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Algebra of the Noncompact Group $O(3,2)$ and the Hydrogen-Atom Radial Functions*

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The bound-state hydrogen-atom radial functions are used to construct a basis for a unitary representation of the algebra $O(3, 2)$. With the use of the $O(3)$ subalgebra of this "radial algebra" matrix elements of r^s between states of different energy are shown to be completely expressible in terms of the matrix elements of r^{-2}. Matrix elements corresponding to the radial matrix elements of the dipole operator are shown to be proportional to the overlap of the radial functions. The continuum radial functions of constant energy are shown to provide a basis for a unitary representation of $O(2, 1)$.

I. INTRODUCTION

The bound-state nonrelativistic hydrogen-atom wave functions $u_{nlm}=R_{nl}Y_{lm}$ were shown by Malkin and Man'ko to be a basis for a representation of the group $O(4, 2)$.[1] The importance of this dynamical group was noted later by Barut and Kleinert, who used it to calculate dipole-transition probabilities.[2] More recently Armstrong used only the radial portion of the wave function, R_{nl}, to define a representation of the group $O(2, 1)$.[3] By defining "tensor" operators he was able to show that radial matrix elements of integer powers of the radial coordinate r between two radial functions of the same principal quantum number are proportional to an $O(2, 1)$ Clebsch-Gordan coefficient. Matrix elements of r^k between radial functions of different principal quantum number have not yet been as easily evaluated.[4] The difficulty in evaluating these "off-diagonal" radial matrix elements by group-theoretical methods lies in the definition of the tensor operators. The tensor operators are not functions of r^k alone but of $D_{(a)}r^k$, where $D_{(a)}$ is the dilatation operator $D_{(a)}f(r)=f(ar)$ on functions of r. When the matrix elements are between radial functions of the same energy, $a=1$ and the difficulty is removed.

The purpose of the present paper is threefold. In Sec. II we generalize the method used by Armstrong to show that a more complete radial dynamical group is $O(3, 2)$. In Sec. III we use the $O(3)$ subalgebra of the "radial algebra" to investigate matrix elements of r^k. While we do not use r^k to define tensor operators, we do show how matrix elements with different values of k are related. In Sec. IV there is a brief discussion of how the $O(3)$ subalgebra becomes $O(2, 1)$ when the methods used are extended to continuum radial functions.

II. $O(3, 2)$ RADIAL ALGEBRA

The method used involves a decomposition of the $|nlm\rangle$ space into the product of two spaces,

$$|nlm\rangle = |lm\rangle\langle\Omega_{nl}|\cdot|\Omega_{nl}\rangle|nl\rangle \ . \tag{1}$$

The $|\Omega_{nl}\rangle$ are unspecified, but if they are chosen such that

$$\langle\Omega_{n'l'}|\Omega_{nl}\rangle = \delta_{nn'}\delta_{l'l} \ , \tag{2}$$

we can use the orthonormal $|\Omega_{nl}\rangle|nl\rangle$ space to investigate the radial portion of the hydrogen-atom wave functions. We shall use a functional form for the $|\Omega_{nl}\rangle$ similar to that used by Armstrong.

The radial coordinate will be $\sigma=rZ$, Z being the nuclear charge. The radial functions R_{nl} are normalized to have the sign $(-)^l$ near the origin, and satisfy

$$\int_0^\infty P_{n'l}P_{nl}\,d\sigma = \delta_{n'n} \ , \tag{3}$$

with $P_{nl}(\sigma)=\sigma R_{nl}(\sigma)$. A space of functions $g_{n\mu}$ is defined by

$$g_{n\mu} = (8\pi^2)^{-1/2}e^{is\eta}e^{i\mu t}P_{nl} \ , \quad 0\le s\le 2\pi, \ 0\le t\le 4\pi, \quad |\mu| = l+\tfrac{1}{2} \ . \tag{4}$$

An important feature of the $g_{n\mu}$ is that there are two $g_{n\mu}$ for each P_{nl} since $\mu=\pm(l+\frac{1}{2})$. With respect to the volume element $d\Omega=d\sigma\,ds\,dt$ the $g_{n\mu}$ are orthonormal,

$$\int g^*_{n',\mu'} g_{n\mu}\, d\Omega = \delta_{n',n}\delta_{\mu',\mu} \ . \tag{5}$$

