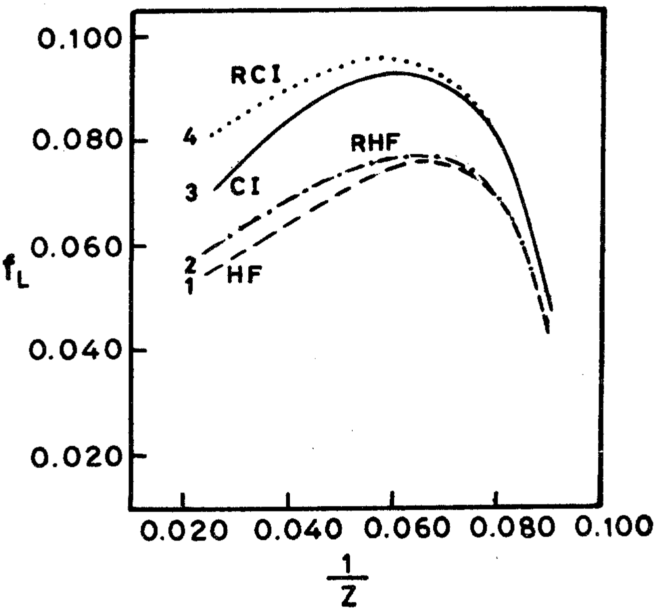

Fig. 1. Theoretical oscillator strengths (f_L) as a function of $1/Z$ for the resonance excitation $1s^22s^22p^63s\ ^2S^e_J \rightarrow 1s^22s^22p^53s^2\ ^2P^o_{J'}$, transition, which leads to autoionization (Auger transition), in Na, Mg^{1+}, Al^{2+}, Si^{3+}, P^{4+}, S^{5+}, Cl^{6+}, Ar^{7+}, K^{8+}, Ca^{2+}, Sc^{10+}, Ti^{11+}, Fe^{15+}, Cu^{18+}, Zn^{19+}, Br^{24+}, and Kr^{25+} ions of the sodium isoelectronic sequence. (1) Hartree–Fock (HF), (2) relativistic Hartree–Fock (RHF), (3) configuration-interaction (CI), (4) relativistic configuration-interaction (RCI).

Several features of importance emerge from Fig. 1. First, it is clear that the HF curve coincides with the RHF curve in the neutral end of the sodium isoelectronic sequence. This indicates that the effect of relativity is negligible for the lowly ionized ions. There is a little disagreement between the HF and RHF curves for the medium and highly ionized ions. It reflects that relativity begins to play a role, but not significantly. Second, the CI curve lies always above the HF and RHF curves. This shows that the correlation enhances the oscillator strengths in all ions of the sodium isoelectronic sequence under consideration. The CI curve does not coincide with the HF curve. This shows the importance of correlation in all systems under consideration. Third, the CI curve tends to move toward the HF curve for the highly ionized ions. This exhibits that the effect of correlation decreases with increase of atomic number (Z). The RCI curve merges with the CI curve for the lowly ionized ions. This is a similar situation to the merging of the HF curve to the RHF curve. This clearly establishes that the effect of relativity is not important in the case of lowly ionized ions. The disagreement between the CI and RCI curves increases with increase of Z. This suggests that the effect of relativity must be included in the scattering as well as the structure calculations in order to obtain reliable results. The RCI curve does not tend to the HF or RHF curve, which shows the dominant role of the relativistic correlation. Finally, it is clear from Fig. 1 that the HF, RHF, CI, and RCI curves exhibit smooth behavior, which reflects the regular and systematic trend of the oscillators strengths.

4. CONCLUSION

Our present theoretical relativistic and nonrelativistic Hartree–Fock and configuration-interaction investigations of the optical oscillator strengths demonstrate (1) there is regular and systematic behavior and (2) it is indispensable to incorporate simultaneously the effects of correlation and relativity in the elaborate calculations in order to obtain accurate results for the inner-shell excitation, which leads to autoionization, in the sodium isoelectronic sequence. We hope that this work will simulate experimental as well as other theoretical investigations.

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