Configuration Mixing and Quadrupole Moments of Odd Nuclei

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The quadrupole moments of odd nuclei are calculated from the standpoint of configuration mixing. The calculations are based upon the simple perturbation theory. The quadrupole moments of odd-neutron nuclei are due to the excitation of one or more protons. The quadrupole moments of odd-proton nuclei also contain the quadrupole moments of the initial configuration. The agreement between the calculated and observed values are fairly good except for the nuclei with very large quadrupole moments.

I. INTRODUCTION

THE fact that the quadrupole moments of nuclei containing one proton outside a closed shell are negative and those of nuclei lacking one proton to a closed shell are positive is a simple consequence of the shell model.[1,2] Further, if p is the number of protons in the shell with total angular momentum $j\hbar$, the quadrupole moment of the j^p configuration (p odd) and spin $J=j$ becomes in this model[3,4]:

$$Q=Q_j(2j+1-2p)/(2j-1), \tag{1}$$

where Q_j is the quadrupole moment of the nucleus with a single proton in the orbit j outside a closed shell:

$$Q_j=-(2j-1)/(2j+2)\cdot\langle r^2\rangle_j. \tag{2}$$

$\langle r^2\rangle_j$ is the expectation value of r^2 for the proton in the outermost orbit j. Thus, quadrupole moments are negative for less than half-filled shells and positive for more than half-filled shells. The observed signs of quadrupole moments are, in general, in agreement with this rule.

The quadrupole moments of some nuclei with an odd number of protons lying between the magic numbers 50 and 82 are so large that one cannot expect to explain them by the shell model. The collective model ascribes these very large quadrupole moments to core deformation.[5,6] According to this model, the magnitude of the quadrupole moments of closed shell $\pm$ one proton nuclei should also be very large—considerably larger than the observed values.[6,7] These are usually two or three times larger than the values given by the simple shell model.

Quadrupole moments of several odd-neutron nuclei show a similar variation with the number of neutrons in the not-closed shell to that shown by odd-proton nuclei with respect to the number of protons. This might be explained by the collective model. Again this model gives too large quadrupole moments for nuclei with a closed shell $\pm$ one neutron. On the other hand, the usual shell model gives zero quadrupole moments for odd-neutron nuclei, since the neutrons carry no charge and since the effect of the recoil of the core is negligibly small except for extremely light nuclei.

We consider the effect of configuration mixing which explains the deviations of magnetic moments of odd nuclei from the Schmidt lines in a reasonable way.[8] As the starting configuration, we adopt again the configuration given by the single-particle model, i.e., assume that the even particles couple to angular momentum zero and the state of the odd particles is that of lowest seniority consistent with the observed spin. Thus, for some of our wave functions the isotopic spin is not a good quantum number. However, introduction of the isotopic spin does not improve the agreement with respect to quadrupole moments[9] and its use does not change the wave function for medium heavy and heavy nuclei.

II. THE QUADRUPOLE MOMENTS DUE TO THE EXCITATION OF PROTONS

In the shell model with strong spin-orbit interaction, even and odd numbers of nucleons in the same orbit j couple in such a way that the resultant angular momenta are $J=0$ and $J=j$, respectively.[1] Although there are a few exceptions under this rule for an odd number of nucleons, it does hold in most cases and will be adopted as the starting point for our considerations. As was mentioned before, if one disregards the intermixing of configurations, the quadrupole moments of odd-proton nuclei in the j^p configuration is given by (1). The quadrupole moments of odd-neutron nuclei are zero in this model.

Let us consider the effects of configuration mixing on quadrupole moments of odd nuclei. If we assume

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[2] E. P. Wigner, Lecture note at Wisconsin University, 1951 (unpublished).

[3] R. G. Sachs, *Nuclear Theory* (Addison-Wesley Press, Cambridge, 1953).

[4] S. A. Moszkowski and C. H. Townes, Phys. Rev. **93**, 306 (1954).

[5] J. Rainwater, Phys. Rev. **79**, 432 (1950).

[6] A. Bohr and B. R. Mottelson, Kgl. Danske. Videnskab. Selskab Mat.-fys. Medd. **27**, No. 16 (1953).

[7] F. J. Milford, Phys. Rev. **93**, 1297 (1954).

[8] A. Arima and H. Horie, Progr. Theoret. Phys. **12**, 623 (1954).

[9] M. Umezawa, Progr. Theoret. Phys. **10**, 505 (1953).

that the admixture of excited configurations to the original one is so small that the effects proportional to the square of the admixture coefficients can be neglected, only the contributions from the nondiagonal elements of the quadrupole moment operator between the excited and ground configurations need be considered. Let us denote the ground configuration given by the shell model by $\Psi_0(jm)$. Let $\Psi_n(jm)$ be a typical excited configuration; j and m are the angular momentum and its z-component, respectively, for these states. Then the whole wave function is given by

$$\Psi_{\text{mixed}}(jm)=\Psi_0(jm)+\sum_n \alpha_n\Psi_n(jm), \tag{3}$$

where the α are the coefficients of mixing. The expectation value of the quadrupole moment operator for the state represented by the first term of (3) with $m=j$ gives the value (1) of the single-particle model, while the main correction caused by the addition of the other terms is given by the cross terms between the first and later terms with $m=j$. Thus, the quadrupole moment caused by the configuration mixing is given by expressions of the form

$$\delta Q=2\alpha_1(\Psi_0(jj),\, Q_{\text{op}}\Psi_1(jj)), \tag{4}$$

where Q_{op} represents the quadrupole moment operator

$$Q_{\text{op}}=\sum_{i=1}^{Z} er_i^2(3\cos^2\theta_i-1). \tag{5}$$

r_i and θ_i are radial and angular variables of the ith proton. The excited configuration $\Psi_1(jm)$ must not differ from the original one $\Psi_0(jm)$ by more than one orbit in order to have a nonvanishing δQ in (4) because the quadrupole operator Q_{op} is a one-particle operator. It is also evident that either the orbital angular momenta of the orbits in which Ψ_0 and Ψ_1 differ must be equal, or their difference must be ± 2. The coefficient of mixing, α, is given by perturbation theory in terms of the nondiagonal element of energy matrix:

$$\alpha_1=-(\Psi_0(jm),\, \sum_{i<k} V_{ik}\Psi_1(jm))/\Delta E, \tag{6}$$

where V_{ik} is the interaction between the ith and kth nucleons and ΔE is the energy difference between the first and second configuration. We assume, for the sake of simplicity, that the radial dependence of the interaction has delta-function character.

