

THE ISOMER SHIFT AND THE STRUCTURE OF METASTABLE STATES OF NUCLEI

V. A. BELYAKOV

Submitted to JETP editor March 13, 1965

J. Exptl. Theoret. Phys. (U.S.S.R.) **49**, 832-840 (September, 1965)

On the basis of the theory of finite Fermi systems the quantity $\Delta\langle R^2 \rangle$, the difference in the mean square radii of the electric charge distributions in the ground and excited states of a nucleus, is calculated. The constant for the volume isotope shift is calculated for the same region of atomic weights. The nature of the excited nuclear states is discussed.

BY the isomer shift we mean a dependence of the energy of the electronic states of the atom on the state of the nucleus (ground or excited state). This dependence is connected with the different spatial distributions of the nuclear charge in the ground and excited states. The study of the isomer shift enables one to investigate delicate effects in the distribution of the electric charge of the nucleus and gives information about the structure of the nucleus which is difficult or impossible to obtain by other methods.

The theoretical treatment of the isomer (isotope) shift has mainly concentrated on the electronic part of the problem, which by now has been well investigated (cf., for example, [1]). For the description of the nuclear part of the problem, extremely crude models have been invoked in the past. In the present paper the study of the nuclear aspects of the problem is carried out in the framework of the theory of finite Fermi systems. [2]

Experimentally the isomer shift was first detected by optical methods. [3] Later it was observed and investigated extensively in experiments on the Mössbauer effect (cf. [4]).

In the optical case the isomer shift manifests itself as a shift of the lines of the optical spectra of isomers. Since only s and $p_{1/2}$ electrons are sensitive to the charge distribution in the nucleus (since their ψ functions are different from zero over the region of the nucleus), the shift can be observed only on lines corresponding to transitions of s and $p_{1/2}$ electrons. The effect is very much smaller for the p electrons, so we shall treat the isomer shift only for s electrons.

The difference in the volume distribution of charge for the isomeric and ground states of the nucleus is characterized by $\Delta\langle R^2 \rangle$, the difference in the mean square radii of the charge distributions in these states. We have

$$\begin{aligned}\Delta\langle R^2 \rangle &= \langle R_e^2 \rangle - \langle R_g^2 \rangle; \\ \langle R_e^2 \rangle &= \int \rho_e(\mathbf{r}) r^2 dV \Big/ \int \rho_e(\mathbf{r}) dV = \frac{1}{Z} \int \rho_e(\mathbf{r}) r^2 dV, \\ \langle R_g^2 \rangle &= \frac{1}{Z} \int \rho_g(\mathbf{r}) r^2 dV,\end{aligned}\quad (1)$$

where $\rho_e(\mathbf{r})$ and $\rho_g(\mathbf{r})$ are the electric charge distributions in the excited and ground states, respectively, and Z is the nuclear charge.

The isomer shift in optical spectra is characterized by the quantity C , which is related to $\Delta\langle R^2 \rangle$ as follows:

$$C = \frac{R_\infty}{3} \left(\frac{1 + \sigma}{\Gamma(1 + 2\sigma)} \right)^2 \left(\frac{2ZR}{\alpha_H} \right)^{2\sigma} \frac{\Delta\langle R^2 \rangle}{R^2}, \quad (2)$$

where R_∞ is the Rydberg constant, α_H is the radius of the first Bohr orbit of hydrogen, $\sigma = [1 - (Z/137)^2]^{1/2}$, and R is the nuclear radius.

In experiments on the Mössbauer effect (resonance absorption of γ quanta) the isomer shift appears if the source and absorber are the same isotope but bound in different chemical compounds. In this case the energy of the emitted γ rays is different from the resonance energy for absorption of the γ rays. The difference in energy is related to the different electron densities at the nucleus in the source and absorber. The energy of the emitted γ quantum is $\epsilon_1 = \epsilon_0 - \Delta T_1$, the energy of the absorbed γ quantum is $\epsilon_2 = \epsilon_0 - \Delta T_2$, where ϵ_0 is the energy of the nuclear transition, ΔT_1 is the change in the energy of the electron shell because of the difference in the charge distributions of the excited and ground states of the source nucleus, and ΔT_2 is the same quantity for the absorber. The energy difference $\Delta E = \Delta T_1 - \Delta T_2$ is expressed in terms of the ψ functions of the s electrons of the source, ψ_s , the absorber, ψ_a , and $\Delta\langle R^2 \rangle/R^2$, by the formula

$$\Delta E = \frac{1}{3} \pi Z e^2 R^2 S(Z) \left[\sum \psi_a^2(0) - \sum \psi_s^2(0) \right] \frac{\Delta\langle R^2 \rangle}{R^2}, \quad (3)$$

where $S(Z)$ is a relativistic factor which is close to unity for light nuclei (cf. [4]).

