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Quadrupole Moments of Odd-Neutron Nuclei

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Without taking into account the effect of configuration mixing, we attempt to calculate electric quadrupole moments of odd-neutron nuclei on the basis of the single configuration model. The quadrupole moments of odd-neutron nuclei are assumed to be due to the promotion of two protons from the zeroth-order proton state of seniority zero to the states of seniority two. These mixing coefficients of the ground state are determined by fitting the wave function to the magnetic moment of the odd-neutron nucleus considered. We have a fairly good agreement between the calculated and observed values except for the nuclei with very large quadrupole moments.

1. Introduction

The extreme single-particle model manifests its most serious deficiency in accounting for the nuclear quadrupole moments, particuiarly, those of odd-neutron nuclei, although there is a definite correlation between nuclear quadrupole moments and nuclear shell structure. The quadrupole moment of the nucleus with a single proton in the orbit j outside a core with zero angular momentum is $Q_j^{(2)}$:

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

On the other hand, the single-particle shell model gives zero quadrupole moments for odd-neutron nuclei, since the neutrons carry no charge and since the quadrupole moment Q_{recoil} induced by the effect of the recoil of the core

$$Q_{recoil} \simeq \frac{Z}{A^2}\cdot Q_j^{(2)} \tag{2}$$

is negligible small except extremely light nuclei. But the facts that the quadrupole moments of odd-neutron nuclei can be just as large as those of odd-proton nuclei and that the behaviour of odd-neutron nuclei with the number of neutrons outside their closed shells is similar to that of odd-proton nuclei with respect to the number of extra protons seem to indicate that the nuclear angular momentum should be shared with the protons. As an explanation of the fact that the odd-neutron nuclei have electric quadrupole moments the following three prescriptions have been proposed by various authors. First, in the individual particle model, indeed, the angular momentum of a nucleus is shared among all nucleons outside closed shells and therefore the odd-neutron nuclei in which there are loose protons outside closed shells can possess electric quadrupole moments. Flowers has calculated as a particular example quadrupole moments of j^3 configurations for which $I=j$, $T=1/2$ and $v=1$, where I is the total angular momentum of a nucleus and T the total isotopic spin and v the seniority quantum number. His results are as follows[1]: for an odd-neutron nucleus

$$Q(1n+2p)=\frac{2j+7}{6j+6}\cdot Q_j^{(2)}, \tag{3}$$

and by the way for an odd-proton nucleus

$$Q(1p+2n)=\frac{4j+5}{6j+6}\cdot Q_j^{(2)}.$$

We find in several light nuclei observations in good agreement with this result. But effects of this kind for heavier nuclei in which the neutron unfilled shell is different from the proton unfilled shell cannot be expressed in the simple form. Secondly, the collective model[2] ascribes quadrupole moments of odd-neutron nuclei to core deformation induced by an extra neutron. However, this model gives too large quadrupole moments for light and medium heavy odd-neutron nuclei. Finally, the mixing of excited configurations to the ground configuration given by the single-particle shell model can also give quadrupole moments for odd-neutron nuclei. In configuration mixing approach, it is assumed that this admixture is so small that the effects proportional to the square of the mixing coefficients can be neglected. The mixing coefficients α's are given by the perturbation theory in terms of the off-diagonal elements of residual nuclear interactions and the energy difference between the ground and excited configurations. All the excited configurations are taken into account for which the off-diagonal elements of the quadrupole moment operator $Q_{op}=\sum_p r_i^2(3\cos^2\theta_i-1)$ do not vanish. The quadrupole moments of odd-neutron nuclei are only the contributions from the off-diagonal elements of the quadrupole moment operator Q_{op} between the ground and excited configurations. Thus, calculated values for the quadrupole moment in configuration mixing are in excellent agreement with the observed values[3].

However, we donot very well know about the nuclear interaction between free two nucleons, still less residual nuclear interactions which should be considered in shell model calculation. And it is difficult to determine precisely the energy difference between the ground and excited configurations. Then, without taking into acccount the effect of configuration mixing, we attempt to calculate electric quadrupole moments of odd-neutron nuclei on the basis of the single configuration model. The quadrupole moments of odd-neutron nuclei are assumed to be due to the promotion of two protons in the unfilled shell from the zeroth-order proton state of seniority zero to the states of seniority two. And it is assumed that in the correct ground state wave function there exists the large admixture of these states. The mixing coefficients of the ground state are determined by fitting the wave function to the magnetic moment of the odd-neutron nucleus considered.

