

Isotopic Spin Impurity. II. Shell Model

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The isotopic spin impurity introduced into nuclear states by the Coulomb interaction is calculated with jj -coupling shell-model wave functions. Upper limits on the impurity present in $N=Z$ nuclei for $4 \leq A \leq 16$ are given and shown to be in agreement with the experimental work of Wilkinson on the isotopic spin selection rule for $E1$ transitions.

I. INTRODUCTION

THE introduction of isotopic-spin impurity into the ground state of light nuclei by the Coulomb potential can be treated most easily by considering the nuclear wave function as a $(J, T=0)$ core of nucleons coupled to a wave function for the nucleons outside the core. The core impurity has been calculated on the Fermi gas model¹ by computing the mixing of excited $T=1$ states with the ground state of an $N=Z$ even-even ($T_z=0, A=4n$) nucleus. This core impurity has been found to exceed by a large factor the isotopic-spin impurity estimated by Radicati² to arise from Coulomb distortion of the wave function for nucleons outside closed shells. This predominance of core impurity will now be verified on the jj -coupling model with harmonic oscillator wave functions, where the core now consists of the shells completely filled with both neutrons and protons.

We shall first perform a more rigorous calculation of the Coulomb mixing of the isotopic-spin states for the nucleons outside closed shells by using a more realistic representation of the nonexchange potential interaction with the core nucleons than the $(1/r)$ dependence of Radicati.² Following this, the calculation will be extended to obtain the isotopic-spin impurity for He^4 and C^{12} , which are closed-shell configurations, $(1s_3)^4$ and $(1s_3)^4(1p_3)^8$ respectively. After giving a simple method of reproducing the shell-model calculations by use of an equivalent potential, we shall have a way of obtaining, from the isotopic-spin impurity of He^4 and C^{12} , estimates of the impurity in the ground states of some $N=Z$ nuclei having open shells.

II. TWO NUCLEONS OUTSIDE CLOSED SHELLS

When there is only one nucleon outside closed shells, there can be no mixing to higher isotopic-spin states unless there is also excitation of the core. With the appearance of two nucleons outside closed shells, however, the possibility arises of mixing between $T=0$ and $T=1$ states as well as between $T=1$ states of different configurations. The first type of mixing produces violations of the isotopic-spin selection rules, while the second type of mixing destroys the displacement prop-

erty of the isotopic-spin operators $T_{\xi \pm i} T_{\eta}$, since the eigenstates of T_z and $T_{z \pm 1}$ are *not* related by

$$(T_{\xi \pm i} T_{\eta}) \Psi_{TT_z} = [(T \mp T_z)(T \pm T_z + 1)]^{\frac{1}{2}} \Psi_{TT_z}. \quad (1)$$

The implications of this circumstance for β decay will be discussed in a later paper. These two types of mixing are produced by the interaction of the extra-shell nucleons, both with each other and with the core. The core interaction is a central potential which commutes with the j of the individual particles and will produce mixing to excited configurations differing from the ground state only in the principal quantum number of one of the nucleons. On the other hand, the nucleon interaction does not commute with the j of the individual nucleons and can mix the ground state to many excited configurations whose parities are the same as the ground state.

For a specific investigation of the two-nucleon mixing we shall consider the $(1p_3)^2$ and $(1p_3)^2$ configurations, and the results will be specifically applicable to the triads at $A=6$ and $A=14$. We do not imply that jj -coupling should be valid for so light a nucleus as Li^6 , but from the results of the calculations on $(1p_3)^2$ will emerge certain general conclusions that are applicable to any configuration j^2 . Indeed the most significant features of the mixing are also present in LS coupling and the configuration l^2 .

The nonexchange potential for the Coulomb interaction of an extrashell proton with the protons in closed shells will be shown to be represented approximately by the potential of a uniform spherical charge distribution,

$$V(r) = \frac{3Ze^2}{2R} \left(1 - \frac{r^2}{3R^2} \right), \quad r \leq R \\ = Ze^2/r, \quad r \geq R \quad (2)$$

Using harmonic-oscillator wave functions, one can show easily that the contribution of the region outside the nucleus to nuclear matrix elements is only a few percent of the contribution from the nuclear volume. In evaluating the perturbation effect of the core potential, we shall therefore use $V(r) = -Ze^2 r^2 / 2R^3$. The total interaction of two nucleons in an open shell with each other and with the core will be taken as

$$V = V_c + V_p; \\ V_c \equiv -(Ze^2/2R^3) \left[\left(\frac{1}{2} - t_{z1} \right) r_1^2 + \left(\frac{1}{2} - t_{z2} \right) r_2^2 \right] \\ V_p \equiv (e^2/r_{12}) \left(\frac{1}{2} - t_{z1} \right) \left(\frac{1}{2} - t_{z2} \right), \quad (3)$$

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¹ W. M. MacDonald, Phys. Rev. **100**, 51 (1955). This paper will be designated as (I).

² L. A. Radicati, Proc. Phys. Soc. (London) **A66**, 139 (1953).

where t_{ζ} is related to the usual spin matrices $\tau = \{\tau_x, \tau_y, \tau_z\}$ by $\mathbf{t} = \frac{1}{2}\tau$ and to T_{ζ} by

$$T_{\zeta} = \sum_{i=1}^A t_{\zeta i} = \frac{1}{2}(N - Z).$$

The decomposition of V_c and V_p into irreducible tensors in isotopic-spin space gives

$$\begin{aligned} V_c &= V_c^{(0)} + V_c^{(10)}; \\ V_c^{(0)} &= -(Ze^2/4R^3)(r_1^2 + r_2^2), \\ V_c^{(10)} &= (Ze^2/2R^3)(t_{\zeta 1}r_1^2 + t_{\zeta 2}r_2^2), \end{aligned} \quad (4)$$

and

$$\begin{aligned} V_p &= V_p^{(0)} + V_p^{(10)} + V_p^{(20)}; \\ V_p^{(0)} &= (e^2/r_{12})(\frac{1}{4} + \frac{1}{3}\mathbf{t}_1 \cdot \mathbf{t}_2), \\ V_p^{(10)} &= -(e^2/2r_{12})(t_{\zeta 1} + t_{\zeta 2}), \\ V_p^{(20)} &= (e^2/r_{12})(t_{\zeta 1}t_{\zeta 2} - \frac{1}{3}\mathbf{t}_1 \cdot \mathbf{t}_2), \end{aligned} \quad (5)$$

where $V^{(kl)}$ is the l th component of a tensor of rank k . For two-nucleon configurations, $V_p^{(10)}$ and $V_p^{(20)}$ can be written in terms of T and T_{ζ} ,

$$\begin{aligned} V_p^{(10)} &= -(e^2/2r_{12})T_{\zeta} \\ V_p^{(20)} &= (e^2/2r_{12})(T_{\zeta}^2 - \frac{1}{3}\mathbf{T}^2). \end{aligned} \quad (6)$$

These expressions clearly exhibit the fact that the interaction of the extra-core nucleons produces no mixing of different isotopic-spin states of the two nucleons.

In calculating the effect of the Coulomb perturbation we shall use only the vector and tensor parts of V , since the scalar part can be included in the nuclear Hamiltonian and T will still be a good quantum number. The perturbation that we shall use in computing isotopic-

TABLE I. Coulomb interaction matrix elements between $(1p_1)^2$ and nearest configurations. The energy separation of $(1p)^2$ from $1p1f$, $(1d)^2$, and $1p2p$ is taken as 30.9 Mev.

