Quasi-spin symmetrized orbital operators for dN configurations

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Classification :
Physics Abstracts
13.00, 13.20.

QUASI-SPIN SYMMETRIZED ORBITAL OPERATORS FOR d^N CONFIGURATIONS

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(*Reçu le 3 décembre 1970*)

Résumé. — Deux opérateurs de particules en orbite, ayant les propriétés de transformation des groupes quasi rotatifs et rotationnels R_5, sont construits. Les effets d'ordre secondaire produits par la corrélation électrostatique des inter-réactions orbitales d'une particule, sont écrites formellement en termes d'opérateurs symétriques. Le calcul des éléments de matrice est discuté ainsi que ses relations au problème du calcul des facteurs isoscalar.

L'application aux inter-réactions électriques quadripolaires infiniment fines est envisagée.

Abstract. — Two particle orbital operators having well-defined transformation properties under the quasi-spin group and the rotational group R_5 are constructed. The second-order effects produced by electrostatic correlation of one particle orbital interactions are formally written in terms of the symmetrized operators. The calculation of the matrix elements is discussed together with its relationship to the problem of calculating isoscalar factors. The possible application to electric quadrupole hyperfine interactions is considered.

Introduction. — The symmetrization of the interactions for many-electron systems into operators having well-defined transformation properties under the groups used to classify the many electron states is well established [1]. Judd [2] has discussed in some detail the analysis of the spin-spin and spin-other-orbit interactions for the d-shell, making particular use of quasi-spin methods [3]. Feneuille [4] has, in a similar fashion, considered the symmetrization of effective three-particle operators for the d-shell. These operators arise in the perturbative treatment of the configuration interaction produced by the Coulomb repulsion [5, 6].

In each of the above cases considered the Hamiltonian is rotationally invariant and thus there was no preferred axis of quantization and hence only scalar interactions arose. There are, however, a number of situations where the Hamiltonian, real or effective, is not rotationally invariant. This is indeed the case for an ion in an external electric or magnetic field or in the presence of a nuclear magnetic dipole or electric quadrupole.

In this paper we first establish the form of the effective operators required to represent electrostatically correlated single particle operators leading to the need to consider the evaluation of the matrix elements of effective two particle operators of the form

$$\mathbf{T}^{(K_1k_1K_2k_2)(Kk)} = \sum_{i<j} (\mathbf{w}_i^{(K_1k_1)}\,\mathbf{w}_j^{(K_2k_2)})^{(Kk)} .$$

In the case of spin-independent interactions, such as arise in crystal field and electric quadrupole hyperfine interactions, we must consider the matrix elements of the operators

$$\mathbf{T}^{(k_1k_2)k} = \sum_{i<j} (\mathbf{v}_i^{(k_1)}\,\mathbf{v}_j^{(k_2)})^{(k)} .$$

The problem of representing these operators in terms of symmetrized operators of pure quasi-spin for the specific case of the d^N configurations is then attacked. Problems related to the calculation of the matrix elements of the quasi-spin symmetrized operators and their application to problems in electric quadrupole hyperfine structure is considered.

I. Electrostatically Correlated Single Particle Interactions.

— Any single particle interaction may be expressed in terms of double tensors [7],

$$\mathbf{T}^{(KK)} = \sum_{i=1}^{N} \boldsymbol{\tau}_i^{(KK)} . \tag{1}$$

Consider the state $|\, A\alpha >$ of a configuration A to be perturbed by the states $|\, B\beta >$ of a configuration B, then to second order we must replace each matrix element

$$< A\alpha \,|\, T_{\pi q}^{(KK)} \,|\, A\alpha' > \tag{2}$$

by

$$(1 + \Delta) < A\alpha \,|\, T_{\pi q}^{(KK)} \,|\, A\alpha' > \tag{3}$$

where

$$\Delta = -\sum_{\beta} (< A\alpha \mid Q \mid B\beta > < B\beta \mid T_{\pi q}^{(KK)} \mid A\alpha' > + < A\alpha \mid T_{\pi q}^{(KK)} \mid B\beta > < B\beta \mid Q \mid A\alpha' >) / < A\alpha \mid T_{\pi q}^{(KK)} \mid A\alpha' > E \quad (4)$$

where E is the positive excitation energy required to transfer a single electron from A $\rightarrow$ B and Q designates the Coulomb interaction between electrons. If we identify the $\mid A\alpha >$'s with the states of a configuration $(nl)^N (n' l')^{4l'+2}$ then we may distinguish three possible configurations B, namely

(1) $(nl)^N (n' l')^{4l'+1} n'' l''$

(2) $(nl)^{N-1} (n' l')^{4l'+2}$

(3) $(nl)^{N+1} (n' l')^{4l'+1}$.

Case (1) has already been considered by Judd [7] who obtains the result

$$\Delta^{(1)} = -\frac{2 < n' l' \| \tau^{(KK)} \| n'' l'' >}{E < nl \| \tau^{(KK)} \| nl >} \left[\frac{2\,\delta(K, 0)}{(2K+1)} \Xi_1^K - \sum_t (-1)^{K+t} \begin{Bmatrix} l & K & l \\ l' & t & l'' \end{Bmatrix} \Xi_2^t \right] \quad (5)$$

where

$$\Xi_1^K = < l \| C^{(K)} \| l > < l'' \| C^{(K)} \| l' > R^K(nln' l' ; nln'' l'') \quad (6a)$$

and

$$\Xi_2^t = < l \| C^{(t)} \| l' > < l'' \| C^{(t)} \| l > R^t(nln' l' ; n'' l'' nl) . \quad (6b)$$

The above result shows that to second-order case (1) leads to a simply linear scaling of the first-order matrix elements. The values of Δ for cases (2) and (3) are of a quite different nature and cannot be so readily accommodated. The relevant summations over the perturbing states may be readily accomplished using the now standard second-quantization methods of Judd [3] to give for case (2)

$$\Delta^{(2)} = -4\sqrt{2} \sum_{k,t} R^k(nlnl ; n' l' nl) < l \| C^{(k)} \| l > < l \| C^{(k)} \| l' > \frac{< n' sl' \| \tau^{(KK)} \| nsl >}{< nsl \| \tau^{(KK)} \| nsl >} \times \begin{Bmatrix} k & K & t \\ l & l & l' \end{Bmatrix} (-1)^K \sqrt{\frac{[t]}{[k]}} < A\alpha \| \sum_{i<j} (\mathbf{w}_i^{(Kt)} \mathbf{w}_j^{(0k)})^{(KK)} \| A\alpha' > / E < A\alpha \| W^{(KK)} \| A\alpha' > . \quad (7)$$

