

\*Research supported by the National Science Foundation Grant No. GP-29522 and the U. S. Atomic Energy Commission Contract No. A.T. 4997-54-13965.

<sup>1</sup>E. P. Harper, Y. E. Kim, and A. Tubis, *Phys. Rev. C* **2**, 877 (1970); *Phys. Rev. C* **2**, 2455(E) (1970). The notation and definitions of this reference will be used throughout this paper. In formula B.5 of this reference, the phase factor should be changed to  $(-1)^{t_i+T_i-T_i}$  and  $t_i$  and  $T_i$  should be interchanged in the  $W$  coefficient. Also in Eqs. (4.12), (4.18), and (4.28),  $-T_2$  should be replaced by  $+T_2$  in the phase factor  $(-1)^{t_2-T_2-T_2}$ , and  $t_1$  and  $t_2$  should be interchanged in the  $W$  coefficient. For trinucleon systems, these corrections to the general formulas have no effect, since  $t_i = \frac{1}{2}$ ,  $T_i = 0, 1$ .

<sup>2</sup>An analysis similar to that of Ref. 1 has also been

carried out by R. A. Malfliet and J. A. Tjon, *Ann. Phys. (N.Y.)* **61**, 425 (1970).

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## Coulomb Forces in the Nuclear $1p$ Shell\*

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Correlated wave functions obtained by solving the Bethe-Goldstone equation with realistic nuclear interactions are employed to calculate Coulomb shifts, isospin mixing, Coulomb energies, and coefficients of the isobaric mass formula in  $1p$ -shell nuclei. Improved agreement with experiment is obtained, particularly for the Coulomb shifts and isospin mixing which are not sensitive to the size parameter. No evidence is found favoring a charge-dependent component in the nuclear force.

### I. INTRODUCTION

The concept of charge-independent nuclear forces is very nearly as old as the discovery of the neutron.<sup>1,2</sup> It is very well established that any charge-dependent component of the nuclear force must be quite weak compared with the basic interactions which bind atomic nuclei. A definitive evaluation of this component is hampered by the presence of the Coulomb interaction. Charge dependent effects clearly exist in nuclei; can they be *precisely* attributed to Coulomb forces?

To answer this question, one obviously requires precise knowledge of nuclear wave functions. Thus, the theoretical investigation of charge-dependent effects in nuclei requires a twofold approach. First one tries to calculate charge-dependent effects from known electromagnetic interactions with a trial wave function, then one must determine if any remaining discrepancies are to be attributed to additional charge-dependent interactions or an inadequate wave function.

The first nuclear  $p$  shell ( $4 < A \leq 16$ ) provides a wealth of charge-dependent data. The differences

in binding energy for a mirror pair,

$$-\Delta(Z) \equiv B.E.(Z, N) - B.E.(Z-1, N+1), \quad (1.1)$$

have received extensive attention in the literature,<sup>3-5</sup> and have proved useful in the investigation of nuclear size. Likewise the alternation of second differences,

$$\Delta\Delta(Z) \equiv \Delta(Z) - \Delta(Z-1), \quad (1.2)$$

with odd-even  $Z$  has been useful in establishing the pairing correlation.<sup>3,6</sup>

More recently there has been considerable interest in the isospin mass formula<sup>7</sup>:

$$E(A; T, T_3) = a + bT_3 + cT_3^2. \quad (1.3a)$$

This formula relates the energies of isobaric analog levels in neighboring isobars. It is valid so long as the charge-dependent part of the interaction between nucleons is strictly of a two-body character and isospin mixing is negligible.

Sufficient data are now available on several multiplets, three of which ( $A=7, 9, 13$ ) are in the first  $p$  shell.<sup>8,9</sup> Usually an empirical fit to the

positions of the levels is made using the formula

$$E(A, T, T_3) = a + bT_3 + cT_3^2 + dT_3^3. \quad (1.3b)$$

Then  $d$  should prove to be very small compared to  $a$ ,  $b$ ,  $c$  (hopefully zero) in order to establish the validity of Eq. (1.3a).

A difficulty existing in all of the above tests is that the Coulomb matrix elements are sharply dependent on the nuclear-size parameters. Two additional types of data are available where this dependence (though still present) turns out to be much less significant. These are the isospin mixing of levels found<sup>10, 11</sup> in  ${}^8\text{Be}$ , and the Coulomb shifts in the positions of analog levels of isobars throughout the shell. In the next section of this paper we shall demonstrate that the key to this lack of sensitivity is in the use of correlated wave functions (obtained as the solutions of the Bethe-Goldstone equation) in the calculation of the two-body matrix elements. This will also prove to be the key for obtaining results in reasonable agreement with experiment.

The main objective of this paper is to investigate the calculation of Coulomb shifts and isospin mixing. The Coulomb energy differences, second differences, and the coefficients of the mass formula will also be calculated with the matrix elements obtained as a further, but less definitive test of the importance of correlated wave functions.

## II. COULOMB MATRIX ELEMENTS

From this point on we shall consider the Coulomb interaction,

$$V_C = \frac{1}{4} \sum_{i < j} (1 + \tau_3^i)(1 + \tau_3^j) \frac{e^2}{r_{ij}}, \quad (2.1)$$

to be the only charge-dependent force within the nucleus. The neglected magnetic interactions may later prove to be essential for quantitative accuracy; however, their effect is probably smaller than certain cross terms between  $V_C$  and the nuclear forces which cannot be treated properly at this point. We will return to this issue in the conclusion.

Now let us see what parameters are needed to describe the effects of  $V_C$  in the  $1p$  shell. To do this we first use the harmonic-oscillator shell-model description as a guide. The expressions can be easily modified to accommodate correlated wave functions later.

The Coulomb interaction of a  $1p$  nucleon with closed  $1s$  core is given by an effective single-particle energy:

$$\epsilon_j = (2j + 1)^{-1} \sum_J (2J + 1) \times \langle s_{1/2} p_j J(T=1) | V_C | s_{1/2} p_j J(T=1) \rangle, \quad (2.2)$$

where one may have  $j = \frac{1}{2}, \frac{3}{2}$ .

The two-body matrix elements representing the interaction of two protons in the  $1p$  shell may be related to just two parameters<sup>12</sup> ( $T = T_3 = 1$ );

$$\langle p^2 {}^1S_0 | V_C | p^2 {}^1S_0 \rangle = L + 2K, \quad (2.3a)$$

$$\langle p^2 {}^3P_J | V_C | p^2 {}^3P_J \rangle = L - 3K, \quad (2.3b)$$

$$\langle p^2 {}^1D_2 | V_C | p^2 {}^1D_2 \rangle = L - K. \quad (2.3c)$$

Since the Coulomb force is purely central,  $L$  and  $K$  are given by

$$L = \int x_1^2 x_2^2 |R_{1p}(r_1)R_{1p}(r_2)|^2 \frac{e^2}{r_{12}} d\vec{r}_1 d\vec{r}_2, \quad (2.4a)$$

$$K = \int x_1 x_2 y_1 y_2 |R_{1p}(r_1)R_{1p}(r_2)|^2 \frac{e^2}{r_{12}} d\vec{r}_1 d\vec{r}_2, \quad (2.4b)$$

where  $R_{1p}$  represents the radial portion of the single-particle orbitals (for oscillator orbitals  $R_{1p}$  is simply a Gaussian function).

Thus, in the context of the shell model, Coulomb effects may be described in terms of four simple parameters ( $\epsilon_{1/2}$ ,  $\epsilon_{3/2}$ ,  $L$ , and  $K$ ). If oscillator functions are insufficiently realistic, one can always refine the calculation by substituting Woods-Saxon wave functions.

What are the major deficiencies of this approach? The single-particle orbitals may be subject to many refinements, even the possibility of variation from one level to another,<sup>8</sup> and the formalism presented above will remain essentially intact. The next logical step is to introduce configuration mixing into the shell-model wave functions.