In both the formulas (2) and (3), the dependences on the nuclear and electronic features of the problem are separated. To find the nuclear factor we must calculate $\Delta\langle R^2 \rangle$. It should be mentioned that we can experimentally get a very accurate value for the product of the two factors, but their individual determination is difficult. The quite good agreement of the theoretical values of $\Delta\langle R^2 \rangle$ with experimental data for the isotope shift (cf. also [5]) leads one to hope that a comparison of theoretical values of $\Delta\langle R^2 \rangle/R^2$ with experimental results for the isomer shift will make it possible, in those cases where the nature of the isomeric states is well understood, to get information about the electronic characteristics of the problem, and in those cases where the electronic characteristics are well known to improve our knowledge of the isomeric states.

CALCULATION OF $\Delta\langle R^2 \rangle$

Let us consider isomers for which the transition to the ground state is a single-particle transition. Such isomeric states can be pictured as the result of adding to the even-even core a nucleon (hole) in a single-particle level with the appropriate spin and excitation energy. The ground state is similarly described as an even-even core plus a particle (hole). The problem of calculating $\Delta\langle R^2 \rangle$ then reduces to computing the difference in the changes in the mean square radii of the charge distributions resulting from adding the nucleon in different single-particle states.

Usually this quantity is calculated for both proton and neutron transitions using the shell model. In order to obtain the redistribution of the charge in neutron transitions, i.e., to take account of the interaction of the odd neutron with the core, a positive effective charge is ascribed to the neutron. In the isotope shift problem this approach gives the correct order of magnitude of the effect. As we shall see, for the isomer shift this approximation usually gives the wrong sign for the effect.

In the present paper the interaction of the odd nucleon (hole) with the core is included by using the theory of finite Fermi systems. [2]

The change δA of some quantity A characterizing the nucleus, as the result of adding a proton, can be expressed in terms of the corresponding vertex $\mathcal{F}^p(A)$ according to the formula

$$\delta A = \sum_{\lambda} a \mathcal{F}_{\lambda\lambda^p}(A) (\tilde{n}_{\lambda} - n_{\lambda}); \quad (4)$$

here λ labels the single-particle states (n, l, j, m),

n_{λ} are the occupation numbers for single-particle states in the initial nucleus, \tilde{n}_{λ} are the occupation numbers in the nucleus obtained by adding a proton and neglecting the interaction of the added proton with the nucleons in the core, $\mathcal{F}_{\lambda\lambda}^p(A)$ is the diagonal matrix element of the vertex between single-particle functions. When a neutron is added, δA is expressed similarly in terms of the vertex $\mathcal{F}^n(A)$.

In the λ representation, the vertex

$$\mathcal{F}(A) = \begin{pmatrix} \mathcal{F}^p(A) \\ \mathcal{F}^n(A) \end{pmatrix}$$

satisfies the equation

$$\begin{aligned} \mathcal{F}(A)_{\lambda\lambda'} &= \mathcal{F}^{\omega}(A)_{\lambda\lambda'} \\ &+ \sum_{\lambda_1\lambda_2} \langle \lambda\lambda' | a^2 \Gamma^{\omega} | \lambda_1\lambda_2 \rangle \left[L_{\lambda_1\lambda_2} \mathcal{F}(A)_{\lambda_1\lambda_2} \right. \\ &\left. - \delta_{\lambda_1\lambda_2} \frac{\Delta_{\lambda_1}^2}{2E_{\lambda_1}^3} (\mathcal{F}(A)_{\lambda_1\lambda_1} - \overline{\mathcal{F}}(A)_{\lambda_1\lambda_1}) \right] \end{aligned} \quad (5)$$

where

$$L = \begin{pmatrix} L^p & 0 \\ 0 & L^n \end{pmatrix}, \quad \Gamma^{\omega} = \begin{pmatrix} \Gamma_{pp}^{\omega} & \Gamma_{pn}^{\omega} \\ \Gamma_{np}^{\omega} & \Gamma_{nn}^{\omega} \end{pmatrix}, \quad \mathcal{F}^{\omega} = \begin{pmatrix} \mathcal{F}_{p}^{\omega} \\ \mathcal{F}_{n}^{\omega} \end{pmatrix}$$

