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ISOTOPE AND ISOMER SHIFTS IN MERCURY[†]

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Abstract: Calculations have been made of the change in the mean square charge radius of the mercury isotopes which results when a neutron is added to an even-even core. Both the ground and isomeric states of the odd-A isotopes were considered. First-order perturbation theory was used to obtain the amplitudes of monopole excitations of the proton core. The calculations were carried out by first assuming a conventional neutron-proton force, and then using various density-dependent interactions. The results show a very marked A-dependence and achieve partial success in explaining the experimental shifts in the optical spectra.

[†] Work performed under the auspices of the U. S. Atomic Energy Commission.

1. Introduction

A number of experiments have been carried out in recent years to measure the optical spectra in sets of isotopes¹). Some of the measurements on odd-N isotopes have been made with the nucleus in an isomeric state, as well as the ground state. Theoretical aspects of these spectra have been described by a number of authors²⁻⁵). In heavy nuclei the differences between these spectra are due mainly to the finite charge distribution of the nucleus²⁻⁵), and these differences are proportional to the changes which occur in the mean square radius of the protons[†]. (For odd-A isotopes we assume that the statistically-weighted mean of each multiplet has been taken.)

[†]The changes arise almost entirely from changes in the electron-nucleus Coulomb energy of s-electrons. If we use point-nucleus wave functions, then for a given s-electron this Coulomb energy is proportional to $[\overline{r_p^{2\rho}}/2\rho(2\rho+1)] + C$, where C is independent of the nuclear radius. Here $\rho = (1-\alpha^2)^{1/2}$, where α is the fine-structure constant. If, on the other hand, we use electron wave functions appropriate to a finite nucleus, then the Coulomb energy is proportional to $[(5/3)\overline{r^2}]^\rho/10 + C$. A full treatment of this effect has been given by Bodmer⁶). The author is grateful to Professor L. Wilets and A. S. Reiner for discussions on this point.

In the mercury isotopes a feature of the experimental results is the fact that the change in the spectrum which occurs when a pair of neutrons is added to an even-N isotope is approximately independent of N, whereas the change which results when a single neutron is added (with the odd-N nucleus in the ground state) varies with N and is, in some cases, considerably less than half the change which results from adding a pair of neutrons. This is known as the odd-even staggering effect¹⁻⁵). The change in the spectrum which occurs when the nucleus is excited from the ground state to an isomeric state is the isomer shift.

There are various mechanisms by which the addition of one or more neutrons can contribute to the changes in the proton wave functions. If a single-particle model is used for the proton wave functions then the neutron-proton force will cause monopole, quadrupole, and higher multipole excitations of the core. Here we shall consider only the first-order effects (i. e., monopole excitations). An additional effect, which is not considered here, results from the modification of the pairing correlations in the proton wave functions caused by changes in the proton single-particle energy levels due to the neutron-proton interaction.

The effect on the proton wave functions of a neutron in a particular orbital depends on the quantum numbers of the orbital. Because of pairing correlations⁷⁻¹⁰) in the neutron wave functions it is, in general, not valid to assume that a neutron can be added into one particular orbital. Instead, the changes in the average number of particles in each of the neutron orbitals near the top of the Fermi sea must be calculated. These changes can then be combined with the results of the perturbation theory calculations to give the isotope and isomer shifts.

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2. Formulation of the Model

The method used to describe the excitation of the core is the particle-hole formalism of Brown^{11, 12}). We assume that the protons form a core, the ground state of which is the vacuum, and we define particle creation and annihilation operators $a_{am}^\dagger$ and a_{am} , where a represents the quantum numbers $n\ell j$, which describe the shell model state, and m is the projection of the angular momentum j on the z -axis. We shall use the following convention with regard to the labels $n\ell jm$ (and am): labels without a subscript refer to neutron states; labels with subscript 1 refer to proton states below the Fermi surface; labels with subscript 2 refer to proton states above the Fermi surface. We represent states of the neutron together with core excitations of angular momentum L by the state vector

$$|a_1 a_2 a' L; jm\rangle = \sum_{m_1 m'} (-1)^{j_1 - m_1} (j_1 - m_1 j_2 m_2 | LM) (j' m' LM | jm) \times a_{a'm'}^\dagger a_{a_2 m_2}^\dagger a_{a_1 m_1} |0\rangle, \quad (1)$$

and the energy of the state is written as $E_{a_1 a_2 a'}$. If the core is in the ground state, we write the state vector as $|00a0; jm\rangle$. The correlated state with angular momentum jm is then given by

$$|jm\rangle = |00a0; jm\rangle + \sum_{a_1 a_2} \sum_{a' L} B_{a_1 a_2 a' L} |a_1 a_2 a' L; jm\rangle. \quad (2)$$