There is a very simple way to introduce configuration mixing into the above equations. Instead of using shell-model wave functions to compute the various matrix elements one could use correlated wave functions from the Brueckner-Bethe-Goldstone formalism:

$$\psi(1, 2) = \phi(1, 2) + \frac{Q}{W - H_0(1, 2)} v_{12} \psi(1, 2). \quad (2.5)$$

Here  $\phi$  is the two-body shell-model wave function appropriately vector coupled to two-body quantum numbers ( $L S J T$ ),  $v_{12}$  is the nuclear interaction between particles 1 and 2,  $H_0(1, 2)$  is the shell-model Hamiltonian (taken here to be just the kinetic energies of the nucleons),  $Q$  is the Pauli operator,  $W$  is the "starting energy" (to be defined more closely later), and  $\psi(1, 2)$  is the correlated (or perturbed) wave function. Details for solving the Bethe-Goldstone equation have been adequately covered elsewhere in the literature.<sup>13-16</sup> In this paper we will only treat those points specifically relevant to this investigation.

The main value of using correlated wave functions to compute two-body Coulomb wave functions can be seen by writing the iterative expansion

$$\begin{aligned} \langle \psi | V_C | \psi \rangle &= \langle \phi | V_C | \phi \rangle + \left\langle \phi \left| V_C \frac{1}{e} v_{12} \right| \phi \right\rangle \\ &+ \left\langle \phi \left| v_{12} \frac{1}{e} V_C \right| \phi \right\rangle \\ &+ \left\langle \phi \left| v_{12} \frac{1}{e} V_C \frac{1}{e} v_{12} \right| \phi \right\rangle + \dots, \end{aligned} \quad (2.6)$$

where  $1/e \equiv Q/(w - H_0)$ . The first term on the right is just the usual shell-model matrix element. The remaining terms are cross terms between the nuclear force and the Coulomb force. These corrections may prove to be very important when one is working in the shell-model formalism. The Coulomb force is normally referred to as a "long-range" force in nuclear physics. When one truncates the set of basis functions by introducing a model space, cross terms between the nuclear and Coulomb forces appear. Essentially the Coulomb force is renormalized:

$$\langle \phi | V_C | \phi \rangle - \langle \psi | V_C | \psi \rangle = \langle \phi | G_C | \phi \rangle, \quad (2.7)$$

where

$$G_C = V_C + v_{12} \frac{1}{e} V_C + V_C \frac{1}{e} v_{12} + v_{12} \frac{1}{e} V_C \frac{1}{e} v_{12} + \dots, \quad (2.8)$$

so that now  $G_C$  contains components that are not so long ranged. Thus, any effect strongly dependent on the long-ranged nature of the Coulomb force may appear sharply modified in a truncated shell-model basis.

To understand how this effect will manifest itself physically, one must have a quantitative measure of what is meant by a "short"- or "long"-range interaction. Such a measure is available<sup>17,18</sup> in the ratio  $K/L$ . For a  $\delta$ -function interaction, one obtains

$$K/L = 1/3 \quad (\text{zero range}) \quad (2.9)$$

to establish a short-range limit, while for an interaction which is simply a constant, one has

$$K/L = 0 \quad (\text{infinite range}) \quad (2.10)$$

as a long-range limit. Nuclear forces yield a ratio of

$$K/L \sim 1.6. \quad (2.11)$$

Thus, one might expect the use of correlated wave functions to be of paramount importance in the calculation of any quantity that depends principally on the value of  $K$ . The Coulomb shifts and the isospin mixing are such quantities.

The introduction of correlated wave functions requires some simple modifications of Eqs. (2.3). So long as single-particle orbitals are used, all five diagonal Coulomb matrix elements ( ${}^1S_0$ ,  ${}^1D_2$ ,  ${}^3P_{0,1,2}$ ) are related to only two parameters ( $L$  and  $K$ ). With correlated wave functions no such relationships exist *a priori*, and one must treat all five matrix elements as being independent.

In particular we note that since the three  ${}^3P_J$  matrix elements are not equal, one now has an "effective noncentral Coulomb interaction." One should note that this particular noncentral dependence is not a Thomas term nor a magnetic correction, but comes about from the cross terms with nuclear noncentral interactions in the truncated shell-model basis.

This is a most interesting effect, as it demonstrates how a term of a given symmetry type may arise in the effective interaction without a counterpart in the realistic potential.<sup>19</sup> Unfortunately, the available data on the noncentral components of the nuclear interaction do not warrant further investigation of this effect here. We suppress it by defining an average central matrix element in the  ${}^3P$  state:

$$\langle p^2 {}^3P | G_C | p^2 {}^3P \rangle \equiv \frac{\sum_J (2J+1) \langle p^2 {}^3P_J | G_C | p^2 {}^3P_J \rangle}{\sum_J (2J+1)}. \quad (2.12)$$

This particular weighted average simply removes the vector and tensor components of the matrix elements, and leaves one with an effective central interaction. To be consistent in suppressing the noncentral Coulomb effects we also take the single-particle energies to be degenerate, and therefore define

$$\epsilon = \epsilon_{1/2} = \epsilon_{3/2}. \quad (2.13)$$

The effect this neglect may have on agreement between theory and experiment will, however, be investigated in the latter part of this paper.

In the following investigation the Coulomb effects are digested into four parameters;  $\epsilon$ ,  $\langle p^2 {}^1S_0 | G_C | p^2 {}^1S_0 \rangle$ ,  $\langle p^2 {}^1D_2 | G_C | p^2 {}^1D_2 \rangle$ , and  $\langle p^2 {}^3P | G_C | p^2 {}^3P \rangle$ . For direct comparison with a conventional shell-model approach it is convenient to define

$$K_{SD} \equiv \frac{1}{3} [\langle p^2 {}^1S_0 | G_C | p^2 {}^1S_0 \rangle - \langle p^2 {}^1D_2 | G_C | p^2 {}^1D_2 \rangle], \quad (2.14a)$$

$$K_{SP} \equiv \frac{1}{5} [\langle p^2 {}^1S_0 | G_C | p^2 {}^1S_0 \rangle - \langle p^2 {}^3P | G_C | p^2 {}^3P \rangle]. \quad (2.14b)$$

If pure single-particle wave functions are used,

TABLE I. Coulomb parameter (in keV) as a function of the starting energy  $W$ . The Hamada-Johnston potential was used.  $\hbar\omega$  is held constant at 17 MeV.

$W$ (MeV)	-26	-28	-30	-32	-34
$L'$	713	708	704	700	696
$K_{SD}$	50	49	48	47	47
$K_{SP}$	64	62	61	60	59

then

$$K = K_{SD} = K_{SP}. \quad (2.15)$$

Departures from Eq. (2.15) found in solving the Bethe-Goldstone equation, and as indicated by the nuclear data, will be indicative of the value of using correlated wave functions in this investigation.

To generate the  $G$  matrix elements we follow the reference-spectrum method.<sup>20</sup> One starts by setting  $Q = 1$  in Eq. (2.5), and rearranges terms to obtain

$$(W - H_0)(\psi - \phi) = v_{12}\psi. \quad (2.16)$$

This nonlinear differential equation can then be solved by well-established procedures.<sup>14-16</sup> The  $G$  matrix elements are then given by

$$\langle \phi | G_C | \phi \rangle = \langle \psi | V_C | \psi \rangle, \quad (2.17)$$

as indicated by Eq. (2.6). The resulting matrix element is not  $Q - 1$  corrected. We shall return to this point in the conclusions.