$T_{\zeta}=0$ (Li ⁶).					
$M = [(1p_1)^2 J T \mathcal{U} 1p_1 2p_1 J T']$ $J=0,2, T=1, T'=0;$					
$= 0.1778$ Mev $J=1,3, T=0, T'=1.$					
$p = M^2 (30.9 \text{ Mev})^{-2} = 3.31 \times 10^{-5}.$					
$[(1p_1)^2 J 1 T_{\zeta} \mathcal{U} j j' J 1 T_{\zeta}] = M(T_{\zeta}).$					
$E_0 - E_1 = 30.9$ Mev. $p = M^2(T_{\zeta}) (30.9 \text{ Mev})^{-2}.$					
$j j'$	J	$M(1)$	p	$M(-1)$	p
$(1p_1)^2$	0	-0.001858		0.003717	
$1p_1 1p_1$	2	0.002230		-0.004456	
$1p_1 1f_{5/2}$	2	-0.01024	1.1×10^{-7}	0.02048	4.4×10^{-7}
$1p_1 1f_{5/2}$	2	0.005474	3.1×10^{-8}	-0.01045	1.3×10^{-7}
$1p_1 1f_{7/2}$	2	-0.01340	1.9×10^{-7}	0.02681	7.5×10^{-7}
$(1d_1)^2$	0	0.02496	6.5×10^{-7}	-0.04993	2.6×10^{-6}
$(1d_1)^2$	2	0.008146	6.7×10^{-8}	-0.01629	2.8×10^{-7}
$1d_1 1d_{5/2}$	2	0.009977	1.0×10^{-7}	-0.01995	4.2×10^{-7}
$(1d_{5/2})^2$	0	0.03700	1.4×10^{-6}	-0.07403	5.7×10^{-6}
$(1d_{5/2})^2$	2	0.03406	1.2×10^{-6}	-0.06812	4.9×10^{-6}
$1p_1 2p_1$	0	-0.00985	1.0×10^{-7}	0.01971	4.1×10^{-7}
$1p_1 2p_1$	2	0.002787	8.1×10^{-9}	-0.005575	3.3×10^{-8}
$1p_1 2p_1$	2	-0.002787	8.1×10^{-9}	0.005575	3.3×10^{-8}
$1p_1 2p_1$	0	-0.2475	6.2×10^{-5}	0.3171	1.0×10^{-4}
$1p_1 2p_1$	2	-0.2363	5.8×10^{-5}	0.2949	9.5×10^{-5}

spin impurity in this case is

$$\mathcal{U} = V_c^{(10)} + V_p^{(10)} + V_p^{(20)}. \quad (7)$$

The evaluation of matrix elements of \mathcal{U} is easily performed by transforming into a representation in which states are characterized by the individual t_{ζ} quantum numbers. In this representation the problem of finding the matrix elements of an isotopic-spin dependent potential between states completely antisymmetric in space, spin, and isotopic-spin coordinates is reduced to the evaluation of matrix elements of several ordinary potentials between wave functions which are *either* symmetric or antisymmetric in the space and spin coordinates of the two nucleons, but which contain no isotopic-spin variables.

We first transform matrix elements of the general form $(\gamma T T_{\zeta} | \mathcal{U} | \gamma' T' T_{\zeta})$, where γ and γ' represent all the auxiliary quantum numbers.

$$\begin{aligned} (\gamma T T_{\zeta} | \mathcal{U} | \gamma' T' T_{\zeta}) &= \sum_{t_{\zeta 1}, t_{\zeta 2}} (T T_{\zeta} | t_{\zeta 1} t_{\zeta 2}) (t_{\zeta 1} t_{\zeta 2} | T' T_{\zeta}) \\ &\quad \times (\gamma t_{\zeta 1} t_{\zeta 2} | \mathcal{U} | \gamma' t_{\zeta 1} t_{\zeta 2}). \end{aligned} \quad (8)$$

Defining $V_{TT'}^{(T_{\zeta})}$ by the equation

$$(\gamma T T_{\zeta} | \mathcal{U} | \gamma' T' T_{\zeta}) \equiv (\gamma | V_{TT'}^{(T_{\zeta})} | \gamma') \quad (9)$$

we find for $V_{TT'}^{(T_{\zeta})}$:

$$\begin{aligned} V_{00}^{(0)} &= 0, \\ V_{01}^{(0)} &= (Ze^2/4R^3)(r_1^2 - r_2^2), \\ V_{11}^{(0)} &= 0, \\ V_{11}^{(-1)} &= -(Ze^2/4R^3)(r_1^2 + r_2^2) + \frac{2}{3}(e^2/r_{12}), \\ V_{11}^{(1)} &= (Ze^2/4R^3)(r_1^2 + r_2^2) - \frac{1}{3}(e^2/r_{12}). \end{aligned} \quad (10)$$

The antisymmetric character of $V_{01}^{(0)}$ arises from the difference in symmetry of the space-spin part of the wave functions for $T=0$ and $T=1$. The sign of $V_{01}^{(0)}$ is determined by the phases of the vector addition coefficients and is not unique. This arbitrariness disappears when one comes to the matrix element of $V_{01}^{(0)}$ since the sign of the antisymmetric space-spin function associated with the $T=1$ state is also determined by the sign of the vector addition coefficients.

The matrix elements of the $V_{TT'}^{(T_{\zeta})}$ between different J states of $(1p_1)^2$ and higher jj configurations can be evaluated by first finding the matrix elements between $(1p)^2$ and higher configurations in the LS representations. As Talmi³ has shown, the Slater integrals $F^{(k)}(n_1 l_1 n_2 l_2; n_3 l_3 n_4 l_4)$ which appear at this point can all be easily evaluated for the case of harmonic-oscillator single-particle wave functions. These functions have the form

$$\psi(r, \vartheta, \phi) = [R_{nl}(r)/r] Y_l^m(\vartheta, \phi), \quad (11)$$

where $Y_l^m(\vartheta, \phi)$ is a surface spherical harmonic and

$$R_{nl}(r) = N_{nl} \exp[-(\nu/2)r^2] r^{l+1} L_{n+l-1}^{l+1}(\nu r^2), \quad n=1, 2, \dots \quad (12)$$

³ I. Talmi, Helv. Phys. Acta 25, 185 (1952).

$L_{n+l-\frac{1}{2}}^{l+\frac{1}{2}}$ being an associated Laguerre polynomial. The parameter ν can be determined by using the relation $\langle r^2 \rangle = R^2$ and the following values would be obtained:

$$\begin{array}{cccc} A & 4 & 12 & 16 \\ \nu & 11/6R^2 & 13/6R^2 & 9/4R^2. \end{array} \quad (13)$$

In working in the $1p$ shell, however, we have found it convenient to use just $(1p|r^2|1p) = R^2$ giving $\nu = 5/2R^2$. The uncertainties in other parts of the calculation (e.g., energy denominators) does not justify concern over the precise value of ν . Having evaluated the LS matrix elements of $V_{TT'}(T_\zeta)$, we obtain the jj -coupling matrix elements by use of the $(LSJM|j_1j_2JM)$ transformation coefficients given by Racah,⁴ or less explicitly by a formula due to Hope and quoted by Edmonds and Flowers.⁵ Using these matrix elements and the energy separations given by the oscillator wave functions for $\nu = 5/2R^2$, we have calculated the squared amplitude of those neighboring jj states which are present in the $(1p_{\frac{3}{2}})^2$ states of He⁶, Li⁶, and Be⁶. These impurities are listed in Table I. The corresponding quantities for the $(1p_{\frac{3}{2}})^2$ states of C¹⁴, N¹⁴, and O¹⁴ are given in Table II. These figures are probably overestimates since the energy separation of two states in different isotopic-spin multiplets is probably larger than the separation given by the extreme single-particle model.

The first observation we make about these Coulomb matrix elements is that no mixing of different isotopic-spin states of $(1p_{\frac{3}{2}})^2$ and $(1p_{\frac{1}{2}})^2$ can occur. All mixing of different isotopic-spin states must therefore occur between states already separated by a large energy (~ 20 – 30 Mev). The nucleon interaction vanishes for $T_\zeta = 0$ components and can mix only $T = 1$ states. The core interaction on the other hand can mix only states of different isotopic spin. In doing this there is an additional selection rule, however, which arises from the central force character of the interaction, $\Delta j_1 = \Delta j_2 = 0$. The result of this selection rule on \mathcal{U} is that the only possible mixing of $T = 0$ and $T = 1$ states is between $(1p_{\frac{3}{2}})^2$ and $1p_{\frac{3}{2}} 2p_{\frac{3}{2}}$ or between $(1p_{\frac{1}{2}})^2$ and $1p_{\frac{1}{2}} 2p_{\frac{1}{2}}$.