(for scalar vertices, a $\mathcal{F}^{\omega}(A) = A$),

$$L_{\lambda\lambda^p} = \frac{E_{\lambda^p} E_{\lambda^p} - \varepsilon_{\lambda^p} \varepsilon_{\lambda^p} + \Delta_{\lambda^p} \Delta_{\lambda^p}}{2E_{\lambda^p} E_{\lambda^p} (E_{\lambda^p} + E_{\lambda^p})}$$

$E_{\lambda}^p = [(\varepsilon_{\lambda}^p)^2 + (\Delta_{\lambda}^p)^2]^{1/2}$, ε_{λ}^p are the proton single particle energy levels, measured from the chemical potential μ^p , $\Delta_{\lambda}^p = a \Delta_{\lambda\lambda}^p$, $\Delta_{\lambda\lambda}^p$ is the diagonal matrix element of the amplitude of transition of a proton particle (hole) to a hole (particle) and condensation of a pair, a is the renormalization constant. $L_{\lambda\lambda}^n$ is expressed similarly in terms of the characteristics of the neutron system having label n .

The matrix elements of Γ^{ω} appearing in (5) have the form

$$\begin{aligned} \langle \lambda_1\lambda_2 | \Gamma_{ik}^{\omega} | \lambda\lambda' \rangle &= \int (\varphi_{\lambda_1}^i(\mathbf{r}_1))^* \varphi_{\lambda_2}^k(\mathbf{r}_2) \Gamma_{ik}^{\omega}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) \\ &\times (\varphi_{\lambda}^k(\mathbf{r}_3))^* \varphi_{\lambda'}^i(\mathbf{r}_4) dV_1 dV_2 dV_3 dV_4; \end{aligned}$$

$\varphi_{\lambda}^i(\mathbf{r})$ are single particle wave functions of nucleons (i, k run through the two values n and p). $\overline{\mathcal{F}}_{\lambda\lambda}$ represents an average over levels close to the Fermi surface of the diagonal matrix element of the vertex (and is independent of λ). For spherical nuclei, to which we shall restrict our treatment, the angular dependence of the total vertex coincides with the angular dependence of \mathcal{F}^{ω} , so the transitions entering in the sum in (5) are determined by the selection rules for the part \mathcal{F}^{ω} .

To find $\Delta\langle R^2 \rangle$, we must solve (5) for $\mathcal{F}(A)$ when $A = r^2$. In this case

$$a\mathcal{F}^\omega = \begin{pmatrix} r^2 \\ 0 \end{pmatrix}.$$

In the equation for $\mathcal{F}(r^2)$ the diagonal terms are small, and also vary in sign, so they can be dropped. The smallness of the diagonal terms is related to the fact that $\mathcal{F}(r^2)_{\lambda\lambda}$ is weakly dependent on λ , and so $|\bar{\mathcal{F}}_{\lambda\lambda} - \mathcal{F}_{\lambda\lambda}| \ll \mathcal{F}_{\lambda\lambda}$. Substituting $A = r^2$ in (5), dropping the diagonal terms in the sum and summing over m , we get

$$\bar{\mathcal{F}}_{\lambda\lambda'} = \mathcal{F}_{\lambda\lambda'} + \sum_{\lambda_1\lambda_2} \frac{a^2}{4\pi} \langle \lambda\lambda' | \Gamma^\omega | \lambda_1\lambda_2 \rangle (2j_1 + 1) L_{\lambda_1\lambda_2} \mathcal{F}_{\lambda_1\lambda_2}. \quad (6)$$

Here the index λ denotes the set of quantum numbers n, l, j , and the matrix elements appearing in (6) are taken between the radial wave functions. The transitions in the sum are determined by the selection rules $\Delta l = 0, \Delta j = 0$.