We define the Hamiltonian for the system consisting of the proton core and the last odd neutron to be

$$\mathcal{H} = \mathcal{H}^0 + V, \quad (3)$$

where V represents the neutron-proton interaction. The coefficients B are then given by

$$B_{a_1 a_2 a' L} = \langle a_1 a_2 a' L; jm | V | 00 a 0; jm \rangle / (E_{00 a} - E_{a_1 a_2 a'}). \quad (4)$$

For convenience we omit the subscripts jm on the B 's. The mean square proton radius is given by

$$\overline{r_p^2} = \langle jm | \frac{1}{Z} \sum r_p^2 | jm \rangle, \quad (5)$$

where the summation is over the Z protons. Substituting from eq. (2) we obtain, to first order in V ,

$$\begin{aligned} \overline{r_p^2} &= \frac{1}{Z} \langle 00 a 0 | \sum r_p^2 | 00 a 0 \rangle \\ &+ \frac{2}{Z} a_1 a_2 \sum_{a' L} B_{a_1 a_2 a' L} \langle 00 a 0; jm | \sum r_p^2 | a_1 a_2 a' L; jm \rangle \\ &= \frac{1}{Z} a_1 \sum_{m_1} \langle a_1 m_1 | r^2 | a_1 m_1 \rangle \\ &+ \frac{2}{Z} a_1 a_2 \sum B_{a_1 a_2 a 0} (2j_1 + 1)^{1/2} \langle a_1 || r^2 || a_2 \rangle, \end{aligned} \quad (6)$$

where the reduced matrix element $\langle a_1 || r^2 || a_2 \rangle$ is equal to the matrix element $\langle a_1 m_1 | r^2 | a_2 m_2 \rangle$ itself since r^2 has no angular dependence. We note that this lack of angular dependence means that to first order in V only the monopole excitations contribute to the expectation value of r_p^2 . For $L=0$ the amplitudes B reduce to a particularly simple form given by

$$B_{a_1 a_2 a' 0} (E_{00a} - E_{a_1 a_2 a'})$$

$$= \delta_{aa'} \delta_{j_1 j_2} \delta_{m_1 m_2} (2j_1 + 1)^{1/2} \langle 0 | a_{a_1 m_1}^\dagger a_{a_2 m_2} a_{a' m'} V_0 a_{am}^\dagger | 0 \rangle, \quad (7)$$

where V_0 is the monopole part of V . Putting

$$V_0 = \frac{1}{2} \sum_{k_1 k_2 k_3 k_4} \langle k_1 k_2 | V_0 | k_3 k_4 \rangle a_{k_2}^\dagger a_{k_1}^\dagger a_{k_3} a_{k_4}, \quad (8)$$

we obtain the two types of matrix elements which are represented diagrammatically in fig. 1. We shall neglect the exchange terms in eq. (7) (since we are dealing with short-range forces) so that we obtain finally

$$B_{a_1 a_2 a' 0} (E_{00a} - E_{a_1 a_2 a'})$$

$$= \delta_{aa'} \delta_{j_1 j_2} \delta_{m_1 m_2} (2j_1 + 1)^{1/2} \langle a m a_1 m_1 | V_0 | a' m a_2 m_2 \rangle. \quad (9)$$

The Kronecker deltas in eq. (9) restrict the contributing particle-hole excitations to those in which a proton is excited by two major shells (increasing n by 1, but keeping the same value of ℓ and j) while the neutron state remains unchanged ($a' = a$).

The second term in eq. (6) represents the change in $\overline{r_p^2}$ which results when the occupation number of the neutron state am is increased by unity. Near the top of the Fermi sea, however, the states of particles in a nucleus are modified by pairing correlations⁷⁻¹⁰). When an odd particle is added, one of the pairs of states which was previously available becomes blocked and all the particles are rearranged. When pairing correlations are taken into account the ground state of the neutrons in an even- N isotope may be written

$$|\tilde{0}\rangle = \prod_{a,m>0} (U_a + V_a a_{am}^\dagger a_{a-m}^\dagger) |0\rangle. \quad (10)$$

For an odd-N isotope the state of angular momentum $j m$ is

$$(U_a a_{am}^\dagger - V_a a_{a-m}) |\tilde{0}\rangle. \quad (11)$$

The U 's and V 's must be calculated for each value of the neutron number N and, in the case of odd- N , for each value of the spin of the nucleus. These wave functions have a disadvantage for isotope shift calculations in that they do not represent a fixed number of particles. This difficulty can be overcome by projecting out the components which do represent a fixed number of particles. Details of this projection have been given previously^{13,14}).