There are several modes of excitation of the proton group which will give rise to quadrupole moments. First of all, we consider the excitation of a proton from one of the orbits filled with an even number of protons to another orbit which is not filled, due to the interaction with the odd nucleons[10] in the outermost orbit. We represent the zeroth-order state of the nucleus given by the single-particle model as

$$\Psi_0(jm)=\Psi(j_1{}^n(0)j^p(j);\, jm),$$

where nucleons in the orbit j_1 are protons and n is an even number not larger than $2j_1+1$; p is the number of nucleons in the outermost orbit. Then a sequence of excited states in which one proton in j_1 orbit jumps to j_2,

$$\Psi_1(jm)=\Psi([j_1{}^{n-1}(j_1)j_2](J)j^p(j);\, jm),$$

can interact with the above state.[11] J is restricted by the condition $|j_1-j_2|\leq J\leq j_1+j_2$. However, it can easily be seen that only the state with $J=2$ gives nonvanishing δQ by (4) and the orbital angular momentum of j_2 must be equal to that of j_1 or differ from it by two units. Hence, the mixed configuration which can give rise to the quadrupole moment is expressed as

$$\Psi(j_1{}^n(0)j^p(j);\, jm)+\alpha\Psi([j_1{}^{n-1}(j_1)j_2](2)j^p(j);\, jm). \tag{I}$$

After a straightforward calculation following the procedure (4) and (6) which is given in Appendix I, δQ is obtained as

$$\delta Q_{\text{I}}=-n[(2j+1-2p)/(2j+2)](j_1\tfrac{1}{2}\,20|\,j_1\,2j_2\,\tfrac{1}{2})^2 \times\langle j_1|r^2|j_2\rangle\begin{cases}(-V_sI)/\Delta E & \text{for odd-proton nuclei}\\ (-\tfrac{1}{2}V_s-\tfrac{3}{2}V_t)I/\Delta E & \text{for odd-neutron nuclei,}\end{cases} \tag{7}$$

where $(j_1\frac{1}{2}\,20|\,j_1\,2j_2\,\frac{1}{2})^2$ is the square of the Clebsch-Gordan coefficient, the values of which are shown in Table I, and V_s and V_t are interaction strengths in the singlet and triplet states, respectively. $\langle j_1|r^2|j_2\rangle$ is a matrix element of r^2 between the radial wave functions of j_1 and j_2 orbits:

$$\langle j_1|r^2|j_2\rangle=\int_0^\infty R(j_1)r^2R(j_2)r^2dr, \tag{8}$$

and I is a Slater integral for a delta-function interaction

$$I=\tfrac{1}{2}\int_0^\infty R^2(j)R(j_1)R(j_2)r^2dr. \tag{9}$$

The R are radial wave functions; their phases do not affect the signs of δQ since each radial wave function appears necessarily an even number of times in Eq. (7).

TABLE I. The values of the square of Clebsch-Gordan coefficient $(j_1\frac{1}{2}\,20|\,j_1\,2j_2\,\frac{1}{2})^2$.

$j_1\backslash j_2$	1/2	3/2	5/2	7/2	9/2	11/2	13/2
1/2	...	2/5	3/5	...	...	...	...
3/2	1/5	1/5	3/35	18/35	...	...	...
5/2	1/5	2/35	8/35	4/105	10/21	...	...
7/2	...	9/35	1/35	5/21	5/231	5/11	...
9/2	...	...	2/7	4/231	8/33	2/143	64/143
11/2	...	...	...	28/65	7/715	35/143	5/429
13/2	...	...	...	...	36/85	8/1105	16/65

[10] In an odd nucleus which has an odd number of protons, the protons are the "odd nucleons." Similarly, the neutrons will be called "odd nucleons" if their number is odd. This notation facilitates the discussion.

[11] The case that j_2 coincides with j in odd proton nuclei will be considered later in the excitation (II).

Although it was assumed that the zeroth-order state contained no proton in the orbit j_2, (7) will be valid also when there are m protons in the orbit j_2 (m even) and if they couple to an angular momentum zero, except that the right side must be multiplied by $(2j_2+1-m)/(2j_2+1)$. Equation (7) and the equation modified in this way are applicable for both odd-proton and odd-neutron nuclei and they correspond to Table I of reference 8 for the case of magnetic moments.

For odd-proton nuclei, there are two other configurations which give a quadrupole moment. In one of these, j_2 coincides with j in (I) and the corresponding mixed configuration is

$$\Psi(j_1{}^n(0)j^p(j);jm) \\ +\sum_J \beta_J\Psi(j_1{}^{n-1}(j_1)j^{p+1}(J);jm), \quad \text{(II)}$$

where β_J is the coefficient of mixing for each J and $J=2, 4, \cdots, 2j-1$ so that $j^{p+1}(J)$ represent the states of seniority two.[12,13] The derivation of the quadrupole moment caused by the configuration mixing (II) is somewhat more complicated than that of (I). However, by making use of the average value of the reciprocals of the zeroth order energy differences between the first and each of the second configurations as $\langle 1/\Delta E\rangle$, we obtain a formula for δQ which is similar to (7) (see Appendix B):

$$\delta Q_{\mathrm{II}}=-n[(2j-p)/(2j+2)] \\ \times(j_1\tfrac{1}{2}\,20|j_1\,2j_2\,\tfrac{1}{2})^2\langle j_1|r^2|j_2\rangle(-V_sI)\langle 1/\Delta E\rangle. \quad (10)$$

The integral I is obtained by putting $j_2=j$ in (9). The factor $(2j-p)$ in (10) reflects the fact that this mode of excitation cannot take place in those odd-proton nuclei in which a single proton is missing from the outermost orbit.

