Original contributions

M1 transition probabilities between fine structure components \( ^2L_J(L \geq 1) \)

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Abstract. Spontaneous emission transition probabilities of the magnetic dipole transitions between states of ground state configurations consisting of one \( nl \) electron (or a hole) outside a closed shell have been calculated by using relativistic terms of order \( \alpha^2 Z^2 \) and using hydrogenic orbitals to calculate the required overlap integrals. The line strengths calculated for the Boron and Fluorine isoelectronic sequences are in excellent agreement with the calculations involving Dirac wavefunctions for all ions upto \( Z = 60 \). The maximum difference at the highest value of \( Z = 92 \) is about 6\%. Our calculated lifetimes for the state \( 2p^5 2p_{1/2} \) for Fluorine-like Mg IV and Fe XVIII are 5.03 s and 51.7 \( \mu s \) respectively which are in excellent accord with corresponding values 5.00 s and 51.0 \( \mu s \) calculated by using sophisticated configuration interaction wavefunctions within the Breit-Pauli approximation. Our calculated value of lifetime for Thalium-like Pb II is 40.0 ms which is in good accord with the experimental value of 41.2 ms. New results are presented for the highly ionized ions in the Al-like and Cl-like isoelectronic sequences. The present analysis can be exploited for all the ions in the isoelectronic sequences of elements of groups III A, III B VII A of the periodic table.

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1 Introduction

In the LS coupling scheme the individual electrons interact predominantly by their mutual Coulomb repulsion. In this scheme magnetic dipole (M1) transitions are possible only between components of the fine structure of one term. For example, the transition between the fine structure components of the ground state term of Boron proceeds via the magnetic-dipole term in the atom-field hamiltonian. The non-relativistic theory predicts that the line strength for M1 transitions is independent of the nuclear charge of the ion. However, this is not the case in the relativistic formulation [1] because the radial integrals involved in the calculation of line strength are not independent of \( Z \). The transition probability for M1 transitions is \( \alpha^2 \) times smaller than the transition probability for electric dipole transitions of the same frequency but it increases rapidly with increasing \( Z \) and M1 transitions are indeed observed for higher members of the isoelectronic sequences of various atoms. These forbidden lines are emitted by highly ionized impurity atoms of tokamak plasmas and have been studied extensively [2, 3]. This study is useful for plasma diagnostic purposes, specially for temperature measurements by Doppler broadening. These forbidden transitions occur at larger wavelengths than the resonant transitions which are often in the ultraviolet region. This allows the use of normal incidence spectrometers which are easier to implement than the grazing incidence measurements for diagnostic studies of the core species of the tokamak plasma. Eidelsberg et al. [4] have published a review of forbidden lines occurring in the hotter \( (T > 2 \times 10^5 \text{ K}) \) astronomical sources.

There is a scarcity of measured transition probabilities of M1 transitions. However, the measured transition wavelengths of these transitions are available. Dalgarno [5] has shown that the effect of relativity is more significant on the transition energy than on the transition matrix element. In this spirit, one can take the relativistic transition energy deduced from the analysis of the spectrum. The calculation of line strength may be performed in an easy way and the transition probabilities can be calculated by making use of the observed transition wavelengths.

Grant [1] has studied the gauge invariance of the relativistic radiative transitions and has given extensive formulas for their transition probabilities. We also refer to other works [6–8] on relativistic transition probabilities.

The present work closely follows the formulation of Grant [1] for M1 transitions. We focus on transitions between fine structure components of the term having a configuration comprising one \( nl \) electron outside a closed shell or subshell. Since the relativistic effects are small in the valence shell of an atom, we seek a representation in which the small components of the eigenvectors of
Dirac Hamiltonian are eliminated [9]. In this representation, the Dirac Hamiltonian is replaced by the Pauli operator, which is the Schrödinger operator with the relativistic corrections. This description is correct through order \((v/c)^2\) in which \(v\) is the average velocity of the electron corresponding to its kinetic energy. We further replace all the orbitals by their hydrogenic form. This yields an analytic formula for the line strength of \(M_1\) transitions for one \(nl\) electron outside a closed shell or subshell atomic system with nuclear charge \(Z\). We present results for the Boron and Fluorine isoelectronic sequences for all ions up to \(Z = 92\) and compare our results with the fully relativistic calculations of Cheng et al. [10].

2 Theory

The spontaneous emission probability per unit time for the transition \(\beta \rightarrow \alpha\) for an electron outside a closed shell is given by the time dependent perturbation theory [1]

\[
A_{\beta \rightarrow \alpha} = 2\pi c^2 \left( \frac{2j_\alpha + 1}{2L + 1} \right) \left( \frac{\langle \beta \mid L \mid \alpha \rangle}{\langle \beta \mid -L \mid \alpha \rangle} \right)^2 \left| \langle \beta \rangle \right|^2
\]

(1)

where the matrix elements \(\langle \beta \rangle\) for a relativistic radiative transition of multipole order \(L\) have been given by Grant [1]. Here \(\langle \rangle\) stands for \(3j\) symbol with arguments \(j_\alpha\) and \(j_\beta\) representing the \(j\) values of the electron in the state \(\alpha\) and \(\beta\) respectively.