Although no mixing of different isotopic spin states can occur when $T_\zeta = \pm 1$, the matrix elements between the $T = 1$ states of different configurations have one interesting feature. We see that mixing can occur to configurations in which the angular momentum j of one or both nucleons is different. The core interaction does not play any role in these matrix elements, which are expected for this reason to be somewhat smaller than those matrix elements to the $1p_{\frac{3}{2}} 2p_{\frac{3}{2}}$ or $1p_{\frac{1}{2}} 2p_{\frac{1}{2}}$ configurations. These latter matrix elements are actually found to be larger by a factor of ~ 10 – 15 and this predominance is not due just to the absence of the core interaction. This result holds in fact for any spin independent "long-range potential" for which the Slater $F^{(0)} \gg F^{(k)}$. Such a potential is approximately diagonal

in the (lj) representation. It is reasonable that the energy separation between states of the same spin J , parity, and isotopic-spin T in $(nj)^2$ and $(nj, n+1j)$ should not be more than two or three times the separation of the same state in $(nj)^2$ and (nj', nj'') . The extreme predominance of the matrix elements between the former configurations then implies that the mixing between these configurations will also predominate.

Two important conclusions have been drawn from the results on the Coulomb mixing of excited states to the ground state of a two-nucleon configuration: (1) only the interaction with core nucleons (protons) introduces isotopic-spin impurity into the two-nucleon state, and this is from excitation of a single nucleon without change of its orbital or total angular momentum; (2) the Coulomb interaction of two nucleons in an open shell has an effect like a central potential in mixing principally to configurations having the same orbital and total angular momenta for the individual nucleons. Although the interaction of the two extra-core nucleons introduces no isotopic-spin impurity into the two-nucleon state, we shall see that such interactions do introduce isotopic-spin impurity into configurations of three or more nucleons. The result (2) for two nucleon interactions then will be seen to determine the excited states which contribute principally to the isotopic-spin impurity of the ground state for three or more nucleons outside closed shells.

III. THREE NUCLEONS OUTSIDE CLOSED SHELLS

The results of the calculation of the mixing of the states of two nucleons outside closed shells disclosed certain interesting general features. The two-nucleon configuration, however, was seen to have the special property that no mixing of isotopic-spin states could be produced by the interaction of the extra-core nucleons. Consequently the efficiency of the particle interaction in mixing states of different isotopic-spin is first to be observed in the case of three nucleons outside closed shells. In addition, in the two nucleon case there was no mixing of different isotopic-spin states belonging to the ground state configuration. Indeed,

TABLE II. Configuration interaction matrix elements between $(1p_{\frac{3}{2}})^2$ and nearest configurations. The energy separation of $(1p)^2$ from $1p 1f$, $(1d)^2$, and $1p 2p$ is taken as 17.7 Mev.

$T_\zeta = 0$ (N^{14}).				
$M = [(1p_{\frac{3}{2}})^2 J T \mathcal{U} 1p_{\frac{3}{2}} 2p_{\frac{3}{2}} J T']$ $J = 0, T = 1, T' = 0;$				
$= 0.403$ Mev, $J = 1, T = 0, T' = 1.$				
$\rho = M^2(17.7 \text{ Mev})^{-2} = 1.52 \times 10^{-4}.$				
$[(1p_{\frac{3}{2}})^2 0 1 T_\zeta \mathcal{U} j j' 0 1 T_\zeta] = M(T_\zeta).$				
$E_0 - E_1 = 17.7$ Mev. $\rho = M^2(T_\zeta)(17.7 \text{ Mev})^{-2}.$				
jj'	$M(1)$	ρ	$M(-1)$	ρ
$(1d_{\frac{3}{2}})^2$	0.03852	4.7×10^{-6}	-0.07707	1.9×10^{-6}
$(1d_{5/2})^2$	0.01287	5.3×10^{-7}	-0.02573	2.1×10^{-6}
$1p_{\frac{3}{2}} 2p_{\frac{3}{2}}$	-0.4942	2.6×10^{-4}	0.4968	6.1×10^{-4}
$1p_{\frac{1}{2}} 2p_{\frac{1}{2}}$	0.002476	1.9×10^{-8}	0.004953	7.9×10^{-6}

⁴ G. Racah, *Physica* **16**, 651 (1950).

⁵ A. R. Edmonds and B. H. Flowers, *Proc. Roy. Soc. (London)* **A214**, 515 (1952).

there was not even a mixing of the ground state with a different isotopic-spin state in the nearest configuration, e.g., $(1p_{3/2})^2$ with $1p_{3/2} 1p_{3/2}$. In order to investigate these aspects of the Coulomb mixing of different isotopic-spin states we shall consider the isotopic-spin impurity of the $T=\frac{1}{2}$ states of the $(1p_{3/2})^3$ configuration, this being the configuration to which the low excited states of Li^7 and Be^7 would belong in jj -coupling.

Matrix elements are needed of the Coulomb interaction \mathcal{U}_3 of the three extra-core nucleons with each other and with the nucleons in closed shells.

$$\begin{aligned}\mathcal{U}_3 &= V_c^{(10)} + V_p^{(10)} + V_p^{(20)}, \\ {}_3V_c^{(10)} &= (Ze^2/2R^3) \sum_{i=1}^3 t_i r_i^2, \\ {}_3V_p^{(10)} &= -e^2 \sum_{i<j} (t_i + t_j) r_{ij}^{-1}, \\ {}_3V_p^{(20)} &= e^2 \sum_{i<j} (t_i t_j - \frac{1}{3} \mathbf{t}_i \cdot \mathbf{t}_j) r_{ij}^{-1}.\end{aligned}\quad (14)$$

The matrix elements of \mathcal{U}_3 between three-nucleon states are reduced by the use of coefficients of fractional parentage⁶ (c.f.p.) to the previously calculated matrix elements of the Coulomb interaction between two nucleon states. This reduction is complicated by the fact that the perturbation is the sum of a vector and of a second-rank tensor operator.⁷

One would expect the greatest impurity in the $T=\frac{1}{2}$ states of $(1p_{3/2})^3$ to arise from the low-lying states unless unusually small matrix elements occur. The nearest states of isotopic-spin $T=\frac{3}{2}$ should belong to $(1p_{3/2})^3$. Using the calculations of Kurath⁸ for a Rosenfeld potential,⁹ the separation of the $T=\frac{1}{2}$ and $T=\frac{3}{2}$ states of $(1p_{3/2})^3$ is found to be 10.3 Mev. This is in agreement with the suggestion by Peaslee and Telegdi¹⁰ that the first $T=\frac{3}{2}$ level in Li^7 lies at 10.8 Mev. From a table of (c.f.p.) for $(1p_{3/2})^3$ we find that the only $T=\frac{3}{2}$ state of $(1p_{3/2})^3$ has spin $J=\frac{3}{2}$. We find, moreover, that the only two-nucleon matrix elements which appear in the expression for the three nucleon matrix elements are $[(1p_{3/2})^2 01T_1 | \mathcal{U}_2 | (1p_{3/2})^2 01T_1]$ and $[(1p_{3/2})^2 21T_1 | \mathcal{U}_2 | (1p_{3/2})^2 21T_1]$ for the states $J, T=0, 1$ and $J, T=2, 1$. These matrix elements appear with coefficients which are equal in magnitude but of opposite sign. Since the matrix elements of ${}_2V_c^{(10)}$ are independent of J , the core interaction contributes nothing to the mixing of these $T=\frac{1}{2}$ and $T=\frac{3}{2}$ states of $(1p_{3/2})^3$. Furthermore the only contributions from ${}_2V_p^{(10)}$ and ${}_2V_p^{(20)}$ are proportional to the Slater integral $F^{(2)}[(1p)^2; (1p)^2]$ in the expansion for the matrix element of r_{12}^{-1} . The reason for this is that the $F^{(0)}$ term arises from the part of

r_{12}^{-1} which can be represented by a central potential, and the coefficient of $F^{(0)}$ must vanish just as does the matrix element ${}_3V_c^{(10)}$. Using an energy separation of 10 Mev, we find very little isotopic-spin impurity arising from the mixing of the $T=\frac{1}{2}$ and $T=\frac{3}{2}$ states of $(1p_{3/2})^3$.