We can define several important operators on $g_{n\mu}$:

$$G = -\frac{i\partial}{\partial t} \ , \tag{6a}$$

$$N = -\frac{i\partial}{\partial s} \ , \tag{6b}$$

$$a_\pm = G \pm \tfrac{1}{2} \ , \tag{6c}$$

$$H = \frac{\partial^2}{\partial\sigma^2} - \frac{a_+ a_-}{\sigma^2} + \frac{2}{\sigma} \ , \tag{6d}$$

$$G_\pm = e^{\pm it}\left(\pm a_\pm \frac{\partial}{\partial\sigma} - \frac{a_\pm^2}{\sigma} + 1\right) N \ , \tag{6e}$$

$$N_\pm = D_{(N\mp 1/N)} e^{\pm is}\left(\pm z_N \frac{\partial}{\partial z_N} + N - \frac{z_N}{2}\right)\left(\frac{N}{N\pm 1}\right) . \tag{6f}$$

The $N_\pm$ are similar to those used by Armstrong (cf. also Ref. 2), the difference arising from his use of a different normalization for the radial functions. The variable $z_N = 2\sigma/N$ and $D(N \mp 1/N)$ is the dilatation operator. Additional operators related to those in (6) are

$$A = \tfrac{1}{2}(G + N) \ , \tag{7a}$$

$$A_\pm = \pm\tfrac{1}{2}[G_\pm,\ N_\pm] \ , \tag{7b}$$

$$B = \tfrac{1}{2}(G - N) \ , \tag{7c}$$

$$B_\pm = \mp[G_\pm,\ N_\mp] \ . \tag{7d}$$

Direct evaluation of the action of the operators on the $g_{n\mu}$ gives

$$Hg_{n\mu} = n^{-2} g_{n\mu} \ , \tag{8a}$$

$$Gg_{n\mu} = \mu g_{n\mu} \ , \tag{8b}$$

$$G_\pm g_{n\mu} = [(p \mp \mu)(p \pm \mu + 1)]^{1/2}\ _{\mu\pm 1}, \qquad p = n - \tfrac{1}{2} \tag{8c}$$

$$Ng_{n\mu} = n g_{n\mu} \ , \tag{8d}$$

$$N_\pm g_{n\mu} = [(n \mp l)(n \pm l \pm 1)]^{1/2} g_{n\pm 1\,\mu} \ . \tag{8e}$$

Defining $a = \frac{1}{2}(n + \mu)$ and $b = \frac{1}{2}(\mu - n)$, (7) and (8) are combined to give

$$Ag_{n\mu} = a g_{n\mu} \ , \tag{9a}$$

$$A_\pm g_{n\mu} = [\tfrac{3}{16} + a(a \pm 1)]^{1/2} g_{n\pm 1\,\mu\pm 1} \ , \tag{9b}$$

$$Bg_{n\mu} = b g_{n\mu} \ , \tag{9c}$$

$$B_\pm g_{n\mu} = [\tfrac{3}{16} + b(b \pm 1)]^{1/2} g_{n\mp 1\,\mu\pm 1} \ . \tag{9d}$$

Investigation of the operators in (8) and (9) shows that their commutation relations are closed, and we note the following four subalgebras:

$$s_1 = \{G,\ G_\pm\}, \quad s_3 = \{A,\ A_\pm\}, \qquad s_2 = \{N,\ N_\pm\}, \quad s_4 = \{B,\ B_\pm\} . \tag{10}$$

The commutation relations of s_1 are seen from (8) to be

$$[G,\ G_\pm] = \pm G_\pm \ , \qquad [G_+,\ G_-] = 2G \tag{11}$$

and those of s_2, s_3, and s_4 are

$$[W,\ W_\pm] = \pm W_\pm \ , \qquad [W_+,\ W_-] = -2W \ , \tag{12}$$

with $W = N$, A, and B, respectively. The relations in (11) are isomorphic to those of the Lie algebra $O(3) \sim SU(2)$, and those in (12) are isomorphic to the commutation relations of $O(2,\ 1) \sim SU(1,\ 1)$. The unitary representations of $O(2,\ 1)$ are well known.[5] They are specified by the invariant $Q_W g_{n\mu} = q \times (q+1) g_{n\mu}$, with

$$Q_W = W(W-1) - W_+ W_- \ . \tag{13}$$

The value of q determines the representation. In addition $W_+ W_-$ is positive definite. For $O(3)$ the well-known invariant is $Q_G g_{n\mu} = p(p+1) g_{n\mu}$, with

$$Q_G = G(G-1) + G_+ G_- \ . \tag{14}$$

The dimension of each irreducible $O(3)$ representation is $2p + 1$.