In getting (6) it was assumed that

$$\begin{aligned} \Gamma_{ik}^\omega(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) \\ = \frac{1}{2} \frac{dn}{d\epsilon_0} f^{ik}(\mathbf{r}_1) \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}_3) \delta(\mathbf{r}_1 - \mathbf{r}_4) \end{aligned} \quad (7)$$

where n is the density of nucleons and ϵ is the Fermi energy.

Equation (6) was solved on a digital computer. The Nilsson scheme^[6] was used for the single-particle levels for both neutrons and protons. Transitions between shells were considered (within one shell the selection rules forbid transitions). For the f^{ik} we used the interpolation formula^[5]

$$f^{ik} = \frac{1}{n_0} \{f_{in}^{ik} n(r) - f_{ex}^{ik} [n(r) - n_0]\}, \quad (8)$$

where $n(r) = n_0/[1 + e^{\alpha(r - R_0)}]$, n_0 is the mean density of nucleons in the nucleus, $\alpha = 1.55 \text{ f}^{-1}$, $R_0 = 1.2 A^{1/3} \text{ f}$. It was assumed that $f^{\text{nn}} = f^{\text{pp}}$.

In the sum in (6) the pairing correlation is important for transitions involving levels close to the Fermi surface. Since there are few such terms in the sum, the inaccuracy in the corresponding $L_{\lambda_1\lambda_2}$ has little effect on the solution. Considering this point, we assumed that $\Delta_\lambda^{\text{p}} \equiv \Delta^{\text{p}}$ and $\Delta_\lambda^{\text{n}} \equiv \Delta^{\text{n}}$ are independent of the indices and are the same constant values for all transitions in a given nucleus. The values of μ^{p} and μ^{n} were found from the approximate solution of the equations

$$\begin{aligned} N &= \sum_\lambda \frac{1}{2} \left\{ 1 - \frac{\epsilon_\lambda^n}{[(\Delta^n)^2 + (\epsilon_\lambda^n)^2]^{1/2}} \right\}, \\ Z &= \sum_\lambda \frac{1}{2} \left\{ 1 - \frac{\epsilon_\lambda^{\text{p}}}{[(\Delta^{\text{p}})^2 + (\epsilon_\lambda^{\text{p}})^2]^{1/2}} \right\} \end{aligned} \quad (9)$$

In choosing numerical values for Δ^{n} and Δ^{p} we used data from the paper of Nemirovskiĭ and

Adamchuk.^[7] The values of f^{pp} and f^{nn} were taken from^[8], where they were obtained from an analysis of the quadrupole moments:

$$f_{in}^{\text{pp}} = 1.3, \quad f_{ex}^{\text{pp}} = -2.9, \quad f_{in}^{\text{np}} = 0.6, \quad f_{ex}^{\text{np}} = -2.3.$$

To check the correctness of our choice of constants, we calculated the constant for the volume isotope shift in the same region of masses for which the isomer shift was treated. The quantity $\Delta\langle R^2 \rangle$ in (2) for the isotope shift is given by the expression

$$\Delta\langle R^2 \rangle = \sum_\lambda a \mathcal{F}_{\lambda\lambda^n}(r^2) (\tilde{n}_\lambda - n_\lambda), \quad (10)$$

where \tilde{n}_λ and n_λ are the occupation numbers in isotopes with $N+2$ and N neutrons, respectively.

The problem of finding \tilde{n}_λ when pairing is taken into account was not solved. The assumption was made that the occupation numbers for neutrons are changed for only one level λ_0 . Then (10) becomes

$$\Delta\langle R^2 \rangle = 2a \mathcal{F}_{\lambda_0\lambda_0}^{\text{n}}. \quad (11)$$

For many of the isotopes considered, as neutrons are added there is competition between different j levels, so that the choice of the state in which the pair of neutrons is added can be made only by comparing the values of the isotope shift constant with experimental values. With the stated values of the constants f^{ik} the calculations are in satisfactory agreement with experiment, and the order of filling of the j levels does not contradict the usually accepted schemes. The computations of the constant for the volume isotope shift are given in Table I.