3. Results

The first calculations were done by using harmonic-oscillator wave functions, both with a zero-range and with a finite-range neutron-proton force. Subsequently the nucleon wave functions were taken to be those of a Woods-Saxon potential^{15,16}). In the zero-range, harmonic-oscillator case, it was possible to write down the matrix elements and amplitudes in closed form. For the finite-range force a Gaussian shape was assumed, and the integrals were calculated numerically on a computer. As a check a calculation was carried out with a range of 0.05fm and the results were found to agree to within 0.1% of the zero-range results. A second computer code was written, using an iterative procedure, to obtain the eigenfunctions in a Woods-Saxon potential.[†] Both codes were written in Fortran II and run on the Columbia University and the Lawrence Radiation Laboratory IBM 7094 computers.

[†]This was based on a method described in ref. ¹⁷).

The results for the change in $\overline{r_p^2}$ which occurs when a neutron is added in various states is shown in Table 1. For the proton wave functions a nuclear potential of Woods-Saxon shape was used, i. e., $V(r) = - \{1 - \exp[(r-r_0 A^{1/3})/a]\}^{-1}$, with $V = 80$ MeV, $r_0 = 1.2$ fm, $a = 0.65$ fm. The Coulomb potential used was that due to a uniformly charged sphere of radius $r_0 A^{1/3}$. For neutrons, r_0 and a were unchanged, with $V = 45$ MeV. The spin orbit force was taken to be 39.5 times the Thomas potential¹⁸). The neutron-proton force was of the form

$$V\left(\begin{smallmatrix} r \\ \underline{m}_n, \underline{m}_p \end{smallmatrix}\right) = f\left(\left|\frac{\underline{r}_n + \underline{r}_p}{2}\right|\right) V \exp\left(-\left|\underline{r}_n - \underline{r}_p\right|^2/\beta^2\right), \quad (12)$$

with $V = -0.625 \times 32.5$ MeV and $\beta = 1.8$ fm¹⁹). The four shapes of f which were used are shown in fig. 2; f_I is the conventional density-independent force; f_{II} has a nuclear-density dependent which is given by $f(x) = c_1 - c_2 \{1 - \exp[(r-R)/a]\}^{-1}$, where R and a are the same as in the nuclear potentials²⁰). The values of c_1 and c_2 are 3.6 and -4.2 respectively. In f_{III} , c_2 is changed to -3.6; f_{IV} has the shape $[c_1 + c_2(r/R)]/c_1 + c_2$, with $c_1 = 1$ and $c_2 = 0.5$.

An example of the wave functions used in the calculation of two particular matrix elements is shown in fig. 3(a). Fig. 3(b) shows why it happens that for a conventional (attractive) force, a 1i neutron causes a negative matrix element while a 3p neutron causes a positive matrix element. Moreover it is easy to see how a force which is repulsive near the centre of the nucleus results in a change in the sign of the matrix element for the case of the 3p neutron.

The numbers of neutrons in different shell-model states of Hg are plotted against N in fig. 4. The discontinuities in slope of the ground-state

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curves occur when the ground-state spin changes.

Table 2 shows the change in the number of neutrons in each orbital which results when the neutron number is changed. These results were obtained by using values of U_j and V_j calculated with a computer programme of G. Struble. The pairing force G was taken to be 0.11 MeV and the single-particle energies were the same as those used by Kisslinger and Sorensen¹⁰).

Using the numbers in Tables 1 and 2 we obtain the isotope shifts shown in figs. 4 and 5. Fig. 6 shows the isomer shift. In converting the line shifts to changes in nuclear radius, the electron wave functions used were taken from a relativistic self-consistent calculation of Cohen^{22, 23}). Since this calculation was carried out for a point-charge nucleus, the wave functions were multiplied by a correction factor for finite charge distributions given by Bodmer⁶).

