Neutron $d_{5/2}{}^n$ Configurations in Zr Isotopes*

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(Received January 17, 1962)

Energy levels of neutron $2d_{\frac{5}{2}}{}^n$ configurations are analyzed by shell model methods. Good agreement is obtained between experimental and calculated energies. The position of the $3/2^+$ level in Zr^{93} is predicted on the basis of this analysis. The energies of these configurations to which a $2p_{\frac{1}{2}}$ is added (in Y isotopes) are also considered by using a closed formula for the energies of j^nj' configurations, with $j'=\frac{1}{2}$, derived in the Appendix.

I. INTRODUCTION

STRONG evidence was recently presented[1] for rather pure $d_{5/2}{}^n$ configurations of neutrons beyond the magic number 50. The evidence, which comes from the analysis of (d,p) and (d,t) reactions, shows that the ground states of Zr^{91} to Zr^{96} belong predominantly to $d_{5/2}{}^n$ configurations. The wave functions of these states contain at most a few percent admixtures of other configurations. The reason for this behavior is clearly demonstrated in reference 1. It is shown there that the single neutron $2d_{5/2}$ level is sufficiently removed from other single-neutron states. For example, in Zr^{91},[2] the $3s_{1/2}$ state lies 1.215 Mev above the $2d_{5/2}$ ground state. The next single-neutron state is the $2d_{3/2}$ at 2.07 Mev and the $1g_{7/2}$ is even higher, at 2.19 Mev above the ground state.

Similar information from stripping reactions exists also about excited states in this region. It was found by $Zr^{91}(d,p)Zr^{92}$ stripping that the 2^+ level at 0.93 Mev belongs to the rather pure $d_{5/2}{}^2$ configuration.[3] In fact, no $l=0$ contribution to the stripping was observed, although this is allowed by the selection rules. The same conclusion about this 2^+ level as well as about the 4^+ level (at 1.49 Mev) of Zr^{92} was obtained in a recent paper.[4]

It is therefore interesting to see whether the energies of the levels observed agree with those predicted for $d_{5/2}{}^n$ configurations. There are enough experimental data available to check the consistency of such a configuration assignment. If we find good agreement between theory and experiment the positions of other levels of $d_{5/2}{}^n$ configurations can be predicted. We consider the neutrons outside the closed shells of 50. We take the proton configuration of the Zr isotopes to be that of closed shells. Strictly speaking, if we consider 38 protons to be in closed shells, the two extra protons are only about 75% in the (closed) $p_{1/2}$ orbit (and the rest in the $g_{9/2}$ orbit).[5] Still, the excitation energy of the 40 protons in Zr^{90} is so high that they can be considered as forming closed shells. It would be interesting to carry out a similar analysis of the Sr isotopes beyond Sr^{88}. Unfortunately, not enough experimental data are known on the spectra of these nuclei.

The $d_{5/2}{}^n$ configurations (of identical particles) are simple enough so that their energies can be expressed in terms of the $d_{5/2}{}^2$ energies, by a closed formula. This formula is derived, using a method due to Racah,[6] in a recent paper.[7] The neutron $d_{5/2}{}^n$ configurations in the oxygen isotopes were recently treated with the help of this closed expression.[8] The results in the present case turn out to be very similar to those obtained for the oxygen isotopes. The situation in the Zr isotopes seems to be more favorable for pure $d_{5/2}{}^n$ configurations. In O^{17} the first-excited single-neutron state is the $2s_{1/2}$ level at 0.87 Mev. This separation is considerably smaller than the corresponding 1.22-Mev separation in Zr^{91}. Moreover, the $d_{5/2}-s_{1/2}$ separation should be compared with the matrix elements which give rise to configuration interaction. The interaction between the outer nucleons in O^{18}, for instance, is far stronger than that in Zr^{92}. This is due to the fact that the $2d_{5/2}$ neutrons in the Zr isotopes are on the average much farther apart than the $1d_{5/2}$ neutrons in the O isotopes. An indication of this effect can be obtained by comparing the interaction energy in the $d_{5/2}{}^2$, $J=0$ state in the O isotopes (about 4 Mev) to that in the Zr isotopes. In Sec. III we shall see that the latter $d_{5/2}{}^2$, $J=0$ interaction energy is only about 1.5 Mev. Therefore, we expect to find rather pure $d_{5/2}{}^n$ configurations in the Zr isotopes as actually demonstrated by the experimental data.