Equation (2.16) contains two parameters which must be chosen theoretically. These are the starting energy  $W$  and the size parameter  $\hbar\omega$  of the oscillator function  $\phi$ . The normal prescription, in a self-consistent calculation, is to take  $W$  to be the sum of two single-hole energies. For  $1p$ -shell nucleons the hole energy may be obtained by comparing the binding energy of  $^{16}\text{O}$  with the two  $1p$ -shell levels of  $^{15}\text{O}$ . The proton hole energy is  $-12.11$  MeV in the  $p_{1/2}$  state and  $-18.44$  MeV for the  $p_{3/2}$  state.

Tables I and II demonstrate the degree of sensitivity of the Coulomb integrals to changes in  $W$

TABLE II. Coulomb parameters (in keV) as a function of  $\hbar\omega$ . The Hamada-Johnston potential is used, with  $W = -30$  MeV.

$\hbar\omega$ (MeV)	9	11	13	15	17
$L'$	524	579	627	668	704
$K_{SD}$	47	50	50	50	48
$K_{SP}$	52	56	59	61	61

TABLE III. Coulomb integrals (in keV) for the Yale, Hamada-Johnston (HJ), Reid hard-core (RHC), and Reid soft-core (RSC) potentials compared with the oscillator value.  $\hbar\omega = 16.2$  MeV and  $W = -30$  MeV. These parameters are employed for all subsequent calculations in this paper.

	Uncorrelated oscillator	Yale	HJ	RHC	RSC
$L'$	588	674	690	690	707
$K_{SD}$	36	42	49	49	54
$K_{SP}$	36	55	61	61	66

and  $\hbar\omega$ . Here we define

$$L' \equiv \frac{1}{3}[\langle p^2 {}^1S_0 | G_C | p^2 {}^1S_0 \rangle + 2\langle p^2 {}^1D_2 | G_C | p^2 {}^1D_2 \rangle], \quad (2.18)$$

for purposes of comparison with the oscillator results. All Coulomb parameters appear to be very insensitive to the starting energy.  $L'$  changes by only 3% while  $W$  is varied by about 30%, while  $K_{SD}$  changes by 3 keV, and  $K_{SP}$  changes by 5 keV. Consequently, the value chosen for the starting energy is not an important factor in any phase of the calculations. We set

$$W = -30 \text{ MeV} \quad (2.19)$$

in all the remaining calculations. When  $\hbar\omega$  is varied the exchange parameters  $K_{SD}$  and  $K_{SP}$  undergo remarkably little change. When pure oscillator orbitals are used  $K$  varies as  $(\hbar\omega)^{-1/2}$ . When correlated functions are employed, however,  $K_{SD}$  varies by only 2% and  $K_{SP}$  by 18%, while  $\hbar\omega$  is nearly doubled.  $L'$ , however, retains a substantial variation with  $\hbar\omega$ . This newfound stability of the exchange integrals is both interesting and useful in the calculations of the following sections.

Table III compares the Coulomb integral calculated with correlated wave functions derived from four modern realistic interactions (Yale,<sup>21</sup> Hamada-Johnston,<sup>22</sup> Reid<sup>23</sup> hard and soft core), and pure oscillator orbitals. The differences are far from negligible.  $K_{SD}$  and  $K_{SP}$  are both greater than the uncorrelated oscillator value, and even differ significantly from each other.  $L'$  is also substantially reinforced by the correlated wave functions. Significant differences in the integrals appear between the realistic interactions.  $K_{SD}$ , for example, is 30% greater in the Reid soft-core calculation compared to the result with the Yale potential.

Thus, one has three parameters of concern in this investigation. In addition to the starting energy and the size parameter, the results are quite sensitive to the choice of nuclear force. Of these, the choice of starting energy is least significant.

TABLE IV. Comparison between experimental and theoretical Coulomb shifts. The parameters used for the results from realistic interactions are given in Table III. The  $\chi^2$  fit refers to the two-parameter fit in Table V. Other notation is explained in the text.

Nuclei	$J_1 T_1$	$J_2 T_2$	$E_1$ (MeV)	$E_2$ (MeV)	Experiment	Coulomb shift (keV)				$\chi^2$ fit
						Osc.	Yale	HJ	RSC	
${}^6\text{Be}$ ${}^6\text{Li}$	2 1	0 1	1.50 5.36	0 3.56	$-298 \pm 200$	-104	-129	-149	-163	-139
${}^7\text{Be}$ ${}^7\text{Li}$	$\frac{1}{2} \frac{1}{2}$	$\frac{3}{2} \frac{1}{2}$	0.43 0.48	0 0	$-47 \pm 1$	-18	-22	-25	-28	-21 <sup>a</sup>
${}^7\text{Be}$ ${}^7\text{Li}$	$\frac{7}{2} \frac{1}{2}$	$\frac{1}{2} \frac{1}{2}$	4.55 4.63	0.43 0.48	$-33 \pm 29$	-52	-68	-78	-85	-80 <sup>a</sup>
${}^7\text{Be}$ ${}^7\text{Li}$	$\frac{5}{2} \frac{1}{2}$	$\frac{7}{2} \frac{1}{2}$	6.51 6.56	4.55 4.63	$30 \pm 188$	8	17	18	19	31 <sup>a</sup>
${}^7\text{Be}$ ${}^7\text{Li}$	$\frac{5}{2} \frac{1}{2}$	$\frac{5}{2} \frac{1}{2}$	7.19 7.48	6.51 6.56	$-240 \pm 184$	-64	-133	-141	-150	-241 <sup>a</sup>
${}^7\text{Be}$ ${}^7\text{Li}$	$\frac{3}{2} \frac{3}{2}$	$\frac{5}{2} \frac{1}{2}$	10.79 11.13	7.19 7.48	$-50 \pm 195$	44	76	83	89	122
${}^9\text{B}$ ${}^9\text{Be}$	$\frac{5}{2} \frac{1}{2}$	$\frac{3}{2} \frac{1}{2}$	2.33 2.43	0 0	$-100 \pm 5$	12	15	17	19	17
${}^9\text{B}$ ${}^9\text{Be}$	$\frac{3}{2} \frac{3}{2}$	$\frac{5}{2} \frac{1}{2}$	14.67 14.39	2.33 2.43	$380 \pm 25$	60	93	102	111	134
${}^{10}\text{C}$ ${}^{10}\text{B}$	2 1	0 1	3.36 5.17	0 1.74	$-70 \pm 23$	0	4	4	4	12 <sup>a</sup>
${}^{10}\text{B}$ ${}^{10}\text{Be}$	2 1	0 1	5.17 3.37	1.74 0	$60 \pm 7$	51	62	71	78	64 <sup>a</sup>
${}^{11}\text{C}$ ${}^{11}\text{B}$	$\frac{1}{2} \frac{1}{2}$	$\frac{3}{2} \frac{1}{2}$	1.99 2.12	0 0	$-129 \pm 4$	-15	-13	-17	-19	-4
${}^{11}\text{C}$ ${}^{11}\text{B}$	$\frac{5}{2} \frac{1}{2}$	$\frac{1}{2} \frac{1}{2}$	4.30 4.44	1.99 2.12	$-10 \pm 11$	25	29	34	37	26 <sup>a</sup>
${}^{11}\text{C}$ ${}^{11}\text{B}$	$\frac{3}{2} \frac{1}{2}$	$\frac{5}{2} \frac{1}{2}$	4.79 5.02	4.30 4.44	$-86 \pm 15$	-23	-21	-26	-29	-9 <sup>a</sup>
${}^{11}\text{C}$ ${}^{11}\text{B}$	$\frac{7}{2} \frac{1}{2}$	$\frac{3}{2} \frac{1}{2}$	6.48 6.74	4.79 5.02	$-38 \pm 15$	-35	-41	-48	-53	-40 <sup>a</sup>
${}^{11}\text{C}$ ${}^{11}\text{B}$	$\frac{5}{2} \frac{1}{2}$	$\frac{7}{2} \frac{1}{2}$	8.42 8.93	6.48 6.74	$-247 \pm 16$	-31	-69	-73	-77	-129
${}^{11}\text{C}$ ${}^{11}\text{B}$	$\frac{1}{2} \frac{3}{2}$	$\frac{5}{2} \frac{1}{2}$	12.45 13.02	8.42 8.93	$-60 \pm 168$	11	20	22	23	32
${}^{12}\text{N}$ ${}^{12}\text{C}$	2 1	1 1	0.97 16.11	0 15.11	$-31 \pm 12$	12	26	27	29	49 <sup>a</sup>
${}^{12}\text{C}$ ${}^{12}\text{B}$	2 1	1 1	16.11 0.95	15.11 0	$47 \pm 6$	4	10	10	11	21 <sup>a</sup>
${}^{13}\text{N}$ ${}^{13}\text{C}$	$\frac{3}{2} \frac{1}{2}$	$\frac{1}{2} \frac{1}{2}$	3.51 3.68	0 0	$-170 \pm 5$	12	13	16	18	11
${}^{13}\text{N}$ ${}^{13}\text{C}$	$\frac{5}{2} \frac{1}{2}$	$\frac{3}{2} \frac{1}{2}$	7.38 7.55	3.51 3.68	$0 \pm 20$	29	22	28	33	-3 <sup>a</sup>
${}^{13}\text{N}$ ${}^{13}\text{C}$	$\frac{1}{2} \frac{1}{2}$	$\frac{5}{2} \frac{1}{2}$	8.93 8.86	7.38 7.55	$240 \pm 59$	53	110	117	124	200 <sup>a</sup>
${}^{13}\text{N}$ ${}^{13}\text{C}$	$\frac{3}{2} \frac{1}{2}$	$\frac{1}{2} \frac{1}{2}$	11.88 11.80	8.93 8.86	$10 \pm 104$	11	24	25	27	44 <sup>a</sup>
${}^{13}\text{N}$ ${}^{13}\text{C}$	$\frac{3}{2} \frac{3}{2}$	$\frac{3}{2} \frac{1}{2}$	15.07 15.11	11.88 11.08	$-121 \pm 66$	-46	-80	-87	-93	-129 <sup>a</sup>