The mixing of the $T=\frac{1}{2}$ states of $(1p_{3/2})^3$ and the $T=\frac{3}{2}$ states of $(1p_{3/2})^2 1p_{3/2}$ can actually occur for the $J=\frac{1}{2}, \frac{3}{2}$, and $5/2$ components of these configurations, and the intermultiplet matrix elements for all these states are given in Table III. The energy separation has been taken as 10 Mev to obtain the estimates of the (maximum) isotopic-spin impurity which are given.

We have remarked that the experimental separation of the $T=\frac{1}{2}$ and $T=\frac{3}{2}$ states of $(1p_{3/2})^3$ is at least 10 Mev. Such a large multiplet separation means that the separation of the $T=\frac{1}{2}$ states of $(1p_{3/2})^3$ from the $T=\frac{3}{2}$ states of $(1p_{3/2})^2 2p_{3/2}$ is probably no more than three or four times the separation of these isotopic-spin states in $(1p_{3/2})^3$. Considering that the Coulomb matrix elements between $(1p_{3/2})^2$ and $1p_{3/2} 2p_{3/2}$ were so large in the two-nucleon case and that the matrix elements between the $T=\frac{1}{2}$ and $T=\frac{3}{2}$ states of $(1p_{3/2})^3$ are proportional only to $F^{(2)}[(1p)^2; (1p)^2]$, we should expect that the mixing of different isotopic-spin states between $(1p_{3/2})^3$ and $(1p_{3/2})^2 2p_{3/2}$ will be at least as large as the mixing of these states within $(1p_{3/2})^3$.

The matrix elements between the $(J, T=\frac{3}{2}, \frac{1}{2})$ states of $(1p_{3/2})^3$ and the two $(J, T=\frac{3}{2}, \frac{3}{2})$ states of $(1p_{3/2})^2 2p_{3/2}$ are given in Table III. The isotopic-spin mixing has been computed using an energy separation equal to the $1p, 2p$ separation of the harmonic oscillator states. A value of $E_0 - E_1 = 28$ Mev has therefore been used. We find that the matrix elements between the above states in $(1p_{3/2})^3$ and $(1p_{3/2})^2 2p_{3/2}$ exceed by a factor of $\sim 12-20$ those between the same states in $(1p_{3/2})^3$. The corresponding isotopic-spin mixing of $(1p_{3/2})^3$ and $(1p_{3/2})^2 2p_{3/2}$ also dominates by a factor of at least fifteen.

Impurities from configurations like $(1p_{3/2})^2 1f_{7/2}$ may also appear and one would like to know the relative magnitudes of the mixing to configurations like this and to $(1p_{3/2})^2 2p_{3/2}$. Using Racah's approach to complex spectra, we can express the three-nucleon matrix elements as linear combinations of two-nucleon matrix elements with coefficients of fractional parentage (c.f.p.).⁶ For configurations of nonequivalent particles the c.f.p. have been discussed by Meshkov¹¹ and Redlich.¹² Using Redlich's notation the c.f.p. have the normalization

$$\sum_{\alpha_1 J_1 T_1} |(\alpha_1 J_1 T_1) j_r | \alpha J T |^2 = 1 \quad (15)$$

where α_1, J_1, T_1 are quantum numbers of a two-nucleon state to which a nucleon of spin j_r is being coupled. The c.f.p. are always less than unity. Since for three

⁶ G. Racah, Phys. Rev. **63**, 367 (1943).

⁷ G. Racah, Phys. Rev. **62**, 438 (1942).

⁸ D. Kurath, Phys. Rev. **88**, 804 (1952).

⁹ L. Rosenfeld, *Nuclear Forces* (Interscience Publishers, Inc., New York, 1948).

¹⁰ D. C. Peaslee and V. L. Telegdi, Phys. Rev. **92**, 126 (1953).

¹¹ S. Meshkov, Phys. Rev. **91**, 871 (1953).

¹² M. G. Redlich, Phys. Rev. **99**, 1427 (1955).

nucleons the sum is distributed over not more than four parent states and the c.f.p. vary among themselves by no more than a factor of two, the relative magnitude of corresponding matrix elements (same J, T) to different configurations is determined mostly by the magnitudes of the matrix elements between two-nucleon parent states. Observing that matrix elements from $(1p_{3/2})^2$ to $1p_{3/2} 2p_{3/2}$ are ~ 10 – 15 times larger than those to all other configurations, one can conclude that the matrix elements from $(1p_{3/2})^3$ to $(1p_{3/2})^2 2p_{3/2}$ will also dominate matrix elements to other three-nucleon configurations. Consequently we can conclude that $(1p_{3/2})^2 2p_{3/2}$ contributes most of the isotopic spin impurity of $(1p_{3/2})^3$.

IV. ISOTOPIC SPIN IMPURITY OF CLOSED SHELLS

In the calculation of the isotopic-spin impurity of the state of two or three nucleons in open shells, we have neglected the excitation of the isotopic-spin $T=0$ state of the core. We have shown, however, that the isotopic-spin impurity of the states for the extra-core nucleons is even smaller than that indicated by the calculations of Radicati² and are negligible compared to the estimate made in (I) of the isotopic-spin impurity of the core. We now purpose to study the excitation of the core and the isotopic-spin impurity of nuclei having closed shells in neutrons and protons.

The problem can be treated by two different methods which illuminate two different aspects of the Coulomb effect upon the isotopic-spin state of closed shells. These two methods are (1) the reduction to two-nucleon matrix elements, and (2) the use of the "equivalent" potential produced by a closed shell. The first approach will show how one may regard the excitation of the isotopic-spin state of the core as an extension of the Coulomb mixing of the states of two nucleons. The second approach leads to a rigorous derivation of the method by which we have introduced the effect of the interaction of the core on two- and three-nucleon states. We shall also show how one can use the method to estimate the impurity of closed shells.

A. Reduction to Two-Nucleon Interactions

In jj coupling the nuclear wave function is an anti-symmetric linear combination of the single particle wave functions $\psi_\nu = \phi_{j, m_\nu}(\mathbf{r}, \sigma) u(t_\zeta)$. The isotopic-spin function $u(t_\zeta)$ is an eigenfunction of t_ζ with eigenvalues $\pm \frac{1}{2}$. The nuclear wave function Ψ_0 for the ground state can be written as a Slater determinant of these wave functions with all the $(2j_\nu + 1)$ values of m_ν appearing for each shell with each isotopic-spin eigenfunction. Excited states Ψ_ν of this nucleus can also be written as a Slater determinant, or a linear combination of Slater determinants, in which one or more of the closed shell wave functions have been replaced by states from the unfilled shells. Since the Coulomb perturbation is a two-particle operator, matrix elements to states Ψ_ν differing from Ψ_0 by more than two single particle

TABLE III. Matrix elements for isotopic-spin mixing with $(1p_{3/2})^3$.