In the computation of $\Delta\langle R^2 \rangle$ for isomeric states, either the proton or neutron vertex appears in (10) depending on whether the odd particle is a proton or neutron. Then \tilde{n}_λ denotes the occupation number for nucleons in the isomeric state. For strictly single-particle (hole) isomeric states, we find from (10)

$$\Delta\langle R^2 \rangle = \pm a (\mathcal{F}_{\lambda_2\lambda_1} - \mathcal{F}_{\lambda_0\lambda_0}), \quad (12)$$

where λ_1 is the set of quantum numbers for the excited state and λ_0 the set for the ground state. The upper sign applies for particle states and the lower sign for hole states. The assumption that the state is a single-particle state is well satisfied for the longlived isomers, in which the isomer shift can be detected optically. The corresponding isomeric transitions are characterized by a large difference of the angular momenta for a small energy difference. The E2 transitions typical for collective states are absent. In the neighboring even-even nuclei no collective excitations near this energy

Table I. Constants for the Volume Isotope Effect

Element	$A_1 - A_2$	λ_0	$C^I, 10^{-3} \text{cm}^{-1}$	$C_T, 10^{-3} \text{cm}^{-1}$	$C_{\text{exp}}, 10^{-3} \text{cm}^{-1}$
³⁷ Rb	85—87	1 $g_{7/2}$	23	12	8±12
³⁸ Sr	84—86	1 $g_{7/2}$	23	12	} ~ 0
	86—88	1 $g_{7/2}$	23	12	
⁴⁴ Ru	96—98	1 $g_{7/2}$	40	22	34 ± 9 averaged over all isotopes
	98—100	1 $g_{7/2}$	40	22	
	100—102	1 $g_{7/2}$	40	22	
	102—104	2 $d_{5/2}$	68	35	
⁴⁶ Pd	106—108	2 $d_{5/2}$	78	38	42±9
	108—110	2 $d_{5/2}$	78	38	36±9
⁴⁷ Ag	107—109	2 $d_{5/2}$	76	38	38±6
⁴⁸ Cd	106—108	2 $d_{5/2}$	100	44	35
	108—110	2 $d_{5/2}$	98	43	32
	110—112	2 $d_{5/2}$	96	42	32±4
	112—114	2 $d_{5/2}$	94	41	30
	114—116	2 $h_{11/2}$	52	27	22
⁵⁰ Sn	—	1 $g_{7/2}$	62	34	
	112—114	2 $d_{5/2}$	100	48	40±10
	114—116	2 $d_{5/2}$	100	48	40±10
	116—118	2 $d_{5/2}$	100	48	30±10
	118—120	3 $s_{1/2}$	100	44	30±10
	120—122	1 $h_{11/2}$	58	30	15±10
	122—124	1 $h_{11/2}$	58	30	15±10
⁵⁶ Ba	134—136	1 $h_{11/2}$	82	44	44±9
	136—138	1 $h_{11/2}$	82	44	67±13
⁵⁴ Xe	132—134	1 $h_{11/2}$	70	38	18±4
	134—136	1 $h_{11/2}$	70	38	26±6

Footnote. C_T is the theoretical value of the isotope shift constant, C^I is the value of C_T obtained from the first iteration of Eq. (2); the experimental data are taken from^[1]. The results for the $1g_{7/2}$ state of Sn⁵⁰ are given to illustrate the possibility of improving the fit of the theoretical values of C_T to experiment by including the pair correlation.

are observed. The results of calculations for such isomers are given in Table II.

For isomers studied by the Mössbauer effect it is difficult to give a unique assignment of the states. But from the calculations of $\Delta\langle R^2 \rangle$ one can get information about the nature of the states if one has reliable experimental values of $\Delta\langle R^2 \rangle$. For these nuclei $\Delta\langle R^2 \rangle$ should be obtained by using formula (10), i.e., taking account of the redistribution of the nucleons over all levels near the Fermi surface.

