and Philbrick,[12] and Kuyat and co-workers[13] have observed many elastic resonances, including one at 23.82 eV. If one assumes additional He^- formation associated with the upper excited states and subsequent 4^1D_2 excitation, one has a partial qualitative explanation of the observed effect. The relatively greater effect for the lower states can be explained in this manner. The fact that the polarization remains depressed to approximately 40 eV and the intensity of I_1 is nearly constant through this energy range are less understandable, although the doubly excited configuration $2p^2$ has been observed[14] at 59.5 eV.

In summary, the near-threshold minimum polarization effect previously observed for several lines in helium has been observed for He 4922 Å under experimental conditions which are believed to rule out the possibility of its being an experimental or instrumental error. Also, high-energy pressure-independent negative polarization has been observed. Although some scatter is measured in the experimental polarization values, nothing indicative of resolved structure has been observed.

The described observations agree with threshold and high-energy polarization theory, but current theory does not predict the near-threshold minimum, as observed.

[12] G. J. Schulz and J. W. Philbrick, Phys. Rev. Letters **13**, 477 (1964).
[13] C. W. Kuyatt, J. A. Simpson, and S. R. Mielczarek, Phys. Rev. **138**, A385 (1965).
[14] *Atomic Energy Levels*, edited by C. E. Moore, Natl. Bur. Std. U.S., Circ. 467 (U. S. Government Printing and Publishing Office, Washington, D. C., 1949), p. 6.

PHYSICAL REVIEW VOLUME 156, NUMBER 1 5 APRIL 1967

Effective Electrostatic Interactions in l^N Configurations*

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(Received 8 August 1966)

A new and simple method is developed for calculating effective interactions produced by interaction between electronic configurations. Also, a classification of the effective-interaction operators is performed, which both generalizes and corrects the previous classification made by Bacher and Goudsmit.

I. INTRODUCTION AND DISCUSSION OF RESULTS

ATOMIC energy levels are generally classified into configurations, corresponding to independent particle motions for the atomic electrons. In fact, different configurations "interact" as a result of the Coulomb repulsion between any two electrons, which is not consistent with independent particle motion. This interaction can often be treated by perturbation theory. In first order, different configurations do not interact; in second order, only those configurations interact which differ in the quantum numbers of at most two electrons.

Bacher and Goudsmit[1] have shown in a classical paper that this second-order effect may be replaced, under certain circumstances, by an effective interaction operator acting only within the perturbed configuration. That is, one can diagonalize the energy matrix including the operator V_{eff} within the configuration, as an alternative to setting up the larger matrix of the true interaction V between all states of both configurations.

The structure of this operator V_{eff} depends on the two configurations. Bacher and Goudsmit showed that when the perturbing configuration has two excited electrons, i.e., if two electron states differ from those of the original configuration, then V_{eff} has the structure of a two-body interaction; whereas a perturbing configuration differing in only *one* electron state leads to a V_{eff} with the structure of a three-particle interaction.

Explicit calculations of these operators have been performed by Rajnak and Wybourne[2] for configurations of N electrons, all of the same l and n, outside closed shells (l^N configurations). Their final results have a very simple form, but the calculations involved in their derivation are fairly complicated. In the present paper, we first develop a different method which makes the calculations as simple as the results,[3] and which exhibits the physical reasons for the form of the effective interactions. Furthermore, we can now both generalize and correct the statements of Bacher and Goudsmit. It turns out that the structure of V_{eff} depends not only on the *number* of "excited electrons," but on the precise nature of their excitation. The method is not limited to l^N configurations, but can be applied to any configuration and to any interaction.

* Work supported in part by the U. S. National Bureau of Standards, Washington, D. C.
† Deceased 28 August 1965.
[1] R. F. Bacher and S. Goudsmit, Phys. Rev. **46**, 948 (1934).
[2] K. Rajnak and B. G. Wybourne, Phys. Rev. **132**, 280 (1963).
[3] As a byproduct, we have been able to check the work of Rajnak and Wybourne (Ref. 2) and to correct a number of minor calculational errors.

If the perturbing configuration B is well separated from the perturbed configuration A, the matrix elements of the second-order perturbation produced by B on A are given by

$$(A\Psi|W_2|A\Psi') = -\sum_{\Psi''}(A\Psi|G|B\Psi'')\times(B\Psi''|G|A\Psi')/\Delta E_c, \quad (1)$$

where G is the Coulomb interaction and ΔE_c is the distance between the centers of gravity of the two configurations. Rajnak and Wybourne wrote the expressions for the matrix elements appearing on the right-hand side of (1) and performed the summation over Ψ'' by using the recoupling identity of Biedenharn.

The fundamental idea of our method is to "curtail" the operator G: In the first factor of the sum (1) we shall substitute for G a "curtailed" operator g whose matrix elements $(A'\Psi|g|B'\Psi'')$ are equal to the matrix elements of G if $A'=A$ and $B'=B$, and vanish in any other case; in the second factor of the sum (1) we shall substitute for G a similarly "curtailed" operator $\tilde{g}$. We then have

$$(A\Psi|W_2|A\Psi') = -\sum_{B'\Psi''}(A\Psi|g|B'\Psi'')\times(B'\Psi''|\tilde{g}|A\Psi')/\Delta E_c; \quad (2)$$

but now the summation over Ψ'' need not be limited to the states of the configuration B, and may be extended to all states of the system. It then follows from the matrix multiplication law that

$$(A\Psi|W_2|A\Psi') = -(A\Psi|g\tilde{g}|A\Psi')/\Delta E_c, \quad (3)$$

and the effective interaction is simply given by

$$W_2 = -g\tilde{g}/\Delta E_c, \quad (4)$$

without any summation over intermediate states. The calculation of the product $g\tilde{g}$ will still need some recoupling identities; but these identities will be much simpler than the identity of Biedenharn, because we need to recouple only products of operators and not products of matrix elements, which are themselves products of operators and of eigenfunctions.