For the case of spin independent interactions $K = 0$ and eq. (7) becomes

$$\Delta'^{(2)} = -4 \sum_{k,t} R^k(nlnl ; n' l' nl) < l \| C^{(k)} \| l > < l \| C^{(k)} \| l' > \frac{< n' l' \| \tau^{(K)} \| nl >}{< nl \| \tau^{(K)} \| nl >} \times \begin{Bmatrix} k & K & t \\ l & l & l' \end{Bmatrix} (-1)^K \sqrt{\frac{[t]}{[k]}} < A\alpha \| \sum_{i<j} (\mathbf{v}_i^{(t)} \mathbf{v}_j^{(k)})^{(K)} \| A\alpha' > / E < A\alpha \| V^{(K)} \| A\alpha' > . \quad (8)$$

In each case $t + K$ is even.

Case (3) gives

$$\Delta^{(3)} = -\Delta^{(2)} - \Delta_1^{(3)} + \Delta_2^{(3)} \quad (9)$$

where

$$\Delta_1^{(3)} = \frac{\delta(l, l')}{(4l+2)} \sum_k R^k(nlnl ; n' l' nl) < l \| C^{(k)} \| l >^2 \times \frac{< n' sl \| \tau^{(Kk)} \| nsl >}{E < nsl \| \tau^{(Kk)} \| nsl >} \quad (10a)$$

and

$$\Delta_2^{(3)} = \delta(K, 0) \frac{R^K(nlnl ; n' l' nl)}{(2K+1)(2l+1)} < l \| C^{(K)} \| l >^2 \times \frac{< n' l' \| \tau^{(0K)} \| nl >}{E < nl \| \tau^{(0K)} \| nl >} . \quad (10b)$$

The last two terms in eq. (9) give rise to a simple scaling of the first order matrix elements. Here, our principal interest will be in the study of the properties of the terms Δ_2 which produce overt effects that cannot be accommodated by any simple scaling of the first order matrix elements.

The application of the above results to practical calculations requires that the single particle interactions be first represented in terms of tensor operators as, for example, outlined by Judd [8]. In the cases of the spin-orbit interaction and the spin part of the magnetic hyperfine structure it is necessary to consider the double tensor operators $\mathbf{W}^{(11)}$ and $\mathbf{W}^{(12)}$ respectively. For the electric quadrupole hyperfine interaction, the orbital part of the magnetic hyperfine interaction, and crystal field interactions the purely orbital operators $\mathbf{V}^{(2)}$, $\mathbf{V}^{(1)}$ and $\mathbf{V}^{(k)}$ ($k = 2, 4, ..., 2l$) are required. The calculation of the electrostatic correlation of these purely orbital interactions necessitates the evaluation of the matrix elements of the two-particle orbital operators

$$\mathbf{T}^{(tk)K} = \sum_{i<j} (\mathbf{v}_i^{(t)} \mathbf{v}_j^{(k)})^{(K)} \quad (11)$$

where k is necessarily even and t and K have the same parity.

In making practical calculations of the matrix elements of $\mathbf{T}^{(tk)K}$ it is useful to be able to represent the operators in terms of operators of well-defined quasi-spin. The advantages gained include not only a simplification of the matrix element calculations but more mportantly, a sharper and more descriptive analysis of the effects of the electrostatically correlated perturbations.

For the particular case of the d-shell we are interested in the matrix elements of the operators $\mathbf{T}^{(22)K}$, $\mathbf{T}^{(42)K}$ and $\mathbf{T}^{(44)K}$ where $K = 2$ or 4. The operators $\mathbf{T}^{(kk)0}$ all have matrix elements that are simply proportional to those of the Coulomb interaction and need not be considered here.

II. **R_5 Symmetrization of the Orbital Operators.** — The states of the d-shell may be profitably classified by their transformation properties under the chain of groups

$$R_{21} \supset R_{20} \supset R_3^Q \times \times (Sp_{10} \supset R_3^S \times R_5 \supset R_3^S \times R_3^L)\,. \quad (12)$$

The operators $\mathbf{V}^{(2)}$ and $\mathbf{V}^{(4)}$ transform together as the [20] representation of R_5 and hence suitable linear combinations of the operators $\mathbf{T}^{(22)K}$, $\mathbf{T}^{(42)K}$ and $\mathbf{T}^{(44)K}$ must transform according to the representations of R_5 contained in the plethysm [1],

$$[20] \otimes \{2\} = [00] + [20] + [22] + [40]\,.$$

Under restriction to the R_3^L subgroup we find that only the [20], [22] and [40] representations yield the representations $D^{(K)}$ ($K = 2$ or 4). Thus we wish to construct six R_5 symmetrized operators $\mathbf{E}[20]^{(K)}$, $\mathbf{E}[22]^{(K)}$, $\mathbf{E}[40]^{(K)}$ ($K = 2$ or 4) as linear combinations of the $\mathbf{T}^{(tk)K}$ ($t, k = 2, 4$) operators. The linear combinations may be readily determined by writing

$$\mathbf{E}[\lambda\mu]^K = = \sum_{t,k} \mathbf{T}^{(tk)K} < [20]\, t + [20]\, k \mid [\lambda\mu]\, K > . \quad (13)$$

The isoscalar factors may be readily determined [1] from the known matrix elements of $\mathbf{V}^{(k)}$ tabulated by Nielson and Koster [9] to give the results of Table I.