In the other configuration which must be considered for the quadrupole moments of odd-proton nuclei the number of protons in the outermost orbit j is larger than 1. It corresponds to the inverse case of the excitation mode (II) and is expressed as

$$\Psi(j_1{}^n(0)j^p(j);jm) \\ +\sum_J \gamma_J\Psi(j_1{}^{n+1}(j_1)j^{p-1}(J);jm), \quad \text{(III)}$$

where the even number n may be equal to zero, and γ_J is the coefficient of mixing. The quadrupole moment caused by the excitation (III) is

$$\delta Q_{\mathrm{III}}=(p-1)[(2j_1+1-n)/(2j_1+2)] \\ \times(j_1\tfrac{1}{2}\,20|j_1\,2j\,\tfrac{1}{2})^2\langle j_1|r^2|j\rangle(-V_sI)\langle 1/\Delta E\rangle, \quad (11)$$

where I is similar to the corresponding integral in (10). Equations (10) and (11) correspond to (11) and (14) of reference 8, respectively.

In addition to the three modes of excitation which were described above, the state $j_1{}^n(0)$ (n even) of protons can be excited into a state $j_1{}^n(J)$. The lowest excited states $j_1{}^n(J)$ are usually assumed to be those of seniority two. Again only the state with $J=2$ can contribute to the quadrupole moment in our approximation.[14] This type of excitation may be taken as a degenerate case of (I) in which j_2 coincides with j_1, so that the result is obtained at once by putting $j_2=j_1$ in (7) and multiplying a factor $(2j_1+1-n)/(2j_1-1)$ which comes from the coefficient of fractional parentage. Hence, the excitation

$$\Psi(j_1{}^n(0)j^p(j)jm)+\alpha'\Psi(j_1{}^n(2)j^p(j)jm), \quad \text{(IV)}$$

gives

$$\delta Q_{\mathrm{IV}}=-n[(2j_1+1-n)(2j+1-2p)/(2j_1-1)(2j+2)] \\ \times(j_1\tfrac{1}{2}\,20|j_1\,2j_1\,\tfrac{1}{2})^2\langle j_1|r^2|j_1\rangle \\ \times\begin{cases}(-V_sI)/\Delta E_2 & \text{for odd-proton nuclei}\\ (-\tfrac{1}{2}V_s-\tfrac{3}{2}V_t)I/\Delta E_2) & \text{for odd-neutron nuclei.}\end{cases} \quad (12)$$

Thus, the corrections to the quadrupole moments in the approximation here considered are given by the sum of (7) and (12) for odd-neutron nuclei, and the sum of (7), (10), (11), and (12) for odd-proton nuclei. They depend on the number p of nucleons in the outermost orbit linearly. Furthermore, the contributions given by (7) and (12) depend on p in the same way as the single-particle model's expression (1). This applies also for odd-neutron nuclei. The other corrections to the odd-proton nuclei, given in (10) and (11), have a different dependence upon p. The former vanishes at the end of the subshell while the latter vanishes at the beginning of the subshell.

III. COMPARISON WITH THE OBSERVED VALUES

(i) Determination of the Parameters

In order to compare the theoretical values for the quadrupole moment, obtained in the preceding section, with the observed values it is necessary to estimate the quantities which appear in (7), (10), (11), and (12). First of all, we assume that the interactions between nucleons are attractive and the attractive force in the triplet state is stronger than in the singlet state so that $|V_t|=1.5|V_s|$. Although this agrees with the experimental data of two-nucleon systems at low energy, it remains an assumption since the interactions in larger nuclei might differ from those in two-nucleon systems. It is possible, in fact, that the integrals I and the matrix elements of r^2 become negative in some cases. It is necessary, therefore, to obtain a somewhat more accurate estimate of these quantities than was necessary for the calculation of the magnetic moments. We assume that the wave functions for nucleons are those of a harmonic oscillator[15]:

$$R_{nl}(r)=N_{nl}\exp(-\nu r^2/2)r^l v_{nl}(r).$$

[12] G. Racah, Phys. Rev. **63**, 367 (1943).
[13] B. H. Flowers, Proc. Roy. Soc. (London) **A212**, 248 (1952).
[14] This type of excitation does not contribute to the magnetic moment in the approximation of reference 8, since there is no low excited state with $J=1$.
[15] For example, I. Talmi, Helv. Phys. Acta **25**, 185 (1952).

N_{nl} is a normalization constant and $v_{nl}(r)$ is an associated Laguerre polynomial

$$v_{nl}(r)=L_{n+l-1/2}{}^{l+1/2}(\nu r^2).$$

The constant ν is determined by evaluating the diagonal elements of r^2. For $n=1$, these are $\langle 1l|r^2|1l\rangle=(2l+3)/2\nu$. If one assumes a uniform nuclear density, the average value of r^2 is $\langle r^2\rangle=(3/5)(1.45A^{1/3})^2\times10^{-26}$ cm^2, A being the mass number. Thus, putting $1/2\nu=c_1A^{2/3}$, the order of magnitude of c_1 becomes 1 to 1.8 times 10^{-27} cm^2 (assuming $l=2\sim5$). Furthermore, the matrix elements of r^2 become

$$\langle j_1|r^2|j_2\rangle=f(j_1;j_2)/(2\nu)=c_1f(j_1;j_2)A^{2/3},$$

where $f(j_1;j_2)$ does not depend on the mass number, and they can be obtained by straightforward integration.