A. Results

In order to be able to describe our results clearly we have to define a "new electronic state."

A state of one electron (in the perturbing configuration) which has quantum numbers (nl) will be called "a new electronic state" if there is no one-electron state in the perturbed configuration with the same n and l; e.g., if the perturbed configuration is $(nl)^N(n'l')$ then the state $n''l''$ (or $n'l$) is "new," while the states nl and $n'l'$ are "old."

The results may be stated as: (1) If two excited electrons are in a new electronic state, then V_{eff} is a two-body interaction. (2) If only one excited electron is in a new electronic state, then V_{eff} is a three-body interaction. (3) Otherwise, V_{eff} is a four-body interaction.

For these rules, a "new hole state" is equivalent to a "new electronic state"; e.g., if the perturbed configuration is p^6d^N (a closed shell p, and N electrons d) and the perturbing configuration is p^5d^Nf, then we have one "new electron" and one "new hole"; therefore, V_{eff} is a two-body interaction.

These simple rules also have a simple interpretation: The effective interaction is described by Eq. (1). The right side of this equation describes how two electrons jump from configuration A to configuration B, and then two from B to A; therefore, in general, four electrons "jump" during the interaction process. But if an electron from A jumps to a new state in B, *the same* electron must jump back to A. Therefore the number of jumping electrons is reduced to three if B contains one new state, and to two if B contains two new states.

The remainder of the paper contains technical details, organized as follows: IIA: Perturbation produced by $l^{N-2}l'^2$; IIB: perturbation caused by $l^{N-2}l'l''$; IIC: perturbation produced by $l^{N-1}l'$; IID: perturbation produced by $l'^{4l'+1}l^{N+1}$; IIE: perturbation produced by $l'^{4l'}l^{N+2}$; IIF: perturbation produced by $l'^{4l'+1}l^Nl''$.

In IID, results differ from (2); check calculations were performed by a different method[4] with identical results.

II. EFFECTIVE INTERACTIONS IN THE CONFIGURATIONS l^N

A. Perturbations produced by $l^{N-2}l'^2$

If we define the tensor operators $\mathbf{u}^{(k)}$, $\mathbf{z}^{(k)}$, and $\mathbf{z}^{(k)T}$ as the tensor operators of order k whose only nonvanishing elements of the reduced matrices are

$$(nl\|u^{(k)}\|nl) = (nl\|z^{(k)}\|n'l') = (n'l'\|z^{(k)T}\|nl) = 1, \quad (5)$$

and also define, following Rajnak and Wybourne, the two quantities

$$X(k;l_al_b,l_cl_d) = (l_a\|C^{(k)}\|l_c)(l_b\|C^{(k)}\|l_d)R^k(l_al_b,l_cl_d) \quad (6)$$

and

$$P(kk';l_al_b,l_cl_d) = X(k;l_al_b,l_cl_d)X(k';l_al_b,l_cl_d)/\Delta E_c \quad (7)$$

then we immediately see that

$$g = \sum_k X(k;ll'l'l')\sum_{i<j}(\mathbf{z}_i^{(k)}\cdot\mathbf{z}_j^{(k)}), \quad (8a)$$

$$\tilde{g} = \sum_{k'} X(k';ll'l'l')\sum_{r<s}(\mathbf{z}_r^{(k')T}\cdot\mathbf{z}_s^{(k')T}), \quad (8b)$$

and that

$$W_2 = -\sum_{kk'} P(kk';ll'l'l')\sum_{i<j}\sum_{r<s}(\mathbf{z}_i^{(k)}\cdot\mathbf{z}_j^{(k)})\times(\mathbf{z}_r^{(k')T}\cdot\mathbf{z}_s^{(k')T}). \quad (9)$$

The operator $(\mathbf{z}_i^{(k)}\cdot\mathbf{z}_j^{(k)})$ acts only on states where the electrons i and j are in the shell l'; since the con-

[4] J. Stein, Ph.D. Thesis, The Hebrew University, Jerusalem, 1967 (unpublished).

figuration l^N does not contain electrons in the shell l', that operator will give a nonvanishing contribution only if the electrons i and j have been brought to the shell l' by the operator $(\mathbf{z}_r^{(k')T}\cdot\mathbf{z}_s^{(k')T})$. This means that the only nonvanishing terms of the sum (9) are those for which $i=r$ and $j=s$, and therefore

$$W_2=-\sum_{kk'} P(kk';ll'l'l')\sum_{i<j}(\mathbf{z}_i^{(k)}\cdot\mathbf{z}_j^{(k)})\times(\mathbf{z}_i^{(k')T}\cdot\mathbf{z}_j^{(k')T}). \quad (10)$$

This expression already shows that the effective interaction is a two-body interaction; but we may still simplify the result by recoupling the product of scalar products according to the identity

$$(\mathbf{A}^{(k)}\cdot\mathbf{B}^{(k)})(\mathbf{C}^{(k')}\cdot\mathbf{D}^{(k')})=\sum_t([\mathbf{A}^{(k)}\times\mathbf{C}^{(k')}]^{(t)}\cdot[\mathbf{B}^{(k)}\times\mathbf{D}^{(k')}]^{(t)}), \quad (11)$$

which follows immediately from the definition of irreducible product and from the orthogonality of the Wigner coefficients, when $\mathbf{B}^{(k)}$ and $\mathbf{C}^{(k')}$ are commutative. It follows moreover from the definitions (5) and from Eq. (15.15) of Fano and Racah[5] that

$$[\mathbf{z}^{(k)}\times\mathbf{z}^{(k')T}]^{(t)}=(-1)^t(2t+1)^{1/2}\begin{Bmatrix}k & k' & t\\ l & l & l'\end{Bmatrix}\mathbf{u}^{(t)}. \quad (12)$$