T_ζ		$((1p_{3/2})^3 \frac{3}{2} \frac{1}{2} T_\zeta \mathcal{U} (1p_{3/2})^3 \frac{3}{2} \frac{3}{2} T_\zeta) = M$	For $A=7$ Nucleus $p=10^{-2}M^2$	
$\frac{1}{2}$		0	0	0
$-\frac{1}{2}$		$\frac{1}{30\sqrt{\pi}} e^2/R$	0.0106 Mev	1.11×10^{-6}
$J \quad T_\zeta$		$((1p_{3/2})^3 J \frac{1}{2} T_\zeta \mathcal{U} (1p_{3/2})^2 1p_{3/2} J \frac{3}{2} T_\zeta) = M$	For $A=7$ Nucleus $p=10^{-2}M^2$	
1/2	$\frac{1}{2}$	0		
	$-\frac{1}{2}$	$-\frac{1}{150} \left(\frac{5}{3\pi}\right)^{\frac{1}{2}} \frac{e^2}{R}$	-0.00272 Mev	7.37×10^{-8}
3/2	$\frac{1}{2}$	0		
	$-\frac{1}{2}$	$-\frac{1}{450} \left(\frac{5}{2\pi}\right)^{\frac{1}{2}} \frac{e^2}{R}$	-0.00111 Mev	1.24×10^{-8}
5/2	$\frac{1}{2}$	0		
	$-\frac{1}{2}$	$\frac{1}{150} \left(\frac{35}{6\pi}\right)^{\frac{1}{2}} \frac{e^2}{R}$	0.00512 Mev	2.61×10^{-7}
$J' \quad T'$		$((1p_{3/2})^3 \frac{3}{2} \frac{1}{2} T'_\zeta \mathcal{U} (1p_{3/2})^2 2p_{3/2} \frac{3}{2} \frac{3}{2} (J'T') T'_\zeta) = M$	For $A=7$ Nucleus $p=M^2/(28 \text{ Mev})^2$	
0	1	$\frac{1}{2} \quad -\frac{Ze^2}{R} \frac{1}{6\sqrt{2}}$	-0.132 Mev	2.2×10^{-6}
	$-\frac{1}{2}$	$-\frac{Ze^2}{R} \frac{1}{6\sqrt{2}} - \frac{23}{72} \left(\frac{1}{2\pi}\right)^{\frac{1}{2}} \frac{e^2}{R}$	-0.233	6.9×10^{-6}
2	1	$\frac{1}{2} \quad -\frac{Ze^2}{R} \frac{1}{6\sqrt{10}}$	-0.0593	4.4×10^{-6}
	$-\frac{1}{2}$	$-\frac{Ze^2}{R} \frac{1}{6\sqrt{10}} - \frac{31}{360} \left(\frac{5}{2\pi}\right)^{\frac{1}{2}} \frac{e^2}{R}$	-0.1203	1.8×10^{-6}

states will vanish. We shall first calculate only the impurities arising from states Ψ_ν , corresponding to single-nucleon excitation and shall neglect the effect of two-nucleon excitation. This approximation will be checked later by calculating the contributions to impurity from states of two-nucleon excitation.

The Coulomb interaction is

$$V = e^2 \sum_{i < j} \left(\frac{1}{2} - t_{\zeta i}\right) \left(\frac{1}{2} - t_{\zeta j}\right) r_{ij}^{-1} \quad (16)$$

and the decomposition into irreducible tensors may be performed just as in (I). Since we are interested only in the mixing of $T=1$ states to the $T=0$ ground state, we need retain only the vector component of V as our perturbation operator

$$\mathcal{C} = -\frac{e^2}{2} \sum_{i < j} (t_{\zeta i} + t_{\zeta j}) r_{ij}^{-1}. \quad (17)$$

The selection rule $0 \rightarrow 0$ on \mathcal{C} insures that all matrix elements of between the $T=0$ ground state and the excited states Ψ_ν will correspond to the addition of isotopic-spin impurity from $T=1$ states.

In Ψ_0 let a nucleon in the individual particle state of angular momentum $j_2 m_2(n_2)$ be excited to the state of momentum $j_3 m_3(n_3)$ to form an excited state. For the

present we suppress the principal quantum numbers n_2 and n_3 . If by ψ_ν we designate the state of the nucleon which is excited to the state ψ_σ , the matrix element of \mathcal{C} is

$$(\Psi_\nu, \mathcal{C}\Psi_0) = -\frac{e^2}{2} \sum_{\omega} \int dr_1 dr_2 \{ \psi_\sigma^*(1) \psi_\omega^*(2) (t_{r_1} + t_{r_2}) r_{12}^{-1} \\ \times [\psi_\nu(1) \psi_\omega(2) - \psi_\nu(2) \psi_\omega(1)] \}. \quad (18)$$

Performing the sum over the isotopic-spin states, which are combined with each $\phi_{j_1 m_1}$ to give two different ψ_ν , we get

$$(\Psi_\nu, \mathcal{C}\Psi_0) = \pm \frac{e^2}{2} \sum_{i_1 m_1} [(j_3 m_3 j_1 m_1 | r_{12}^{-1} | j_2 m_2 j_1 m_1) \\ - (j_3 m_3 j_1 m_1 | r_{12}^{-1} | j_1 m_1 j_2 m_2)]. \quad (19)$$

The plus sign corresponds to the excitation of a proton; the minus sign, to the excitation of a neutron from the same state. The quantity in square brackets can be interpreted as a matrix element between the isotopic-spin triplet states in the (jm) representation.

$$(\Psi_\nu, \mathcal{C}\Psi_0) = \sum_{i_1, m_1} (n_3 j_3 m_3 n_1 j_1 m_1 T T_z) \\ \times | -T_z e^2 / 2 r_{12} | n_2 j_2 m_2 n_1 j_1 m_1 T T_z \rangle. \quad (20)$$

We transform Eq. (19) to the J, M representation:

$$(\Psi_\nu, \mathcal{C}\Psi_0) = -\frac{e^2}{2} \sum_{J, i_1} \frac{2J+1}{2j_1+1} [(n_2 j_2 n_1 j_1 J | r_{12}^{-1} | n_3 j_2 n_1 j_1 J) \\ - (-1)^{J-i_1-i_2} (n_1 j_1 n_2 j_2 J | r_{12}^{-1} | n_3 j_2 n_1 j_1 J)]. \quad (21)$$

The conditions $j_2 = j_3$, $m_2 = m_3$ which emerge from this transformation can be understood by observing that the excited state can be regarded as a shell with a single hole in the state $j_2 m_2$ coupled to a nucleon in the state $j_3 m_3$. But unless $j_2 = j_3$ and $m_2 = m_3$ the state Ψ_ν cannot have spin $J=0$, and the matrix element $(\Psi_\nu, \mathcal{C}\Psi_0)$ must vanish. The individual terms of Eq. (21) are not matrix elements between properly antisymmetrized jj -states, but between individual jj -states coupled to a state of total angular momentum J .

The principal contributions to isotopic-spin impurity are seen from Eq. (21) to come from the excitation of a neutron or a proton from the state $n_2 j_2$ to the state n_2+1, j_2 . There are $2(2j_2+1)$ equal matrix elements $(\Psi_{n_2 j_2}, \mathcal{C}\Psi_0)$ corresponding to the perturbation of the wave functions for nucleons in the shell j_2 . The total isotopic-spin impurity which is introduced into the ground state Ψ_0 by mixing with excited states formed by excitation of one nucleon is then just

$$p = \sum_{j_2} 2(2j_2+1) | (\Psi_{n_2 j_2}, \mathcal{C}\Psi_0) |^2 [E_0 - E(n_2 j_2)]^{-2}, \quad (22)$$

where $E - E(n_2 j_2)$ is the appropriate energy denominator for the nuclear matrix element $(\Psi_{n_2 j_2}, \mathcal{C}\Psi_0)$.