II. Calculation of matrix elements for the electric quadrupole moments of odd-neutron nuclei

Firstly, we explain the essential-features of our method in the simplest case, i.e. the system consisting of one neutron and two protons outside closed shells. Let us denote the zeroth-order ground state given by the single-particle model by

$$\psi_0(j,\ j_1^2 v=0(0),\ J=M=j)\ ,$$

where j is the total angular momentum of the odd neutron and j_1 those of the extra protons. Then we represent the excited states in which two j_1-protons in the unfilled shell promote from the zeroth-order ground state of seniority zero to the states of seniority two as

$$\psi(j,\ j_1^2 v=2(J'),\ J=M=j)$$

where J' is even and restricted by the conditions $2j_1-1\geq J'\geq 2,\ j+J'\geq j\geq |j-J'|$. However, it can easily be seen that only the state with $J'=2$ gives nonvanishing off-diagonal elements of Q_{op} between it and the zeroth-order ground state given by the shell model. In the present paper we assume that the correct ground state wave function is the linear combination

$$\psi(J=M=j)=\alpha\,\psi_0(j,j_1^2 v=0(0),J=M=j)+\beta\psi(j,\ j_1^2 v=2(2),J=M=j). \quad (4)$$

In order to calculate the matrix elements of the quadrupole moment operator Q_{op} we transform the wave functions in Eq. (4) as follows:

$$\begin{aligned}\psi(j,\ j_1^2(J'),\ J=M=j)&=\sum_{J''}\psi(j,\ j_1(J'')j_1,\ J=M=j)\langle jj_1(J'')j_1,\ j|j,\ j_1^2(J')J=j\rangle\\&=\sum_{J''}U(jj_1jj_1;\ J''J')\psi(jj_1(J'')j_1,\ J=M=j)\\&=\sum_{J''}\sum_{M'',m}U(jj_1\ jj_1;\ J''J')\langle J''j_1M''m|J''j_1J=jM=j\rangle\\&\quad\times\psi(jj_1J''M'')\phi(j_1m)\ ,\end{aligned}\quad (5)$$

where U is the modified Racah coefficient defined by Jahn[4] and $\langle J''jM''m|J''jJ=jM=j\rangle$ is the Clebsch-Gordan Coefficient. Using this expression for the wave function, we can easily calculate the diagonal matrix elements of Q_{op} as follows:

$$\begin{aligned}\langle Q^{(2)}\rangle&=(j,\ j_1^2(J')J=M=j=|Q_{op}^{(2)}|\,j,\ j_1^2(J')J=M=j)\\&=2\sum_{J''}\sum_{M''m_1}U^2(jj_1jj_1;\ J''J')\,|\langle J''j_1M''m_1|J''j_1jj\rangle|^2\langle j_1 2m_1 0|\,j_1 2j_1m_1\rangle\\&\quad\times(2j_1+1)^{-\frac{1}{2}}(j_1\|Q^{(2)}\|j_1)\\&=2(2j+1)(j_1\|Q^{(2)}\|j_1)\sum_{J''}U^2(jj_1\ jj_1;\ J''J')\sum_{M''m_1}(-1)^{j_1-m_1}V(J''j_1j;\ M''m_1-j)\\&\quad\times V(J''jj_1;\ -M''j-m_1)V(j_12j_1;\ -m_10m_1)\\&=2(2j+1)(j_1\|Q^{(2)}\|j_1)\sum_{J''}(-1)^{2j}U^2(jj_1\,jj_1;\ J''J')W(J''j_1j2;\ jj_1)\times V(j2j;\ j0-j)\ .\end{aligned}$$

On the other hand,

$$(j_1\|Q^{(2)}\|j_1)=[(2j_1+3)(2j_1+2)(2j_1+1)/(2j_1)(2j_1-1)]^{\frac{1}{2}}Q_{j_1}^{(2)},$$
$$V(j2j;\ j0-j)=(-1)^{2j}[(2j)(2j-1)/(2j+1)(2j+2)(2j+3)]^{\frac{1}{2}}.$$

Then,

$$\begin{aligned}\langle Q^{(2)}\rangle &= \frac{2(2j+1)!}{(2j_1)!}\Big[\frac{(2j_1+3)!(2j_1-2)!}{(2j+3)!(2j-2)!}\Big]^{\frac{1}{2}}(2J'+1)Q_{j_1}^{(2)}\sum_{J''}(2J''+1)W(jj_1\,jj_1;J''J')\\ &\quad\times W(j_1\,jj_1j;J''J')W(J''j_1j2;\ jj_1)\\ &=(-1)^{2J'}2(2J'+1)\frac{(2j+1)!}{(2j_1)!}\Big[\frac{(2j_1+3)!(2j_1-2)!}{(2j+3)!(2j-2)!}\Big]^{\frac{1}{2}}W(jj2J';J'j)W(j_1j_12J';J'j_1)\\ &\quad\times Q_{j_1}^{(2)}\\ &=(-1)^{2J'}\frac{2J'(J'+1)\{3J'(J'+1)-3-4j_1(j_1+1)\}\{3J'(J'+1)-3-4j(j+1)\}Q_{j_1}^{(2)}}{(2J'+3)(2J'-1)(2j+3)(2j+2)(2j_1)(2j_1-1)}.\end{aligned}\tag{6}$$