If we define, according to Rajnak and Wybourne,

$$M(t;l_al_b,l_cl_d)=\sum_{kk'}\begin{Bmatrix}k & k' & t\\ l_a & l_b & l_c\end{Bmatrix}\begin{Bmatrix}k & k' & t\\ l_a & l_b & l_d\end{Bmatrix}P(kk';l_al_b,l_cl_d), \quad (13)$$

then Eq. (10) reduces to

$$W_2=-\sum_t(2t+1)M(t;ll'l'l')\sum_{i<j}(\mathbf{u}_i^{(t)}\cdot\mathbf{u}_j^{(t)}), \quad (14)$$

in agreement with Eq. (14) of Rajnak and Wybourne. The difference in the phase factor $(-1)^t$ depends only on a different convention in the definition of the scalar product. Rajnak and Wybourne use the old definition of Racah,[6] while we are using throughout the phase conventions of Fano and Racah,[5] and in this particular case their Eq. (6.5).

B. Perturbations produced by $l^{N-2}l'l''$

In this case we also need the tensor $\mathbf{y}^{(k)}$ whose only nonvanishing element of the reduced matrix is

$$(nl\|y^{(k)}\|n''l'')=1; \quad (15)$$

then

$$g=\sum_k X(k;ll'l'')\sum_{i\neq j}(\mathbf{z}_i^{(k)}\cdot\mathbf{y}_j^{(k)}), \quad (16)$$

and proceeding in the same way as before we get

$$W_2=-\sum_t(2t+1)M(t;ll'l'')\sum_{i\neq j}(\mathbf{u}_i^{(t)}\cdot\mathbf{u}_j^{(t)})=-2\sum_t(2t+1)M(t;ll'l'')\sum_{i<j}(\mathbf{u}_i^{(t)}\cdot\mathbf{u}_j^{(t)}). \quad (17)$$

The factor 2 is not mentioned by Rajnak and Wybourne. It seems that they overlooked the fact that when we substitute $l'l''$ for l'^2, their Eq. (9) should be multiplied by $\sqrt{2}$, according to Eq. (6⁸17) of Condon and Shortley.[7]

C. Perturbations produced by $l^{N-1}l'$

In this case,

$$g=\sum_k X(k;llll')\sum_{i\neq j}(\mathbf{u}_i^{(k)}\cdot\mathbf{z}_j^{(k)}), \quad (18)$$

but it is more convenient to write

$$g=\sum_k X(k;llll')\Big(\sum_{ij}(\mathbf{u}_i^{(k)}\cdot\mathbf{z}_j^{(k)})-\sum_j(\mathbf{u}_j^{(k)}\cdot\mathbf{z}_j^{(k)})\Big), \quad (19a)$$

and

$$\tilde{g}=\sum_{k'} X(k';llll')\Big(\sum_{rs}(\mathbf{z}_r^{(k')T}\cdot\mathbf{u}_s^{(k')})-\sum_r(\mathbf{z}_r^{(k')T}\cdot\mathbf{u}_r^{(k')})\Big). \quad (19b)$$

Now the nonvanishing terms of the product $g\tilde{g}$ will only have to satisfy the requirement $j=r$, and therefore, the effective interaction will contain three-body interactions

$$W_2=-\sum_{kk'} P(kk';llll')\Big(\sum_{ijs}(\mathbf{u}_i^{(k)}\cdot\mathbf{z}_j^{(k)})(\mathbf{z}_j^{(k')T}\cdot\mathbf{u}_s^{(k')})-\sum_{js}(\mathbf{u}_j^{(k)}\cdot\mathbf{z}_j^{(k)})(\mathbf{z}_j^{(k')T}\cdot\mathbf{u}_s^{(k')})-\sum_{ij}(\mathbf{u}_i^{(k)}\cdot\mathbf{z}_j^{(k)})\times(\mathbf{z}_j^{(k')T}\cdot\mathbf{u}_j^{(k')})+\sum_j(\mathbf{u}_j^{(k)}\cdot\mathbf{z}_j^{(k)})(\mathbf{z}_j^{(k')T}\cdot\mathbf{u}_j^{(k')})\Big). \quad (20)$$

The convenient recoupling formula is now

$$(\mathbf{A}^{(k)}\cdot\mathbf{B}^{(k)})(\mathbf{C}^{(k')}\cdot\mathbf{D}^{(k')})=\sum_{k''}(-1)^{k+k'+k''}(2k''+1)^{1/2}\times[\mathbf{A}^{(k)}\times[\mathbf{B}^{(k)}\times\mathbf{C}^{(k')}]^{(k'')}\times\mathbf{D}^{(k')}]^{(0)}. \quad (21)$$

Taking into account (12) and the fact that k and k' are even, we get

$$W_2=-\sum_{kk'k''}P(kk';llll')(2k''+1)\begin{Bmatrix}k & k' & k''\\ l & l & l'\end{Bmatrix}\times\Big(\sum_{ijs}[\mathbf{u}_i^{(k)}\times\mathbf{u}_j^{(k'')}\times\mathbf{u}_s^{(k')}]^{(0)}-\sum_{js}[\mathbf{u}_j^{(k)}\times\mathbf{u}_j^{(k'')}\times\mathbf{u}_s^{(k')}]^{(0)}-\sum_{ij}[\mathbf{u}_i^{(k)}\times\mathbf{u}_j^{(k'')}\times\mathbf{u}_j^{(k')}]^{(0)}+\sum_j[\mathbf{u}_j^{(k)}\times\mathbf{u}_j^{(k'')}\times\mathbf{u}_j^{(k')}]^{(0)}\Big). \quad (22)$$

[5] U. Fano and G. Racah, *Irreducible Tensorial Sets* (Academic Press Inc., New York, 1959).