For later calculations it is also useful to construct the R_5 symmetrized operators $\mathbf{O}[20]\,K$, $\mathbf{O}[22]\,K$ ($K = 2, 4$) from linear combinations of the operators $\mathbf{T}^{(tk)K}$ where $t, k = 1, 3$. The appropriate isoscalar factors are given in Table II. The complete set of R_5 symmetrized operators appears in Table III. These results may then be readily inverted by either solving the linear equations or more simply by inversion of eq. (13) to give the operators $\mathbf{T}^{(tk)K}$ as linear combinations of the R_5 symmetrized operators as given in Table IV. Thus we have a set of R_5 symmetrized two particle operators and must now study their properties with respect to the other groups appearing in eq. (12).

TABLE I

Table of Normalized Isoscalar Factors for d^N Configurations

t	k	$<[20]t+[20]k\mid[20]2>$	$<[20]t+[20]k\mid[20]4>$	$<[20]t+[20]k\mid[22]2>$	$<[20]t+[20]k\mid[22]4>$	$<[20]t+[20]k\mid[40]2>$	$<[20]t+[20]k\mid[40]4>$	$<[20]t+[20]k\mid[22]0>$
2	2	$-\frac{\sqrt{15}}{21}$	$\frac{4\sqrt{15}}{63}$	$-\frac{3\sqrt{2}}{7}$	$\frac{8\sqrt{11}}{42}$	$\frac{4\sqrt{66}}{42}$	$\frac{\sqrt{2\,145}}{63}$	$\frac{3\sqrt{14}}{14}$
4	2	$\frac{4\sqrt{3}}{21}$	$\frac{5\sqrt{66}}{63}$	$\frac{\sqrt{10}}{7}$	$\frac{\sqrt{10}}{42}$	$\frac{\sqrt{330}}{42}$	$-\frac{2\sqrt{78}}{63}$	0
2	4	$\frac{4\sqrt{3}}{21}$	$\frac{5\sqrt{66}}{63}$	$\frac{\sqrt{10}}{7}$	$\frac{\sqrt{10}}{42}$	$\frac{\sqrt{330}}{42}$	$-\frac{2\sqrt{78}}{63}$	0
4	4	$\frac{\sqrt{330}}{21}$	$\frac{\sqrt{429}}{63}$	$-\frac{\sqrt{11}}{7}$	$-\frac{4\sqrt{65}}{42}$	$-\frac{4\sqrt{3}}{42}$	$\frac{20\sqrt{3}}{63}$	$-\frac{\sqrt{70}}{14}$

TABLE II

Table of Normalized Isoscalar Factors for d^N Configurations

t	k	$<[11]t+[11]k\mid[20]2>$	$<[11]t+[11]k\mid[20]4>$	$<[11]t+[11]k\mid[22]2>$	$<[11]t+[11]k\mid[22]4>$	$<[11]t+[11]k\mid[00]0>$	$<[11]t+[11]k\mid[22]0>$
1	1	$\frac{-\sqrt{7}}{5}$	0	$\frac{\sqrt{14}}{5}$	0	$\frac{\sqrt{30}}{10}$	$\frac{-\sqrt{70}}{10}$
3	1	$\frac{2\sqrt{2}}{5}$	$\frac{-\sqrt{30}}{15}$	$\frac{1}{5}$	$\frac{\sqrt{330}}{30}$	0	0
1	3	$\frac{2\sqrt{2}}{5}$	$\frac{-\sqrt{30}}{15}$	$\frac{1}{5}$	$\frac{\sqrt{330}}{30}$	0	0
3	3	$\frac{\sqrt{2}}{5}$	$\frac{-\sqrt{165}}{15}$	$\frac{3}{5}$	$\frac{-4\sqrt{15}}{30}$	$\frac{\sqrt{70}}{10}$	$\frac{\sqrt{30}}{10}$

TABLE III

R_5 Symmetrized Operators for d^N

$$\mathbf{E}[20]^{(2)} = \frac{-\sqrt{3}}{21}(\sqrt{5}\,\mathbf{T}^{(22)2} - 8\,\mathbf{T}^{(42)2} - \sqrt{110}\,\mathbf{T}^{(44)2})$$

$$\mathbf{E}[22]^{(2)} = \frac{-1}{7}(3\sqrt{2}\,\mathbf{T}^{(22)2} - 2\sqrt{10}\,\mathbf{T}^{(42)2} + \sqrt{11}\,\mathbf{T}^{(44)2})$$

$$\mathbf{E}[40]^{(2)} = \frac{1}{21}(2\sqrt{66}\,\mathbf{T}^{(22)2} + \sqrt{330}\,\mathbf{T}^{(42)2} - 2\sqrt{3}\,\mathbf{T}^{(44)2})$$

$$\mathbf{E}[20]^{(4)} = \frac{\sqrt{3}}{63}(4\sqrt{5}\,\mathbf{T}^{(22)4} + 10\sqrt{22}\,\mathbf{T}^{(42)4} + \sqrt{143}\,\mathbf{T}^{(44)4})$$

$$\mathbf{E}[22]^{(4)} = \frac{1}{21}(4\sqrt{11}\,\mathbf{T}^{(22)4} + \sqrt{10}\,\mathbf{T}^{(42)4} - 2\sqrt{65}\,\mathbf{T}^{(44)4})$$

$$\mathbf{E}[40]^{(4)} = \frac{1}{63}(\sqrt{2\,145}\,\mathbf{T}^{(22)4} - 4\sqrt{78}\,\mathbf{T}^{(42)4} + 20\sqrt{3}\,\mathbf{T}^{(44)4})$$

$$\mathbf{O}[20]^{(2)} = -\frac{1}{5}(\sqrt{7}\,\mathbf{T}^{(11)2} - 4\sqrt{2}\,\mathbf{T}^{(31)2} - \sqrt{2}\,\mathbf{T}^{(33)2})$$

$$\mathbf{O}[22]^{(2)} = \frac{1}{5}(\sqrt{14}\,\mathbf{T}^{(11)2} + 2\,\mathbf{T}^{(31)2} + 3\,\mathbf{T}^{(33)2})$$

$$\mathbf{O}[20]^{(4)} = \frac{-\sqrt{15}}{15}(2\sqrt{2}\,\mathbf{T}^{(31)4} + \sqrt{11}\,\mathbf{T}^{(33)4})$$

$$\mathbf{O}[22]^{(4)} = \frac{2\sqrt{15}}{30}(\sqrt{22}\,\mathbf{T}^{(31)4} - 2\,\mathbf{T}^{(33)4}).$$

