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Theoretical Study to Calculate OOS Calculations of the Inner Shell of Ion

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ABSTRACT

In this paper, we present the theory to find or calculate OOS. The optical oscillator strengths (f), of atoms and positive atomic ions is needed in astrophysics, atmospheric physics, laser physics, plasma physics, radiation physics, gas discharge, mass spectroscopy, space research, and fusion research. The most serious problem in fusion research with magnetically confined high-temperature plasmas (eg. Tokamaks) is caused by plasma impurities, eg., highly ionized metal atoms. It is, therefore vital to determine and reduce the impurity concentration. For this purpose, the values of f are required. The abundance of the chemical elements in the sun is of considerable interest because they contain information about the creation of the solar system term.

Keywords : CI Configuration, Hartee-Fock, Optical Strength

I. INTRODUCTION

Our investigation shows that the inclusion of correlation is indispensable to obtain reliable results. From the survey of the literature, it is clear that neither experimental observations nor theoretical predictions for OSS are available for the inner-shell excitation transition, which leads to auto-ionization in P4+ ions.

Recently, we[1-9] have calculated the transition energies (ΔE in atomic unit) and OSS of both length and velocity forms for several transitions like Li atom using the HF as well as CI wave functions for both initial and final states. In our earlier work, we have reported the excitation energies and oscillator strengths, of both length and velocity forma (f_L and f_v respectively), for the resonance transition and non-resonance transitionas in several ions of the sodium isoelectronic sequence. We have also calculated the ΔE, f_L, and f_v values for several outer-shell transitions as well as the inner-shell excitation transition in P^4 ion which leads to auto-ionization using non-relativistic HF and large Cl wavefunctions for both initial and final states involved in the transition. However, there is a considerable discrepancy between the length and velocity forms of the oscillator strengths.

It is well known that the relativistic effects play an extremely important role in obtaining accurate results. Consequently, it is indispensable to incorporate the relativistic effects into the study of atomic structure in order to generate reliable results. In our earlier work we have calculated the oscillator strengths using the non-relativistic Cl wavefunction. In this work we have taken into account the relativistic effects which may then be used to calculate transitions that are forbidden in purely L - S coupling.

II. THEORY TO CALCULATE OOS

Concerning the increasing accuracy of experimental data obtained from high-resolution techniques, it becomes really necessary to introduce relativistic effects into the reliable study of atomic structure. For this, there are so many methods but a general method of evaluating relativistic effects in atomic structure problems is described, which may be used to calculate transitions that are forbidden in purely L-S coupling [12-20].

The relativistic corrections to the non-relativistic energy may be determined to order $(\alpha Z)^2$ in terms of the Breit operator (H_B) by first-order perturbation theory, Bethe and Salpeter[21]. That is these corrections are given as the expectation value of the Breit operator concerning the zero-order wave function Φ_0 which satisfies

$$H_0 \Phi_0 = \sum_i h_i + \sum_{i<j} \frac{1}{r_{ij}} \Phi_0 = E_0 \Phi_0 \qquad (1)$$

where, h_i is a one electron Dirac operator and α is the fine structure constant. Bethe and Salpeter point out that the further development of the perturbation treatment, in which the full Hamiltonian is taken as (H_0+H_B) leads to higher order corrections which are of the wrong order of magnitude. As a consequence, the use of the resulting Breit equation to determine the corresponding correction to the wave function is therefore unjustified. This point is emphasised by Detrich[22] who develops an alternative perturbation formulism in which the relativistic energy corrections are not given in terms of an effective Hamiltonian H_B.

In the calculation of transition probabilities, it is not sufficient that the energy corrections are treated properly. The corrections to the wavefunction must also be included as well as possible. For fairly low value of Z the Pauli approximation is satisfactory. In this approximation the chief contribution to the fine structure splitting are the nuclear spin- orbit term and the spin-other-orbit and spin-spin-terms. If indeed the correct wavefunction is given as an eigenfunction of H_0 and not of (H_0+ H_B), then in the Pauli approximation, one must determine the wavefunction as an eigenfunction of the non-relativistic Hamiltonian plus the nuclear spin- orbit operator. The spin other term should not be included. For low Z, all relativistic effects are small, but the nuclear spin-orbit and the spin other orbit terms are of comparable order of magnitude. It seems at best anomalous to determine the wavefunction by including one but not the other in the full Hamiltonian.

Since relativistic efffects are small, they should have little in- fluencee on the form of the radial functions. The time consuming optimisation of these functions may thus be determined in a non-relativistic approximation.

The corresponding relativistic corrections to transition probabilities have been derived from quantum electrodynamics by Drake[23-24]. He finds that in the Pauli approximation, the multipole matrix element should be evaluated between eigenfunctions of (H_0 + H_B) provided that only terms up to relative order $(\alpha Z)^2$ are retained Higher-order powers of αZ will necessarily be included in a variational treatment of (H_0 + H_B), but the errors should be small when αZ is small.