For magnetic multipoles, \(\langle \beta \rangle\) can be written to lowest order \(O(1/c)\) as [1]

\[
\langle \beta \rangle = \left( 1 - \frac{\alpha^2}{4} \right) \left( 1 - \frac{d^2}{2d^2 + l(l+1)} \right) P_{nl}(r)
\]

(2)

where

\[
K_\alpha = -(l+1) \quad \text{for} \quad j = l+1/2
\]

\[
K_\beta = l \quad \text{for} \quad j = l-1/2.
\]

(3)

It is known that up to lowest order \((v/c)^2\), we can replace \(R_{nl}\) by [11]

\[
R_{nl} = \left( 1 - \frac{T_i}{4c^2} \right) P_{nl} + O(1/c^4) P_{nl}
\]

(4)

where \(T_i\) is the effective kinetic energy operator

\[
T_i = -\frac{d^2}{2d^2 + l(l+1)} \frac{l(l+1)}{2r^2}.
\]

(5)

In (4) \(P_{nl}\) represents the Schrödinger radial orbital.

For magnetic dipole transitions with \(L = 1\), we can express the transition probability \(A_{\beta \rightarrow \alpha}\) in terms of the line strength \(S_{M_1}\) as follows [10]

\[
A_{\beta \rightarrow \alpha}^{M_1} = \frac{2.69735 \times 10^{13}}{(2j_\alpha + 1)\lambda^3} S_{M_1}\quad \text{(in s}^{-1})
\]

(6)

where \(\lambda\) is the transition wavelength in Angstroms. \(S_{M_1}\) is given (in Bohr magneton units) by

\[
S_{M_1} = \frac{1}{4} \left( \frac{2j_\alpha + 1}{2j_\beta + 1} \right) \left( \frac{\langle \beta \mid L \mid \alpha \rangle}{\langle \beta \mid -L \mid \alpha \rangle} \right)^2 \left[ \langle K_\alpha + K_\beta \rangle (1 - K_\alpha - K_\beta) \right]^2 I^2
\]

(7)

where

\[
I = \int_0^\infty R_{nl}^2 R_{nl} dr.
\]

(8)

The line strength \(S_{M_1}\) is symmetrical with respect to \(\alpha\) and \(\beta\). The overlap integral \(I\) for transitions between levels of the same configuration is unity for non-relativistic orbitals. However, when the lowest order relativistic correction is taken into account, the overlap integral is less than unity due to the contraction of the orbits. Now

\[
R_{nl} = \left( 1 - \frac{\alpha^2}{4} \left( 1 - \frac{d^2}{2d^2 + l(l+1)} \right) \right) P_{nl}(r).
\]

(9)

We now replace \(P_{nl}\) by a hydrogenic orbital and since

\[
\left( -\frac{1}{2} \frac{dr^2}{d^2 + l(l+1)} \right) P_{nl}(r) = \left( \frac{Z}{r} - \frac{Z^2}{2n^2} \right) P_{nl}(r)
\]

(10)

we get

\[
I = \int_0^\infty \left( 1 - \frac{\alpha^2 Z}{2r} - \frac{Z^2}{2n^2} \right) P_{nl}^2(r) \, dr.
\]

(11)

Using [12] \(\langle 1/r \rangle = \frac{Z}{n^2}\), we finally get

\[
I^2 = \left( 1 - \frac{\alpha^2 Z^2}{2n^2} \right)^2.
\]

(12)

Since \(j_\alpha\) and \(j_\beta\) differ by unity, we can simplify the evaluation of the \(3j\) symbol by using the relation [13]

\[
\frac{(a + 1)(a + x + 1)}{(a + 1)(a + x + 1)} = \frac{(a + 1)(a + x + 1)(a + 2x + 3)}{(a + 1)(a + x + 1)}.
\]

(13)

Also noting that \(K_\alpha + K_\beta = -1\), we finally get \(S_{M_1}\) to lowest order as

\[
S_{M_1} = \frac{(J_\beta + 1/2)(J_\beta + 3/2)}{(J_\beta + 1)} \left( 1 - \frac{\alpha^2 Z^2}{2n^2} \right)^2
\]

(14)

where \(J_\beta\) stands for the smaller value of \(J_\alpha\) and \(J_\beta\), respectively. Since we are dealing with one electron outside a closed shell or subshell, the effective field experienced by the valence electron is centrally symmetric because the filled shells have a total orbital angular momentum and total spin equal to zero. Asymptotically, the electron moves in the field of the residual charge \(z = Z - N + 1\) where \(N\) is the number of electrons in the atomic system. Near the nucleus, there is no screening and the electron moves in the field of nuclear charge \(Z\). The effect of the core can be included in the line strength by replacing \(Z\) by \(z\) and \(n\) by \(n^* = n - \mu\) where \(\mu\) is the quantum defect of the valence orbital. The value of \(\mu\) does not depend upon \(n\) but varies with the nuclear charge. The lifetime can be computed by the relation

\[
\tau_{\beta \rightarrow \alpha} = (A_{\beta \rightarrow \alpha})^{-1} \text{(in s)}.
\]

(15)