TABLE IV

Expansion of $T^{(tk)K}$ in terms of R_5 symmetrized tensors

$$\mathbf{T}^{(22)2} = \frac{-1}{21}(\sqrt{15}\,\mathbf{E}[20]^{(2)} + 9\sqrt{2}\,\mathbf{E}[22]^{(2)} - 2\sqrt{66}\,\mathbf{E}[40]^{(2)})$$

$$\mathbf{T}^{(42)2} = \frac{1}{42}(8\sqrt{3}\,\mathbf{E}[20]^{(2)} + 6\sqrt{10}\,\mathbf{E}[22]^{(2)} + \sqrt{330}\,\mathbf{E}[40]^{(2)})$$

$$\mathbf{T}^{(44)2} = \frac{1}{21}(\sqrt{330}\,\mathbf{E}[20]^{(2)} - 3\sqrt{11}\,\mathbf{E}[22]^{(2)} - 2\sqrt{3}\,\mathbf{E}[40]^{(2)})$$

$$\mathbf{T}^{(22)4} = \frac{1}{63}(4\sqrt{15}\,\mathbf{E}[20]^{(4)} + 24\sqrt{11}\,\mathbf{E}[22]^{(4)} + \sqrt{2\,145}\,\mathbf{E}[40]^{(4)})$$

$$\mathbf{T}^{(42)4} = \frac{1}{126}(10\sqrt{66}\,\mathbf{E}[20]^{(4)} + 3\sqrt{10}\,\mathbf{E}[22]^{(4)} - 2\sqrt{78}\,\mathbf{E}[40]^{(4)})$$

$$\mathbf{T}^{(44)4} = \frac{1}{63}(\sqrt{429}\,\mathbf{E}[20]^{(4)} - 6\sqrt{65}\,\mathbf{E}[22]^{(4)} + 20\sqrt{3}\,\mathbf{E}[40]^{(4)})$$

$$\mathbf{T}^{(11)2} = \frac{-\sqrt{7}}{5}(\mathbf{O}[20]^{(2)} - \sqrt{2}\,\mathbf{O}[22]^{(2)})$$

$$\mathbf{T}^{(31)2} = \frac{1}{5}(2\sqrt{2}\,\mathbf{O}[20]^{(2)} + \mathbf{O}[22]^{(2)})$$

$$\mathbf{T}^{(33)2} = \frac{1}{5}(\sqrt{2}\,\mathbf{O}[20]^{(2)} + 3\,\mathbf{O}[22]^{(2)})$$

$$\mathbf{T}^{(31)4} = \frac{-\sqrt{30}}{30}(2\,\mathbf{O}[20]^{(4)} - \sqrt{11}\,\mathbf{O}[22]^{(4)})$$

$$\mathbf{T}^{(33)4} = \frac{-\sqrt{15}}{15}(\sqrt{11}\,\mathbf{O}[20]^{(4)} + 2\,\mathbf{O}[22]^{(4)})$$

III. **Symplectic Symmetry.** — The operators $\mathbf{W}^{(0k)}$ and $\mathbf{W}^{(1k+1)}$ ($k = 2, 4$) transform together as the $\langle 1^2 \rangle$ representation of Sp_{10} [10, 11] and hence the two particle operators constructed from these operators must transform according to the representations of Sp_{10} contained in the plethysm

$$\langle 1^2 \rangle \otimes \{2\} = \langle 0 \rangle + \langle 1^2 \rangle + \langle 1^4 \rangle + \langle 2^2 \rangle .$$

Under the reduction $Sp_{10} \to R_3^S \times R_5$ we find [1] that the $^1[40]$ representation occurs only with $\langle 2^2 \rangle$ and thus the operators $\mathbf{E}[40]^{(K)}$ have pure symplectic symmetry. The $^1[22]$ representation occurs in the reduction of both $\langle 1^4 \rangle$ and $\langle 2^2 \rangle$ while the $^1[20]$ representation occurs in the reduction of $\langle 1^2 \rangle$, $\langle 1^4 \rangle$ and $\langle 2^2 \rangle$ and hence the operators $\mathbf{E}[22]^{(K)}$ and $\mathbf{E}[20]^{(K)}$ are not symmetrized with respect to Sp_{10}.

The operators $\mathbf{W}^{(0k+1)}$ and $\mathbf{W}^{(1k)}$ ($k = 0, 2, 4$) transform together as the $\langle 2 \rangle$ representation of Sp_{10} and hence two particle operators constructed from them must transform according to representations of Sp_{10} contained in the plethysm

$$\langle 2 \rangle \otimes \{2\} = \langle 0 \rangle + \langle 1^2 \rangle + \langle 2^2 \rangle + \langle 4 \rangle .$$

Operators transforming as $\langle 4 \rangle$ will have vanishing matrix elements when evaluated between electron states and need not be considered further. The $^1[22]$ representation occurs only in the reduction of the $\langle 2^2 \rangle$ representation and thus the operator $\mathbf{O}[22]^{(K)}$ has symplectic symmetry $\langle 2^2 \rangle$. The operator $\mathbf{O}[20]^{(K)}$ has mixed symplectic symmetry since $^1[20]$ occurs in the reduction of both $\langle 1^2 \rangle$ and $\langle 2^2 \rangle$. The symplectic symmetries of the **E** and **O** operators are collected together in Table V. While we could in principle form linear combinations of the **E** and **O**

TABLE V

Symplectic Symmetries of the R_5 Symmetrized Operators

Operator	Symplectic Symmetry
$\mathbf{E}[20]^{(K)}$	$<1^2>, <1^4>, <2^2>$
$\mathbf{E}[22]^{(K)}$	$<1^4>, <2^2>$
$\mathbf{E}[40]^{(K)}$	$<2^2>$
$\mathbf{O}[20]^{(K)}$	$<1^2>, <2^2>$
$\mathbf{O}[22]^{(K)}$	$<2^2>$

operators, together with certain additional operators, to give operators of well-defined symplectic symmetry it proves to be more useful to proceed directly to the construction of operators having pure quasi-spin.