The properties of the four subalgebras are listed in Table I. For each of the $O(2,\ 1)$ subalgebras the representation is either a positive or negative discrete series, labeled $\mathfrak{D}^\pm_{-q}$.

We shall not list the additional commutation relations except to note that the subalgebra $s_3 + s_4$ is isomorphic to that of $O(2,\ 1) \times O(2,\ 1)$ since $[s_3,\ s_4] = 0$. The above properties of the Lie algebra $S = \{G,\ G_\pm,\ N,\ N_\pm,\ A_\pm,\ B_\pm\}$ are sufficient to establish that the commutation relations of S are isomorphic to those of $O(3,\ 2)$.[6]

It should be emphasized that the generators of the radial $O(3,\ 2)$ are defined only on the $g_{n\mu}$ space. For instance, using G_+ and G_- from (6) we see that (11) should actually read

$$[G_+,\ G_-] = 2IG \ , \tag{15}$$

with $I = HN^2$ being a representation of the identity operator on $g_{n\mu}$.

Direct computation shows also that $[G,\ H]$

TABLE I. Radial $O(3,2)$ subalgebras.

Subalgebra	$q(q+1)$	Spectrum of diagonal element	Representation
$s_1 = O(3)$	$n^2 - \frac{1}{4}$	$\mu = \pm\frac{1}{2},\ \pm\frac{3}{2},\ \ldots,\ \pm(n - \frac{1}{2})$	dimension $= 2n$
$s_2 = O(2,1)$	$l(l+1)$	$n = l+1,\ l+2,\ \ldots$	$\mathfrak{D}^+_{l+1}$
$s_3 = O(2,1)$	$\frac{3}{16}$	$a = \frac{1}{4},\ \frac{5}{4},\ \ldots$	$\mathfrak{D}^+_{1/4}$
	$\frac{3}{16}$	$a = \frac{3}{4},\ \frac{7}{4},\ \ldots$	$\mathfrak{D}^+_{3/4}$
$s_4 = O(2,1)$	$\frac{3}{16}$	$b = -\frac{1}{4},\ -\frac{5}{4},\ \ldots$	$\mathfrak{D}^-_{1/4}$
	$\frac{3}{16}$	$b = -\frac{3}{4},\ -\frac{7}{4},\ \ldots$	$\mathfrak{D}^-_{3/4}$

$=[G_\pm, H]=0$. That G_+ and G_- commute with the radial Hamiltonian H suggests that they are related to the Runge-Lenz operator, which is associated with the $O(4)$ symmetry of the complete bound-state–hydrogen-atom wave functions $|nlm\rangle$.[7,8] This is indeed the case, and investigation of the reduced matrix elements of the Runge-Lenz operator with respect to the $O(3)$ rotation group results in radial operators similar to those of $G_\pm$.

We should note also that the recursion relations on the P_{nl} obtained with the $G_\pm$ operators are well known from the factorization method of Infeld and Hull.[9]

III. RADIAL $O(3)$ AND RADIAL INTEGRALS

Matrix elements on $g_{n\mu}$ are easily evaluated, but some care must be taken when transforming the results in this space to the space of functions P_{nl}. This point is best illustrated with an example. Let m and d be integers and define $f=e^{idt}e^{ims}\sigma^k$. Then

$$\langle n'\mu'|f|n\mu\rangle=\int g^*_{n',\mu'}(fg_{n\mu})\,d\Omega$$

$$=\langle n+m\,\mu+d|f|n\mu\rangle\delta_{n',n+m}\delta_{\mu',\mu+d}\,. \tag{16}$$

The identification of (16) with a radial integral of the type

$$(n'l'|\sigma^k|nl)=\int P_{n',l'}\sigma^k P_{nl}\,d\sigma \tag{17}$$

depends upon the sign of $\mu+d$, since $|\mu|=l+\frac{1}{2}$. Thus (16) becomes

$$\langle n+m\,\mu+d|f|n\mu\rangle=(n+m\,l'|\sigma^k|nl)\,, \tag{18}$$

with $l'=l+d$ if $\mu+d>0$, and $l'=-(l+d+1)$ if $\mu+d<0$.