V is defined by Racah and W is the Racah coefficient.[5)]
Similarly, off-diagonal elements of the quadrupole moment operator Q_{op} between $\psi(j,\ j_1^2(0), J=M=j)$ and $\psi\ (j,\ j_1^2(J'), J=M=j)$ are easily obtained as

$$\begin{aligned}&(j,\ j_1^2(0),\ J=M=j\,|Q_{op}|\,j,\ j_1^2(J'),J=M=j)\\ &=2(-1)^{J'}\Big[\frac{(2J'+1)(2j)(2j+1)(2j-1)(2j_1+3)(2j_1+2)(2j_1+1)}{(2j+2)(2j+3)(2j_1)(2j_1-1)}\Big]^{\frac{1}{2}}W(jj2J';\ 0j)\\ &\quad\times W(j_1\ j_12J';\ 0j_1)Q_{j_1}^{(2)}.\end{aligned}\tag{7}$$

From the triangle conditions among the arguments of the Racah coefficients in Eq. (7) it can easily be seen that only in the case of $J'=2$ we have non-vanishing elements. Then,

$$\begin{aligned}&(j,\ j_1^2(0),J=M=j\,|Q_{op}|\,j,\ j_1{}^2(J'=2),J=M=j)\\ &\qquad=\Big[\frac{4(2j)(2j-1)(2j_1+3)(2j_1+2)}{5(2j_1)(2j_1-1)(2j+3)(2j+2)}\Big]^{\frac{1}{2}}\cdot Q_{j_1}^{(2)}.\end{aligned}\tag{8}$$

Now, let us consider the system consisting of an odd number of neutrons in the orbit j and an even number of protons in the orbit j_1 outside the closed shells. We write down the zeroth-order ground state of the odd-neutron nucleus given by the single-particle model as

$$\psi_0(j^n v=1(J_n=j),\ j_1{}^p v=0(J_p=0),\ J=j=M)\,.$$

Then we represent the states in which two protons in the unfilled j_1 -shell promote the zeroth-order state of seniority zero to the states of seniority two as

$$\psi(j^n v=1(J_n=j),\ j_1^p v=2(J_p\neq 0),\ J=j=M)\,.$$

Here, also we assume that the correct ground state wave function is the linear combination

$$\Psi(j^n j_1^p J=j=M)=\alpha\psi_0(j^n v=1(J_n=j),\ j_1^p v=0(J_p=0), J=j=M)$$
$$+\beta\psi(j^n v=1(J_n=j),\ j_1^p v=2(J_p=2),\ J=j=M)\,. \qquad (4')$$

In order to calculate the matrix elements we transform the wave functions as follows:

$$\psi(j^n v=1(J_n=j),\ j_1^p v_1(J_p),\ J=j=M)$$
$$=\sum_{J'v'}\psi(j^n v=1(J_n=j),\ [j_1^{p-1}v'J',\ j_1](J_p),\ J=j=M)(j_1^{p-1}v'J',\ j_1,\ j_1^p v_1(J_p)|\}j_1^p v_1(J_p))$$
$$=\sum_{v'J'}\sum_{J''}\psi([j^n v=1(J^n=j),\ j_1^{p-1}v'J'](J''),\ j_1,\ J=j=M)$$
$$\times\langle jJ'(J''),\ j_1,\ J=j|j,\ J'j_1(J_p),\ J=j\rangle(j_1^{p-1}v'J',\ j_1,\ j_1^p v_1(J_p)|\}j_1^p v_1(J_p))$$
$$=\sum_{v'J'}\sum_{J''M''}\sum_{m_1}\psi(j^n v=1(J_n=j),\ j_1^{p-1}v'(J'),\ J''M'')\phi(j_1 m_1)$$
$$\times\langle J''j_1M''m_1|J''j_1J=jM=j\rangle U(jJ'jj_1;J''J_p)(j_1^{p-1}v'J',\ j_1,\ j_1^p v_1(J_p)|\}j_1^p v_1(J_p))\,.$$