IV. **Quasi-spin Symmetrization.** — If our operators are symmetrized with respect to the quasi-spin group R_3^Q then the dependence of their matrix elements upon the number of electrons N and the seniority v is simply proportional to a 3-j symbol involving N, v and l. Judd [12] has shown that for r-particle operators we may restrict our attention to representations $[1^{2x}]$ of R_{8l+4} where $0 \leqslant x \leqslant r$. Thus in the case of the d-shell we may restrict our attention to the quasi-spin states arising in the reduction $R_{20} \to R_3^Q \times Sp_{10}$.

$$\begin{aligned}
&[0] \to {}^1<0> \\
&[1^2] \to {}^1<2> + {}^3(<0> + <1^2>) \\
&[1^4] \to {}^1(<0> + <1^2> + <2^2>) + \\
&\qquad + {}^3(<1^2> + <2> + <21^2>) \qquad (14)\\
&\qquad + {}^5(<0> + <1^2> + <1^4>)
\end{aligned}$$

where we write the quasi-spin multiplicity $2\,Q + 1$ as a left superscript. Inspection of the above decompositions shows that operators transforming as $<2^2>$ under Sp_{10} have quasi-spin $Q = 0$ and thus $\mathbf{E}[40]^{(K)}$ and $\mathbf{O}[22]^{(K)}$ are pure quasi-spin $Q = 0$ operators.

The operators $\mathbf{E}[20]^{(K)}$, $\mathbf{E}[22]^{(K)}$ and $\mathbf{O}[20]^{(K)}$ are clearly of mixed quasi-spin. We may however form operators of pure quasi-spin by construction of suitable linear combinations. It appears at first that the operator $\mathbf{O}[20]^{(K)}$ will involve $Q = 0$, 1 and 2. However, $\mathbf{O}[20]^{(K)}$ is constructed from operators $\mathbf{T}^{(tk)K}$ (t, $k = 1$, 3) and we may write

$$\mathbf{T}^{(tk)K} = \frac{1}{2}\left\{(\mathbf{V}^{(t)}\,\mathbf{V}^{(k)})^{(K)} - (2\,K+1)^{1/2}\begin{Bmatrix} t & k & K \\ l & l & l \end{Bmatrix}\mathbf{V}^{(K)}\right\}. \quad (15)$$

Since t and k are odd while K is even we find that the operators $\mathbf{T}^{(tk)K}$ can only couple states with $\Delta v = 0$, $\pm\,2$ and hence $\mathbf{O}[20]^{(K)}$ cannot contain a non-vanishing part with quasi-spin $Q = 2$.

The operators $\mathbf{E}[22]^{(K)}$ and $\mathbf{O}[22]^{(K)}$ may be combined to form an operator

$$\mathbf{X}[22]^{(K)} = \mathbf{E}[22]^{(K)} + a\mathbf{O}[22]^{(K)} \qquad (16)$$

with pure quasi-spin $Q = 2$ where a is independent of K. The value of a may be readily fixed by demanding that the reduced matrix element

$$< d^4[00]^1\,S \parallel X^{(2)} \parallel d^4[22]^1\,D > = 0\,.$$

This matrix element may be readily determined by use of eq. (15) and the table of Nielson and Koster [9]. We then find that $a = -\sqrt{3}/3$.

The results of Tables I and II may be used to obtain the quasi-spin $Q = 2$ operator

$$\mathbf{X}[22]^{(0)} = \frac{\sqrt{14}}{14}(3\,\mathbf{T}^{(22)0} - \sqrt{5}\,\mathbf{T}^{(44)0}) + \frac{\sqrt{30}}{30}(\sqrt{7}\,\mathbf{T}^{(11)0} - \sqrt{3}\,\mathbf{T}^{(33)0})\,. \quad (17)$$

This operator is simply proportional to Judd's [8] $e_2 + \Omega'$ operator, in fact

$$\mathbf{X}[22]^{(0)} = \frac{\sqrt{70}}{420}(e_2 + \Omega')\,. \qquad (18)$$

The operator $\mathbf{O}[20]^{(K)}$ is of mixed quasi-spin 0 and 1. The single operators $\mathbf{V}^{(K)}$ (K even) are pure quasi-spin 1 operators. The operators $\mathbf{O}[20]^{(K)}$ and $\mathbf{V}^{(K)}$ may be combined to form a pure quasi-spin zero operator

$$\mathbf{Y}[20]^{(K)} = \mathbf{O}[20]^{(K)} + b\mathbf{V}^{(K)}\,, \qquad (19)$$

where b is independent of K. The constant b may be readily determined by demanding that the reduced matrix element

$$< d^2[00]^1\,S \parallel Y[20]^{(2)} \parallel d^2[20]^1\,D > = 0$$

to yield $b = -\sqrt{3}/4$. Finally we may construct a pure quasi-spin 2 operator by forming the linear combination

$$\mathbf{Z}[20]^{(K)} = \mathbf{E}[20]^{(K)} + d\mathbf{O}[20]^{(K)} + e\mathbf{V}^{(K)}\,. \quad (20)$$

The constants d and e are readily fixed by demanding that the reduced matrix elements

$$< d^5[20]^4\,D \parallel Z[20]^{(2)} \parallel d^5[20]^4\,D > = 0$$

and

$$< d^4[10]^5\,D \parallel Z[20]^{(K)} \parallel d^4[10]^5\,D > = 0$$

to give $d = \sqrt{5}/3$ and $e = 2\sqrt{15}/15$. Thus we have the quasi-spin symmetrized operators of Table VI.