The integrals I are inversely proportional to the mass number A since they involve four wave functions. For harmonic oscillator wave functions, they have the form

$$I(jj_1;jj_2)=\tfrac{1}{2}F(jj_1;jj_2)(\nu^3/\pi)^{1/2},$$

where $F(jj_1;jj_2)$ does not depend upon ν or A, while the factor $\nu^{3/2}$ provides an A^{-1} dependence because of the proportionality of ν to $A^{-2/3}$. The average value of V_sI can be estimated from the difference of binding energies of odd and even nuclei[1,8] to be $-25/A$ Mev. Hence, we obtain from

$$V_sI(jj_1;jj_2)=-c_2F(jj_1;jj_2)/2A,$$

200 to 300 Mev for the order of magnitude of c_2 at $A\sim200$ because the values of F for $2d$, $1g$, and $1h$ orbits are 0.260, 0.213, and 0.176, respectively. This gives the estimate $c_1c_2=(0.3$ to $0.6)\times10^{-24}$ cm^2 Mev. Actually, the value $c_1c_2=0.5\times10^{-24}$ cm^2 Mev was used in the calculations.

(ii) Determination of the Energy Denominators

The energy difference ΔE consists of two parts. One is the difference between the single-particle levels in which the ground and excited configurations differ, and the other is that between the energies caused by the interaction between nucleons in each configuration. The estimate of the latter is complicated and it will be ignored in the actual calculation. Even if we restrict ourselves only to the energy differences of the single-particle levels, it is not easy to determine completely on the basis of conventional potentials, spin-orbit interactions, and the observed values of nuclear spins. The oscillator potential gives strongly degenerate states with different principal and azimuthal quantum numbers, and the square well potential with finite or infinite well depth does not always provide the order of levels which, together with plausible doublet splittings, would yield the observed values of the nuclear spins. Therefore, we attempted to construct a level scheme by using both empirical data and theoretical information.

TABLE II. Doublet splitting assumed in the calculation. The splitting $1d_{3/2}-1d_{5/2}$ is taken from the experimental data on O^{17}.[17] The others are estimated by the formula by determining the proportionality constant by the doublet splitting of O^{17}.

	$\Delta E_{\text{doublet}}$ in Mev	$\bar{A}$
$1p_{1/2}-p_{3/2}$	3	17
$1d_{3/2}-d_{5/2}$	5	...
$1f_{5/2}-f_{7/2}$	3	60
$2p_{1/2}-p_{3/2}$	1.5	60
$1g_{7/2}-g_{9/2}$	2.5	105
$2d_{3/2}-d_{5/2}$	1.5	120
$1h_{9/2}-h_{11/2}$	2	200
$2f_{5/2}-f_{7/2}$	1.5	200
$3p_{1/2}-p_{3/2}$	0.5	200
$1i_{11/2}-i_{13/2}$	2	260

First of all, the doublet splittings are estimated by the simple formula of Inglis[16]: $\Delta E_{\text{doublet}}=K(2l+1)A^{-2/3}$, where A and K are the mass number and a proportionality constant with the dimension of energy. If we employ the observed value[17] of the splitting $1d_{5/2}-1d_{3/2}$ in O^{17}, we obtain $K=6.6$ Mev. However, the doublet splitting was assumed to be constant for a subshell and the mass number A adopted for calculating it was the average A of those nuclei the observed spins of which indicate that they contain this subshell partially filled. The assumed doublet splittings obtained in this way are given in Table II and the above-mentioned mass numbers are shown under $\bar{A}$. The values adopted will be seen to be considerably in excess of the excitation energy of isomeric levels. This was not considered to be an inconsistency because the isomeric levels are probably not single-particle levels but result from many-body effects.

The position of the $1s$ level relative to the $1p$ levels cannot be obtained directly from the experimental data. However, as the contribution from the excitation of a $1s$ proton can be seen to be small, the estimate obtained from the square well potential[2] was considered to be sufficiently accurate. The spacing is given as 15.5 Mev and 9.2 Mev by the potential with infinite depth if one assumes a mass number 17 and 37, respectively (and corresponding nuclear radii). These figures are the two extreme mass numbers in which the $1s$ level plays a role in our calculation. Therefore, we assume the $1s-1p$ energy difference to be 12 Mev. Then the $1p_{3/2}$ level is assumed to be lower than the center of gravity of the $1p$ levels by 1 Mev and the $1p_{1/2}$ higher by 2 Mev. These numbers were obtained by dividing the doublet splitting 3 Mev in the ratio 1 to 2.

The observed levels of C^{13} and N^{13} give the spacings between $1p_{1/2}$ and $1d_{5/2}$ as 3.86 Mev and 3.56 Mev, respectively.[17] We assume the $1d_{5/2}-1p_{1/2}$ spacing to be 3 Mev for nuclei, the mass number of which are larger than 20. The position of the $2s_{1/2}$ level relative to the $1d_{5/2}$ is assumed in accordance with the observed levels

[16] D. R. Inglis, Revs. Modern Phys. **25**, 390 (1953).
[17] F. Ajzenberg and T. Lauritsen, Revs. Modern Phys. **27**, 77 (1955).

TABLE III(a). Spacing of even-parity levels which was used in our calculation.

	$1d_{5/2}$	$2s$	$1d_{3/2}$	$1g_{9/2}$	$1g_{7/2}$	$2d_{5/2}$	$2d_{3/2}$	$3s$	$1i_{13/2}$	$1i_{11/2}$
$1s$	17	···	22	···	···	32	33.5	···	···	···
$1d_{5/2}$		1	5	12	14.5	15	16.5	16.75	···	···
$2s$			4	···	···	14	15.5	···	···	···
$1d_{3/2}$				7	9.5	10	11.5	11.75	···	···
$1g_{9/2}$					2.5	3	4.5	4.75	8.5	10.5
$1g_{7/2}$						0.5	2	2.25	6	8
$2d_{5/2}$							1.5	1.75	···	···
$2d_{3/2}$								0.25	···	···
$3s$									···	···
$1i_{13/2}$										2

TABLE III(b). Spacing of odd-parity levels which was used in our calculation.