[6] G. Racah, Phys. Rev. **62**, 438 (1942).

[7] E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Cambridge University Press, New York, 1935).

The last three terms in the brackets may still be simplified by performing the products $[\mathbf{u}_j^{(k)}\times\mathbf{u}_j^{(k'')}]^{(k')}$ and $[\mathbf{u}_j^{(k'')}\times\mathbf{u}_j^{(k')}]^{(k)}$ by formulas like (12), and then summing over k'' with the help of the orthogonality relations of the $6j$ symbols. In the last term we may also take into account the relation

$$(\mathbf{u}^{(k)}\cdot\mathbf{u}^{(k)})=(-1)^k/(2l+1). \quad (23)$$

If we define, as usual,

$$\mathbf{U}^{(k)}=\sum_i \mathbf{u}_i^{(k)}, \quad (24)$$

then the final result is

$$W_2=-\sum_{kk'k''}P(kk';lll')(2k''+1)\begin{Bmatrix}k & k' & k''\\ l & l & l'\end{Bmatrix}\times[\mathbf{U}^{(k)}\times\mathbf{U}^{(k'')}\times\mathbf{U}^{(k')}]^{(0)}+\delta(ll')/(2l+1)\times\sum_{kk'}P(kk';lll')[(\mathbf{U}^{(k)}\cdot\mathbf{U}^{(k)})+(\mathbf{U}^{(k')}\cdot\mathbf{U}^{(k')})-N/(2l+1)], \quad (25)$$

in agreement with Rajnak and Wybourne.

In these summations, k and k' are restricted to even values only, but k'' may assume both even and odd values. It should be remarked, however, that for $k+k'+k''$ odd the triple scalar products are antisymmetric, while on the other hand, owing to the symmetry of $P(kk';lll')$ with respect to k and k', they always appear in pairs;

$$[\mathbf{U}^{(k)}\times\mathbf{U}^{(k'')}\times\mathbf{U}^{(k')}]^{(0)}+[\mathbf{U}^{(k')}\times\mathbf{U}^{(k'')}\times\mathbf{U}^{(k)}]^{(0)}. \quad (26)$$

If the $\mathbf{U}^{(k)}$ were commutative, the contribution of these pairs would vanish for odd k'; since the $\mathbf{U}^{(k)}$ are not commutative, it may be shown that the expressions (26) do not vanish, but reduce for odd k'' to

$$2\begin{Bmatrix}k & k' & k''\\ l & l & l\end{Bmatrix}[(\mathbf{U}^{(k)}\cdot\mathbf{U}^{(k)})+(\mathbf{U}^{(k')}\cdot\mathbf{U}^{(k')})+(\mathbf{U}^{(k'')}\cdot\mathbf{U}^{(k'')})]. \quad (27)$$

Therefore the only terms in (25) which actually give effective three-body interactions are those for which k, k', and k'' are all even.

The assumption that the perturbed configuration does not contain electrons in the l' shell was an essential step in our calculation. Although the calculation of Bacher and Goudsmit is not explicitly limited to this case, the same limitation is implicitly contained in their paper. Their Eqs. (47) and (48) do not hold for $m=A$ or $n=A$, and their Eqs. (46) and (49) do not hold for $n=A$ or $n=B$. This oversight is the reason for the difference in the general rules concerning the structure of the effective interaction between their paper and the present one.

In the following sections the essential assumption will be that the l' shell is completely full, and we shall therefore use techniques which are similar to those used in the theory of holes.

D. Perturbations produced by $l'^{4l'+1}l^{N+1}$

In this case,

$$g=\sum_k X(k;lll')\sum_{i\neq j}(\mathbf{u}_i^{(k)}\cdot\mathbf{z}_j^{(k)T})+\sum_k X(k;l'l'l'l)\sum_{i\neq j}(\mathbf{u}_i'^{(k)}\cdot\mathbf{z}_j^{(k)T}), \quad (28)$$

where $\mathbf{u}'^{(k)}$ is the tensor whose only nonvanishing element of the reduced matrix is

$$(n'l'\|u'^{(k)}\|n'l')=1. \quad (29)$$

It can be easily shown that the second term of (28) is a scalar proportional to $\mathbf{Z}^{(0)T}$, and therefore its contribution to W_2 is of the form $A+\sum_k B^k(\mathbf{U}^{(k)}\cdot\mathbf{U}^{(k)})$, where k is restricted to even values, and A, B_k are *new* radial parameters (functions of $X(k;l'l'l'l)$). The coefficients of these parameters are proportional to those of the usual Slater parameters and therefore cannot be distinguished from them empirically. We shall not consider them further in this work.