<sup>a</sup> Level was used in the  $\chi^2$  fit to determine  $K_{SD}$  and  $K_{SP}$ .

Choice of size parameter will be important for any physical quantity involving the direct integral, but is not critical for those quantities (Coulomb shifts and isospin mixing) that involve only  $K_{SD}$  and  $K_{SP}$ . Tables I, II, and III imply that the most critical over-all choice is that of the appropriate nuclear force. This is probably the most important result of this investigation. It is not so surprising as it may appear at first glance. We shall discuss it in detail in the Conclusions. For now, the only reasonable course open is to compute each result with all four available modern potentials and compare them. We note from Table III that the Hamada-Johnston and Reid hard-core potentials yield identical Coulomb integrals. Consequently, we shall not quote the values for the Reid hard-core potential separately any further.

Because of the strong dependence of the results on the chosen nuclear interaction, it does not seem to be warranted to use  $\hbar\omega$  as a parameter to fit experiment. In all subsequent calculations, we simply choose  $\hbar\omega = 16.2$  MeV, a convenient number which yields a reasonable fit<sup>18</sup> to the electron scattering data of <sup>16</sup>O.

To obtain the appropriate matrix elements for more than two nucleons in the shell, the CFP<sup>24</sup> program described in a previous paper<sup>25</sup> was employed. The intermediate-coupling vectors used for the  $1p$ -shell nuclei are also those of the 4BNC fit of Ref. 25, unless otherwise stipulated.

### III. COULOMB SHIFTS

Insofar as the theory presented in the preceding section is valid, the Coulomb shift depends only on the exchange integrals. To illustrate this important fact let us consider the  $1p$ -shell levels of  $A=6$  with  $T=1$ . The well-established levels with these quantum numbers are the  $J=0$  (the ground state of <sup>6</sup>He and <sup>6</sup>Be and the 3.56-MeV level of <sup>6</sup>Li) and the  $J=2$  (1.80-MeV excitation in <sup>6</sup>He, 5.36 MeV in <sup>6</sup>Li, and 1.5 MeV in <sup>6</sup>Be) levels.

The interesting feature, which originally motivated this investigation, is that the separation of the  $J=0$  and  $J=1$  levels in <sup>6</sup>He and <sup>6</sup>Li are nearly identical at 1.80 MeV, while in <sup>6</sup>Be this separation is  $1.5 \pm 0.2$  MeV.  $LS$  coupling holds in  $A=6$  to a very good approximation, so that the  $J=0$  level can be taken as  $^1S_0$  and the  $J=2$  level as  $^1D_2$  to an accuracy near 99%. Equations (2.3a) and (2.3b) then indicate that the Coulomb force will tend to compress the levels in question of <sup>6</sup>Be by an amount

$$\langle p^2 ^1S_0 | G_C | p^2 ^1S_0 \rangle - \langle p^2 ^1D_2 | G_C | p^2 ^1D_2 \rangle = 3K, \quad (3.1)$$

in the oscillator model. This compression is ab-

sent, however, in <sup>6</sup>Li and <sup>6</sup>He where there is no Coulomb repulsion between the two  $1p$ -shell nucleons. Thus, the value  $K \approx 0.1$  MeV will explain the observed Coulomb shift in  $A=6$ .

This interpretation is almost certainly oversimplified. There are several other effects which may also contribute to this Coulomb shift. The most obvious of these, still in the context of the oscillator model, is a change in size parameter in going from the  $0^+$  to the  $2^+$  level in <sup>6</sup>Be. Such a change, in fact, would seem likely, since the separation energy for the process <sup>6</sup>Be  $\rightarrow$  <sup>3</sup>Li +  $p$  appears between these levels. Wilkinson<sup>8</sup> has previously emphasized the importance of using different single-particle orbitals to obtain a precise evaluation of the Coulomb energy under these circumstances.

Furthermore, in order to obtain  $K=0.10$  MeV in the oscillator model, one would have to use orbitals corresponding to a value of  $\hbar\omega$  well over 100 MeV; certainly an unreasonable size parameter. Table III shows that  $K_{SD}=0.054$  MeV with the Reid soft-core potential ( $\hbar\omega=16.2$  MeV), yielding over one half (0.162 MeV) the observed Coulomb shift. Use of intermediate-coupling wave functions,<sup>25</sup> which incorporate an admixture of  $^3P$  into each level, then yields a Coulomb shift of 0.163 MeV; a very small correction.

Nevertheless, this effect does account for more than one half the Coulomb shift in <sup>6</sup>Be. We must remember that, because of the appearance of the threshold for proton emission between these two levels, this case is exceptionally unfavorable, and the Coulomb shift comparatively large. Furthermore, the critical 1.5-MeV level in <sup>6</sup>Be has an exceptionally large experimental error ( $\pm 0.2$  MeV). This illustration is presented here only because of the relative simplicity of the two-nucleon case.

Table IV compares theoretical and experimental Coulomb shifts for the data available in the  $1p$  shell. All possible pairs of levels were not used, since this would be redundant and be likely to lead to confusion. In order to minimize the effects of size variations, neighboring  $1p$ -shell levels were selected. Thus in  $A=7$ , for example, we take the Coulomb shift of the first excited level relative to the ground state, the second excited level relative to the first excited level, and so on. The Coulomb shift is defined by

$$\delta_C \equiv (E_1 - E_2)_{Z+1} - (E_1 - E_2)_Z. \quad (3.2)$$

A few cases exist for  $T=1$  levels where sufficient experimental information exists to make comparison. Again, in order to avoid redundancy and minimize the effect of size variations, we chose pairs differing by only one unit in  $Z$ .