Finding n_λ and \tilde{n}_λ requires the solution of the system of equations for Δ_λ (cf.^[2]). The approximation $\Delta_\lambda \equiv \Delta$, it seems, will be unsatisfactory here. For example in this approximation Δ for the excited state is greater than for the ground state.^[10] Therefore, in calculating $\Delta\langle R^2 \rangle$ the assumption was made that in the excited state of the nucleus the only occupation numbers that are changed are those for the states λ_0 and λ_1 . Then

from the condition of conservation of nucleons we get

$$\sum_m (n_{n_0 l_0 j_0 m} - \tilde{n}_{n_0 l_0 j_0 m}) = \sum_m (\tilde{n}_{n_1 l_1 j_1 m} - n_{n_1 l_1 j_1 m}) = \xi, \quad (13)$$

where ξ characterizes the number of "redistributed" nucleons. Expression (10) changes to

$$\Delta\langle R^2 \rangle = a\xi(\mathcal{F}_{\lambda_1 \lambda_1} - \mathcal{F}_{\lambda_0 \lambda_0}), \quad (14)$$

where $\xi = 1$ corresponds to a particle transition and $\xi = -1$ to a hole transition.

The results of computations for these isotopes when $|\xi| = 1$ are shown in Table III.

We note that in general the number of redistributed nucleons is different from unity, so that the values of $\Delta\langle R^2 \rangle$ given in Table III correspond only to the limiting case of strict single-particle transitions. Although in finding ξ the dependence of Δ_λ on λ is important, still in evaluating ξ for the transitions considered here one can assume that

Table II. Isomer Shift Constant

Isotope	λ_0	λ_1	ΔE , keV	τ	C , 10^{-3} cm $^{-1}$	$C_{s.p.}$, 10^{-3} cm $^{-1}$
$^{30}\text{Zn}^{69}$	$2p_{1/2}$	$1g_{7/2}$	436	13.8 h	-3	4
$^{36}\text{Kr}^{85}$	$-1g_{7/2}$	$-2p_{1/2}$	305	4.4 h	-4	6
$^{38}\text{Sr}^{87}$	$-1g_{7/2}$	$-2p_{1/2}$	390	2.8 h	-4	8
$^{39}\text{Y}^{87}$	$2p_{1/2}$	$1g_{7/2}$	384	14 h	+2	23
$^{39}\text{Y}^{89}$	$2p_{1/2}$	$1g_{7/2}$	913	14 sec	+2	23
$^{39}\text{Y}^{91}$	$2p_{1/2}$	$1g_{7/2}$	555	51 min	+2	23
$^{40}\text{Zn}^{89}$	$-1g_{7/2}$	$-2p_{1/2}$	588	4.4 min	-4	8
$^{48}\text{Cd}^{113}$	$3s_{1/2}$	$1h_{11/2}$		5.1 y	-10	19
$^{49}\text{In}^{113}$	$-1g_{7/2}$	$-2p_{1/2}$	390	1.73 h	-7	+48
$^{49}\text{In}^{115}$	$-1g_{7/2}$	$-2p_{1/2}$	335	4.5 h	-7	+48
$^{52}\text{Te}^{127}$	$-2d_{3/2}$	$-1h_{11/2}$	88,5	113 d	3	-20
$^{52}\text{Te}^{129}$	$-2d_{3/2}$	$-1h_{11/2}$	106	34 d	3	-20
$^{52}\text{Te}^{133}$	$-2d_{3/2}$	$-1h_{11/2}$	300	63 min	3	-20
$^{54}\text{Xe}^{133}$	$-2d_{3/2}$	$-1h_{11/2}$	232	2.3 d	4	-24
$^{54}\text{Xe}^{135}$	$-2d_{3/2}$	$-1h_{11/2}$	520	15.3 min	4	-24
$^{56}\text{Ba}^{135}$	$-2d_{3/2}$	$-1h_{11/2}$	269	28.7 h	5	-28
$^{56}\text{Ba}^{137}$	$-2d_{3/2}$	$-1h_{11/2}$	661	2.6 min	5	-28

Footnote. λ_0 is the ground state, λ_1 is the isomeric state, ($-\lambda$ denotes a hole state), ΔE is the transition energy, τ the lifetime of the isomeric state. The last column gives the single-particle estimate of C based on the radial moments from^[9]. The effective charge of the neutrons was set equal to Ze/A .

Table III.