Since $(\mathbf{u}_i^{(k)}\cdot\mathbf{z}_i^{(k)T})$ vanishes identically also for $l=l'$ (if, of course, $n\neq n'$), the first term of g can be written

$$g'=\sum_k X(k;lll')\sum_{ij}(\mathbf{u}_i^{(k)}\cdot\mathbf{z}_j^{(k)T})=\sum_k X(k;lll')(\mathbf{U}^{(k)}\cdot\mathbf{Z}^{(k)T}), \quad (30a)$$

and similarly,

$$\tilde{g}'=\sum_{k'} X(k';lll')\sum_{rs}(\mathbf{z}_r^{(k')}\cdot\mathbf{u}_s^{(k')})=\sum_{k'} X(k';lll')(\mathbf{Z}^{(k')}\cdot\mathbf{U}^{(k')}). \quad (30b)$$

It follows that

$$W_2=-\sum_{kk'}P(kk';lll')(\mathbf{U}^{(k)}\cdot\mathbf{Z}^{(k)T})(\mathbf{Z}^{(k')}\cdot\mathbf{U}^{(k')})=-\sum_{kk'k''}P(kk';lll')(-1)^{k''}(2k''+1)^{1/2}\times[\mathbf{U}^{(k)}\times[\mathbf{Z}^{(k)T}\times\mathbf{Z}^{(k')}]^{(k'')}\times\mathbf{U}^{(k')}]^{(0)}. \quad (31)$$

In order to evaluate this expression, we shall exchange the order of $\mathbf{Z}^{(k)T}$ and $\mathbf{Z}^{(k')}$. It follows from the symmetry of the tensor product that

$$[\mathbf{z}_j^{(k)T}\times\mathbf{z}_r^{(k')}]^{(k'')}=(-1)^{k''}[\mathbf{z}_r^{(k')}\times\mathbf{z}_j^{(k)T}]^{(k'')}\quad(j\neq r), \quad (32)$$

but this relation does not hold for $j=r$, because the two factors do not commute. In this case we have from (12) that

$$[\mathbf{z}_j^{(k)T}\times\mathbf{z}_j^{(k')}]^{(k'')}=(-1)^{k''}[\mathbf{z}_j^{(k')}\times\mathbf{z}_j^{(k)T}]^{(k'')}+\mathbf{x}_j^{(k'')}, \quad (33)$$

where

$$\mathbf{x}^{(k'')}=-(2k''+1)^{1/2}\begin{Bmatrix} k & k' & k'' \\ l & l & l' \end{Bmatrix}\mathbf{u}^{(k'')} +(-1)^{k''}(2k''+1)^{1/2}\begin{Bmatrix} k & k' & k'' \\ l' & l' & l \end{Bmatrix}\mathbf{u}'^{(k'')}. \quad (34)$$

From (32), (33), and (34) we get

$$[\mathbf{Z}^{(k)T}\times\mathbf{Z}^{(k')}]^{(k'')} =(-1)^{k''}[\mathbf{Z}^{(k')}\times\mathbf{Z}^{(k)T}]^{(k'')}+\mathbf{X}^{(k'')}, \quad (35)$$

with

$$\mathbf{X}^{(k'')}=-(2k''+1)^{1/2}\begin{Bmatrix} k & k' & k'' \\ l & l & l' \end{Bmatrix}\mathbf{U}^{(k'')} +(-1)^{k''}(2k''+1)^{1/2}\begin{Bmatrix} k & k' & k'' \\ l' & l' & l \end{Bmatrix}\mathbf{U}'^{(k'')}, \quad (36)$$

and (31) becomes

$$W_2=-\sum_{kk'k''}P(kk';lll')\Bigg((2k''+1)^{1/2}[\mathbf{U}^{(k)}\times[\mathbf{Z}^{(k')}\times\mathbf{Z}^{(k)T}]^{(k'')}\times\mathbf{U}^{(k')}]^{(0)}+(-1)^{k''+1} \times(2k''+1)\begin{Bmatrix} k & k' & k'' \\ l & l & l' \end{Bmatrix}[\mathbf{U}^{(k)}\times\mathbf{U}^{(k'')}\times\mathbf{U}^{(k')}]^{(0)} +(2k''+1)\begin{Bmatrix} k & k' & k'' \\ l' & l' & l \end{Bmatrix}[\mathbf{U}^{(k)}\times\mathbf{U}'^{(k'')}\times\mathbf{U}^{(k')}]^{(0)}\Bigg). \quad (37)$$

When acting on the configuration $l'^{4l'+2}l^N$, the first term vanishes because the operator $\mathbf{Z}^{(k)T}$ wants to transfer an electron from the l shell into the l' shell which is already filled. When acting on a closed shell the operator $\mathbf{U}'^{(k'')}$ also vanishes unless $k''=0$; in this last case it is a scalar and has the value $2(2l'+1)^{1/2}$. We may therefore write

$$\mathbf{U}'^{(k'')}=2(2l'+1)^{1/2}\delta_{k''0}, \quad (38)$$

and the final result is

$$W_2=-\sum_{kk'k''}P(kk';lll')(-1)^{k''+1}(2k''+1) \times\begin{Bmatrix} k & k' & k'' \\ l & l & l' \end{Bmatrix}[\mathbf{U}^{(k)}\times\mathbf{U}^{(k'')}\times\mathbf{U}^{(k')}]^{(0)} -2\sum_k P(kk;lll')(\mathbf{U}^{(k)}\cdot\mathbf{U}^{(k)})/(2k+1). \quad (39)$$

This result agrees with Eq. (45) of Rajnak and Wybourne, if two misprints are corrected: The term $N\delta(\Psi,\Psi')/[l]$ should be preceded by a plus sign, and the last $P(kk';lll')$ should read $P(kk;lll')$. The same result can be obtained by transforming Eq. (30a) to the complementary configurations l^{4l+2-N} and $l^{4l+1-N}l'$ and using the results of Sec. IIC. In this case one has only to remember that $\mathbf{z}^{(0)}(nl,n'l)$ transforms like a tensor and not like a scalar (Ref. 6, Eq. 74).