II. ENERGIES OF $d_{5/2}{}^n$ CONFIGURATIONS

The energy of a state in the $d_{5/2}{}^n$ configuration with spin J and seniority v is given by[7]

$$nC+\frac{n(n-1)}{2}a+\left[J(J+1)-\frac{35}{4}n\right]b+\frac{(n-v)(8-n-v)}{2}c. \quad (1)$$

* This work was supported by the U. S. Atomic Energy Commission and the Higgins Scientific Trust Fund.
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In this expression, C is the single $d_{5/2}$ neutron energy. It is equal to the sum of the kinetic energy and interaction with the closed shells of a $d_{5/2}$ neutron. The constants a, b, and c are certain linear combinations of the interaction energies, $V_J=V_J(d_{5/2}{}^2)$, in the $d_{5/2}{}^2$ configuration. They are uniquely determined from the following equations, obtained from Eq. (1) by putting $n=2$, $v=0$, $J=0$ and $n=2$, $v=2$, $J=2$ or 4.

$$\begin{aligned} V_0&=a-(35/2)b+6c,\\ V_2&=a-(23/2)b,\\ V_4&=a+(5/2)b. \end{aligned} \tag{2}$$

The spacings between energy levels, as given by Eq. (1), are determined from the values of b and c only. Therefore, if we know the positions of the $J=2$ and $J=4$ levels above the $J=0$ ground state of the $d_{5/2}{}^2$ configuration, we can calculate energy spacings in every case.

The levels of the $d_{5/2}{}^2$ configuration can be taken from Zr^{92}. The levels with $J=2$ and $J=4$ are 0.93 and 1.49 Mev, respectively, above the $J=0$ ground state. The $d_{5/2}{}^4$ configuration, expected in Zr^{94}, has two $d_{5/2}$ neutrons missing from the closed shell and is complementary to the $d_{5/2}{}^2$ configuration. This $d_{5/2}{}^{-2}$ configuration should have the same level spacings as the $d_{5/2}{}^2$ configuration as also follows from Eq. (1). In fact, the first-excited 2^+ level in Zr^{94} lies 0.92 Mev above the ground state.[9] The level at 1.47 Mev in that nucleus has been recently identified as a 4^+ level.[10] This agrees rather well with the corresponding 0.93 Mev and 1.49 Mev spacings in Zr^{92} and supports the configuration assignments.

More interesting is the $d_{5/2}{}^3$ configuration expected for Zr^{93}. There are three states in this configuration, the $J=5/2$ state with $v=1$ and the $J=3/2$, $9/2$ states with $v=3$. We take the values $V_0-V_2=0.93$ Mev and $V_0-V_4=1.49$ Mev from Zr^{92} (for convenience, we take the binding energies to be *positive* numbers). We then find from Eq. (1) that the ground state has $J=5/2$ and that the position of the $J=3/2$ level is given by

$$\begin{aligned} V(d_{5/2}{}^3, v=1, J=5/2)&-V(d_{5/2}{}^3, v=3, J=3/2)\\ &=5b+4c=1/42[55(V_0-V_2)-27(V_0-V_4)]\\ &=0.26\text{ Mev}. \end{aligned} \tag{3}$$

Turning now to the experimental data, we see that the ground state of Zr^{93} is indeed a $5/2^+$ state.[1,9] At 0.267 Mev above it there is a level with a probable $3/2^+$ assignment.[9] The energy spacing is in excellent agreement with the calculated value. The 0.267-Mev level is apparently not excited by a (d,p) stripping reaction. This is in agreement with its having the $d_{5/2}{}^3$ configuration and only a negligible amount of $d_{3/2}$ admixture. Another check on the purity of the configuration would be the lifetime of the $3/2^+$ level. No $M1$ transition can occur within the j^n configuration of identical particles[7] and therefore the $3/2^+\rightarrow 5/2^+$ $M1$ transition should be strongly attenuated (as in O^{19} or V^{51}).

The occurrence of a low lying state with $J=j-1$ (and $v=3$) in the j^3 configuration is a common feature of nuclear spectra. In O^{19} there is a similar low-lying $3/2^+$ level. Low-lying $5/2^+$ levels are found in $1f_{7/2}{}^3$ configurations and $7/2^+$ levels in $1g_{9/2}{}^3$ configurations. This phenomenon is due to the fact that the levels of the j^2 configuration are, more or less, evenly spaced. This is clearly demonstrated, for the present case, in Eq. (3). On the other hand, if short-range (δ-type) forces are used, the levels with seniority $v=2$ in the j^2 configuration are closely spaced and lie far above the $v=0$, $J=0$ ground state. The situation is even more drastic for a "pairing interaction" where all $v=2$ levels are degenerate. In the case of such interactions, all states with seniority $v=3$, of the j^3 configuration, including the $J=j-1$ state, lie closely, far above the $v=1$ $J=j$ ground state. In the present case of the $d_{5/2}{}^3$ configuration, a pairing interaction leads to degenerate $J=3/2$ and $J=9/2$ levels in addition to degenerate $J=2$ and $J=4$ levels of the $d_{5/2}{}^2$ configuration.