TABLE VI

Quasi-spin symmetrized orbital operators for the d-shell

$Q = 0$	$\mathbf{E}[40]^{(K)}$
	$\mathbf{O}[22]^{(K)}$
	$\mathbf{Y}[20]^{(K)} = \mathbf{O}[20]^{(K)} - \frac{\sqrt{3}}{4}\mathbf{V}^{(K)}$
$Q = 1$	$\mathbf{V}^{(K)}$
$Q = 2$	$\mathbf{X}[22]^{(K)} = \mathbf{E}[22]^{(K)} - \frac{\sqrt{3}}{3}\mathbf{O}[22]^{(K)}$
	$\mathbf{Z}[20]^{(K)} = \mathbf{E}[20]^{(K)} + \frac{\sqrt{5}}{3}\mathbf{O}[20]^{(K)} + \frac{2\sqrt{15}}{15}\mathbf{V}^{(K)}$

(K *even*)

V. Matrix Elements. — The reduced matrix elements of the operators $\mathrm{T}^{(tk)\mathrm{K}}$ may be readily evaluated for a l^2 configuration using the result [13]

$$< l^2\,\mathrm{SL} \,\|\, T^{(tk)\mathrm{K}} \,\|\, l^2\,\mathrm{SL}' > = \\ = [\mathrm{L}, \mathrm{L}', t, k, \mathrm{K}]^{1/2} \begin{Bmatrix} l & l & \mathrm{L} \\ l & l & \mathrm{L}' \\ t & k & \mathrm{K} \end{Bmatrix} . \quad (21)$$

Linear combinations were then formed to give the reduced matrix elements of the R_5 symmetrized operators (for $\mathrm{K} = 2$) for the d^2 configuration shown in Table VII. The results of Table VI were then used to give the reduced matrix elements of the quasi-spin symmetrized operators given in Table VIII.

TABLE VII

Matrix elements of the R_5 symmetrized orbital operators for d^2

$\mathrm{E}[20]^{(2)}$	^{1}S	^{1}D	^{1}G	^{3}P	^{3}F
^{1}S	0	$\frac{3\sqrt{15}}{10}$	0	0	0
^{1}D	$\frac{3\sqrt{15}}{10}$	$-\frac{\sqrt{3}}{42}$	$\frac{2\sqrt{15}}{105}$	0	0
^{1}G	0	$\frac{2\sqrt{15}}{105}$	$\frac{\sqrt{66}}{42}$	0	0
^{3}P	0	0	0	$\frac{3\sqrt{7}}{10}$	$-\frac{3\sqrt{2}}{5}$
^{3}F	0	0	0	$-\frac{3\sqrt{2}}{5}$	$-\frac{3\sqrt{2}}{10}$

$\mathrm{E}[22]^{(2)}$	^{1}S	^{1}D	^{1}G	^{3}P	^{3}F
^{1}S	0	0	0	0	0
^{1}D	0	$\frac{3\sqrt{10}}{14}$	$-\frac{5\sqrt{2}}{14}$	0	0
^{1}G	0	$-\frac{5\sqrt{2}}{14}$	$\frac{\sqrt{55}}{14}$	0	0
^{3}P	0	0	0	$-\frac{\sqrt{210}}{10}$	$-\frac{\sqrt{15}}{10}$
^{3}F	0	0	0	$-\frac{\sqrt{15}}{10}$	$-\frac{3\sqrt{15}}{10}$

TABLE VII (Contd)

$\mathrm{E}[40]^{(2)}$	^{1}S	^{1}D	^{1}G	^{3}P	^{3}F
^{1}S	0	0	0	0	0
^{1}D	0	$\frac{2\sqrt{330}}{21}$	$\frac{5\sqrt{66}}{42}$	0	0
^{1}G	0	$\frac{5\sqrt{66}}{42}$	$-\frac{2\sqrt{5}}{21}$	0	0
^{3}P	0	0	0	0	0
^{3}F	0	0	0	0	0

$\mathrm{O}[20]^{(2)}$	^{1}S	^{1}D	^{1}G	^{3}P	^{3}F
^{1}S	0	$\frac{\sqrt{3}}{2}$	0	0	0
^{1}D	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{15}}{14}$	$-\frac{2\sqrt{3}}{7}$	0	0
^{1}G	0	$-\frac{2\sqrt{3}}{7}$	$-\frac{\sqrt{330}}{14}$	0	0
^{3}P	0	0	0	$-\frac{\sqrt{35}}{10}$	$\frac{\sqrt{10}}{5}$
^{3}F	0	0	0	$\frac{\sqrt{10}}{5}$	$\frac{\sqrt{10}}{10}$

$\mathrm{O}[22]^{(2)}$	^{1}S	^{1}D	^{1}G	^{3}P	^{3}F
^{1}S	0	0	0	0	0
^{1}D	0	$\frac{3\sqrt{30}}{14}$	$-\frac{5\sqrt{6}}{14}$	0	0
^{1}G	0	$-\frac{5\sqrt{6}}{14}$	$\frac{\sqrt{165}}{14}$	0	0
^{3}P	0	0	0	$\frac{\sqrt{70}}{10}$	$\frac{\sqrt{5}}{10}$
^{3}F	0	0	0	$\frac{\sqrt{5}}{10}$	$\frac{3\sqrt{5}}{10}$

The reduced matrix elements given in Table VIII form the basis for calculating the matrix elements for all d^{N} matrix elements since if $T^{(\mathrm{K})}$ is an arbitrary two particle operator we have the well known results [13, 14]

$$< l^N \alpha SL \parallel T_i^{(K)} \parallel l^N \alpha' SL' > = \frac{1}{2} N(N-1) [L, L']^{1/2} \sum (-1)^{L+\tilde{L}+l+K} \times \begin{Bmatrix} L & K & L' \\ \hat{L}' & \tilde{L} & \hat{L} \end{Bmatrix}$$

$$(l^N \alpha SL \{ | l^{N-2} \tilde{\alpha}\tilde{S}\tilde{L} ; l^2 \hat{S}\hat{L}) (l^{N-2} \tilde{\alpha}\tilde{S}\tilde{L} ; l^2 \hat{S}\hat{L}' | \} l^N \alpha' SL') \times < l^2 \hat{S}\hat{L} \parallel T_i^{(K)} \parallel l^2 \hat{S}\hat{L}' > \quad (22a)$$

$$= \frac{N}{N-2} [L, L']^{1/2} \sum (-1)^{L+\tilde{L}+l+K} \begin{Bmatrix} L & K & L' \\ \tilde{L}' & l & \tilde{L} \end{Bmatrix} (l^N \alpha SL \{ | l^{N-1} \tilde{\alpha}\tilde{S}\tilde{L}) \times$$

$$\times (l^{N-1} \tilde{\alpha}' \tilde{S}' \tilde{L}' | \} l^N \alpha SL') < l^{N-1} \tilde{\alpha}\tilde{S}\tilde{L} \parallel T_i^{(K)} \parallel l^{N-1} \tilde{\alpha}' \tilde{S}\tilde{L}' > \quad (22b)$$