E. Perturbations produced by $l'^{4l'}l^{N+2}$

In this case,

$$g=\sum_k X(k;ll'l'l')\sum_{i<j}(\mathbf{z}_i^{(k)T}\cdot\mathbf{z}_j^{(k)T}), \quad (40)$$

and since again $(\mathbf{z}_i^{(k)T}\cdot\mathbf{z}_i^{(k)T})$ vanishes identically, we may write

$$g=\tfrac{1}{2}\sum_k X(k;ll'l'l')(\mathbf{Z}^{(k)T}\cdot\mathbf{Z}^{(k)T}), \quad (41)$$

and

$$W_2=-\tfrac{1}{4}\sum_{kk'}P(kk';ll'l'l')(\mathbf{Z}^{(k)T}\cdot\mathbf{Z}^{(k)T})(\mathbf{Z}^{(k')}\cdot\mathbf{Z}^{(k')}). \quad (42)$$

Using (21) and (35), we get

$$(\mathbf{Z}^{(k)T}\cdot\mathbf{Z}^{(k)T})(\mathbf{Z}^{(k')}\cdot\mathbf{Z}^{(k')}) =\sum_{k''}(2k''+1)^{1/2}[\mathbf{Z}^{(k)T}\times[\mathbf{Z}^{(k')}\times\mathbf{Z}^{(k)T}]^{(k'')}\times\mathbf{Z}^{(k')}]^{(0)} +\sum_{k''}(-1)^{k''}(2k''+1)^{1/2}[\mathbf{Z}^{(k)T}\times\mathbf{X}^{(k'')}\times\mathbf{Z}^{(k')}]^{(0)}. \quad (43)$$

Changing again the coupling of the first term and changing also the name of the summation variable in the second term, we have

$$(\mathbf{Z}^{(k)T}\cdot\mathbf{Z}^{(k)T})(\mathbf{Z}^{(k')}\cdot\mathbf{Z}^{(k')}) =\sum_t([\mathbf{Z}^{(k)T}\times\mathbf{Z}^{(k')}]^{(t)}\cdot[\mathbf{Z}^{(k)T}\times\mathbf{Z}^{(k')}]^{(t)}) +\sum_t(-1)^t(2t+1)^{1/2}[\mathbf{Z}^{(k)T}\times\mathbf{X}^{(t)}\times\mathbf{Z}^{(k')}]^{(0)}. \quad (44)$$

By calculations similar to those which led to Eq. (35) it may be shown that for $k+k'$ even,

$$[\mathbf{X}^{(t)}\times\mathbf{Z}^{(k')}]^{(k)}=(-1)^t[\mathbf{Z}^{(k')}\times\mathbf{X}^{(t)}]^{(k)}-(2k+1)^{1/2} \times(2t+1)^{1/2}\left(\begin{Bmatrix} k & k' & t \\ l & l & l' \end{Bmatrix}^2+\begin{Bmatrix} k & k' & t \\ l' & l' & l \end{Bmatrix}^2\right)\mathbf{Z}^{(k)}, \quad (45)$$

and therefore,

$$(\mathbf{Z}^{(k)T}\cdot\mathbf{Z}^{(k)T})(\mathbf{Z}^{(k')}\cdot\mathbf{Z}^{(k')}) =\sum_t([\mathbf{Z}^{(k)T}\times\mathbf{Z}^{(k')}]^{(t)}\cdot[\mathbf{Z}^{(k)T}\times\mathbf{Z}^{(k')}]^{(t)}) +\sum_t([\mathbf{Z}^{(k)T}\times\mathbf{Z}^{(k')}]^{(t)}\cdot\mathbf{X}^{(t)})-\sum_t(-1)^t(2t+1) \times\left(\begin{Bmatrix} k & k' & t \\ l & l & l' \end{Bmatrix}^2+\begin{Bmatrix} k & k' & t \\ l' & l' & l \end{Bmatrix}^2\right)(\mathbf{Z}^{(k)T}\cdot\mathbf{Z}^{(k)}). \quad (46)$$

For the reasons discussed in Sec. IID, when acting on the configuration $l'^{4l'+2}l^N$ the tensorial product $[\mathbf{Z}^{(k)T}\times\mathbf{Z}^{(k')}]^{(t)}$ may be replaced by $\mathbf{X}^{(t)}$, and for very similar reasons the scalar product $(\mathbf{Z}^{(k)T}\cdot\mathbf{Z}^{(k)})$ may be replaced by $(4l+2-N)/(2l+1)$. If we also take into account that

$$\sum_t(-1)^t(2t+1)\begin{Bmatrix}k & k' & t\\ l' & l' & l\end{Bmatrix}^2 =\sum_t(-1)^t(2t+1)\begin{Bmatrix}k & k' & t\\ l & l & l'\end{Bmatrix}^2=\begin{Bmatrix}k & l & l'\\ k' & l & l'\end{Bmatrix}, \tag{47}$$

then we get

$$W_2=-\tfrac{1}{2}\sum_{kk't}P(kk';ll'l')\bigg((\mathbf{X}^{(t)}\cdot\mathbf{X}^{(t)}) -(-1)^t(2t+1)\begin{Bmatrix}k & k' & t\\ l & l & l'\end{Bmatrix}^2\frac{4l+2-N}{2l+1}\bigg). \tag{48}$$

Introducing the expression (36) of $\mathbf{X}^{(t)}$ and remembering also (23) and (38), we obtain

$$W_2=-\sum_t(2t+1)M(t;ll'l')\times\bigg(\sum_{i<j}(\mathbf{u}_i^{(t)}\cdot\mathbf{u}_j^{(t)})-(-1)^t\frac{2l+1-N}{2l+1}\bigg) -2\frac{2l+1-N}{2l+1}\sum_k\frac{P(kk;ll'l')}{2k+1}, \tag{49}$$

which is equivalent to the results of Rajnak and Wybourne.