Using the value $\nu = 5/2R^2$ to calculate the impurity in C^{12} , we find for the nuclear matrix elements

$$(\Psi_{1p_3}, \mathcal{C}\Psi_0) = \pm 0.624e^2/R, \\ (\Psi_{1s_3}, \mathcal{C}\Psi_0) = \pm 0.343e^2/R. \quad (23)$$

These matrix elements lead to an isotopic-spin impurity for C^{12} of

$$p = 3.59(e^2/R)^2 (E_0 - E)^{-2}, \quad (24)$$

where we have taken $E_0 - E_{1p_3} \approx E_0 - E_{1s_3} \approx E_0 - E$. This value for p can be compared with the result for the Fermi gas model¹

$$p = 9.0(e^2/R)^2 (E_0 - E_1)^{-2}. \quad (25)$$

The agreement between Eqs. (24) and (25) is good, but the numerical value found from Eq. (24) will be somewhat lower than the upper limit on isotopic spin impurity of C^{12} given in (I). The $E_0 - E$ in Eq. (24) is equal to the separation of the $(1s_3)^4 (1p_3)^8$ $J, T=0$ ground state of C^{12} from a $J, T=0, 1$ excited state belonging to $(1s_3)^4 (1p_3)^7 2p_3$ or to $(1s_3)^3 2s_3 (1p_3)^8$. Where we took $E_0 - E_1 \sim 15$ Mev in (I), we shall use the energy separation ~ 19 Mev of the $1p$ and $2p$ orbits of the harmonic oscillator and thus obtain an *upper limit* of 1.9×10^{-3} on the impurity of C^{12} . This should be compared with the previously estimated limit of $\sim 7.5 \times 10^{-3}$.

The impurity of the alpha particle is very easily found by using just $(\Psi_{1s_3}, \mathcal{C}\Psi_0)$.¹³ If we use a $1s, 2s$ separation for He^4 of ~ 35 Mev, the *upper limit* on the impurity of the ground state of He^4 emerges as $p \sim 1.3 \times 10^{-5}$. Such a small impurity justifies considering the alpha particle as having zero total isotopic spin for most nuclear reactions involving emission or absorption of an alpha particle.

B. Contributions to Impurities from Doubly Excited Shells

The contributions to impurity from excited states $\Psi_{\mu\nu}$ formed by the excitation of two nucleons in states ψ_μ and ψ_ν has been assumed to be much smaller than contributions from states Ψ_ν of single nucleon excitation. We shall investigate this assumption by first deriving a general expression for the impurity introduced from states of two nucleon excitation. Analogous to Eq. (15) we now have

$$(\Psi_{\mu\nu}, \mathcal{C}\Psi_0) = -\frac{e^2}{2} \int dr_1 dr_2 \{ \psi_\sigma^*(1) \psi_\omega^*(2) (t_{r_1} + t_{r_2}) r_{12}^{-1} \\ \times [\psi_\mu(1) \psi_\nu(2) - \psi_\mu(2) \psi_\nu(1)] \}. \quad (26)$$

The only nonvanishing matrix elements are then

$$(\Psi_{\mu\nu}, \mathcal{C}\Psi_0) = \pm (e^2/2) [(n_3 j_3 m_3 n_4 j_4 m_4 | r_{12}^{-1} | n_1 j_1 m_1 n_2 j_2 m_2) \\ - (n_3 j_3 m_3 n_4 j_4 m_4 | r_{12}^{-1} | n_2 j_2 m_2 n_1 j_1 m_1)]. \quad (27)$$

This matrix element can be formed for all permissible values of m_1, m_2, m_3 , and m_4 . The total impurity due to

¹³ Contributions from $1p_1$ nucleons must be omitted.

the excitation of nucleons from the shells n_1j_1 and n_2j_2 to the shells n_3j_3 and n_4j_4 will be found by summing the square of the nuclear matrix elements given by Eq. (27) over all possible values of the magnetic quantum numbers with appropriate energy denominators. If we use the same average energy denominator for all terms of the sum over magnetic quantum numbers, the total isotopic-spin impurity of the nucleus arising from the mixing with excited states formed by exciting two nucleons is

$$p_2 = 2 \sum_{i_3, i_4}^{\text{open shells}} \sum_{i_1, i_2}^{\text{closed shells}} S(j_1, j_2; j_3, j_4) \times [E_0 - E(j_1, j_2; j_3, j_4)]^{-2}, \quad (28)$$

where

$$\begin{aligned} S(j_1, j_2; j_3, j_4) &= \sum |\langle \Psi_{\mu\nu} | \mathcal{O} \Psi_0 \rangle|^2 \quad (\text{sum over magnetic} \\ &\quad \text{quantum numbers}) \quad (29) \\ &= \sum_J (2J+1) \{ (n_3 j_3 n_4 j_4 J | e^2 / 2r_{12} | n_1 j_1 n_2 j_2 J)^2 \\ &\quad - 2(n_3 j_3 n_4 j_4 J | e^2 / 2r_{12} | n_1 j_1 n_2 j_2 J) \\ &\quad \times (n_4 j_4 n_3 j_3 J | e^2 / 2r_{12} | n_1 j_1 n_2 j_2 J) (-1)^{J-j_3-j_4} \\ &\quad + (n_4 j_4 n_3 j_3 J | e^2 / 2r_{12} | n_1 j_1 n_2 j_2 J)^2 \}. \quad (30) \end{aligned}$$

Conservation of parity greatly limits the number of excited states which contribute significantly to the isotopic spin impurity. The matrix elements which contribute principally to p_2 in C^{12} are listed in Table IV. In evaluating these matrix elements we again do not know the relative energy separations of the ground state from states of two-nucleon excitation. Accordingly we shall use the separation of the individual harmonic-oscillator states, neglecting the spin-orbit splittings. Where matrix elements are between states degenerate on this model, we use the $T=0$ to $T=1$ multiplet separation in C^{12} of ~ 15 Mev. We find $p_2 \sim 9.4 \times 10^{-5}$, a 5% correction to the isotopic-spin impurity from mixing with states of single-nucleon excitation.

C. The Equivalent Potential

If we return to Eq. (19) we can see that if the sum over the states $\phi_{j_1 m_1}$ were performed, we should have for the first term a matrix element for the excitation of a single nucleon moving in the potential produced by all the nucleons in the closed shells. The second term, which we call the "exchange term," is actually equal to the first term when $n_1 j_1 m_1 = n_2 j_2 m_2$ and reduces the sum over m_1 when $j_1 = j_2$ by a factor $2j_1 / (2j_1 + 1)$. This means that if one wishes to calculate p by neglecting the small contributions from true "exchange" integrals in the second term of Eq. (19), one must reduce the sum over the $j_1 = j_2$ terms by this factor, i.e., by $\frac{2}{3}$ when $j_1 = j_2 = 1p_{\frac{1}{2}}$ or by $\frac{1}{2}$ when $j_1 = j_2 = 1s_{\frac{1}{2}}$. This can be regarded as merely subtracting the self-perturbation effect. The terms of the second sum have no simple interpretation in terms of an equivalent

TABLE IV. Matrix elements for isotopic-spin impurity from two nucleon excitation.

$M = (n_1 j_1 n_2 j_2 011 T_1 r_{12}^{-1} n_3 j_3 n_4 j_4 011)$		
$n_1 j_1 n_2 j_2$	$n_3 j_3 n_4 j_4$	M
$(1p_{\frac{1}{2}})^2$	$(1p_{\frac{1}{2}})^2$	0.00425 Mev
$(1p_{\frac{1}{2}})^2$	$1p_{\frac{1}{2}} 2p_{\frac{1}{2}}$	0.0166
$(1s_{\frac{1}{2}})^2$	$(1p_{\frac{1}{2}})^2$	-0.162
$(1s_{\frac{1}{2}})^2$	$1p_{\frac{1}{2}} 2p_{\frac{1}{2}}$	-0.463

potential when $j_1 m_1 \neq j_2 m_2$. The corresponding "exchange" integrals will be much smaller than the "direct" integrals.