Using this expression for the wave function, we can calculate the matrix elements of Q_{op} in the same way as in the simple case. The results are as follows:

$$(j^n v=1(J_n=j),\ j_1^p v_1(J_p),\ J=j=M|Q_{op}|j^n v=1(J_n=j),\ j_1^p v_1(J_p),\ j=j=M)$$
$$=p(2J_p+1)\frac{(2j+1)!}{(2j_1)!}\Big[\frac{(2j_1+3)!(2j_1-2)!}{(2j+3)!(2j-2)!}\Big]^{\frac{1}{2}}\sum_{v'J'}|(j_1^{p-1}v'(J'),\ j_1,\ j_1^p v_1(J_p)|\}j_1^p v_1(J_p))|^2$$
$$\times W(j_1J'2J_p;\ J_pj_1)W(jj2J_p;J_pj)Q_{j_1}^{(2)}\,, \qquad (9)$$

$$(j_n v=1(J_n=j),\ j_1^p v_1=0(0), J=j=M|Q_{op}|j^n v=1(J_n=j),\ j_1^p v_1=2(J_p=2),\ J=j=M)$$
$$=(-1)^{J_p}\frac{(2j+1)!}{(2j_1)!}\Big[\frac{(2J_p+1)(2j_1+3)!(2j_1-2)!}{(2j+3)!(2j-2)!}\Big]^{\frac{1}{2}}W(jj2J_p;\ 0j)W(j_1j_12J_p;\ 0j_1)$$
$$\times p(j_1^{p-1}v'=1(J'=j_1)j_1,\ j_1^p v_1(J_p)|\}j_1^p v_1(J_p))Q_{j_1}^{(2)}$$
$$=p\Big[\frac{(2j)(2j-1)(2j_1+3)(2j_1+2)}{5(2j+2)(2j+3)(2j_1)(2j_1-1)}\Big]^{\frac{1}{2}}(j_1^{p-1}v'=1(J'=j_1)j_1,\ j_1^p v_1(J_p)|\}j_1^p v_1(J_p))Q_{j_1}^{(2)}. \qquad (10)$$

III. Comparison with the observed values and discussions

The mixing coefficients of the ground state wave functions (4) and (4′) are determined by fitting the wave functions to the magnetic moment of the odd-neutron nucleus considered. The expectation value of the magnetic moment operator

$$\vec{\mu}=g_j\sum^{n}\vec{j}_i+g_{j_1}\sum_{k}^{p}\vec{j}_k$$

for the state (4′) is

$$(j^n j_1^p J=j=M|\mu_z|j^n j_1^p J=j=M)$$
$$=\alpha^2 g_j\cdot j+\beta^2[2(j+1)]^{-1}\{2g_i\cdot j(j+1)+(g_{j_1}-g_j)J_p(J_p+1)\}\,, \quad (11)$$

where $\beta^2=1-\alpha^2$, g_j and g_{j_1} are the g factor of a j-neutron and that of the j_1-proton. By fitting the theoretical magnetic moment (11) to the observed value we cannot determine the sign of the mixing coefficients α and β. In principle, the mixing coefficients should be determined by solving the secular determinant equation for residual neutron-proton interactions. If residual neutron-proton interactions are attractive as usual, α and β are equal sign for the ground state. Then, we assume that both α and β are positive.

The calculation of the quadrupole moments was carried out only for the odd-neutron nuclei with normal coupling by using those α and β and the results obtained in the preceding section. We obtain the values listed in Table 1. The value of the parameter r_0 for the nuclear radius was assumed to be 1.45×10^{-13}cm. We have a fairly good agreement between the calculated and observed values for light and medium heavy odd-neutron nuclei.

The validity of the assumption that in the correct ground state wave function there exists the large admixture between the zeroth-order state given by the single particle shell model with the proton state of seniority zero and the excited proton state of seniority two, i. e. the validity of the assumption that those states are almost degenerate and therefore the first order perturbation theory for the degenerate states applicable, must be considered in detail.[6]

Table 1. Calculated and observed values of quadrupole moments of oddneutron nuclei. $<r^2> = 0.6A^{2/3}r_0^2$, $r_0 = 1.45\times10^{-13}$cm. The $Q_{B.M.}$'s are the hydrodynamical estimate of the collective model (reference 2). The $Q_{C.M.}$'s are the calculated values by configuration mixing (reference 3)

Nucleus	Configuration		Q_{obs}	Q_{cal}	$Q_{C.M.}$	$Q_{B.M.}$
	neutron	proton				
S^{33}	$(d_{3/2})^1$	$(d_{3/2})^2$	−0.064	−0.03	−0.09	−0.22
S^{35}	$(d_{3/2})^{-1}$	$(d_{3/2})^{-2}$	+0.035	+0.03	+0.09	+0.22
Ge^{73}	$(g_{9/2})^1$	$(p_{3/2})^2$	−0.21 ±10	−0.12	{−0.43, −0.27}	−1.2
Kr^{83}	$(g_{9/2})^{-3}$	$(p_{3/2})^{-2}$	+0.15	+0.14	+0.28	…
Kr^{85}			+0.23	+0.14	…	…
Xe^{131}	$(d_{3/2})^1$	$(g_{7/2})^4$	−0.1	−0.07	−0.26	…
Hg^{201}	$(p_{3/2})^1$	$(h_{11/2})^2$	+0.42	+0.17	+0.70	…

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