4. Conclusions

The calculations show that the monopole excitations of the proton core produce a large change in the radius. Both the conventional density-independent force and the linearly varying force (IV) give the wrong sign for the isotope and the isomer shifts. The Migdal force (II) and the modified Migdal force (III) give the right sign for the isotope shift but only the former will reproduce the positive isomer shift for ¹⁹⁷Hg. It is in the isomer shift that these calculations are expected to be most reliable, since the particle number is not changed. The numbers in Table 2 could also be used to obtain the shift corresponding to the addition of a pair of neutrons to an even-N nucleus. The resultant shifts are less than twice the shift due to adding a single neutron (whereas the experimental ratios are usually greater than two).

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This indicates that there are non-negligible contributions which have been ignored here.

Although the whole picture of isotope shifts has not yet been satisfactorily explained, these calculations do show how it is possible to achieve an A-dependence and do reproduce the puzzling change in the sign of the isomer shift which occurs at about $A = 195$. It is apparent that the monopole excitations contribute significantly to the isotope shift and that they must be taken into account in any complete explanation of the phenomenon.

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Table 1
Change in $\overline{r_p^2}$ caused by adding a neutron (in fm²)

State of added neutron	Force I	Force II	Force III	Force IV
$1i_{13/2}$	0.025	0.054	0.059	0.028
$3p_{3/2}$	-0.131	0.128	0.045	-0.096
$2f_{5/2}$	-0.085	0.103	0.046	-0.063
$3p_{1/2}$	-0.127	0.127	0.043	-0.093

Table 2

(a) Average change in occupation of different subshells caused by adding an odd neutron

Neutron subshell	Mass number of resultant isotope											
	193	193*	195	195*	197	197*	199	199*	201	201*	203	203*
13/2	0.35	0.74	0.16	-0.09	0.12	-0.54	0.08	-0.74	0.15	-0.83	0.12	-0.88
3/2	0.75	0.16	-0.04	0.63	0.02	0.81	0.09	0.75	-0.18	0.59	0.49	0.48
5/2	-0.09	0.10	-0.08	0.46	-0.09	0.71	-0.10	0.98	1.05	1.24	0.45	1.41
1/2	-0.01	0.00	0.97	0.01	0.95	0.01	0.93	0.01	-0.02	0.00	-0.07	-0.01
Nuclear spin	3/2	13/2	1/2	13/2	1/2	13/2	1/2	13/2	3/2	13/2	5/2	13/2

(b) Average change in occupation of different subshells caused by adding a pair of neutrons.

Neutron subshell	Mass number of resultant isotope					
	194	196	198	200	202	
13/2	1.44	0.71	0.35	0.20	0.14	
3/2	0.29	0.68	0.80	0.71	0.57	
5/2	0.26	0.60	0.83	1.07	1.27	
1/2	0.01	0.02	0.02	0.02	0.02	

Figure Captions

Fig. 1. Diagrammatic representation of the matrix elements in eq. (7).

Fig. 2. Shapes of density-dependent factor in eq. (12).

Fig. 3. (a) shows four of the shell-model wave functions used in the calculation of the matrix elements of V . From the top downwards they are: $R_{2p}^{(p)}$ and $R_{3p}^{(p)}$ for protons and $R_{1i}^{(n)}$ and $R_{3p}^{(n)}$ for neutrons. (b) shows the functions $R_{2p}^{(p)} R_{3p}^{(p)} (R_{1i}^{(n)})^2 / r^2$ and $R_{2p}^{(p)} R_{3p}^{(p)} (R_{3p}^{(n)})^2 / r^2$, which are the corresponding integrands for the matrix elements of V in the case of a zero-range neutron-proton force.

Fig. 4. The numbers of particles, n_j , in the $j = 13/2$, $j = 3/2$, $j = 5/2$ and $j = 1/2$ subshells for different Hg isotopes.

Fig. 5. Curves showing theoretical isotope shifts for odd Hg isotopes, both for the case of a conventional force (f_I) and for a density-dependent-dependent neutron-proton force (f_{II}). The isomeric states have spin $13/2$ and the spins of the ground states are given in Table 2. The experimental points are from ref. ¹).

Fig. 6. Theoretical isotope shifts calculated using density-dependent factors f_{III} and f_{IV} .

Fig. 7. Isomer shifts for odd Hg isotopes. The crosses represent experimental values taken from ref. ¹). The full circles are values from ref. ²¹).

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Fig. 1

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Fig. 2

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Fig. 3

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Fig. 4

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Fig. 5

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Fig. 6

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Fig. 7

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