The parameters  $K_{SD}$  and  $K_{SP}$  used in Table IV are just those given in Table III. No attempt was made to alter the size parameter or the starting energy, as  $K_{SD}$  and  $K_{SP}$  are insensitive to their selection. In order to check how far the procedure can be pushed a  $\chi^2$  fit for the exchange parameters was performed on 15 of the 23 pieces of data in Table IV. The parameters  $K_{SD}$  and  $K_{SP}$  are adjusted to minimize the function

$$\chi^2 = \sum (\delta_c^{\text{theory}} - \delta_c^{\text{experiment}})^2. \quad (3.3)$$

Table V compares the various results. Two  $\chi^2$  fits were made; one with the restriction that  $K_{SD} = K_{SP}$ , while in the other,  $K_{SD}$  and  $K_{SP}$  were allowed to vary independently. The one-parameter fit ( $K_{SD} = K_{SP} \equiv K$ ) yields an rms deviation from the experimental values which is poorer than the results obtained with one of the modern realistic potentials. The two-parameter fit is only slightly better than the result with the Reid soft-core potential. In all, the  $\chi^2$  fits offer very little in comparison with the straightforward results with realistic potentials. We present them here only to demonstrate that this calculation cannot be pushed much further when better nuclear forces are found. As the calculations stand the Reid soft-core potential accounts for roughly 50% of the observed Coulomb shifts, on the average. A discussion of the possible origin of the remainder will be presented in the conclusions.

The remaining examples of Table IV which are not used in the  $\chi^2$  fit display substantial discrepancies between the theoretical and accepted experimental Coulomb shift. In at least three of these cases the experimental value is significantly in doubt. Harrison<sup>26</sup> has reported finding the lowest  $T = \frac{3}{2}$  level in  ${}^7\text{Li}$  at 11.00 MeV. If this position is correct, the Coulomb shift would be in excellent agreement with theory. In most other cases exhibiting poor agreement, an important threshold for charged proton or  $\alpha$  emission occurs between the levels. This was the case in  ${}^6\text{Be}$ , as emphasized previously. A second striking example is the five Coulomb shifts observed in  ${}^{13}\text{N}$ - ${}^{13}\text{C}$ . All are in excellent agreement except the shift between the ground state and first excited state. The threshold for  ${}^{13}\text{N} \rightarrow {}^{12}\text{C} + p$  occurs at an energy intermediate between these two levels. The only discrepancy unaffected by one of these thresholds is the shift between the ground state and first excited  $p$ -shell state of  ${}^{11}\text{C}$ - ${}^{11}\text{B}$ . It must be pointed out, however, that a charged-particle threshold does not always cause a discrepancy. The  ${}^7\text{Be} \rightarrow {}^6\text{Li} + p$  threshold, for example, appears to have no effect on the good agreement found for the  $J, T = \frac{7}{2}, \frac{1}{2}$  and  $\frac{5}{2}, \frac{1}{2}$  levels in  ${}^7\text{Li}$ - ${}^7\text{Be}$  (although this shift has a significant experimental error).

TABLE V. Results of a  $\chi^2$  fit for the parameters  $K_{SD}$  and  $K_{SP}$  to 15 selected Coulomb shifts, compared with various theoretical values where no attempt was made to fit the parameters. The one-parameter fit yielded  $K_{SP} \equiv K_{SD} = 86$  keV, while one obtains  $K_{SD} = 40$  keV and  $K_{SP} = 78$  keV if the two parameters are allowed to vary independently.

Method for choosing parameters	rms deviation $\equiv (\chi^2/15)^{1/2}$
$K_{SD} = K_{SP} = 0$	0.102
Oscillator	0.076
Yale potential	0.055
Hamada-Johnston (or RHC potential)	0.053
RSC potential	0.051
One-parameter fit	0.059
Two-parameter fit	0.037

In several cases one (or more) members of an isospin multiplet have not been identified experimentally. Table VI shows predictions for some of these levels, based on the parameters derived with the Reid soft-core potential. This estimate was made using the nearest identified  $p$ -shell level of lower energy.

#### IV. ISOSPIN MIXING

Isospin is generally regarded as a fairly good quantum number for most light nuclei. A notable exception occurs in the  $2^+$  (16.63 and 16.93 MeV),  $1^+$  (17.64 and 18.15 MeV), and  $3^+$  (19.05 and 19.22 MeV) levels of  ${}^8\text{Be}$ ; for which considerable mixing of  $T=0$  and  $T=1$  is known to exist.<sup>27-29</sup> As is the case with the Coulomb shift, the off-diagonal

TABLE VI. Predicted excitation energies for unobserved members of isospin multiplets, using the Reid soft-core potential.

Observed member			Unseen member		
Nucleus	$J$	$T$	$E$ (MeV)	Nucleus	$E$ (MeV)
${}^7\text{Be}$	$\frac{3}{2}$	$\frac{1}{2}$	9.90	${}^7\text{Li}$	10.2
${}^9\text{Be}$	$\frac{1}{2}$	$\frac{1}{2}$	3.00	${}^9\text{B}$	2.9
${}^9\text{Be}$	$\frac{7}{2}$	$\frac{1}{2}$	6.66	${}^9\text{B}$	6.63
${}^{10}\text{B}$	2	1	7.48	${}^{10}\text{Be}$	5.70
				${}^{10}\text{C}$	5.63
${}^{12}\text{C}$	0	1	17.77	${}^{12}\text{B}$	2.60
				${}^{12}\text{N}$	2.61
${}^{13}\text{C}$	$\frac{7}{2}$	$\frac{1}{2}$	12.40	${}^{13}\text{N}$	12.35

TABLE VII. Off-diagonal matrix elements of the Coulomb perturbation, in keV. Computed values are obtained with oscillator wave functions and with correlated wave functions for the Yale, Hamada-Johnston, Reid hard-core, and Reid soft-core potentials. The experimental values are those deduced by Barker, using the wave functions of Ref. 30.

State	Exp.	Osc.	Yale	HJ	RSC	Ref.
$2^+$	149	67	111	123	133	a
		61	103	114	123	b
$1^+$	120	53	91	100	108	a
		28	52	57	61	b
$3^+$	63	32	69	74	78	a
		30	65	69	74	b

<sup>a</sup> Using the wave functions of Ref. 30.

<sup>b</sup> Using the wave functions of Ref. 25.

matrix element

$$W_J = \langle J, T=0 | V_C | J, T=1 \rangle \quad (4.1)$$

which produces the mixing depends only on the exchange integrals  $K_{SD}$  and  $K_{SP}$ , and consequently is not very sensitive to the size parameter or starting energy.

Barker<sup>30</sup> has deduced the  $W_J$  directly from experiment, and we compare with these values in Table VII. The matrix elements ( $W_J$ ) derived from correlated wave functions are found to be about twice those yielded by oscillator orbitals. Excellent agreement is found for  $W_2$ , where both the shell-model basis function and the experimental data are well established. The experimental value of  $W_3$  is not so well established. Neverthe-

TABLE VIII. Ground-state Coulomb energy differences for mirror nuclei (in MeV). The single-particle energy  $\epsilon$  [defined in Eq. (2.13)] has been adjusted to yield minimum rms deviation from experiment for each set of theoretical calculations.