TABLE VIII

Reduced Matrix Elements of $\mathbf{X}[22]^{(2)}$, $\mathbf{Y}[20]^{(2)}$ *and* $\mathbf{Z}[20]^{(2)}$ *for* d^2

$\mathbf{X}[22]^{(2)}$	^1S	^1D	^1G	^3P	^3F
^1S	0	0	0	0	0
^1D	0	0	0	0	0
^1G	0	0	0	0	0
^3P	0	0	0	$\frac{-2\sqrt{210}}{15}$	$\frac{-2\sqrt{15}}{15}$
^3F	0	0	0	$\frac{-2\sqrt{15}}{15}$	$\frac{-2\sqrt{15}}{5}$

$\mathbf{Y}[20]^{(2)}$	^1S	^1D	^1G	^3P	^3F
^1S	0	0	0	0	0
^1D	0	$\frac{5\sqrt{15}}{28}$	$\frac{-5\sqrt{3}}{7}$	0	0
^1G	0	$\frac{-5\sqrt{3}}{7}$	$\frac{-5\sqrt{330}}{28}$	0	0
^3P	0	0	0	$\frac{\sqrt{35}}{20}$	$\frac{-\sqrt{10}}{10}$
^3F	0	0	0	$\frac{-\sqrt{10}}{10}$	$\frac{-\sqrt{10}}{20}$

$\mathbf{Z}[20]^{(2)}$	^1S	^1D	^1G	^3P	^3F
^1S	0	$\frac{11\sqrt{15}}{15}$	0	0	0
^1D	$\frac{11\sqrt{15}}{15}$	$\frac{-4\sqrt{3}}{21}$	$\frac{16\sqrt{15}}{105}$	0	0
^1G	0	$\frac{16\sqrt{15}}{105}$	$\frac{4\sqrt{66}}{21}$	0	0
^3P	0	0	0	$\frac{-4\sqrt{7}}{15}$	$\frac{8\sqrt{2}}{15}$
^3F	0	0	0	$\frac{8\sqrt{2}}{15}$	$\frac{4\sqrt{2}}{15}$

where in (22*a*) the sum is over the two-particle coefficients of fractional parentage (c. f. p.) and in (22*b*) over the one-particle c. f. p. Tables of both types of c. f. p. are available for the d^N configurations [9, 13, 15].

Equations (22*a*) and (22*b*) are strictly valid only for two particle operators whereas some of the operators in Table VI include one particle operators. These cases may be readily handled by assuming eq. (22*a*) and (22*b*) are valid for one- and two-particle operators and then *subtracting* from the result the matrix elements of the one particle operators.

Equation (22*b*) may be readily used to evaluate the matrix elements for the states of maximum multiplicity to give, for example, the results of Table IX. The matrix elements all vanish for the ^6S state of d^5 while for the ^5D state of d^4 the only non-zero two-particle quasi-spin symmetrized matrix element with $K = 2$ is

$$< d^4\ ^5D \parallel Y[20]^{(2)} \parallel d^4\ ^5D > = \frac{3\sqrt{15}}{4}.$$

TABLE IX

Reduced matrix elements for d^3

$\mathbf{O}[22]^{(2)}$	^4P	^4F
^4P	$\frac{\sqrt{70}}{10}$	$\frac{\sqrt{5}}{10}$
^4F	$\frac{\sqrt{5}}{10}$	$\frac{3\sqrt{5}}{10}$

$\mathbf{X}[22]^{(2)}$	^4P	^4F
^4P	$\frac{-2\sqrt{210}}{15}$	$\frac{-2\sqrt{15}}{15}$
^4F	$\frac{-2\sqrt{15}}{15}$	$\frac{-2\sqrt{15}}{5}$

$\mathbf{Y}[20]^{(2)}$	^4P	^4F
^4P	$\frac{\sqrt{35}}{20}$	$\frac{-\sqrt{10}}{10}$
^4F	$\frac{-\sqrt{10}}{10}$	$\frac{-\sqrt{10}}{20}$

$\mathbf{Z}[20]^{(2)}$	^4P	^4F
^4P	$\frac{2\sqrt{7}}{15}$	$\frac{-4\sqrt{2}}{15}$
^4F	$\frac{-4\sqrt{2}}{15}$	$\frac{-2\sqrt{2}}{15}$

There is, in principle, no difficulty in calculating the matrix elements of the quasi-spin symmetrized orbital operators for all the states of the d-shell. Such a calculation would provide a rich source of isoscalar factors [16].

VI. **Isoscalar Factors.** — The Wigner-Eckart theorem leads to substantial simplifications in the calculation of the reduced matrix elements of the quasi-spin symmetrized operators. Application of the Wigner-Eckart theorem gives

$$< d^N[\lambda]\, SL \parallel T[\lambda'']^{(K)} \parallel d^N[\lambda']SL' > = \sum_\alpha A_\alpha < \alpha[\lambda]\, L \mid [\lambda'']\, K + [\lambda']\, L' > \quad (23)$$

where A_α is independent of K, L and L′ and α distinguishes those cases where $[\lambda]$ occurs more than once in the Kronecker product $[\lambda''] \times [\lambda']$. Thus the entire dependence upon L, L′ and K of the reduced matrix elements is contained in the R_5 isoscalar factor

$$< \alpha[\lambda]\, L \mid [\lambda'']\, K + [\lambda']\, L' > .$$

Judd [8, 12] has discussed a number of applications of isoscalar factors in atomic shell theory. For example, since the Kronecker product [11] × [11] contained [20] and [22] just once we conclude immediately that the reduced matrix elements of $\mathbf{Y}[20]^{(K)}$, $\mathbf{V}^{(K)}$, $\mathbf{Z}[20]^{(K)}$, and of $\mathbf{O}[22]^{(K)}$ and $\mathbf{X}[22]^{(K)}$, among the states of maximum multiplicity of d^2 and d^3 differ by at most a proportionality constant. In a similar fashion the matrix elements for d^2 of the operators with $K = 4$ can be obtained from those found for $K = 2$ by use of the isoscalar factors of Tables I and II.