There is an additional level scheme from which it is possible to obtain a check on the configuration assignments of the $5/2^+$ ground state and $3/2^+$ state of Zr^{93}. If we consider the Y isotopes beyond Y^{89}, we expect to find a $p_{1/2}$ proton and a $d_{5/2}{}^n$ neutron configuration outside closed shells. It is shown in the Appendix that the eigenstates of such configurations are characterized by the quantum numbers J_0 and J, where J is the total spin and J_0 is the spin of a state of the $d_{5/2}{}^n$ configuration. The $p_{1/2}-d_{5/2}$ interaction energy is completely determined by J_0 and J and states with different values of J_0 do not interact even if they have the same value of J. If there is only one $d_{5/2}$ neutron there are two states of the $p_{1/2}d_{5/2}$ configuration with spins 2^- and 3^-. These two states are actually observed in Y^{90}, the 2^- is the ground state and the 3^- state lies 0.20 Mev above it.[9] In Y^{92} there are three $d_{5/2}$ neutrons which have $J_0=5/2$ in their ground state. Therefore, the order and spacing of the two states of $p_{1/2}d_{5/2}{}^3$ $(J_0=5/2)$, with spins 2^- and 3^-, should be the same as in Y^{90}. The two states built on the first-excited state of the $d_{5/2}{}^3$ configuration, with $J_0=3/2$, have spins 1^- and 2^-. The interaction energy in all these states are obtained from (A5) and (A6) to be given, above the interaction in the $J_0=5/2$, $J=2$ state, by

$$J_0=5/2,\ J=3: 0.20\text{ Mev};\quad J_0=5/2,\ J=1: 0.03\text{ Mev};$$
$$J_0=5/2,\ J=2: 0.17\text{ Mev}.$$

In order to find the relative positions of these four states, the states with $J_0=3/2$ should be raised by 0.27 Mev which is the position of the parent state with $J_0=3/2$ of the $d_{5/2}{}^3$ configuration above the $J_0=5/2$ ground state.

We thus obtain that the ground state of Y^{92} should be the 2^- state with $J_0=5/2$. The next state should be the 3^- state (with $J_0=5/2$) at 0.20 Mev. The states

[9] *Nuclear Data Sheets*, National Academy of Sciences, National Research Council (U. S. Government Printing Office, Washington, D. C.).

[10] R. B. Day and D. A. Lind (to be published).

with $J_0=3/2$ should be higher: the 1^- state at $0.03+0.27=0.30$ Mev and the 2^- state at $0.17+0.24=0.44$ Mev. The ground state of Y^{92} is indeed a 2^- state. Excited states were observed at 0.23 Mev and 0.44 Mev above the ground state,[9] which agree very well with the predicted energies. It would be quite interesting to have spin assignments for these levels as well as to have more information on the possible existence of a 1^- state at 0.30 Mev so that comparison with the above predictions can be made.

Coming back to Zr^{93}, the position of the other state, with $J=9/2$, of the $d_{5/2}{}^3$ configuration is given by

$$V(d_{5/2}{}^3, v=3, J=3/2)-V(d_{5/2}{}^3, v=3, J=9/2) = -21b=\tfrac{3}{2}(V_2-V_4)=0.83 \text{ Mev}. \quad (4)$$

Therefore, the $9/2^+$ level is expected to lie about 1.1 Mev above the Zr^{93} ground state. No such possible level has been experimentally observed. Obviously, a level with such a high spin value would be impossible to obtain from beta decay of Y^{93} (with spin $1/2^-$). Further experiments are necessary in order to find the $9/2^+$ level in Zr^{93} and compare its position with the predicted one.

III. BINDING ENERGIES OF THE Zr ISOTOPES

No other excited states, apart from those considered above, exist in the $d_{5/2}{}^n$ configurations considered. In order to further determine the agreement between theory and experiment we must consider energies of ground states. The separation energies of the last neutron in the Zr isotopes considered here are known reasonably well experimentally. It is possible to check whether the experimental energies can be reproduced by the theoretical expression. In the case of ground states, with $v=0$, $J=0$ for n even and $v=1$, $J=j$ for n odd, Eq. (1) is simplified into

$$nC+\frac{n(n-1)}{2}(a-c)+[n/2][7c-(35/2)b]. \quad (5)$$

Here $[n/2]$, the largest integer not exceeding $n/2$, is a step function that gives the pairing term. The expression Eq. (5) is the sum of single nucleon energies and the mutual interaction of the $nd_{5/2}$ neutrons. It should be, therefore, equal to the difference in binding energies between the nucleus considered and Zr^{90} which contains closed shells only.