The many electron Dirac-Hamiltonian (H_D) for an N-electron system is in atomic unit.

$$H_D = \sum_{i=1}^{N}\{c^2\beta_i + \alpha_i[cP_i + A(r_i)] - \Phi(r_i)\} + \sum_{i<j}\frac{1}{r_{ij}} \qquad (2)$$

where Pi is the momentum operator;

$\Phi(r_i)$ and $A(r_i)$ denotes the scalar and vector potentials of the external electromagnetic field, respectively; c is the sped of light; $r_{ij} = |r_i - r_j|$ is the distance between the i the j th electrons; r_i = position vector of the ith electron and β are the Dirac matrices, written, respectively, in terms of the Pauli 2 x 2 matrices and the 2 x 2 unit matrix

$$I = \begin{pmatrix} o & \sigma \\ \sigma & 0 \end{pmatrix}_i \; and \; \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \qquad (3)$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \; \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \; (4)$$

In the theory of atomic structure we are concerned with electrons interacting with each other as well as with an electromagnetic field. The Dirac theory is not sufficient. The most commonly used approximation for describing the relativistic interaction between electrons in an approximate way is the Breit Hamiltonian, Breit.[25,26]

$$H = H_D + H_B \qquad (5)$$

where,

$$H_B = -\frac{1}{2}\sum_{i<i}\frac{1}{r_{ij}}\left(\alpha_i.\alpha_j\right) + \frac{(\alpha_i r_{ij})(\alpha_j r_{ij})}{r_{ij}^2} \qquad (6)$$

The interaction, equation (5), is of the order $(\alpha Z)^2$ relative to the Coulomb interaction and terms of higher order in (αZ) are omitted.

Provided that the velocities of the electrons in the system are sufficiently low that terms of orders higher than $(\alpha^2 Z^2)$ may be neglected the Breit Hamiltonian for the case where there is no external field becomes

$$H_{BP} = H_{NR} + H_R \qquad (7)$$

where

$$H_{NR} = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - Z\sum_{i=1}^{N}\frac{1}{r_i} + \sum_{i<j}\frac{1}{r_{ij}} \qquad (8)$$

is the non-relativistic Hamiltonian and

$$HR = H_{SO} + H_{mass} + H_{D_1} + H_{SOO} + H_{SS} + H_{OO} + H_{D_2} + H_{SSC} \qquad (9)$$

is the relativistic correction. HBP is the Breit-Pauli Hamiltonian for low Z [Z < < 137}

For derivation of the Breit-Pauli Hamiltonian we refer the reader to Bethe and Salpeter[21], Slater[28], Iroh[29], Akhiezer and Berestetky[30], and Amstrong and Feneuille.[31]

$$H_{SO} = \frac{\alpha^2 Z}{2}\sum_{i=1}^{N}\frac{1}{r_i^3}(I_i.S_i) \qquad (10)$$

represents the one-body spin interaction of each electron's magnetic moment with the magnetic field arising from the electron's own motion in the Coulomb field of the nucleus;

$$H_{mass} = -\frac{\alpha^2}{8}\sum_{i=1}^{N}\nabla_i^4 \qquad (11)$$

is the relativistic mass correction;

$$H_{D_1} = -\frac{\alpha^2 z}{8}\sum_{i=1}^{N}\nabla_i^2\left(\frac{1}{r_i}\right) \qquad (12)$$

is the one body Darwin term; the relativistic correction to the potential energy;

$$H_{SOO} = -\frac{\alpha^2}{2}\sum_{i\neq j}\left(\frac{r_{ij}}{r_{ij}^3}\times P_i\right).(S_i + 2S_j) \qquad (13)$$

represents the spin other orbit interaction and is made up of two parts.

The first one, containing the factor Si, is the spin-orbit coupling of electron i in the Coulomb field of electron j.

The second, with the factors $2s_j$ comes from the interaction of the spin magnetic moment of electron j with the orbital current of electron i;

$$H_{SS} = \alpha^2 \sum_{i<j} \frac{1}{r_{ij}^3}\left(S_i.S_j\right) - 3\frac{(S_i.S_{ij})(S_j.S_{ij})}{r_{ij}^2} \qquad (14)$$

is the ordinary dipole interaction of the spin magnetic moments of two electrons[32-33];

$$H_{00} = -\frac{\alpha^2}{2}\sum_{i<j}\left\{\frac{P_iP_j}{r_{ij}} + \frac{r_{ij}(r_{ij}.P_i).P_j}{r_{ij}^3}\right\} \qquad (15)$$

is the orbit-orbit interaction

$$H_{D_2} = \frac{\alpha^2}{4}\sum_{i<j}\nabla_i^2\left(\frac{1}{r_{ij}}\right) \qquad (16).$$

is the two-body Darwin term; the relativistic correction to the potential energy.

$$H_{SSC} = -\frac{8\pi\alpha^2}{3}\sum_{i<j}\left(s_i.s_j\right)\delta(r_i.r_j) \qquad (17)$$

is the electron-spin-contact term.

we can re-write equation (7) as

H_{BP} = non fine structure + fine structure (18)

where,

non fine structre = H_{NR} + H_{mass}+ H_{D_1} + H_{OO} + H_{D_2} + H_{SCC} (19)

and,

Fine structure = H_{SO} + H_{SOO} + H_{SS} (20)

The non-fine structure interactions commute with S^2, S_Z, L^2 and L_Z can therefore be considered in the $|\alpha LSM_LM_S>$ representation.

The fine-structure interactions only commute with L^2; S^2, J^2 and Jz where J and Jz are the total angular momentum and its azimuuthal component, respectively. For these we use the $|\alpha LSJM_j>$ representation.

J-dependent CI expansion takes the form

$$\Psi(J, M_J) = \sum_j a_j \Phi_j(\alpha_j L_j S_j J M_j) \qquad (21)$$

where $\{\phi_i\}$ denotes a set of single configuration wavefunctions, α_j defines the coupling of the angular momenta of the electrons,

J = L + S (22)

for each j, and $\{a_j)$ are determined as the components of the appropriate eigenvector of the Hamiltonian matrix with basis $\{\phi_j\}$. The Hamiltonian consists of the usual non-relativistic terms plus the relativistic corrections.

The Hamiltonian matrix with typical element is

$H_{ij} = < \psi_i |H| \psi_j>$ (23)

Once we have the J-independent and J-dependent CI wave functions, we can calculate the oscillator strengths.

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