F. Perturbations produced by $l'^{4l'+1}l^Nl''$

In this case,

$$g=\sum_k X(k;ll'll'')\sum_{ij}(\mathbf{u}_i^{(k)}\cdot\mathbf{w}_j^{(k)}) +\sum_k X(k;ll'l''l)\sum_{ij}(\mathbf{y}_j^{(k)}\cdot\mathbf{z}_i^{(k)T}), \tag{50}$$

where $\mathbf{w}^{(k)}$ is the tensor whose only nonvanishing element of the reduced matrix is

$$(n'l'\|w^{(k)}\|n''l'')=1. \tag{51}$$

The effective interaction therefore contains three terms;

$$\begin{aligned}W_2=&-\sum_{kk'}P(kk';ll'll'')\sum_{ijs}(\mathbf{u}_i^{(k)}\cdot\mathbf{w}_j^{(k)})(\mathbf{w}_j^{(k')T}\cdot\mathbf{u}_s^{(k')})\\ &-\sum_{kk'}P(kk';ll'l')\sum_{ijs}(\mathbf{y}_j^{(k)}\cdot\mathbf{z}_i^{(k)T})(\mathbf{z}_s^{(k')}\cdot\mathbf{y}_j^{(k')T})\\ &-\sum_{kk'}M(k,k')\sum_{ijs}[(\mathbf{y}_j^{(k)}\cdot\mathbf{z}_i^{(k)T})(\mathbf{w}_j^{(k')T}\cdot\mathbf{u}_s^{(k')})\\ &+(\mathbf{u}_i^{(k')}\cdot\mathbf{w}_j^{(k')})(\mathbf{z}_s^{(k)}\cdot\mathbf{y}_j^{(k)T})],\end{aligned} \tag{52}$$

where $M(k,k')$ is defined, according to Rajnak and Wybourne, by

$$M(k,k')=X(k;ll'l''l)X(k';ll'll'')/\Delta E_c. \tag{53}$$

According to (21) and to an equation similar to (12), the first term is

$$C(1)=-\sum_{kk't}P(kk';ll'll'')(2t+1)\begin{Bmatrix}k & k' & t\\ l' & l' & l''\end{Bmatrix}\times[\mathbf{U}^{(k)}\times\mathbf{U}'^{(t)}\times\mathbf{U}^{(k')}]^{(0)}, \tag{54}$$

and reduces, because of (38), to

$$C(1)=-2\sum_k P(kk;ll'll'')(\mathbf{U}^{(k)}\cdot\mathbf{U}^{(k)})/(2k+1). \tag{55}$$

The second term is

$$C(2)=-\sum_{kk't}P(kk';ll'l''l)(-1)^t(2t+1)^{1/2}\times\sum_j[\mathbf{y}_j^{(k)}\times[\mathbf{Z}^{(k)T}\times\mathbf{Z}^{(k')}]^{(t)}\times\mathbf{y}_j^{(k')T}]^{(0)};$$

as in Secs. IID and IIE, the product $[\mathbf{Z}^{(k)T}\times\mathbf{Z}^{(k')}]^{(t)}$ may be replaced by $\mathbf{X}^{(t)}$, and because of (36), (24), and (38), we get

$$\begin{aligned}C(2)=&\sum_{kk't}P(kk';ll'l'')(-1)^t(2t+1)\begin{Bmatrix}k & k' & t\\ l & l & l'\end{Bmatrix}\times\sum_{ij}[\mathbf{y}_j^{(k)}\times\mathbf{u}_i^{(t)}\times\mathbf{y}_j^{(k')T}]^{(0)}\\ &-2\sum_k P(kk;ll'l'')\sum_j(\mathbf{y}_j^{(k)}\cdot\mathbf{y}_j^{(k)T})/(2k+1).\end{aligned} \tag{56}$$

Since for $i=j$ the product $[\mathbf{y}_j^{(k)}\times\mathbf{u}_i^{(t)}]^{(k')}$ vanishes identically, and for $j\neq i$ the tensors $\mathbf{y}_j^{(k)}$ and $\mathbf{u}_i^{(t)}$ commute, we have

$$\begin{aligned}\sum_{ij}[\mathbf{y}_j^{(k)}\times\mathbf{u}_i^{(t)}\times\mathbf{y}_j^{(k')T}]^{(0)} &=\sum_{i\neq j}[\mathbf{y}_j^{(k)}\times\mathbf{u}_i^{(t)}\times\mathbf{y}_j^{(k')T}]^{(0)}\\ &=(-1)^t\sum_{i\neq j}[\mathbf{u}_i^{(t)}\times\mathbf{y}_j^{(k)}\times\mathbf{y}_j^{(k')T}]^{(0)}.\end{aligned} \tag{57}$$

The tensor product $[\mathbf{y}_j^{(k)}\times\mathbf{y}_j^{(k')T}]^{(t)}$ is given by a formula similar to (12), while the scalar product $(\mathbf{y}_j^{(k)}\cdot\mathbf{y}_j^{(k)T})$ has the value $(2l+1)^{-1}$; therefore,

$$C(2)=2\sum_t(-1)^tM(t;ll'l'')\sum_{i<j}(\mathbf{u}_i^{(t)}\cdot\mathbf{u}_j^{(t)}) -2N\sum_k P(kk;ll'l'')/(2k+1)(2l+1). \tag{58}$$