The equivalent potential is given by the sum

$$V_E(r_2) = e^2 \sum_{j, m_j} \int d\mathbf{r}_1 \phi_{jm}^*(1) r_{12}^{-1} \phi_{jm}(1) \quad (31)$$

over all closed shells in the nucleus. The integral in this expression can be written in terms of the angular momentum eigenfunctions,

$$\chi_{nl}^{m_l} = [R_{nl}(r)/r] Y_l^m(\theta, \phi)$$

by the transformation

$$\begin{aligned} V_E(r_2) &= e^2 \sum_{j m_j} \sum_{l m_l, m_l', m_s} (l \frac{1}{2} j m_j | l m_l \frac{1}{2} m_s) (l m_l' \frac{1}{2} m_s | l \frac{1}{2} j m_j) \\ &\quad \times \int d\mathbf{r}_1 \chi_{nl}^{m_l}{}^*(1) r_{12}^{-1} \chi_{nl}^{m_l'}(1). \quad (32) \end{aligned}$$

Make a Slater-type expansion of the integral

$$\begin{aligned} \int d\mathbf{r}_1 \chi_{nl}^{m_l}{}^*(1) r_{12}^{-1} \chi_{nl}^{m_l}(1) \\ = \sum_k \mathfrak{N}^{(k)}(l, l) (l m_l | P_k(\cos \omega_{12}) | l m_l), \quad (33) \end{aligned}$$

where

$$\begin{aligned} \mathfrak{N}^{(k)}(l, l) &\equiv \frac{2k+1}{2} \int R_{nl}(1) R_{nl}(1) r_{12}^{-1} \\ &\quad P_k(\cos \omega_{12}) d(\cos \omega_{12}) dr_1, \quad (34) \\ \cos \omega_{12} &\equiv \cos(\mathbf{r}_1, \mathbf{r}_2). \end{aligned}$$

Now choose the coordinate system so that $\theta_2 = 0$ and $\cos \omega_{12} = \cos \theta_1$. From Eqs. (42) and (52) of Racah⁶

$$\begin{aligned} (l m_l | P_k(\cos \omega_{12}) | l m_l) \\ = (-1)^{m_l} (2l+1) V(lk; 000) V(lk; -m_l m_l, 0), \quad (35) \end{aligned}$$

where the $V(abc; \alpha\beta\gamma)$ are functions related to the vector addition coefficients. With this expansion $V_E(r_2)$ becomes

$$\begin{aligned} V_E(r_2) &= e^2 \sum_{j, k} \mathfrak{N}^{(k)}(l, l) (2l+1) V(lk; 000) (2j+1) \\ &\quad \times W(lj l j; \frac{1}{2} k) \sum_{m_j} (-1)^{m_j+1/2} V(jjk; -m_j m_j, 0), \quad (36) \end{aligned}$$

with $W(lj l j; \frac{1}{2} k)$ a Racah coefficient. In summing over j the l values also change. Only even k appear in the

TABLE V. Coulomb potential produced for He⁴ and C¹².

He ⁴			
$\xi = \nu^2/R^2$	Uniform sphere potential $\times e^2/R$	Oscillator model potential $\times e^2/R$ $\nu = 3/2R^2$	Oscillator model potential $\times e^2/R$ $\nu = 5/2R^2$
0	3.00	2.77	3.57
0.2	2.96	2.76	3.49
0.4	2.84	2.56	3.14
0.6	2.64	2.35	2.74
0.8	2.36	2.09	2.31
1.0	2.00	1.84	1.95
1.4	1.43	1.41	1.43
1.8	1.11	1.11	1.11

C ¹²		
$\xi = \nu^2/R^2$	Uniform sphere potential $\times e^2/R$	Oscillator model potential $\times e^2/R$ $\nu = 5/2R^2$
0	9.00	8.33
0.2	8.88	8.20
0.4	8.52	7.84
0.6	7.92	7.23
0.8	7.08	6.47
1.0	6.00	5.65
1.4	4.29	4.28
1.8	3.33	3.33

sum since $V(lk; 000)$ vanishes unless $l+l'+k \equiv 2g$ is even.

The sum in Eq. (36) has been carried out over all the states which protons (and neutrons) occupy in the closed-shell nucleus and therefore $V_E(r)$ is the electrostatic potential produced by protons in the nucleus. We shall calculate now $V_E(r)$ for the simple closed-shell nuclei He⁴ and C¹² to compare this $V_E(r)$ with the electrostatic potential produced by a uniform sphere of charge. In this way we shall justify the use of this latter potential in the calculation of the perturbation of the states of two or three nucleons outside a core consisting of filled shells.

We shall derive $V_E(r)$ for C¹² first and shall immediately be able to give $V_E(r)$ for He⁴ also. Since for C¹² k can only be 0, 2 the sum in Eq. (36) reduces to

$$\begin{aligned}
V_E(r)/e^2 = & 12\mathfrak{N}^{(0)}(1p, 1p)V(110; 000)W(1 \frac{1}{2} 1 \frac{3}{2}; \frac{1}{2} 0) \\
& \times \sum_{m_j=-\frac{3}{2}}^{\frac{3}{2}} (-1)^{m_j+\frac{1}{2}} V(\frac{3}{2} \frac{3}{2} 0; -m_j m_j 0) \\
& + 12\mathfrak{N}^{(0)}(1p, 1p)V(112; 000)W(1 \frac{3}{2} 1 \frac{3}{2}; \frac{1}{2} 0) \\
& \times \sum_{m_j=-\frac{3}{2}}^{\frac{3}{2}} (-1)^{m_j+\frac{1}{2}} V(\frac{3}{2} \frac{3}{2} 2; -m_j m_j 0) \\
& + 2\mathfrak{N}^{(0)}(1s, 1s)V(000; 000)V(0 \frac{1}{2} 0 \frac{1}{2}; \frac{1}{2} 0) \\
& \times \sum_{m_j=-\frac{1}{2}}^{\frac{1}{2}} (-1)^{m_j+\frac{1}{2}} V(\frac{1}{2} \frac{1}{2} 0; -m_j m_j 0). \quad (37)
\end{aligned}$$

The sum over the $V(\frac{3}{2} \frac{3}{2} 2; -m_j m_j 0)$ in the second term can be shown to vanish, so one has only terms in which $k=0$. One can show that

$$\begin{aligned}
(2l+1)V(l0; 000)W(ljlj; \frac{1}{2} 0) \\
= \sum_{m_j=-j}^j (-1)^{m_j+\frac{1}{2}} V(jj 0; -m_j m_j 0) = 1, \quad (38)
\end{aligned}$$

and from this derive the result that

$$V_E(r) = e^2\{4\mathfrak{N}^{(0)}(1p, 1p) + 2\mathfrak{N}^{(0)}(1s, 1s)\} \quad (39)$$

for C¹². The potential for He⁴ is clearly

$$V_E(r) = 2\mathfrak{N}^{(0)}(1s, 1s). \quad (40)$$

Performing the indicated integrations in Eq. (34) we find

$$\begin{aligned}
\mathfrak{N}^{(0)}(1s, 1s) &= (e^2/R) \text{Erf}(R\xi\sqrt{\nu})/\xi, \\
\mathfrak{N}^{(0)}(1p, 1p) &= e^2 2(\nu/\pi)^{\frac{1}{2}} \left[-\frac{1}{3} \exp(-\nu R^2 \xi^2) \right. \\
&\quad \left. + \frac{1}{2} (\pi/\nu)^{\frac{1}{2}} \text{Erf}(R\xi\sqrt{\nu})/\xi \right], \\
\xi &\equiv r_2/R. \quad (41)
\end{aligned}$$

These values of $\mathfrak{N}^{(0)}(1s, 1s)$ and $\mathfrak{N}^{(0)}(1p, 1p)$ can be inserted in Eqs. (39) and (40) to find the effective potentials for C¹² and He⁴. The potentials are given in Table V for $\nu = 5/2R^2$ for the 1p orbits and $\nu = 3/2R^2$, $5/2R^2$ for the 1s orbits.