Isotope	λ_0	λ_1	Q_T , b	Q_T^* , b	Q_{exp}	Q_{exp}^*	ΔE , keV	τ , 10^{-9} sec	$10^2 \left(\frac{\Delta \langle R^2 \rangle}{R^2} \right)_T$	$10^2 \left(\frac{\Delta \langle R^2 \rangle}{R^2} \right)_{s.p.}$
$^{28}\text{Ni}^{61}$	$2p_{3/2}$	$1f_{7/2}$	-0.14	-0.13			68	5.2	-15	25
$^{30}\text{Zn}^{67}$	$-1f_{7/2}$	$-2p_{3/2}$	0.10	0.11	0.16		93	9500	-16	25
$^{50}\text{Sn}^{119}$	$3s_{1/2}$	$2d_{3/2}$	0	-0.10	0	-0.08	24	18	-2.5	4
$^{52}\text{Te}^{125}$	$-3s_{1/2}$	$-2d_{3/2}$	0	0.16	0	0.20	35	1.4	2.8	-4
$^{53}\text{I}^{129}$	$1g_{7/2}$	$2d_{3/2}$	-0.30	-0.36	-0.50	-0.69 ^[13]	27	10	15	-40
$^{54}\text{Xe}^{129}$	$3s_{1/2}$	$2d_{3/2}$	0	-0.13	0	± 0.48 ^[14]	40	0.7	-2	3
$^{54}\text{Xe}^{131}$	$2d_{3/2}$	$3s_{1/2}$	-0.13	0	-0.12		80	0.3	2	-3

Here Q and Q^* are the quadrupole moments of the ground and excited states, $-\lambda$ denotes a hole state. The last column gives single-particle estimates based on the radial moments from^[9], with the effective charge of the neutrons set equal to Ze/A . Unless otherwise stated, the experimental data are from^[11]. The subscripts exp denote experimental and T theoretical values.

$\Delta_\lambda \equiv \Delta$ and that Δ is the same for the ground and excited states. With these assumptions we find for transitions with $\Delta E \ll \Delta$:

$$\xi = u_{\lambda_0}^2 - v_{\lambda_0}^2, \quad v_{\lambda^2} = 1/2 [1 - \epsilon_\lambda / (\Delta^2 + \epsilon_\lambda^2)^{1/2}],$$

$$u_{\lambda^2} + v_{\lambda^2} = 1. \quad (13')$$

Evaluation of (13') gives $\xi \sim 1/2$.

DISCUSSION OF RESULTS

Comparison of the theoretical values of C with experimental data for the isotope shift shows that the values of f^{pp} and f^{np} obtained^[8] from the analysis of quadrupole moments give a satisfactory explanation of the isotope shift. One can improve the agreement between the theoretical and experimental values of C if one takes account of the

“smearing out” of the added neutrons over different states λ , i.e., if one takes account of pair correlations. In Table I, to illustrate this possibility we give values of $\mathcal{F}_{\lambda\lambda}^{\text{np}}$ for all the values of λ entering in the shell of Sn^{119} which is being filled. Comparison of the exact solution of (6) with the first iteration shows that in finding $\Delta \langle R^2 \rangle$ one cannot stop at the first iteration, since it gives much too high results.

Going on to a discussion of isomers, we note that the accuracy in the computation of $\Delta \langle R^2 \rangle$ is lower for proton transitions than for neutron transitions, since for proton transitions $\Delta \langle R^2 \rangle$ involves, in addition to the difference of the integral terms, the difference of the individually large single particle matrix elements $r_{\lambda\lambda}^2$. Thus the accuracy of the calculation depends essentially on how accurately the single-particle scheme gives the

relative change of $r_{\lambda\lambda}^2$ for different states. Calculations of the isomer shift constants (Table II) lead to the conclusion that the experimental detection of the effect for these isomers by optical methods would be difficult, since the magnitude of the effect is at the limit of feasibility.^[12] For nuclei which can be studied by the Mössbauer effect there is a great deal of (partially contradictory) data on the isomer shift. Let us discuss these nuclei in more detail.