	$1p_{1/2}$	$1f_{7/2}$	$2p_{3/2}$	$1f_{5/2}$	$2p_{1/2}$	$1h_{11/2}$	$1h_{9/2}$	$2f_{7/2}$	$2f_{5/2}$	$2p_{3/2}$	$2p_{1/2}$
$1p_{3/2}$	3	13	15.5	16	17	···	···	24.5	26	26.75	27.25
$1p_{1/2}$		···	12.5	13	···	···	···	···	23	23.75	···
$1f_{7/2}$			2.5	3	···	9	11	11.5	13	13.75	···
$2p_{3/2}$				0.5	1.5	···	···	9	10.5	11.25	11.75
$1f_{5/2}$					1	6	8	8.5	10	10.75	11.25
$2p_{1/2}$						···	···	···	9	9.75	···
$1h_{11/2}$							2	2.5	4	4.75	5.25
$1h_{9/2}$								0.5	2	2.75	3.25
$2f_{7/2}$									1.5	2.25	2.75
$2f_{5/2}$										0.75	1.25
$3p_{3/2}$											0.5

for O^{17} so that the $2s$ level is higher than the $1d_{5/2}$ by 1 Mev.[17] The spacing between $1f_{7/2}$ and $1d_{3/2}$ is assumed to be 2 Mev, since the corresponding spacings of S^{33} and K^{41} appear to be 2.85 Mev and 1.37 Mev, respectively.[18] Although the spacing between the $2p_{3/2}$ and $1f_{7/2}$ levels seems to be 2 Mev from the observed data on Ca^{41}, we use the value of 2.5 Mev for this spacing in order to bring the $2p_{3/2}$ level close to $1f_{5/2}$. It is known that $2p_{3/2}$ and $1f_{5/2}$ are close to each other from the change of spins in Rb isotopes.

The pair of levels $2p_{1/2}$ and $1g_{9/2}$ often change position in isomeric nuclei. However, the inversion seems to take place on account of the large pairing energy of the $1g_{9/2}$ nucleons. Hence we adopt the energy difference observed in ${}_{39}Y^{89}$ which might be free from this effect. The observed data indicate that the $1g_{9/2}$ is higher than $2p_{1/2}$ by 0.913 Mev,[19] and we assume the spacing as 1 Mev. The situation is similar with respect to the $1g_{7/2}$ and $2d_{5/2}$ levels. Fortunately, as the contribution to the quadrupole moment from the jump of a proton between these levels is much smaller than the contribution from other excitations (see Table I), the relative position of these levels does not influence the calculated results critically. We assume on the basis of the observed energy differences of 0.66, 0.15 and 0.33 Mev for Mo^{99}, Sb^{123} and Sb^{125}, respectively,[19] that the $2d_{5/2}$ level lies 0.5 Mev above the $1g_{7/2}$ level.

The spacings between $1h_{11/2}$, $2d_{3/2}$, and $3s$ are known to be small from isomeric transitions. It was pointed out by Mihelich and de-Shalit[20] that it is uncertain whether the isomeric transitions between these states are "particle transitions" or "hole transitions." Fortunately, the energy differences $2d_{3/2}-1h_{11/2}$ and $3s-1h_{11/2}$ do not affect the calculated values of the quadrupole moments. We assume that the $1h_{11/2}$ level is lowest, the $2d_{3/2}$ second, and the $3s_{1/2}$ level highest, and that the spacing $2d_{3/2}-1h_{11/2}$ is 0.5 Mev and $3s-2d_{3/2}$ is 0.25 Mev. The order of magnitude of the former is inferred from the level of Ba^{137} at 0.66 Mev and the latter is taken from the 0.26-Mev level[19] in Au^{197}.

The spacing between $1h_{9/2}$ and $2f_{7/2}$ levels is expected to be small but no experimental data are available. Since the spin of ${}_{83}Bi^{209}$ is 9/2, we assume that $h_{9/2}$ is slightly lower than $2f_{7/2}$; the spacing is tentatively assumed to be 0.5 Mev. We note in passing that no case is known in which a $h_{9/2}$ proton jumps to the $2f_{7/2}$ level.

The position of the $2f_{5/2}$, $1i_{13/2}$ and $3p_{3/2}$ levels must be determined for estimating the contribution of the excitation of protons from lower levels even though these levels appear only as the neutron levels in actual nuclei. Therefore, we obtain their relative positions from the levels of odd-neutron nuclei. The analysis of isomeric states[20] of Hg, Au, and Pt indicates that $1i_{13/2}$ is higher than $2f_{5/2}$ by about 0.5 Mev and that $3p_{3/2}$ is higher than $2f_{5/2}$ by almost the same amount; the spacing $3p_{3/2}-1i_{13/2}$ is assumed as 0.25 Mev. It might be mentioned that this level scheme is somewhat different from that obtained recently[21] for Pb^{207}. However, our results are not seriously affected by our assumptions concerning the positions of these levels.

The assumed position of all the levels is summarized in Tables III(a) and (b). The former gives the spacings between levels with even parity and the latter of those with odd parity. The values given in these tables are assumed to give the energy differences between levels for all nuclei, regardless of their masses. This might seem to be a crude approximation because the level spacings decrease with increasing A. However, only limited numbers of level spacings affect the calculated values and most level spacings have very little effect on our results. The uncertainties which appeared in the determination of high levels might give rise to some ambiguities in the calculated quadrupole moments of heavier nuclei, but it is not likely that our results could be changed substantially by assuming different level spacings.