A similar evaluation of matrix elements of the operators

$$[G_\pm a_\pm,\ \sigma^k e^{ims}e^{idt}N],\quad e^{ims}e^{idt}[G_+G_-,\ \sigma^k],$$

and

$$[G_+G_-,\ e^{ims}N^2\sigma^k]$$

leads, respectively, to the following relationships:

$$(l'-l-k-1)(n'l'|\sigma^{k-1}|nl)=A_{nl}(n'l'|\sigma^k|nl+1)-A_{n',l'-1}(n'l'-1|\sigma^k|nl)-\frac{(l'-l-1)}{l'(l+1)}(n'l'|\sigma^k|nl)\,, \tag{19}$$

$$(E'-E)(n'l'|\sigma^k|nl)=\frac{-2k}{l+1}(n'l'|\sigma^{k-1}|nl)+2kA_{nl}(n'l'|\sigma^{k-1}|nl+1)+(l+k-l')(l+k+l'+1)(n'l'|\sigma^{k-2}|nl), \tag{20}$$

and for $n\neq n'$,

$$w(n'l|\sigma^k|nl)=kA_{nl}(n'l|\sigma^{k-1}|nl+1)-kA_{n',l}(n'l+1|\sigma^{k-1}|nl)\,, \tag{21}$$

with

$$E=n^{-2},\quad A_{nl}=\frac{[(n+l+1)(n-l-1)]^{1/2}}{n(l+1)}\,,\quad w=(A^2_{nl}-A^2_{n',l})\,.$$

Equations (19)–(21) are valid for any real k, but our primary concern is with the integer values of k. There are two cases of interest.

(i) σ^{-s}, $s=2,\ 3,\ldots$: With repetitive application of (19) to the matrix elements of σ^{-2}, it is evident that nearly all matrix elements $(n'l'|\sigma^{-s}|nl)$ may be expressed in terms of those with $s=2$. The exceptions are those elements with $l=l'=0$, but they present no problem since they are infinite for $s\geq 3$.

In addition, for $k=0$, (20) reduces to

$$[(l-l')(l+l'+1)](n'l'|\sigma^{-2}|nl)=(E'-E)(n'l'|nl)\,, \tag{22}$$

a result previously derived by Feinberg.[10] When $n=n'$, (22) becomes the familiar result that the matrix elements $(nl'|\sigma^{-2}|nl)$ vanish unless $l=l'$. This is of interest because repeated use of either (19) or (20) when $n=n'$ shows immediately that if $s\geq 2$,

$$(nl'|\sigma^{-s}|nl)=0\ \text{ if }\ |l'-l|\geq s-1\,. \tag{23}$$

This is the orthogonality property of Pasternack and Sternheimer,[11] which was shown by Armstrong to be a selection rule resulting from the use of radial $O(2,1)$ tensor operators.[3]

(ii) σ^s, $s=-1,\ 0,\ 1,\ldots$: Of interest are the matrix elements with $n\neq n'$. By letting $k\to k-1$ in (19) and substituting this equation into the right-hand side of (20), we obtain for $l'\neq 0$

$$(E'-E)(n'l'|\sigma^s|nl)=\frac{(l'+l+1)(l'-l-s-1)}{l'(l+1)}(n'l'|\sigma^{s-1}|nl)-(l'+l-s+1)A_{nl}(n'l'|\sigma^{s-1}|nl+1)+(l'+l+s+1)A_{n',l'-1}(n'l'-1|\sigma^{s-1}|nl)\,. \tag{24}$$

The matrix elements with $l=l'=0$ may be obtained using (21). Thus just as was the case with σ^{-s}, we see that with repetitive application of (21) and (24)

all matrix elements of σ^s for $n \neq n'$ may be expressed in terms of the matrix elements of σ^{-2}.

A case of special interest is the matrix element $(n'l+1|\sigma|nl)$. The corresponding reduction of (24) for $s=1$ is to

$$(n'l+1|\sigma|nl) = 2[(l+1)(E-E')]^{-1}(n'l+1|nl) . \tag{25}$$

These matrix elements of σ are of importance because their square is a linear factor in expressions for the electric-dipole-transition probability. Thus (25) confirms for the hydrogen atom the intuitive notion that transition probabilities are proportional to the square of the overlap of the radial functions.[12]

We emphasize that the results of this section are not dependent on any group-theoretical arguments since they may be obtained from the results of Infeld and Hull.[9] In particular we note the work of Feneuille,[13] who obtained Eqs. (20) and (23) in this manner.