Nuclei	Exp.	Osc.	$\Delta(Z)$		
			Yale	HJ	RSC
${}^6\text{Be}-{}^6\text{He}$	2.34	2.59	2.49	2.49	2.48
${}^7\text{Be}-{}^7\text{Li}$	1.64	1.59	1.58	1.59	1.59
${}^8\text{B}-{}^8\text{Li}$	3.54	3.54	3.48	3.48	3.47
${}^9\text{B}-{}^9\text{Be}$	1.85	1.96	1.91	1.90	1.89
${}^{10}\text{C}-{}^{10}\text{Be}$	4.62	4.50	4.47	4.46	4.45
${}^{11}\text{C}-{}^{11}\text{B}$	2.76	2.56	2.58	2.59	2.60
${}^{12}\text{N}-{}^{12}\text{B}$	5.54	5.53	5.58	5.59	5.59
${}^{13}\text{N}-{}^{13}\text{C}$	3.00	2.97	2.98	2.97	2.97
${}^{14}\text{O}-{}^{14}\text{C}$	6.55	6.52	6.62	6.63	6.64
${}^{15}\text{O}-{}^{15}\text{N}$	3.54	3.56	3.64	3.65	3.67
$\epsilon$		0.976	0.884	0.870	0.852
rms deviation					
from experiment		0.117	0.104	0.105	0.106

less the values obtained with the realistic interactions are in very good agreement with the estimate made by Barker. The empirical value of  $W_1$  is seen to be in good agreement with Barker's shell-model basis functions (when realistic forces are used to compute  $K_{SD}$  and  $K_{SP}$ ), but a substantial discrepancy exists when the basis functions of Norton and Goldhammer are used. The primary difficulty lies in the fact that the  $J=1$ ,  $T=0$  basis state is poorly determined by the shell-model fits. The overlap between the Barker and the Norton-Goldhammer basis functions is only 53%. In addition, isospin mixing for the pair of  $J=1^+$  levels is found to be 94/6, and consequently the empirically deduced value of  $W_1$  is most sensitive to any experimental error in this ratio.

The observed isospin mixing in  ${}^8\text{Be}$  is found to be very well accounted for by the Coulomb interaction alone, when correlated wave functions derived from realistic potentials are employed in the calculation. The Reid soft-core potential yields matrix elements modestly larger (and in better agreement with experiment) than the other interactions tested.

A systematic search for other cases where substantial isospin mixing is favorable was made throughout the shell. Negative results were obtained. In all cases we found the mixing to be quite small. For example, in both  ${}^7\text{Be}$  and  ${}^{11}\text{C}$ , we estimate a ground-state admixture of  $T=\frac{3}{2}$  of only about one part in a million. Since the matrix elements providing this mixing are quite small (on the order of 10 to 200 keV), it is necessary that a pair of levels lie very close in energy (about 20 to 400 keV) if isospin mixing is to be sufficiently large to be observed.

There are several cases in odd- $A$  nuclei ( $A=7$ , 9, and 11) where shell-model calculations<sup>25</sup> predict a level with  $T=\frac{1}{2}$  sufficiently close to the lowest  $T=\frac{3}{2}$  level (and with identical  $J$ ) so that mixing may occur. Unfortunately, we predict rather small matrix elements between the levels of different  $T$  in these cases. The most favorable (and most interesting) possibility is in  ${}^7\text{Be}$ . The lowest  $T=\frac{3}{2}$  level is at an excitation energy of 10.79 MeV, with  $J=\frac{3}{2}$ . The shell-model calculations<sup>25</sup> predict a  $J=\frac{3}{2}$ ,  $T=\frac{1}{2}$  level which should be found between 11 and 12 MeV excitation. The off-diagonal matrix element is predicted to be -63 keV with the Reid soft-core potential. Thus if the levels should lie within about 300 keV, measurable isospin mixing would occur. The amusing aspect of this example is that no such mixing is predicted in  ${}^7\text{Li}$ , with the approximations made in this paper. Such mixing is possible, however, either due to a term like  $\tau_3 \vec{1} \cdot \vec{s}$  or through the mediation of core excitation.<sup>31</sup>

TABLE IX. Ground-state Coulomb second energy differences (in keV) for adjacent mirror nuclei with odd  $A$ .

Nuclei	$\Delta\Delta(Z)$				
	Exp.	Osc.	Yale	HJ	RSC
$({}^9\text{B}-{}^9\text{Be})-({}^7\text{Be}-{}^7\text{Li})$	207	374	331	312	299
$({}^{11}\text{C}-{}^{11}\text{B})-({}^9\text{B}-{}^9\text{Be})$	912	597	670	689	708
$({}^{13}\text{N}-{}^{13}\text{C})-({}^{11}\text{C}-{}^{11}\text{B})$	240	409	398	384	376
$({}^{15}\text{O}-{}^{15}\text{N})-({}^{13}\text{N}-{}^{13}\text{C})$	539	589	658	676	693

## V. GROUND-STATE COULOMB ENERGIES

Tables VIII and IX compare theoretical and experimental values of  $\Delta(Z)$  and  $\Delta\Delta(Z)$ , respectively, for ground states of mirror nuclei in the  $1p$  shell. Unfortunately, the theoretical calculations cannot be performed in as clean a manner as was available for the Coulomb shifts and isospin mixing. There are two reasons for this.

First, both  $\Delta$  and  $\Delta\Delta$  depend on the direct integral  $L'$ , as well as the exchange integrals ( $K_{SD}$  and  $K_{SP}$ ). While the exchange integrals are not very sensitive to the size parameter, Table II shows that  $L'$  is still roughly proportional to  $(\hbar\omega)^{1/2}$ . In addition,  $\Delta$  will also depend on the single-particle energy  $\epsilon$ , which accounts for the Coulomb interaction between a  $1p$ -shell nucleon with the  $\alpha$ -particle core.

Nevertheless, all matrix elements needed to calculate ground-state Coulomb energies had previously been computed in the first part of this investigation, and it would be capricious not to exploit them. To avoid excessive parameter fitting (and for consistency) we simply use the parameters displayed in Table III. The single-particle energy was adjusted, however, in each data set to yield minimum rms deviation from experiment.

The results agree surprisingly well with experiment. Theoretical values of  $\Delta$  deviate from experiment by a mean value of only 106 keV for the Reid soft-core potential. Fluctuation in the comparison shows a maximum deviation of only 6%. Agreement is not quite so good for  $\Delta\Delta$ , but the well-known alternation of magnitude is nicely reproduced. The larger errors encountered in the second differences are not surprising. It must be remembered that we are analyzing exactly the same data set. Each time one invokes a difference between pieces of data, errors are compounded. Second differences are very hard to reproduce, simply because they are relatively small.

To emphasize this we also display the absolute Coulomb energies (relative to the  $\alpha$  core) in Table X. "Experimental" values have been deduced by assuming the total Coulomb energy is a function of  $Z$  only,<sup>32</sup> and consistently using the (truly)

TABLE X. Absolute ground-state Coulomb energies (in MeV), relative to the  $\alpha$ -particle core. Theoretical results are given only for the parameters obtained with the Reid soft-core potential. The value of  $\epsilon$  (0.932 MeV) has again been adjusted to yield the best fit with experiment.

Nucleus	Coulomb energy	
	Exp.	Theory
Li <sup>a</sup>	1.01	0.93
${}^6\text{Be}$		2.63
${}^7\text{Be}$	2.65	2.60
${}^8\text{Be}$		2.60
${}^9\text{Be}$		2.59
${}^{10}\text{Be}$		2.61
${}^8\text{B}$		4.57
${}^9\text{B}$	4.50	4.57
${}^{10}\text{B}$		4.56
${}^{11}\text{B}$		4.56
${}^{12}\text{B}$		4.54
${}^{13}\text{B}$		4.56
${}^9\text{C}$		7.24
${}^{10}\text{C}$		7.23
${}^{11}\text{C}$	7.27	7.24
${}^{12}\text{C}$		7.26
${}^{13}\text{C}$		7.24
${}^{14}\text{C}$		7.23
N <sup>a</sup>	10.27	10.29
O <sup>a</sup>	13.81	14.04

<sup>a</sup> In Li, N, and O there is no fluctuation of the Coulomb energy with neutron number.

experimental Coulomb differences for mirror nuclei with odd  $A$ . Such a procedure is not exactly correct, in that it fails to account for different parentages in the various isotopes of a given element. To evaluate the possible magnitude of the error induced we display theoretical values of the Coulomb energy obtained for several isotopes in Table X. We see, for example, that the Coulomb energies of  ${}^9\text{B}$  and  ${}^{10}\text{B}$  differ by 10 keV theoretically; while in deducing experimental values they are assumed to be identical. Thus, we estimate a possible error of no more than 100 keV in the Coulomb energy of  ${}^{16}\text{O}$ . This is an error of less than 1%, and need not be taken too seriously. Absolute Coulomb energies are then found to be in excellent agreement with experiment.