For the excitation modes (II) and (III) the average value $\langle 1/\Delta E\rangle$ would be needed. These are assumed to be equal to $1/\Delta E$ for the sake of simplicity. On the other hand, the ΔE_2 in the excitation mode (IV) is the

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energy difference between $J=0$ and $J=2$ states of the j_1^n configuration (n=even, $0<n<2j_1+1$). Theoretically, this energy difference does not depend upon the numbers n of nucleons[22] and we estimate it from the experimental data near the closed shell. It decreases from 2 to 0.5 Mev as the mass number increases.[23,24]

(iii) Comparison with the Observed Values

The calculation of the quadrupole moments was carried out only for the nuclei with normal coupling; the quadrupole moments of Na^{23}, Mn^{55}, Se^{79}, and Eu^{153} were not calculated.[4] Those nuclei with mass numbers less than 16 were also omitted because the approximation adopted might break down. The observed values for the quadrupole moments were obtained from the compilations of Klinkenberg[25] and Murakawa and Kamei[26] and the configurations adopted are based upon the tables of Klinkenberg,[25] unless otherwise stated. The results for odd-neutron nuclei are given in the fourth column of Table IV. The fifth column of this table gives the hydrodynamic estimates of the collective model (reference 6, Table IX). Our calculated values are for odd neutron nuclei (except for Er^{167}) in general somewhat larger than the observed values. For O^{17}, the assumption that the interaction has delta-function character might not be valid. Two zeroth-order configurations are tried for Ge^{73} because there is a competition between the $p_{1/2}$ and $g_{9/2}$ neutron levels. The calculated values of the magnetic moment following the treatment of reference 8, are -1.72 and -0.76 nm for the configurations $(p_{1/2})^2\, g_{9/2}$ and $(g_{9/2})^3$, respectively. The observed value is -0.88 nm. Hence, the latter configuration gives better agreement both for magnetic and quadrupole moments. The large quadrupole moment of Er^{167} cannot be explained by the present calculation. Some remarks concerning such large quadrupole moments which appear also in odd-proton nuclei will be given in the next section. The detailed contribution of each type of configuration mixing is shown in Table V for S^{33} as an example. The largest contribution comes from the excitation mode $(1d_{5/2})^6 \rightarrow (1d_{5/2})^5\, 1g_{9/2}$ for protons and the probability of this excited configuration is 2.8%. This justifies the use of the first order perturbation theory; the reduction of the zeroth order configuration is negligible at least in most cases.

TABLE IV. Calculated and observed values of quadrupole moments of odd-neutron nuclei. $c_1c_2=0.5\times10^{-24}$ cm² Mev. The $Q_{\text{B.M.}}$'s are the hydrodynamical estimate of the collective model (reference 6).

Nucleus	Configuration proton	neutron	Q_{obs}	Q_{calc}	$Q_{\text{B.M.}}$
$_8O^{17}$	···	$d_{5/2}$	−0.004	−0.04	−0.16
$_{16}S^{33}$	···	$d_{3/2}$	−0.064	−0.09	−0.22
$_{16}S^{35}$	···	$(d_{3/2})^3$	0.045	0.09	0.22
$_{32}Ge^{73}$	···	$(p_{1/2})^2\, g_{9/2}$	−0.2±0.1	−0.43	−1.2
	···	$(g_{9/2})^3$		−0.27	···
$_{36}Kr^{83}$	$(f_{5/2})^4$	$(g_{9/2})^7$	0.15	0.28	···
$_{54}Xe^{131}$	$(g_{7/2})^4$	$d_{3/2}$	−0.12	−0.26	···
$_{60}Er^{167}$	$(h_{11/2})^4$	$(f_{7/2})^7$	10.2	0.70	···

For odd-proton nuclei, we obtain the values listed in Table VI. The value of the parameter c_1 was assumed to be 1.2×10^{-27} cm² for the calculation of the quadrupole moment (1) due to the normal configuration. The only nucleus for which the calculation gives a quadrupole moment with the wrong sign is V^{51}. However, if the normal configuration is assumed to be $(d_{3/2})^{-2}(f_{7/2})^5$ in this case, the calculated value becomes positive in agreement with the observed value. It might be recalled that the $(d_{3/2})^{-2}(f_{7/2})^3$ proton configuration gives a much better value than the $(f_{7/2})^1$ configuration for magnetic moment of Sc^{45}. However, this configuration assignment is difficult to reconcile with the magic character of nuclei with 20 protons. For Tc^{99}, the value calculated for the configuration $(g_{9/2})^5$ is much smaller than the observed value. The experimental moment is, however, somewhat ambiguous. Two configurations are examined for Pr^{141}. One of these gives a large negative, the other a small positive quadrupole moment. Therefore, it is likely that the zeroth-order wave function is a mixture of both. The observed value is obtained by assuming that the main configuration is $(d_{5/2})^3$ with a small admixture of $(g_{7/2})^2 d_{5/2}$. This is consistent with the value of the magnetic moment $\mu_{obs}=4.0$, since the $(d_{5/2})^3$ and $(g_{7/2})^2\, d_{5/2}$ configurations give 3.95 nm and 4.53 nm, respectively. From Eu^{153} to Re^{187}, the observed values are much larger than the calculated values, just as in the case of Er^{167}. The values given by the collective model are in general much larger than the observed values for the shell ± one nuclei for both odd-proton and odd-neutron nuclei.

TABLE V. Contributions from the individual mode of excitation of protons for the quadrupole moment of S^{33}. The zeroth-order proton configuration is $(1s)^2(1p_{3/2})^4(1p_{1/2})^2(1d_{5/2})^6(2s)^2$.

Excitation modes of protons	Q
$(1s)^2 \rightarrow (1s)\, 1d_{3/2}$	−0.004
$(1p_{3/2})^4 \rightarrow (1p_{3/2})^3\, 1f_{7/2}$	−0.007
$(1p_{3/2})^4 \rightarrow (1p_{3/2})^3\, 1f_{5/2}$	−0.001
$(1p_{3/2})^4 \rightarrow (1p_{3/2})^3\, 2p_{3/2}$	0.001
$(1p_{3/2})^4 \rightarrow (1p_{3/2})^3\, 2p_{1/2}$	0.001
$(1p_{1/2})^2 \rightarrow (1p_{1/2})\, 1f_{5/2}$	−0.005
$(1p_{1/2})^2 \rightarrow (1p_{1/2})\, 2p_{3/2}$	0.001
$(1d_{5/2})^6 \rightarrow (1d_{5/2})^5\, 1d_{3/2}$	−0.015
$(1d_{5/2})^6 \rightarrow (1d_{5/2})^5\, 1g_{9/2}$	−0.042
$(1d_{5/2})^6 \rightarrow (1d_{5/2})^5\, 1g_{7/2}$	−0.003
$(1d_{5/2})^6 \rightarrow (1d_{5/2})^5\, 2d_{5/2}$	0.004
$(1d_{5/2})^6 \rightarrow (1d_{5/2})^5\, 2d_{3/2}$	0.001
$(2s)^2 \rightarrow (2s)\, 1d_{3/2}$	−0.021
Sum	−0.090

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TABLE VI. Calculated and observed values of quadrupole moments of odd proton nuclei. $c_1=1.2\times10^{-27}$ cm^2 and $c_1c_2=0.5\times10^{-24}$ cm^2 Mev. $Q_{s.p.}$ and $Q_{B.M.}$ are the values given by the single-particle model and the hydrodynamic estimates of the collective model (reference 6), respectively.