The Coulomb potential produced by the core protons is seen to be quite well represented by the potential produced by a uniform sphere of charge. The agreement of the two potentials is a justification of the method by which the interaction of the nucleons outside closed shells with nucleons in the closed shells was included in the calculation of the isotopic-spin mixing of two- and three-nucleon states.

The potential given by Eq. (39) is that produced by the protons in C¹². The equivalent potential which is to be used in calculating $(\Psi_{j_1, \mathcal{C}}\Psi_0)$, however, is derived from Eq. (39) by subtracting the contribution of the nucleon being excited, this subtraction arising from the second term of Eq. (19) when $j_1, m_1 = j_2, m_2$. Consequently to calculate $(\Psi_{1p\frac{3}{2}, \mathcal{C}}\Psi_0)$ use

$$\mathcal{U}_{1p\frac{3}{2}} = -\frac{e^2}{2} [3\mathfrak{N}^{(0)}(1p, 1p) + 2\mathfrak{N}^{(0)}(1s, 1s)] \quad (42)$$

while for $(\Psi_{1s\frac{3}{2}, \mathcal{C}}\Psi_0)$

$$\mathcal{U}_{1s\frac{3}{2}} = -\frac{e^2}{2} [4\mathfrak{N}^{(0)}(1p, 1p) + \mathfrak{N}^{(0)}(1s, 1s)]. \quad (43)$$

The nuclear matrix elements then emerge as

$$\begin{aligned}
(\Psi_{1p\frac{3}{2}, \mathcal{C}}\Psi_0) &= (2p | \mathcal{U}_{1p\frac{3}{2}} | 1p) \\
(\Psi_{1s\frac{3}{2}, \mathcal{C}}\Psi_0) &= (2s | \mathcal{U}_{1s\frac{3}{2}} | 1s). \quad (44)
\end{aligned}$$

These equations can be combined with Eq. (22) to calculate the approximate isotopic-spin impurity of a nucleus having closed shells in neutrons and protons much more easily than by the use of Eqs. (21) and (22). The error in the isotopic-spin impurity p made by neglecting the exchange integrals for which $j_1 m_1 \neq j_2 m_2$ in Eq. (19) will be less than 6% for C¹². This is satisfactory in view of the uncertainties in the energy denominators.

This approach of an equivalent potential has been used to calculate the isotopic-spin impurity of O^{16} with the result that $p \sim 6.7 \times 10^{-3}$.

D. Impurities for Some Nuclei with Open Shells

Having discussed separately the isotopic-spin impurity for the ground states of two nucleons outside a closed shell and of the ground state of a closed-shell nucleus, we are now in a position to estimate the isotopic-spin impurity in a nucleus with two extra nucleons or two holes. We have so far shown that the principal contribution to the isotopic-spin impurity of both the core and an outside two- or three-nucleon state arises from the promotion of the principal quantum number of single nucleon states. We have further shown that the nuclear matrix elements for such isotopic-spin impurity can be approximately calculated as the matrix elements of an equivalent central potential between the excited and ground states for single nucleons. The equivalent central potential can be very easily calculated for the ground states of $N=Z$ nuclei and the corresponding isotopic-spin impurities immediately obtained. Using some average energy denominator for all the excited states formed by exciting a single nucleon from (n, j) to $(n+1, j)$ we have derived some upper limits on the isotopic-spin impurity of Li^6 , Be^8 , B^{10} , and N^{14} . The energy denominator used for the upper limits is the separation $2h\nu/M$ of two harmonic oscillator states differing by unity in the principal quantum number with $\nu = \frac{3}{2}R^2$ for He^4 and $\nu = 5/2R^2$ through the entire p shell. All the estimates of isotopic-spin impurity obtained from the shell model calculations of this paper are then summarized in Table VI.

E. Summary

These numbers can be compared with the estimates obtained from the Fermi gas model for the upper limit on the isotopic spin impurity of the ground states of even-even $N=Z$ nuclei. The isotopic-spin impurities obtained from the shell model for the ground states of Be^8 and C^{12} are approximately $\frac{1}{5}$ the upper limits provided by the Fermi gas model. A factor of $\sim \frac{1}{2}$ arises from the use of the $(nl) - (n+1, l)$ level separation instead of the multiplet separation. A second factor of $\sim \frac{2}{3}$ arises from the decrease in the interaction of $1p$ and $1s$ nucleons through the Coulomb potential. This decrease corresponds to the decreased overlap of the shell model wave functions relative to the free-particle wave functions of the Fermi gas model.

It should be remarked that the estimates of impurities given in Table VI are probably still over-estimates since, for example, the separation of the $T=0, J=0$ state of $(1s_3)^4(1p_3)^8$ from the $T=1, J=0$ state of $(1s_3)^4(1p_3)^7 2p_3$ surely exceeds the separation of the $1p$ and $2p$ harmonic oscillator states.

TABLE VI. Isotopic spin impurities from the shell model.

Nu- cleus	He ⁴	Li ⁶	Be ⁸	B ¹⁰	C ¹²	N ¹⁴	O ¹⁶
$E_0 - E_1$ (Mev)	35	30.9	25	22	19.1	17.7	16.1
p	1.3×10^{-5}	1.0×10^{-4}	4.4×10^{-4}	1.0×10^{-3}	1.9×10^{-3}	3.1×10^{-3}	6.7×10^{-3}

The estimates of Table VI were only derived for ground states. A simple consideration based on Eq. (44) suggests that the matrix elements between low-lying $T=0$ states and excited isotopic spin $T=1$ states should not be greatly different from the matrix elements between the ground state and excited isotopic spin states. The amount of isotopic spin impurity in these excited states will then depend mostly on the energy separation of states of different isotopic spin which have the same total angular momentum parity. Therefore we do not expect the impurity of states of a few Mev excitation to be very different from the estimates of Table VI. The isotopic spin impurity of states of high excitation (>10 Mev), however, is probably much larger.

The amount of mixing of different nuclear isotopic spin eigenstates produced by the Coulomb interaction can be compared with the amount of isotopic spin impurity deduced from violations of the isotopic spin selection rule.¹⁴ The limits on isotopic spin impurity which have been found in this way by D. H. Wilkinson and collaborators are in agreement with the impurity estimated to be introduced by the Coulomb interactions.

The electric dipole selection rule observed in self-conjugate nuclei has also been shown to be a consequence of charge parity.¹⁵ The principal effect of the Coulomb potential in such nuclei is the mixing of $T=0$ and $T=1$ states, which are states of different charge parity. Consequently, the calculations of this paper show that the violations of the charge parity selection rule on $E1$ transitions can also be attributed to the effects of the Coulomb interactions.

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¹⁴ W. M. MacDonald, Phys. Rev. **98**, 60 (1955). In $Q_{1m}^{(1)}$ on page 65 the coefficient before curly brackets should be $(-k^2/10)$. Four lines below this $(kR) \approx (\hbar\omega/\text{Mev})A^{1/3}/137$. The ratio $|Q_{1m}^{(1)}/Q_{1m}^{(0)}|^2$ is correctly given by $(2/15)^2(kR)^4$ but the numerical value for $\hbar\omega = 10$ Mev in C^{12} is $\sim 10^{-5}$, not $\sim 10^{-6}$. It should be pointed out that the radial transition contributes to $Q_{1m}^{(1)}$. The ratio of this contribution to the contribution from $\varphi_a^* \varphi_b$, calculated in the paper, is easily estimated ($\nu/c = \hbar/MRc$) to be $60A^{-3}/(\hbar\omega/\text{Mev}) = 1$ for the transition considered. For lower energies the transition current is relatively more important; for higher energies, relatively less important. The magnitude of these retardation corrections for this energy is therefore given by the term considered.

¹⁵ G. Morpurgo, Nuovo cimento **12**, 60 (1954).