This quality of agreement was unexpected, since no attempt was made to fit the size parameter. At least in part, it must be attributed to the fact that  $\epsilon$  has been fitted to the data. Attempts were made to derive  $\epsilon$  directly from the Coulomb interaction of a  $1p$  nucleon with the  $\alpha$ -particle core. Tables XI–XIII summarize the results. The single-particle energy is not sensitive to the starting energy, but has a strong dependence on  $\hbar\omega$ . The latter makes calculation of a reliable value difficult. We note, however, that both fits to the data and

TABLE XI. Sensitivity of  $\epsilon$  to the starting energy ( $W$ ). Calculations were made with the Reid soft-core potential, with  $\hbar\omega = 16.2$  MeV.

$W$ (MeV)	-40	-50	-60	-70	-80	-90	-100
$\epsilon$ (MeV)	1.182	1.167	1.155	1.145	1.138	1.132	1.126

the  $G$ -matrix calculation define an  $\epsilon$  in the range

$$\epsilon = 1.00 \pm 0.18 \text{ MeV}, \quad (5.1)$$

so that one has a reasonable degree of consistency.

The  $G$ -matrix calculations yield a value for  $\epsilon$  which appear a bit too large. It must be noted that these calculations are strongly dependent on the odd-parity components of the nuclear force, which are not well established.

## VI. MASS FORMULA

The isobaric mass formula

$$E(T_3) = a + bT_3 + cT_3^2 \quad (6.1)$$

was implicit in the early work of Wigner.<sup>7</sup> Only recently, however, has adequate experimental data been made available to test this relationship (see Ref. 8 for a review). The formula applies to all members of an isobaric multiplet,

$$\psi(\alpha T, T_3 + 1) \sim (T_1 + iT_2)\psi(\alpha T, T_3) \quad (6.2)$$

(where  $\alpha$  relates to all nuclear quantum numbers except the isospin), and relates the energies of the states belonging to the same  $\alpha T$ .

There are two necessary conditions for this formula to be valid:

- (1) Isospin must be a good quantum number. This is meant in the strictest sense that Eq. (6.2) must hold precisely. Not even the size parameter is permitted to vary from one isobar to the next.
- (2) The charge-dependent part of the nucleon interaction is a two-body operator.

It is important to note that empirical verification of Eq. (6.1) by no means implies that nuclear forces are charge independent. A two-body charge-dependent component of the nuclear force would simply modify the values of  $a$ ,  $b$ , and  $c$ . The only way to verify charge independence of the nuclear force is through the derivation of the observed values of  $a$ ,  $b$ , and  $c$  from the Coulomb interactions.<sup>8</sup>

The formula is trivial for  $T \leq 1$ , since one has three parameters to fit no more than three pieces

TABLE XII. Sensitivity of  $\epsilon$  to  $\hbar\omega$ . The Reid soft-core potential is used, with  $W = -70$  MeV.

$\hbar\omega$ (MeV)	9	11	13	15	17	19
$\epsilon$ (MeV)	0.846	0.940	1.025	1.103	1.175	1.242

TABLE XIII. Single-particle energies obtained with various interactions ( $\hbar\omega = 16.2$  MeV,  $W = -70$  MeV).

$\epsilon$ (MeV)	Osc.	Yale	HJ	RSC
	1.080	1.126	1.128	1.145

of data. In this case the investigation reduces to an examination of the Coulomb shifts, as was done in Sec. III. To critically test Eq. (6.1) one must know the energies of at least four levels of a multiplet with  $T \geq \frac{3}{2}$ . Three such multiplets have been established in the  $1p$  shell. These are the lowest  $T = \frac{3}{2}$  levels of  $A = 7, 9$ , and  $13$ . The experimental data have been reviewed by Garvey<sup>33</sup> and Cerny.<sup>34</sup>

Theoretical values for  $b$  and  $c$  are compared with experiment in Tables XIV and XV. The theoretical calculation for  $c$  depends only on the values of  $L'$ ,  $K_{SD}$ , and  $K_{SP}$  from Table III. The calculation of  $b$  also involves the single-particle energy  $\epsilon$ , which has been adjusted to yield an optimum fit. The resulting values of  $\epsilon$  are a bit ( $\sim 4\%$ ) smaller than those obtained in Table VIII by fitting ground-state Coulomb energy differences, but are quite consistent with Eq. (5.1). The coefficient  $a$  depends primarily on nuclear forces, and consequently will not be discussed here.

Both  $b$  and  $c$  depend on  $L'$ , and are consequently sensitive to the size parameter of the starting function. Nevertheless, the parameters of Table III were employed in the calculations, with no attempt to adjust the size parameter to an optimum fit. It seems that insufficient data exist to warrant an elaborate parameter fit, particularly since one is forced to adjust the value of  $\epsilon$  in the evaluation of  $b$ .

Thus, the theoretical calculations for  $b$  and  $c$  cannot be considered as reliable as the calculation of Coulomb shifts and isospin mixing. In spite of this difficulty Tables XIV and XV show that agreement with experiment is quite respectable. In view of the difficulty with the size parameter better agreement would, in fact, be an embarrassment. One may conclude that; if the re-

TABLE XIV. Experimental (Ref. 33) and theoretical values of  $b$  in the isospin mass formula.  $\epsilon$  has been adjusted to fit the data.

$A$	Experiment	$b$ (MeV)			
		Osc.	Yale	HJ	RSC
7	$0.594 \pm 0.028$	0.681	0.636	0.631	0.621
9	$1.3185 \pm 0.0022$	1.209	1.204	1.205	1.205
13	$2.180 \pm 0.0049$	2.203	2.253	2.257	2.266
$\epsilon$ (MeV)		0.934	0.849	0.836	0.818
rms deviation (MeV)		0.082	0.082	0.082	0.084

TABLE XV. Experimental (Ref. 33) and theoretical values of  $c$  in the isospin mass formula.

A	Experiment	$c$ (MeV)			
		Osc.	Yale	HJ	RSC
7	$0.270 \pm 0.027$	0.215	0.285	0.289	0.293
9	$0.267 \pm 0.002$	0.264	0.283	0.287	0.291
13	$0.256 \pm 0.010$	0.265	0.285	0.289	0.293

maining discrepancies are due to a charge-dependent component in the nuclear force, then this component is certainly much weaker than the Coulomb force.

## VII. CONCLUSIONS

Let us summarize the approximations and assumptions made in this paper. These are:

- (a) the neglect of magnetic interactions;
- (b) the suppression of all noncentral effects;
- (c) the Pauli principle has not been accounted for properly in the correlated wave function;
- (d) uncertainty in the size parameter and starting energy;
- (e) higher-order terms in the  $G$ -matrix expansion are neglected;
- (f) the intermediate-coupling shell-model basis used may not exact;
- (g) finite-charge distribution of the proton.<sup>35</sup>

Magnetic effects have been estimated by Wilkinson,<sup>8</sup> and probably amount to no more than a 3% correction to absolute Coulomb energies. This means, however, that they could be much more significant in the Coulomb shifts and in  $\Delta\Delta(Z)$ . This effect is obscured by the suppression of noncentral terms in the nuclear force [Eqs. (2.12) and (2.13)]. Both approximations yield similar effects, and it would be difficult to distinguish between them in an analysis of the data. This is, in fact, a basic reason why no refinement of Eq. (2.12) was attempted.