Nucleus	Proton configuration	Q_{obs}	Q_{calc}	$Q_{s.p.}$	$Q_{B.M.}$
$_{13}Al^{27}$	$(d_{5/2})^5$	0.156 $\pm$ 3	0.16	0.04	0.30
$_{17}Cl^{35}$	$d_{3/2}$	-0.07894 $\pm$ 2	-0.08	-0.04	-0.26
$_{17}Cl^{37}$	$d_{3/2}$	-0.06213 $\pm$ 2	-0.08	-0.04	-0.26
$_{23}V^{51}$	$(f_{7/2})^3$	0.3 $\pm$2	-0.03	-0.03	...
$_{27}Co^{59}$	$(f_{7/2})^7$	0.5 $\pm$2	0.19	0.11	...
$_{29}Cu^{63}$	$p_{3/2}$	-0.157	-0.11	-0.07	-0.48
$_{29}Cu^{65}$	$p_{3/2}$	-0.147	-0.11	-0.07	-0.48
$_{31}Ga^{69}$	$(p_{3/2})^3$	0.2318 $\pm$ 23	0.15	0.07	0.53
$_{31}Ga^{71}$	$(p_{3/2})^3$	0.1461 $\pm$ 15	0.15	0.07	0.53
$_{33}As^{75}$	$(f_{5/2})^3(p_{3/2})^3$	0.32 $\pm$ 5	0.18	0.08	...
$_{35}Br^{79}$	$(f_{5/2})^4(p_{3/2})^3$	0.26 $\pm$ 8	0.19	0.08	...
$_{35}Br^{81}$	$(f_{5/2})^4(p_{3/2})^3$	0.21 $\pm$ 7	0.19	0.08	...
$_{41}Nb^{93}$	$g_{9/2}$	-0.4	-0.33	-0.20	...
$_{43}Tc^{99}$	$(g_{9/2})^5$	0.34 $\pm$17	0.03	0.00	...
$_{49}In^{113}$	$(g_{9/2})^9$	1.144	0.41	0.22	2.4
$_{49}In^{115}$	$(g_{9/2})^9$	1.161	0.42	0.23	2.4
$_{51}Sb^{121}$	$d_{5/2}$	-0.52 $\pm$10	-0.26	-0.18	-1.5
$_{51}Sb^{123}$	$g_{7/2}$	-0.67 $\pm$10	-0.39	-0.22	-2.1
$_{53}I^{127}$	$(g_{7/2})^2d_{5/2}$	-0.72 $\pm$ 2	-0.31	-0.19	...
$_{53}I^{129}$	$(g_{7/2})(d_{5/2})^2$	-0.43 $\pm$15	-0.42	-0.22	...
$_{57}La^{139}$	$(g_{7/2})^7$	0.9 $\pm$1	0.44	0.24	...
$_{59}Pr^{141}$	$d_{5/2}$	-0.05	-0.30	-0.20	...
	$(g_{7/2})^{-2}(d_{5/2})^3$		0.02	0.00	...
$_{63}Eu^{151}$	$(d_{5/2})^5$	1.2	0.36	0.21	...
$_{71}Lu^{175}$	$(h_{11/2})^8(g_{7/2})^7$	5.9	0.74	0.28	...
$_{73}Ta^{181}$	$(h_{11/2})^{10}(g_{7/2})^7$	6	0.65	0.28	...
$_{75}Re^{185}$	$(d_{5/2})^5$	2.8	0.39	0.24	...
$_{75}Re^{187}$	$(d_{5/2})^5$	2.6	0.40	0.25	...
$_{77}Ir^{191}$	$(h_{11/2})^{10}(d_{3/2})^3$	1.0 $\pm$5	0.40	0.18	...
$_{77}Ir^{193}$	$(h_{11/2})^{10}(d_{3/2})^3$	1.0 $\pm$5	0.40	0.18	...
$_{79}Au^{197}$	$(d_{3/2})^3$	0.56	0.29	0.18	...
$_{83}Bi^{209}$	$h_{9/2}$	-0.4	-0.53	-0.39	-5.6

IV. DISCUSSION AND CONCLUSION

There are isotopes with equal spins but somewhat different quadrupole moments. These will not be discussed in detail; one can explain such a situation by assuming a mixture for the zeroth-order wave function. This was shown for Pr^{141} in the preceding section. The configuration interaction of this kind has been discussed concerning beta transitions with anomalous ft values and the first excited states of even-even nuclei by other authors.[24,27]

The harmonic oscillator wave functions might not be the appropriate nucleon wave functions in the heavy nuclei. The wave functions for potentials similar to the square well will presumably give larger quadrupole moments for heavier nuclei by virtue of the increased matrix element of r^2. In general, our calculated values for odd-neutron nuclei are somewhat larger, those for odd-proton nuclei somewhat smaller, than the observed values. This holds even for closed shell $\pm$ one nuclei. It is likely that this discrepancy is due to our assumption concerning the interaction between nucleons. The quadrupole moments due to the excitation of the proton group of odd-neutron and odd-proton nuclei are proportional to $\frac{1}{2}(V_s+3V_t)$ and V_s, respectively, if a delta-function interaction is assumed. Hence, a better agreement could be obtained by decreasing V_t/V_s. However, one cannot determine this ratio exactly, although some indications have been obtained from the ground-state spins of odd-odd nuclei.[28]

The treatment by first-order perturbation theory appears justified, at least in most cases. This was shown in the example of S^{33}. However, it should be noted that the estimate of the energy denominators is not sufficiently accurate. The observed level spacing between $J=0$ and $J=2$ states of even-even nuclei decreases to as little as 0.1 Mev in heavy nuclei between the magic numbers. If this is true also for the states of the even groups of odd nuclei, the treatment by perturbation theory will break down. The large quadrupole moments in the rare earth region, which cannot be explained by the present treatment, may be caused by such a mechanism. In order to interpret the large quadrupole moments in this way, it will be necessary to investigate the level spacings given by the model underlying the present article.