IV. CONTINUUM RADIAL FUNCTIONS

For the continuum hydrogen radial functions we define the space of functions $f_{n\mu}$ by

$$f_{n\mu} = (4\pi)^{-1/2} e^{i\mu t} P_{nl}, \quad 0 \le t \le 4\pi, \quad |\mu| = l + \tfrac{1}{2} . \tag{26}$$

The radial Hamiltonian in this space is

$$h = -\frac{\partial^2}{\partial\sigma^2} + \frac{a_+ a_-}{\sigma^2} - \frac{2}{\sigma}, \tag{27}$$

with $a_\pm$ defined in (6). The P_{nl} are chosen to be energy normalized,[14] and have the sign $(-)^l$ near the origin. The label n is defined by

$$h f_{n\mu} = n^{-2} f_{n\mu}, \quad 0 < n < \infty . \tag{28}$$

For subspaces of constant energy we define the $G_\pm$ in (8) to be

$$G_\pm = e^{\pm it}\left(\pm a_\pm \frac{\partial}{\partial\sigma} - \frac{a_\pm^2}{\sigma} + 1\right) n , \tag{29}$$

with $[G_\pm, h] = [G, h] = 0$, and

$$[G, G_\pm] = \pm G_\pm , \tag{30a}$$

$$[G_+, G_-] = -2IG . \tag{30b}$$

I is the identity operator on $f_{n\mu}$, $I = hn^2$. By comparing (30) with (11) we see that the $O(3)$ subalgebra for bound-state radial functions becomes $O(2, 1)$ for the continuum radial functions. By direct calculation,

$$G f_{n\mu} = \mu f_{n\mu}, \tag{31a}$$

$$G_\pm f_{n\mu} = [(\mu \pm 1)\mu - p(p+1)]^{1/2} f_{n\mu\pm1} , \tag{31b}$$

with $p = -\frac{1}{2} \pm in$, a complex number. Using (13) we see also that the $O(2, 1)$ invariant $Q_G = p(p+1)$. From Ref. 5 the corresponding unitary representation of $O(2, 1)$ is found to be the principal series, with the G spectrum being $\mu = \pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$. As the energy approaches infinity $n \to 0$, and for $n = 0$ the principal series splits into two discrete series $\mathfrak{D}^\pm_{1/2}$. This suggests that the solutions $P^0_{nl} e^{i\mu t}(4\pi)^{-1/2}$ of the radial Hamiltonian

$$h^0 = -\frac{\partial^2}{\partial\sigma^2} + \frac{a_+ a_-}{\sigma^2} \tag{32}$$

might provide a basis for discrete representations of $O(2, 1)$. This is indeed the case, although we shall not discuss the matter other than to give the generators which commute with h^0,

$$G^0_\pm = (h^0)^{-1/2} e^{\pm it}(\pm a_\pm \partial/\partial\sigma - a_\pm^2/\sigma) . \tag{33}$$

The continuum radial functions will not be discussed further in this paper.

V. DISCUSSION

We have shown how radial matrix elements of integer powers of the radial coordinate σ between states of different energy may be expressed in terms of the matrix elements of σ^{-2}. Use was made of the generators of the $O(3)$ subalgebra of an $O(3, 2)$ radial algebra. While this is a significant step towards evaluating the matrix elements group theoretically, we have not answered the question of how tensor operators may be defined in order to facilitate the evaluation. The $O(2, 1)$ subalgebras s_3 and s_4 might be of use in such an investigation. The $O(2, 1)$ algebra used by Armstrong corresponds to the subalgebra s_2 in this paper.

An interesting feature of the decomposition of $|nlm\rangle$ in (1) is that there is a symmetrical counterpart

$$|nlm\rangle = |nl\rangle\langle\Omega|\cdot|\Omega\rangle|lm\rangle , \tag{34}$$

which suggests that the spherical harmonics are a basis for a representation of a group larger than $O(3)$. This is indeed the case, and it may be shown that the corresponding group is $O(3, 2)$. A discussion of this point will be given elsewhere.