The values of the binding energies (over and above that of Zr^{90}) were obtained from recent papers.[11] These energies are listed in the second column of Table I. The numbers given are the binding energies of the nuclei considered minus the Zr^{90} binding energy. Unlike the total binding energies, these differences are known to better than 0.1 Mev. A least squares fit was carried out to determine the parameters, C, a–c and $7c-(35/2)b$ which best reproduce the experimental energies. These

[11] This information was received from Professor B. L. Cohen to whom the author is very grateful.

TABLE I. Experimental and calculated binding energies (in Mev).

Nucleus	Binding energy minus Zr^{90} binding energy: Experimental	Calculated
${}_{40}Zr_{51}{}^{91}$	7.25	7.28
${}_{40}Zr_{52}{}^{92}$	15.95	15.88
${}_{40}Zr_{53}{}^{93}$	22.75	22.80
${}_{40}Zr_{54}{}^{94}$	31.03	31.03
${}_{40}Zr_{55}{}^{95}$	37.55	37.57
${}_{40}Zr_{56}{}^{96}$	45.45	45.43

best values were substituted in Eq. (5) to give the calculated energies listed in the last column of Table I. The agreement between calculated and experimental energies is very good as seen by comparing the last two columns of Table I. The three theoretical parameters reproduce very accurately the six binding energy differences.

The best values of the single $d_{5/2}$ neutron energy and the interaction energies are:

$$C=7.28,\ a-c=-0.185,\ 7c-(35/2)b=1.50 \text{ Mev}. \quad (6)$$

The coefficient of the quadratic term in Eq. (5) turns out to be repulsive (negative in our convention) as it should be. This is the term that makes nuclei with more nucleons of the same kind less stable. The interaction energies in Eq. (6) are only two linear combinations of the three interaction energies V_0, V_2, and V_4. Therefore, they cannot be used to determine the positions of both $J=2$ and $J=4$ states above the $J=0$ ground state of the j^2 configuration. The parameters in Eq. (6) can determine only the position of the center of mass of the $J=2$ and $J=4$ levels. The comparison of this position, predicted from Eq. (6), with the actual spectrum of Zr^{92} gives an additional check on the configuration assignments.

From Eq. (1) follows the relation,

$$V_0-(1/14)[5V_2+9V_4] = (6/7)[7c-(35/2)b]=1.29 \text{ Mev}. \quad (7)$$

In Eq. (7), the value of $7c-(35/2)b$ taken from Eq. (6) was used. The position of the center of mass of the 2^+ and 4^+ levels above the ground state of Zr^{92} is $(5\times0.93+9\times1.49)/14=1.29$ Mev. The agreement between this position and the calculated value Eq. (7) is striking. The position of the corresponding center of mass in Zr^{94} turns out to be 1.27 Mev which agrees equally well with Eq. (7). This may show that in the cases where the agreement between experimental and calculated binding energy differences is good, some information on the excited states can be obtained. This information is limited, however, to the position of the center of mass of the $v=2$ levels.

APPENDIX. ENERGIES OF j^nj' CONFIGURATIONS WITH $j'=1/2$

The interaction energy between a j particle and the j' particle can be expanded in terms of scalar products

of irreducible tensor operators as follows:

$$V_{12}=F^0(\mathbf{u}_1{}^{(0)}\cdot\mathbf{u}_2{}^{(0)})+F^1(\mathbf{u}_1{}^{(1)}\cdot\mathbf{u}_2{}^{(1)}). \tag{A1}$$

In Eq. (A1) the $\mathbf{u}^{(k)}$ are any irreducible tensors of degree k. No higher values of k appear in the expansion Eq. (A1) since k must satisfy $0\leq k\leq 2j$ as well as $0\leq k\leq 2j'=1$. The expansion Eq. (A1) is quite general and applies to all kinds of possible interactions. It applies to the direct as well as to the exchange terms if the j particles are identical with the j' particles.