While the matrix elements of the tensor operators $\mathbf{V}^{(K)}$ provide a rich source of isoscalar factors their range is limited by the fact that the operators all transform under R_5 as [11] (K odd) or [20] (K even). Furthermore, since we only have one species of operator of a given symmetry type we do not have a natural means of distinguishing those isoscalar factors where there is a multiplicity problem. Calculations of Kronecker products [1] of R_5 for those representations describing the transformation properties of d^N electron states never involve multiplicities of > 3, the multiplicity 3 occurring only for the [21] and [31] representations that arise in the Kronecker product [21] × [21]. Clearly the calculation of the matrix elements of the quasi-spin symmetrized operators $\mathbf{E}[40]^{(K)}$, $\mathbf{O}[22]^{(K)}$ and $\mathbf{X}[22]^{(K)}$ could greatly extend our knowledge of R_5 isoscalar factors while calculations of the matrix elements of $\mathbf{Y}[20]^{(K)}$ and $\mathbf{Z}[20]^{(K)}$ would overcome the multiplicity problem in computing many isoscalar factors.

We would suggest that the calculation of symmetrized two-particle operators constitutes a useful approach to the extension of our knowledge of isoscalar factors. Clearly there is scope for the construction of other symmetrized orbital and indeed spin-orbital operators to allow the investigation of other isoscalar factors.

VII. **Electrostatically Correlated Electric Quadrupole Hyperfine Interactions.** — In the case of the electric quadrupole hyperfine interaction we have in eq. (1) $K = 0$ and $K = 2$ and hence in describing the effects of electrostatic correlation eq. (8) is required and the matrix elements of the operator

$$Q = \sum_t \sqrt{[t]} \begin{Bmatrix} k & 2 & t \\ l & l & l' \end{Bmatrix} \mathbf{T}^{(tk)2} \quad (24)$$

need to be considered. Since k is necessarily even we must also have only even values of t. The term with $t = 0$ simplifies to just

$$\frac{\sqrt{5}\, \delta(k, l)\, (N - 1)}{10(2\, l + 1)} \mathbf{V}^{(2)} . \quad (25)$$

Thus this term has the effect of simply screening the normal first order electric quadrupole effect without changing its angular momentum dependence. The terms with $t > 0$ clearly introduce overt effects that cannot be accommodated by a simple modification of $< r^{-3} >$.

The values of t and k are limited by the usual triangular conditions for 6-j symbols and thus the terms arising in eq. (24) depend on the value of l'. For the d^N shell we are limited to one-electron excitations where $l' = s$, d or g. The relevant operators, to within an obvious proportionality constant, are listed in Table X together with their expansion into R_5 symmetrized operators. The corresponding expansion into quasi-spin symmetrized operators follows directly from Table VI.

Contributions from single electron excitations of the type $d^N \to d^{N-1}\, s$ and $d^N \to d^{N+1}\, s^{-1}$ are likely to be dominant through out the transition elements. For states of maximum multiplicity the matrix elements of $\mathbf{E}[40]^{(2)}$ must vanish leaving just those of $\mathbf{E}[20]^{(2)}$. But the representation [20] occurs at most once in the relevant Kronecker product and hence the matrix elements of $\mathbf{E}[20]^{(2)}$ must be simply proportional to

TABLE X

Electrostatically Correlated Operators for Electric Quadrupole Hyperfine Structure

$d^N \to d^{N-1}\, s$ $\quad \sqrt{5}\, \mathbf{T}^{(22)2} + 3\, \mathbf{T}^{(42)2} =$

$$= \frac{\sqrt{3}}{6} (2\, \mathbf{E}[20]^{(2)} + \sqrt{110}\, \mathbf{E}[40]^{(2)})$$

$d^N \to d^{N-1}\, d'$ $\quad \sqrt{5}\, \mathbf{T}^{(22)2} - 4\, \mathbf{T}^{(42)2} =$

$$= -\, (\sqrt{3}\, \mathbf{E}[20]^{(2)} + \sqrt{10}\, \mathbf{E}[22]^{(2)})$$

$4\sqrt{5}\, \mathbf{T}^{(42)2} + 5\sqrt{22}\, \mathbf{T}^{(44)2} =$

$$= (6\sqrt{15}\, \mathbf{E}[20]^{(2)} - 5\sqrt{2}\, \mathbf{E}[22]^{(2)})$$

$d^N \to d^{N-1}\, g$ $\quad 12\sqrt{5}\, \mathbf{T}^{(22)2} + \mathbf{T}^{(42)2}$

$$= \frac{-1}{6} (16\sqrt{3}\, \mathbf{E}[20]^{(2)} + 30\sqrt{10}\, \mathbf{E}[22]^{(2)} - \sqrt{330}\, \mathbf{E}[40]^{(2)})$$

$$\sqrt{110}\, \mathbf{T}^{(42)2} + 3\, \mathbf{T}^{(44)2} = \frac{1}{3} (\sqrt{330}\, \mathbf{E}[20]^{(2)} - {} + 3\sqrt{11}\, \mathbf{E}[22]^{(2)} + 7\sqrt{3}\, \mathbf{E}[40]^{(2)}) .$$

those of $\mathbf{V}^{(2)}$ which arises in the calculation of the unperturbed electric quadrupole hyperfine structure [17]. Thus if the d $\leftrightarrow$ s excitations are dominant it should still be possible to fit the electric quadrupole hyperfine structure associated with the states of maximum multiplicity with a single value of $< r^{-3} >$. However, detailed calculations must await the computation of the relevant energy denominators and radial integrals.

VIII. **Conclusion.** — Quasi-spin symmetrized orbital operators have been constructed to aid the calculation of electrostatically correlated orbital interactions and their matrix elements computed for the d^2 configuration and the states of maximum multiplicity for d^3 and d^4. The calculation of the matrix elements of the symmetrized operators for the d-shell will provide a new source of isoscalar-factors which in turn could give more light on the subject of atomic shell theory.

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