The third term is

$$C(3)=-\sum_{kk't} M(k,k')(-1)^{k+t}(2t+1)^{1/2}$$
$$\times\sum_j\Big([\mathbf{y}_j^{(k)}\times[\mathbf{Z}^{(k)T}\times\mathbf{w}_j^{(k')T}]^{(t)}\times\mathbf{U}^{(k')}]^{(0)}$$
$$+[\mathbf{U}^{(k')}\times[\mathbf{w}_j^{(k')}\times\mathbf{Z}^{(k)}]^{(t)}\times\mathbf{y}_j^{(k)T}]^{(0)}\Big). \quad (59)$$

By calculations similar to those which led to Eq. (35) it may be shown that

$$[\mathbf{Z}^{(k)T}\times\mathbf{w}_j^{(k')T}]^{(t)}=(-1)^{k+t}[\mathbf{w}_j^{(k')T}\times\mathbf{Z}^{(k)T}]^{(t)}$$
$$-(2t+1)^{1/2}\begin{Bmatrix} k & k' & t\\ l'' & l & l'\end{Bmatrix}\mathbf{y}_j^{(t)T}, \quad (60a)$$

and

$$[\mathbf{w}_j^{(k')}\times\mathbf{Z}^{(k)}]^{(t)}=(-1)^{k+t}[\mathbf{Z}^{(k)}\times\mathbf{w}_j^{(k')}]^{(t)}$$
$$-(2t+1)^{1/2}\begin{Bmatrix} k & k' & t\\ l'' & l & l'\end{Bmatrix}\mathbf{y}_j^{(t)}. \quad (60b)$$

Since we have already seen that the contribution of $\mathbf{Z}^{(k)T}$ vanishes when this operator acts on a configuration where the l' shell is filled, and the same holds for $\mathbf{Z}^{(k)}$ acting on the left on such a configuration, we get

$$C(3)=\sum_{kk't} M(k,k')(-1)^{k+t}(2t+1)$$
$$\times\begin{Bmatrix} k & k' & t\\ l'' & l & l'\end{Bmatrix}\sum_j\Big([\mathbf{y}_j^{(k)}\times\mathbf{y}_j^{(t)T}\times\mathbf{U}^{(k')}]^{(0)}$$
$$+[\mathbf{U}^{(k')}\times\mathbf{y}_j^{(t)}\times\mathbf{y}_j^{(k)T}]^{(0)}\Big)$$
$$=2\sum_{kk't} M(k,k')(-1)^{k+t}(2t+1)$$
$$\times\begin{Bmatrix} k & k' & t\\ l'' & l & l'\end{Bmatrix}\begin{Bmatrix} k & k' & t\\ l & l'' & l\end{Bmatrix}(\mathbf{U}^{(k')}\cdot\mathbf{U}^{(k')})$$
$$=2\sum_{kk'} M(k,k')\begin{Bmatrix} l & l & k'\\ l' & l'' & k\end{Bmatrix}(\mathbf{U}^{(k')}\cdot\mathbf{U}^{(k')}). \quad (61)$$

The expressions of $C(1)$ and $C(2)$ agree with those of Rajnak and Wybourne; the expression of $C(3)$ agrees only if the sign of $N\delta(\Psi,\Psi')/[l]$ is changed to plus, and the whole expression (37) is multiplied by 2.

ACKNOWLEDGMENT

We would like to express our thanks to Professor J. M. Blatt for his helpful comments and his invaluable help in the preparation of the manuscript.

PHYSICAL REVIEW VOLUME 156, NUMBER 1 5 APRIL 1967

Hyperfine Structure of Nine Levels in Two Configurations of V^{51}. I. Experimental*

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(Received 2 November 1966)

The hyperfine structure of the $3d^34s^2\ {}^4F_{3/2,5/2,7/2,9/2}$ and $3d^4({}^5D)4s\ {}^6D_{1/2,3/2,5/7,7/2,9/2}$ levels in V^{51} has been studied in detail by the atomic-beam magnetic-resonance technique. Evidence of substantial J mixing within each multiplet is found. This paper discusses the experiment itself; the following paper discusses the theoretical considerations, corrections to the raw data, and the final results.

I. INTRODUCTION

Atomic ground-state hyperfine-structure (hfs) studies have been made for many atoms in recent years, and values of the nuclear moments have been extracted from the data. While these studies are of great value, their interpretation is not always so simple as it might appear. In particular, the composition of the atomic state (which must be known for the extraction of nuclear moments) is difficult to estimate reliably unless several states of the same configuration are examined and compared. In the case of the nuclear electric-quadrupole moment, measurement in several states of at least two different configurations is desirable.

An attractive atom from this point of view is V^{51}, which has a nuclear spin of $\frac{7}{2}$. Because of the low Z, the $3d$ electrons involved in the low even-parity configurations behave nonrelativistically, and the departure from the LS limit is very small. For the purposes of the present experiment, the $3d^34s^2\ {}^4F_{3/2,5/2,7/2,9/2}$ and $3d^44s\ {}^6D_{1/2,3/2,5/2,7/2,9/2}$ levels were sufficiently populated by thermal excitation alone.

The principal results of the investigation are, in addition to the many hyperfine-interaction constants and electronic g factors measured, the value of the ground-state nuclear electric-quadrupole moment as

* Work performed under the auspices of the U. S. Atomic Energy Commission.