If we use Eq. (A1) in the j^nj' configuration, the matrix elements of $\mathbf{u}_1{}^{(k)}$ are taken between states of the j particle and those of $\mathbf{u}_2{}^{(k)}$ between states of the j' particle. The tensors with $k=0$ are therefore just constants. Due to the Wigner-Eckart theorem (or its special case known as the Lande formula), the matrix elements of any tensor $\mathbf{u}^{(1)}$ taken between states with the same value of j, are proportional to the corresponding matrix element of $\mathbf{j}$. We can thus replace any interaction (A1), within j^nj' configurations (with fixed j and $j'=1/2$ but for any n), by

$$V_{12}=a+2(\mathbf{j}\cdot\mathbf{j}')b, \tag{A2}$$

with appropriately chosen constants a and b. All the physical properties of the interaction, within the given configurations, are characterized by the values of a and b.

The $j-j'$ interaction in the j^nj' configuration is given by summing (A2) over-all j particles:

$$\begin{aligned}na+2b\sum_{i=1}^{n}(\mathbf{j}_i\cdot\mathbf{j}')&=na+2b(\mathbf{J}_0\cdot\mathbf{j}')\\&=na+b[(\mathbf{J}_0+\mathbf{j}')^2-\mathbf{J}_0{}^2-\mathbf{j}'^2].\end{aligned} \tag{A3}$$

We thus see that we should take an eigenstate of the j^n configuration, specified by the value of its total spin J_0 (and additional quantum number α if necessary) and couple to it $j'=1/2$ to obtain states with spin $J=J_0\pm1/2$. Due to Eq. (A3), also the $j-j'$ interaction will be diagonal in these states and will have the eigenvalues

$$na+b[J(J+1)-J_0(J_0+1)-\tfrac{3}{4}]. \tag{A4}$$

Thus, J_0 (and α) and J are good quantum numbers which characterize completely the eigenstate of the interaction within the j^nj' configuration with $j'=1/2$. The nondiagonal matrix elements of the interaction Eq. (A3) between two orthogonal states with different values of J_0 (or α) vanish due to the vanishing of the matrix element of the constant a and the vector $\mathbf{J}_0$ between such states.

The eigenvalues (A4) in the two possible cases, $J=J_0+1/2$ and $J=J_0-1/2$, are given by

$$\begin{aligned}V(J=J_0+1/2)&=na+J_0b,\\V(J=J_0-1/2)&=na-(J_0+1)b.\end{aligned} \tag{A5}$$

The constants a and b can be expressed in terms of the interaction energies in the two-particle jj' configuration. We obtain in that case, from Eq. (A5),

$$\begin{aligned}V(jj'J=j+1/2)&=V_{j+1/2}=a+jb,\\V(jj'J=j-1/2)&=V_{j-1/2}=a-(j+1)b,\end{aligned} \tag{A6}$$

which yield

$$\begin{aligned}a&=\frac{1}{2j+1}[(j+1)V_{j+1/2}+jV_{j-1/2}],\\b&=\frac{1}{2j+1}[V_{j+1/2}-V_{j-1/2}].\end{aligned} \tag{A7}$$

One simple consequence of Eq. (A5) concerns states of odd-odd nuclei. If n is odd the ground state of the j^n configuration of neutrons, say, has usually $J_0=j$. If an odd proton is in a $j'=1/2$ state, the ground state will be a doublet, with $J=j\pm1/2$, the spacing of which is independent of n. This result holds always in the j^nj' configuration and is independent of any additional quantum numbers which may be required to specify uniquely the state with $J_0=j$ in the j^n configuration. The spacings of such doublets in actual nuclei are usually small compared to the separation of other levels and thus can be detected. An example of this behavior is discussed in Sec. II above. Another example is offered by the Tl isotopes. In Tl there is one $3s_{1/2}$ proton missing from the closed shells of 82. Beyond neutron number 126 the $2g_{9/2}$ orbit is being filled. The ground state of Tl^{208}, with one $g_{9/2}$ neutron has spin 5^+ and 0.04 Mev above it there is a 4^+ state (presumably of the same configuration). In Tl^{210}, with the $g_{9/2}{}^3$ neutron configuration, there is an excited level, 0.05 Mev above the ground state. No spins or parities are known in this case but the close agreement between the two spacings is probably indicative of the validity of the configuration assignments. *Note added in proof.* Y. E. Kim, D. J. Horen, and J. M. Hollander consider in Nuclear Phys. **31**, 447 (1962) the Y^{86} spectrum. The $p_{1/2}$ proton is presumably coupled to the $J=9/2$ state of the $g_{9/2}{}^{-3}$ neutron configuration to give states with spins 4^- (ground state) and 5^- (at 0.208 Mev). In Y^{88}, with one hole in the neutron $g_{9/2}$ shell, the ground state is known to have spin 4^-. It would be interesting to measure the position of the corresponding 5^- state.