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Origin of the Silver L-Series X-Ray Spectrum*

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Using recently calculated values of radiative, Coster-Kronig, and Auger transition rates, and the hypothesis that the satellite structure arises from doubly ionized atoms (with L and N holes), and an assumed incident x-ray spectrum, we calculate the relative intensities of the Ag L-series x-ray spectrum. The calculations are in best agreement with Parratt's measurements when Ag L_1-$L_3M_{4,5}$ Coster-Kronig transitions are forbidden. Comparison of the calculations with the satellite components leads to unsatisfactory agreement. Reasons for this are discussed. Modified values of f_{12}, f_{13}, and ω_1 for the Ag and Sn L shells are reported.

I. INTRODUCTION

In a 1937 review article on x-ray satellite structure,[1] Richtmyer pointed out that while a multiple-ionization theory[2] could adequately account for the $K\alpha$ satellite spectrum it was unable to predict the peculiar phenomena associated with L-shell satellite spectra. To account for the latter, Richtmyer argued that Auger processes were necessary. However, it is only recently[3-7] that reliable calculated Auger transition rates have become available. In the future, we plan an extensive comparison of calculated and experimental satellite structure but for the present we confine our examination to silver. Parratt[8] has made a precision measurement of the Ag L-series x-ray spectrum. As an indication of the sensitivity involved, Parratt measured the intensity of the L_2-N_1 line as 0.28 compared to the L_3-M_5 line with intensity 100. As we shall see, the calculation leads to 0.30 for the intensity of L_2-N_1 when L_3-M_5 is set equal to 100. The motivation for this study arose neither from the diagram line intensities nor from the satellite structure but rather from the value of the width (lifetime) of an L_1 hole. Parratt measured an average width for the L_1-$M_{2,3}$ transition as 6.25 eV, while for the much weaker L_1-$M_{4,5}$ transition (a nondipole transition) he found a width of 5.8 eV. The author has recently calculated the $M_{4,5}$ and $M_{2,3}$ widths as 0.44 and 3.80 eV.[3] Thus, from the measured L_1-$M_{2,3}$ width one deduces 2.45 eV as the width due to the lifetime of the L_1 hole; yet from the L_1-$M_{4,5}$ width one deduces an L_1 width of 5.4 eV. In addition, the author has calculated[4] an L_1 width of 9.03 eV while Crasemann *et al.*[6] obtain 7.56 eV. The calculated values are so large because it is assumed L_1-$L_3M_{4,5}$ Coster-Kronig transitions are energetically allowed. An inaccurate way of estimating the continuum electron energy in an nl-$n'l'n''l''$ Auger transition is to use

$$\epsilon_1(Z) = -E_{nl}(Z) + E_{n'l'}(Z) + E_{n''l''}(Z) \quad , \tag{1}$$

where E_{nl} is a one-electron ionization threshold and ϵ_1 is the estimated energy of the continuum Auger electron. Three more accurate procedures are

$$\epsilon_2(Z) = -E_{nl}(Z) + E_{n'l'}(Z) + E_{n''l''}(Z+1), \tag{2}$$

$$\epsilon_3(Z) = -E_{nl}(Z) + E_{n'l'}(Z+1) + E_{n''l''}(Z), \tag{3}$$

$$\epsilon_4(Z) = -E_{nl}(Z) + \tfrac{1}{2}[E_{n'l'}(Z) + E_{n'l'}(Z+1) + E_{n''l''}(Z) + E_{n''l''}(Z+1)] \quad . \tag{4}$$

For instance, estimate (1) would allow a large L_1-L_3M_5 Coster-Kronig transition rate at $Z = 73$. The other estimates indicate such a transition is energetically forbidden. Experimental measurements on $f_{1,3}$ indicate the transitions do not occur.[4] For the silver L_1-$L_3(M_4, M_5)$ transition estimate (2) leads to $\epsilon_2 = (+44$ eV, $+51$ eV) for the continuum electron energy, where we use the ESCA[9] tabulation of ionization thresholds. Estimate (3) leads to $\epsilon_3 = (-105$ eV, -99 eV), while estimate (4) leads to $\epsilon_4 = (-31$ eV, -27 eV). Thus two of the estimates predict the transition is energetically forbidden, one predicts it is allowed. The point of this paper is to examine the effect of the presence or absence of