We did attempt to refine Eq. (2.13) by introducing an additional single-body charge-dependent term

$$V_{so} \sum \tau_3^i l_i \cdot s_i, \quad (7.1)$$

which will split  $\epsilon_{3/2}$  and  $\epsilon_{1/2}$ . This attempt led to negative results. If one tries to fit the strength parameter ( $V_{so}$ ) to the Coulomb shifts of Table IV, one finds negligible improvement. The reason simply is that this term generally has a large coefficient when the discrepancy between theory and experiment is small, and a small coefficient where this discrepancy is comparatively large (the only exception to this was, curiously enough, the  $1p$ -hole doublet in  $^{15}\text{N}$ - $^{15}\text{O}$ ). Thus, we have

suppressed this effect for the simple reason that it appears to be of little help in the interpretation of the data.

The Pauli operator  $Q$  was set equal to unity in solving Eq. (2.5) by reference-spectrum method, and this approximation has not been corrected in this paper. Proper treatment of  $Q$  would lead to a renormalization of the exchange parameters  $K_{SD}$  and  $K_{SP}$ . To test the possible importance of the renormalization the  $\chi^2$  fit of  $K_{SD}$  and  $K_{SP}$  to the Coulomb shifts was made, and has already been discussed in Sec. III. The fit led to only modest improvement over those calculations made with realistic potentials and no adjustable parameters, and relatively small renormalization of the exchange integrals. This makes sense, since one is dealing with matrix elements of the  $^1S$ ,  $^1D$ , and  $^3P$  states where  $Q - 1$  corrections are found to be relatively small.<sup>16</sup> A refined treatment of the Pauli operator would probably not be warranted as yet because of larger uncertainties in other aspects of using the correlated wave functions.

The greatest uncertainty is the selection of an appropriate size parameter (Table I shows the various Coulomb integrals to be relatively insensitive to the starting energy). The Coulomb integrals of Table III were used in the calculation of all physical quantities, and no attempt was made to adjust the size parameter to fit the data. Fortunately, the Coulomb shifts and isospin mixing are very insensitive to the size parameter when correlated wave functions are used. Consequently, we think of these as relatively "clean" calculations. All other physical quantities tested involve the absolute Coulomb energies in such a way that they are sensitive to the size parameter, nevertheless, the quality of agreement with experiment obtained is quite respectable.

Table X shows a maximum deviation from experiment of only 2% (if one neglects the *unbound* ground state of  $^5\text{Li}$ ). Even though  $\epsilon$  was adjusted to optimize the fit this quality of agreement is surprising.

Actually, it is not possible to discuss the size parameter in the context of this calculation without bringing in consideration of higher-order terms in the  $G$ -matrix expansion. The reason is that if one did a *complete* calculation of the nuclei involved, correct results for all physical quantities would be obtained independent of the selection of the size parameters of the starting function. If one selects an "unrealistic" size parameter, then the higher-order corrections will be enhanced.

Which higher-order terms will be most important in the calculation of the Coulomb effects? None of them have been calculated, but it is not hard to guess. The leading corrections to Eq. (2.6)

are almost certainly terms of the type

$$\left\langle \phi \left| \frac{1}{r_{12}} \frac{1}{e} g_{13} \right| \phi \right\rangle = \left\langle \phi \left| \frac{1}{r_{12}} \frac{1}{e} v_{13} + \dots \right| \phi \right\rangle. \quad (7.2)$$

Two other classes of higher-order terms should be considered. The first involves two or more Coulomb insertions such as

$$\left\langle \phi \left| \frac{1}{r_{12}} \frac{1}{e} g_{12} \frac{1}{e} \frac{1}{r_{12}} \right| \phi \right\rangle. \quad (7.3)$$

These are expected to be small, since the Coulomb force is comparatively weak, and consequently a perturbation expansion in powers of  $1/r$  should converge rapidly. The second competitor will involve additional  $G$ -matrix insertions such as

$$\left\langle \phi \left| g_{12} \frac{1}{e} g_{13} \frac{1}{e} \frac{1}{r_{12}} \frac{1}{e} g_{23} \right| \phi \right\rangle. \quad (7.4)$$

Hopefully, this class of diagrams will also be small compared with the effect in Eq. (2.6) because the three-body  $T$ -matrix contribution is small in nuclear matter.<sup>36</sup>

Terms like those in Eq. (7.2) (i.e., one Coulomb insertion and one  $G$ -matrix insertion for a different pair of nucleons) may yield substantial corrections. The reason is that the Coulomb potential is long ranged, so that it is not obvious that the term in Eq. (7.2) is small compared with

$$\left\langle \phi \left| \frac{1}{r_{12}} \frac{1}{e} g_{12} \right| \phi \right\rangle. \quad (7.5)$$

Likewise, it is certainly not much larger. Consequently, such matrix elements are not to be expected to amount to more than about 30 keV. Indeed, these are small corrections, but they may produce significant contributions to the Coulomb shifts and isospin mixing. Calculation of these terms has not yet been attempted, and would be much more difficult than the work done in this paper.

All of the physical quantities calculated in this paper are sensitive to the intermediate-coupling shell-model wave functions used. Many different fits to the positions of energy levels were made in Ref. 25. Several of these sets were used to calculate the Coulomb shifts, which are most sensitive to the wave functions. The result was that, so long as the original shell-model fit was good, little difference was found in the computed Coulomb shifts. Consequently, all results reported in this paper were calculated with the best (4BNC) fit of Ref. 25. We must add, however, that a few of the wave functions for highly excited states not in the 4BNC data selection are not well determined by

the shell-model fit. A good example of this was found in the calculation of the isospin mixing for the  $J=1$  levels of  ${}^8\text{Be}$ . These levels were not in the 4BNC fit, and the computed value for  $W_J$  is nearly one half the value obtained when Barker's<sup>30</sup> shell-model wave function is used. This is the only case in all the data analyzed in which we found such a striking discrepancy.

No evidence was found in any phase of this investigation that would suggest a nonvanishing charge-dependent component in the nuclear force. To be sure, we still find discrepancies between theoretical calculations performed with the Coulomb interaction and the charge-dependent data in  $1p$ -shell nuclei. The discrepancies are generally quite small, however, and most likely due to the various approximations that have been made. Certainly any conclusion pointing to charge-dependent nuclear forces is completely unwarranted. One may in fact conclude that if a charge-dependent component of the nuclear force does exist it is definitely far weaker than the Coulomb force.

The best single piece of evidence for this conclusion lies in the calculation of the isospin mixing for the  $J=2$  levels of  ${}^8\text{Be}$ . The experimental data are well established for this case. The theoretical result has no strong dependence on size parameter. The most questionable part of this calculation is the parentage of the shell-model basis functions, which again seem well determined for these states. This calculation then sets an approximate *upper limit* for the charge-dependent component of the nuclear force at 15% the strength of the Coulomb force.

An additional uncertainty lies in the nuclear interaction used in the Bethe-Goldstone equation. Table III reveals this consideration to be far from trivial in this calculation. In fact, the use of a realistic nuclear interaction to compute the cross terms appears to be at least as critical as the selection of an appropriate size parameter. This is one strong reason why we made no attempt to adjust the size parameter to optimize the fit.

This result is not surprising. The nuclear force is strong, and should be expected to have sizable cross terms with the Coulomb force.

The calculations for Coulomb shifts and isospin mixing showed a dramatic improvement when correlated wave functions derived from realistic forces were used in place of the simple oscillator functions of the shell model. Calculations involving absolute Coulomb energies were not so clear cut, most likely because of the uncertainty in the appropriate size parameter. Nonetheless, the necessity of using correlated wave functions in *all* phases of this investigation is firmly established through Table III.

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