In order to characterize the isomeric transitions we have used, in addition to the spin of the excited state and the type of transition, data on the magnitudes and signs of the quadrupole moments Q and Q^* in the ground and excited states. Comparison of the experimental values of the quadrupole moments with single-particle estimates and computations of Q and Q^* assuming a particle (hole) state give additional information about the nature of the states and permit one to judge how good the single-particle assumption is. Depending on the signs of Q and Q^* , the transitions are interpreted either as particle or hole. Negative signs correspond to particle and positive signs to hole transitions.

Let us consider some examples:

$^{28}\text{Ni}^{61}$. The spins and parities of the ground and excited states are $3/2^-$ and $5/2^-$, M1 transition. There are no data on the quadrupole moment. In accordance with the single-particle level scheme, this is a particle transition. $\Delta\langle R^2 \rangle/R^2 = -1.5 \times 10^{-3}$.

$^{30}\text{Zn}^{67}$. Spins $5/2^-$, $1/2^-$, M1 transition; $Q = 0.18$ b, which is about twice the single-particle estimate. According to the single-particle level scheme this is a hole transition, $\Delta\langle R^2 \rangle/R^2 = -1.6 \times 10^{-3}$.

$^{50}\text{Sn}^{119}$. Spins $1/2^+$, $3/2^+$, M1 transition; $Q = 0$, $Q^* = -0.08$ b,^[13] of the order of the single-particle estimate (-0.11 b). We regard this as a particle transition. $\Delta\langle R^2 \rangle/R^2 = -2.5 \times 10^{-4}$. This result is in contradiction to the data of Shirley,^[4] who gives a preliminary value of $+1.2 \times 10^{-4}$.

$^{52}\text{Te}^{125}$. Spins $1/2^+$, $3/2^+$, M1 transition; $Q = 0$, $Q^* = 0.20$ b,^[14] which is twice the single particle estimate (0.11 b). This is classified as a hole transition. $\Delta\langle R^2 \rangle/R^2 = 2.8 \times 10^{-4}$, which agrees with Shirley^[4] in order of magnitude, his preliminary value being $\sim 8 \times 10^{-4}$.

$^{53}\text{I}^{129}$. Spins $7/2^+$, $5/2^+$; $Q = -0.5$ b, $Q^* = -0.69$ b.^[15] The quadrupole moments are three times the single-particle values (-0.18 b). In this nucleus we are treating a transition of an odd proton. In accordance with the signs of the quadrupole moments this is classified as a particle transition. We get an interesting result for I^{129} . If we calculate $\Delta\langle R^2 \rangle$ from the shell model we get a negative

value, which is in contradiction with the experimental data.^[15] Including interactions changes the sign, with $\Delta\langle R^2 \rangle/R^2 = 1.5 \times 10^{-3}$.

$^{54}\text{Xe}^{129}$. Spins $1/2^+$, $3/2^+$, M1 transition; $Q = 0$, $|Q^*| = 0.48$ b.^[16]

$^{54}\text{Xe}^{131}$. Spins $3/2^+$, $1/2^+$, M1 transition; $Q = -0.12$ b, $Q^* = 0$. The single-particle estimate gives $Q = -0.11$ b.

In both the Xe isotopes the transition is classified as particle. The values found for $\Delta\langle R^2 \rangle/R^2$ are equal and opposite, -2×10^{-4} for Xe^{129} and $+2 \times 10^{-4}$ for Xe^{131} .

We note that the values given for $\Delta\langle R^2 \rangle/R^2$ are obtained without making use of the picture of a deformation of the nucleus as a whole.

Comparison of the calculations with single-particle estimates (cf. Tables II and III) shows that the effective charge approximation is completely inapplicable to the problem of the isomer shift. Thus, for neutron transitions this approximation even gives the wrong sign for $\Delta\langle R^2 \rangle$. For isomers with proton transitions, including the interaction of the odd proton with the core is also extremely important: the magnitude of the effect is much less than the single-particle estimate. Sometimes one may find the situation already cited for I^{129} —the single-particle estimates give the wrong sign for $\Delta\langle R^2 \rangle$. In these cases the effect associated with the polarization of the core by the proton is larger than the effect produced by the proton itself.

In conclusion I express my gratitude to Prof. A. B. Migdal for his interest in the work and thank M. O. Mikulinskiĭ for valuable discussions.

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Translated by M. Hamermesh

110