It follows from the calculations here presented that the quadrupole moments of odd-neutron nuclei can be explained as resulting from the excitation of the proton group and that the additional quadrupole moments of odd-proton nuclei due to the same cause are rather large. The agreement between the calculated and observed values of the quadrupole moments of odd nuclei is fairly good except for nuclei with very large quadrupole moments.

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APPENDIX A. DERIVATION OF EQ. (7)

The derivation of (7) is given only briefly since the derivation of a similar equation for magnetic moments has been given before.[8] The methods of Racah[12,29] are employed for the calculation of the various matrix elements.

The matrix element in (4) can be expressed in terms of the double-barred element

$$(j_1{}^n(0)j^p(j);jj|Q_{\mathrm{op}}|[j_1{}^{n-1}(j_1)j_2](2)j^p(j);jj)$$
$$=[j(2j-1)/(j+1)(2j+1)(2j+3)]^{\frac{1}{2}}$$
$$\times(j_1{}^n(0)j^p(j);j\|Q_{\mathrm{op}}\|[j^n{}_1{}^{-1}(j_1)j_2](2)j^p(j);j).$$

The double-barred element is reduced to that of the single particle by making use of the coefficients of fractional parentage and Racah coefficients:

$$(j_1{}^n(0)j^p(j);j\|Q_{\mathrm{op}}\|[j_1{}^{n-1}(j_1)j_2](2)j^p(j);j)$$
$$=[n(2j+1)/5(2j_1+1)]^{\frac{1}{2}}(j_1\|r^2(3\cos^2\theta-1)\|j).$$

One can show in general that

$$(j'\|C^{(k)}\|j)=(-1)^{j-\frac{1}{2}}[(2j+1)(2j'+1)/(2k+1)]^{\frac{1}{2}}$$
$$\times(j'\tfrac{1}{2}\,j-\tfrac{1}{2}|j'jk0),$$

where $C_q{}^{(k)}$ is an unnormalized spherical harmonic: $C_q{}^{(k)}=[4\pi/(2k+1)]^{\frac{1}{2}}\Theta(kq)\Phi(q)$, and the difference of the orbital angular momenta of j and j' must have the same parity as k. In our case, because of $3\cos^2\theta-1=2C_0{}^{(2)}$, the double-barred matrix element of the last equation can be given in terms of a Clebsch-Gordan coefficient with $k=2$.

The calculation of the nondiagonal matrix element of the interaction in (6) is somewhat lengthy. The matrix element between many-particle configurations can be expressed in terms of matrix elements for two-particle configurations:

$$(j_1{}^n(0)j^p(j);jm|\sum_{i>k}V_{ik}|[j_1{}^{n-1}(j_1)j_2](2)j^p(j);jm)$$
$$=[(2j+1-2p)/(2j-1)]\times[5n/(2j+1)(2j_1+1)]^{\frac{1}{2}}$$
$$\times\textstyle\sum_J(2J+1)W(Jjj_22;j_1j)(j_1jJ|V|j_2jJ).$$

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

The summation over J extends herein over the possible angular momenta of the j_1j and j_2j configurations. The matrix elements of the interaction between two-particle configurations can then be obtained in a usual way. The assumption of the delta-function interaction makes the calculation relatively simple and the summation over J can be carried out without difficulty. If the particles in the orbits j and j_1 are both protons, the exclusion principle must be taken into account.

APPENDIX B. DERIVATION OF EQ. (10)

For the wave function (II), the matrix element of the quadrupole moment operator becomes

$$(j_1{}^n(0)j^p(j);jj|Q_{\mathrm{op}}|j_1{}^{n-1}(j_1)j^{p+1}(J);jj)$$
$$=[2nj(2j-p)(2J+1)/(j+1)(2j+3)(2j_1+1)]^{\frac{1}{2}}$$
$$\times(j_1\|r^2(3\cos^2\theta-1)\|j)\times W(j_1jjj;J2).$$

The explicit formulas for the coefficients of fractional parentage were used when deriving this equation. The phase factors are cancelled by the phase factors in the following formula. The nondiagonal energy matrix element for the delta-function interaction is[8]

$$(j_1{}^n(0)j^p(j);jm|\sum_{i<k}V_{ik}|j_1{}^{n-1}(j_1)j^{p+1}(J);jm)$$
$$=(-1)^{j+j_1}[2n(2j-p)(2J+1)/(2j-1)$$
$$\times(2j+1)(2j_1+1)]^{\frac{1}{2}}(j_1jJ|V|jjJ).$$

If the energy denominators are replaced by their average value and factored out, the summation with respect to J in (II) can be carried out by means of the property of Racah coefficient and the delta-function character of the interaction:

$$\textstyle\sum_J(2J+1)W(j_1jjj;J2)(j_1jJ|V|jjJ)$$
$$=V_sI[(2j_1+1)(2j+1)^3]^{\frac{1}{2}}$$
$$\times(j_1-\tfrac{1}{2}j\tfrac{1}{2}|j_1j20)(j\tfrac{1}{2}j-\tfrac{1}{2}|jj20)/20.$$

The J in this formula run over the allowed states of j^{p+1} configuration with seniority two and restricted by $|j_1-j|\leq J\leq j_1+j$. The derivation of (11) is quite similar.